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1960 Design and Engineering of Carbon Defects in TiO₂ Nanoparticle Architectures

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1965 Chiral Nanomaterials

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1994 Tailoring the plasmonic response of Ag/NiO heterostructures by solid state dewetting for spintronic applications

Mrs. Carmen del Pino-Batlles¹, Cayetano Hernández-Gómez¹, Pilar Prieto², Jesús López-Sánchez¹, Juan Rubio-Zuazo^{3,4}, Dóra Zalka⁵, Alba Berja¹, Latiff Ullah Khan⁶, Messaoud Harfouche⁶, Alexey Maximenko⁵, Noemí Carmona⁷, José Francisco Fernández¹, Adrián Quesada¹, Aída Serrano¹

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2021 The use of artificial intelligence to rapidly optimize nanomaterials production

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2027 Fabrication and Nanosecond Laser Processing of TiN Nanoislands for Robust Plasmonic Applications

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2050 Study of the evolution of AgxAu plasmonic nanoparticles on NiO antiferromagnetic layers for spintronics applications

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2067 FeCoNi nanowires as candidates for 3D magnetic memory units

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2119 Physics-based simulations and machine learning for nano-materials and nano-devices

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2139 Pr3+-ACTIVATED NaY9Si6O26 LUMINESCENT NANOPOWDERS: PREPARATION, STRUCTURE, MORPHOLOGY, AND PHOTOLUMINESCENCE

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2140 Electrophoretic deposition of Pr3+-doped Lu2SiO5 thin films for antimicrobial applications

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2154 A bottom-up approach for multifunctionality optimization in nanoreinforced polymers

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2161 Numerical simulations of the elastic energy associated with a buried hexagonal network of dislocations and its application to semiconductor heterostructures

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2173 Thermohydraulic Performance and Optimization of a Double-Pipe Heat Exchanger with Perforated Annular Fins and clove functionalized GNP nanofluids

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2176 TEM investigation of hybrid MXene coatings of Ti3C2Tx and Nb2CTx for lubrication

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A3 Porous materials and metal organic frameworks

426 Compressive strength as a screening tool for quality control of tubular honeycomb ceramic filters

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428 Assessing the mechanical strength of multi-channelled flat-sheet ceramic filters

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558 Investigation of phase transformation in zeolitic imidazolate frameworks (ZIFs) under operating conditions using in-situ TEM

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565 Metal-organic frameworks for Li-S batteries

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609 Sustainable water purification using UiO-66 MOF gels for PFAS remediation

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618 Bulk nano-structured porous martensitic alloys: a sustainable synthesis attempt via reactive vapor phase dealloying-alloying

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657 Mixed-matrix membranes modified with nano-SiO₂ for technical applications

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714 Silica derived from Industrial Waste as Catalyst Support: Characterization of Morphological and Surface Properties.

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719 Hierarchical pore formation in iron nitride foils investigated at nano-scale by phase-contrast tomography

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741 Porous and luminescent coordination networks from new tailored ligands

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824 Unraveling Ion-Exchange behavior in ZnAl LDH: The Impact of Functional Substituents and Isomeric Variations

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908 Metal-Organic Frameworks for the Production of Radionuclides of Medical Interest

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922 Optimizing MOF morphology for enzyme immobilization: Insights from Nanoscale Characterization
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1025 Smart food packaging based on Metal-Organic Frameworks: one platform with multiple possibilities

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1040 Synthesis of novel porphyrin-based MOFs for environmental remediation

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1101 Lanthanide and bi-lanthanide loaded zeolites for wastewater treatment

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1256 Electrospun Lignin/ZIF-8 Hybrid Nanofibers for Sustainable Catalysis and Environmental Applications

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1325 Porosity evolution along simultaneous synthesis and sintering of zinc orthostannate

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1329 Design and optimization of zeolite-CZA tandem catalysts for CO₂-to-ethylene conversion: towards green polymer production

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1397 Aerogels and Xerogels from Biogenic Phenols and Furfural

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1540 Hydrogen storage in nanoporous carbons: A path towards sustainable and scalable solutions

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1564 Fixed-bed column adsorption of activated biochar towards purification of landfill leachate

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1683 Electromagnetic Interference Shielding: Carbon-Based Materials and aluminosilicate Ceramic Fiber Composites

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1695 MOF-Polymer Composites for Enhanced Atmospheric Water Harvesting

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1702 Influence of Microstructure on Dealloying Kinetics and Nanoporosity in AgAu Thin Films for Electrocatalytic Applications

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1723 Accelerating MOF Synthesis Through AI: Building the Lab-of-the-Future

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1825 Exploiting the potential of Metal-Organic Frameworks to improve the therapeutic efficiency of Glycodrugs

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1856 Nanosized Porphyrinic Metal-Organic Frameworks for the Construction of Transparent Membranes as a Multiresponsive Optical Gas Sensor

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1868 Exploiting Cross-Responsiveness of Fluorescent Interpenetrated Zirconium–Organic Frameworks Integrated in Polymeric Membranes as a Multi-Analyte Gas Sensor Array

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1875 Immobilization of Lipase on Hafnium based MOF for heterogenous biocatalysis

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1927 The structure-mechanical properties relations of nanoporous Ag as obtained from molecular dynamics simulations

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1949 Synthesis and characterization of hybrid composites for marine biotoxins by surface-enhanced Raman scattering (SERS)

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1995 Covalent Organic Frameworks for the Efficient Adsorption and Detection of Contaminants of Emerging Concern in Runoff Waters

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2022 Covalent Organic Framework in combination with Surface-enhanced Raman scattering for Ultrasensitive Antibiotic Detection

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2026 Integrated SERS-based microdroplet platform for antibiotics detection in water

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2039 Improving the electrocatalytic behaviour of ZIF-67 nanomaterials via fast eco-friendly cold plasma treatments

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2124 Exploring CO2 capture dynamics in CALF-20 using positron annihilation lifetime spectroscopy

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2195 Optimizing Electrospun Ceramic Fibers: A Direct Aqueous Approach for Cost-Effective Production

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A4 Smart materials

33 Development of Sustainable and Functional Materials from Textile Waste for the Circular Economy

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196 4D Printing of a Transformable Exoskeleton Protector using Shape Memory Polymer

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209 Next generation of stimuli responsive materials for 4D macro- and microprinting

Moritz Hopp¹, Duc Tran¹, Philipp Mainik¹, Mr. Finn Kröger¹, Prof. Dr. Eva Blasco¹, Dr. Christoph A. Spiegel¹

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271 Comparative Analysis of NiTi SMAs Powder Produced via Ultrasonic Atomization: Virgin Powder vs. Re-Powder from 3D Printed Parts

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272 Pioneering NiTi-Cu Shape Memory Alloys via Binder Jetting Additive Manufacturing: Process Optimization and Microstructural Refinement

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488 Development of Bio-Based Photocurable Resins for High-Resolution 3D Printing with the Incorporation of Quantum Dots for Advanced Photonic Applications

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637 Exploring the Influence of Stimuli on 4D Printed Components: A taxonomy of Stimulus, Smart Materials and Transformation Effects

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729 Transforming Jewelry Design: Shape Memory Polymers and the Advances of three- and four-dimensional Printing

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735 In-depth Mechanism of Corrosion and Mechanical behavior of Ni-rich NiTi Alloys through Optimized Heat Treatment and Phase Transformation

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1036 A new generation of bio-renewable vitrimer based on vanillin

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1038 Improving the thermal hysteresis of NiTi Melt-spun ribbons for faster actuation with the Cu addition and optimized annealing time.

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1132 Phase and microstructure formation of α'' Ti-Nb: Laser powder bed fusion (LPBF) vs. single track laser melting

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1133 A sustainable approach to design electrode in structural battery composite applications

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1169 Multi-functional Rotating triangular metamaterial for vibration isolation and energy harvesting applications

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1260 Effect of printed material stiffness on the curvature of 4D textiles: experimental and computational analysis

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1315 Carbon-Nanotubes Embedded Strain Sensors for Monitoring of Structural Carbon Fibre Composites

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1349 Bioinspired approach to autonomous deployment of 4D-printed structures for space applications

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1402 Oxidation resistance of self healing carbon ceramic nanocomposites

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1519 Elastocaloric effect on laser-sintered thermoplastic polyurethanes

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1537 Superelastic Behavior Improvements of Ti–Nb–Mo Alloys via Heat Treatment

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1568 Melt-electrowritten smart light-responsive lamellar structure with carbon nanoparticles incorporated into polymer matrix

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453 Ambient deposition of single atoms for enhancement of nanostructured metal oxide electrodes
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480 High Power Factor Silver Selenide thin films deposited at low temperature by pulsed hybrid reactive magnetron sputtering (PHRMS)

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521 Development of Silicide Thermoelectric Devices for Energy Harvesting based on Recyclable Silicon from PV industry

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603 Nitrogen-based polymeric solid electrolytes for next-generation multivalent batteries: An environmental impact analysis.

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610 Direct Ink Writting of NiFe electrodes for the Oxygen Evolution Reaction

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653 Improvement in the production of green hydrogen from a freeze-cast porous Fe₂O₃ material by the use of small amounts of Al₂O₃ and TiO₂

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660 Intercalation-Conversion Hybrid Cathode Enabled by MXene-Driven TiO₂/TiS₂ Heterostructure for High-Energy-Density Li-S Battery

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739 PHASE CHANGE MATERIALS IN INSULATING ELEMENTS TO INCREASE BUILDING ENERGY EFFICIENCY AND THERMAL CONFORT

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751 Towards Efficient Energy Harvesting: Flexible Piezoelectric Fibrous Mat with PDA@Modified Nanofillers

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753 Experimental assessment of computationally designed Complex Concentrated Alloys (CCAs) for Molten Salt Reactors (MSR)

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788 Investigation of Co-doped Iron Oxide Electrocatalysts for AEM Electrolysis

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851 Novel Na_{0.75}(Ni_{0.2}Co_{0.2}Mn_{0.2}Fe_{0.2}Ti_{0.2})O₂ high entropy cathodes for sodium-ion batteries with superior capacity and stability

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893 Enhanced triboelectric performance in 3D-nanonetworks biodegradable PLA metamaterials

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918 Toward High-rate Carbon-based Supercapacitors: New Insights into the Structural Characterization and Electrochemical Performance of Hierarchical Porous Carbons

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921 High-performance lithium-ion battery electrodes based on ion-implanted germanium thin films

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946 Thermoelectric efficiency enhancement of sputtered L21 Fe₂VAI, Fe₂V_{0.8}AlW_{0.2} and Ti-doped Fe₂VAI (100) and (110) epitaxial thin films

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1015 Novel Polypyrenediimide-Based Organic Cathodes with Graphene-Like Structures for Calcium Multivalent Secondary Batteries.

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1070 Fabrication and characterization of 3D printed ceria structures for solar thermochemical water splitting reactors

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1107 Utilization of Waste Triglycerides and Sulfur for the Production of Triboelectric Nanogenerators

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1200 Development of high porosity bifunctional materials for Sorption Enhanced Steam Reforming (SESR) of ethanol using colloidal process and freezes-casting technique.

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1257 Optical properties of Sb-Ge and Ge-Se thin films for applications in photovoltaic devices

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1281 Scalable Hybrid Organic-Inorganic Solid-Solid Phase Change Materials for Thermal Management in Lithium-Ion Batteries

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1302 Fluorine-Free Materials for Sustainable-By-Design Electrolysis Cells

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1346 The catalytic effect of cobalt and influence of mechanical milling on hydrogen storage system MgH₂ – Co using small milling time

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1377 Electrospun PEO-based membrane enriched with recovered lignin: towards sustainable solid-state electrolytes for Li-ion batteries

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1395 Cu-Mo-O mixed oxides as anodes in high performance lithium-ion batteries

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1396 Lignin-Derived Ionic Conducting Membranes for solid-state energy storage devices

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1410 A comparative study of the effect of the active phase (Rh, Ru, Ir and Ni) and catalyst support on CO₂ methanation reaction

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1458 Selective Lithium Extraction from Geothermal Brines using Advanced Adsorbent Materials

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1491 ZnSnN₂ films with improved optoelectronic features grown by High-Power Impulse Magnetron Sputtering for next-generation tandem solar cells

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1518 The effect of the replacement of La by Sr in La_{1-x}Sr_xMnO₃ perovskite on the catalytic oxidation of light hydrocarbons

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1533 Reversible interfacial Li-oxide formation on germanium and silicon anodes revealed by time-resolved microgravimetry

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1572 Exploring the role of non-metal and metalloid inclusions in transition-metal electrocatalysts for direct seawater splitting

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1578 Lignin-Derived Hard Carbon-MoS₂ Composite as a Potential Anode Material for High-Performance Energy Storage Devices

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1606 DFT calculations of the electrochemical curve of LiMn_{1.5}Ni_{0.5}O₄: influence of the functional and comparison with experiments

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1623 High-temperature creep behavior in 8YSZ and 8YSZ-1wt%rGO composites

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1647 Understanding electrocatalyst degradation at the atomic scale

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1649 Improving the Performance of Wood Templated Nanogenerators through Functionalization and Elastomer Impregnation

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1762 Lignocellulosic solid-state electrolyte for energy storage devices

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1783 Thermomagnetic properties of multi-principal elements Cu-Fe-Mn-Ni-Sn-Ti alloys for waste heat recovery

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1805 Influence of Chemical Composition of FexZn1-xS on The Efficiency of Organic-Inorganic Hybrid Solar Cells

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1824 Advanced SiOx anodes for Li-ion batteries produced by metallothermal reduction of microalgae exoskeletons

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1832 Operando analysis of lead batteries by wavelength-selective neutron imaging

Miguel Rodríguez-Gómez¹, Javier Campo¹, Fernando de la Fuente², Jesús Valenciano², Holger Fricke², Daniel S. Hussey³, Anders Kaestner⁴, Florencia Malamud⁴, Markus Strobl⁴, Dr. Angel Larrea¹

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1867 Evaluation of the remaining service life of district heating preinsulated pipes: In-depth study of a method based on the thermogravimetric analysis of the insulating polymeric foam

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1914 COMPOSITE ANODES OF Si/SnS₂ FOR Li-ION BATTERIES: PHASE RELATIONS AND CRYSTAL STRUCTURE INVESTIGATIONS OF THE QUATERNARY SYSTEM

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1920 Towards nearly zero energy buildings (nZEBs) with smart optical materials

Dr. Amador Menéndez-Velázquez¹, Dr. Ana Belén García-Delgado¹, Dr. Dolores Morales¹

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1946 Poly(vinylidene fluoride) enhanced multisource energy harvesting via Plasma and Vacuum-processed 1D nanoarchitectures.

Ph.D. Juan Delgado Álvarez¹, Ph.D. Xabier García-Casas¹, Dr. Francisco Javier Aparicio Rebollo¹, Dr. Víctor López-Flores^{2,1}, Dr. Hari Krishna Mishra¹, Dr. Juan Ramón Sánchez-Valencia¹, Dr. Ángel Barranco Quero¹, Dra. Ana Borrás Martos¹

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1952 Optimizing Composite Phase Change Material Thermal Performance via Nanoparticle-Enhanced PCM Properties

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1957 Half-Heusler thermoelectrics based on TiFe_{0.5}Ni_{0.5}Sb compounds synthesized via mechanical alloying

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1958 Tuning Wetting and Triboelectrical Properties for Water Energy Harvesting

Ph.D. Nicolo' Giuseppe Di Novo¹, Dr. Fernando Núñez Gálvez¹, Dr. Jaime del Moral¹, PhD Victor Joaquin Rico-Gavira¹, Luis Angurel², Carmen Lopez Santos^{1,3}, Juan Ramón Sánchez Valencia¹, Ana Borrás¹

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1991 Enhancing Structural Stability and Energy Density in MgO-NaNO₃ Composite Phase Change Materials Through SiO₂ Nanoparticle Incorporation

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2007 Eco-friendly tribo- and piezoelectric nanogenerators based on bionanocomposites

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2035 The effect of vanadium content on microstructure and magnetic properties of FeSi electrical steels

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2168 Scalable Fabrication of Flexible Perovskite Solar Modules via Roll-to-Roll Two-Step Deposition and Tailored Photonic Annealing

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74 Effect of doping on the structure and mechanical properties of anti-wear TiB₂ coatings

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97 Thermomechanical response and microstructural characterization of Nitinol alloy produced by laser powder bed fusion

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Mrs. Maria D'Aloia^{1,2,3}, Dr. Ignazio Roppolo^{1,3}, Dr. Francesca Frascella¹

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361 4D Printable Metamaterial and Terahertz: A Pathway to Next-Generation Devices for 6G Technologies

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367 Modifications of furan-based polyesters and copolyesters - a silver bullet for developing novel and sustainable materials

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418 Halide Perovskite Thin Films for Neutron Detection

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421 Formation Mechanism of J-Aggregates in Two Types of Molecularly-Oriented Bisazo Dye Films

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422 Formation and Emission Properties of J-Aggregates in Molecularly-Oriented Bisazo Dye Films

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427 Novel air-jet spinning-assisted 3D printing of porous scaffolds for tissue engineering applications

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442 Bio-Based Photocatalytic Nanocellulose-based Aerogels: A Sustainable Solution for Microplastic Capture and Degradation

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449 Deposition of combinatorial oxide thin films by Spatial Atomic Layer Deposition for optoelectronic applications

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476 Synthesis and characterization of polycationic Sn clathrates via ball milling

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492 Methods of Compound Drug Delivery via Porous Collagen Scaffolds

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552 Metal/polymer nanofluids prepared by nanoparticle-beam deposition for unconventional resistive switching

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629 Advanced multifunctional hybrid carbon nanocomposites

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656 Multifunctional composites based on covalent adaptable networks modified with recycled carbon fiber

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707 Modified Carbon Aerogels as Fe-N-C catalysts

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804 From local agrifood waste to advanced materials for sensing

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813 Composites comprising additively manufactured lattice structures and resorcinol-formaldehyde xerogels

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826 Enhancement of Corrosion Resistance of MAO/Polydopamine/Poly(lactic Acid)-Coated AZ31 Magnesium Alloy for Biomedical Applications

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836 A new synthetic route for the production of well-structured PEDOT-MXene hybrid nanoparticles

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855 From pure element powders to protective coatings in industrial applications based on thin W-Ta-B films obtained by SPS-HiPIMS method

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900 Novel Printable Microwave Metasurfaces for Energy Harvesting Applications

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906 Corrosion resistance of water borne epoxy/carbon dots coatings on aluminium alloy

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935 Controllable Delamination in Multi-Material Multilayer Plastic Packages Using the Addition of oxide particles at the Interface

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942 Rosin-Derived Materials for Active Packaging: A Sustainable Solution for Meat Preservation

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959 Process parameters optimization for L-PBF of a NiTi alloy: a combined analytical and experimental investigation

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981 A paper-based, gasochromic Pd-WO₃ sensor for hydrogen detection

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1022 Functional All-Cellulose Composites for Innovative Sustainable Textiles

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1099 Multifunctional oxide coatings with zeolites prepared by plasma electrolytic oxidation

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1122 Smart Polymer Coatings for Safety Applications in Battery Systems: Exploiting Click Chemistry and Diels-Alder Reactions

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1164 Investigation of the thermoelectric behavior of the ternary composite: Polypyrrole – Ionic liquid – Graphene

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1174 Healing effect of nanochitosan, collagen, keratin and hialuronic acid electrospun membranes in a pre-clinical study

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1179 A bespoke atmospheric pressure plasma process for the fabrication of three-dimensional glutathione-silver nanoparticle-poly(lactic acid) composites for skin regenerative applications

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1206 LDH synthesis on AZ31 alloy: effect of microstructural modifications of substrate processed by ECAP

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1356 SELF-HEALING GLASS SEAL FOR HTE/SOFC

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1365 Ultrafast-laser powder bed fusion of Nb₂O₅-TiO₂ mixtures for emerging environmental applications

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1384 Development of a functional membrane for island and coastal desalination device

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1392 Ultrafast Laser Functionalization of Doped Zinc Oxide Films

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1393 3D PRINTABLE IONIC CONDUCTIVE HYDROGELS AND ORGANOHYDROGELS FOR WEARABLE SENSOR APPLICATIONS

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1399 Polarization dependence on the emission of Nd doped bioactive W-TCP coatings on directionally solidified eutectic Calcium Zirconate-Calcium Stabilized Zirconia

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1400 Encapsulation of Clove Essential Oil into Sepiolite for Active Food Packaging Applications

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1424 Influence of substrate temperature and annealing on the conductivity of ZnO thin films

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1461 3D-Printed Colorimetric Chemosensors Using Natural Dyes for Sustainable Environmental Monitoring

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1494 Water sorption, conversion rate and fracture toughness of liquid rubber modified dental composites

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1545 Influence of porosity on the electrical and thermal conductivity of sintered metal compacts

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1590 Development of Doxorubicin Selective Electrochemical Sensors based on Surfactant-Modified ZnO-Nanoparticles

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1621 Functional phosphate glasses for daily applications

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1661 Oxetanes as a new class of additives for PEDOT:PSS providing high conductivity and water-resistance

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1699 In situ monitoring of Ag-BaTiO₃ CerMet sintering process for tuning the metacomposite properties

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1710 Customizing Luminescence in REPO₄ Nanocrystals via chemical synthesis routes

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1910 Synthesis and characterization of thermochromic VxW1-xO₂ coatings: A scalable approach using multilayer co-deposition and flash annealing

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1916 Synthesis of functionalized polyphosphazene-based materials for decontamination of anionic pollutants from wastewater

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1918 Functionalization of Phthalocyanines for their use as crosslinkers in 3D-printable photopolymer systems

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1941 Solvent-free Remote Plasma Assisted Vacuum Deposition of Organic Nanometric thin films with Tailored Dielectric Properties

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2020 Novel Sulfur-rich polymers from inverse vulcanization as functional materials for all-polymer photonic structures and metamaterials

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2049 Synthesis of KNN with tailored morphology to be used as fillers in composite materials for piezoelectric applications

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B1 Advanced steels

34 Influence of Nitride-forming Elements Al, B, and Ti on the Kinetics of Austenite Grain Growth in Microalloyed Steel

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64 Alteration of phase transformation behavior due to elevated tramp element concentrations in a hypoeutectoid steel

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77 Optimal Chemical Composition Ratio of Nb and Ti on the Mechanical Properties of Cold Rolled High Strength Low Alloy Steels

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78 Toward enhanced tensile and impact properties in low alloy multiphase TRIP-assisted steels

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138 Multi-Objective Optimization of the Thermo-Mechanical Control Process in HSLA Plate Steels

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151 Phase Stability and Impurity Detection in TiO₂(B) Synthesized by Soft Chemical Route: Implications for Preparation and Application

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172 Selective oxidation in ternary Fe-Al-Mn model alloys

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180 Fundamental study on grain boundary segregation in Fe-Zn system using in-situ heating transmission electron microscopy

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257 On the mechanism of nucleation of static recrystallization in austenite: a combined experimental and modelling approach

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294 Alloy design strategy for the development of nanostructured bainitic surface layer in gear steels for wind turbines applications

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321 Solid-state phenomena in advanced bainitic steel through in-situ S/TEM observations

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342 Convergence of Pathways to Equilibrium During Tempering of Bainitic and Martensitic Structures in a High-Si Medium Carbon Steel.

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447 Impact of Steelmaking Route and Rolling Strategy on Nb Solubility in Reinforcement Bars Production

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477 Characterization of high-strength medium manganese zinc-coated steels for the automotive industry

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484 Design of high-strength medium manganese zinc-coated steel for the automotive industry

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502 Mechanical performance of Al-alloyed medium-Mn steels following IA and QP treatments in the continuous annealing regime

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518 Additive Manufacturing of low alloyed 90MnCrV8 tool steel

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536 Role of cementite precipitation in lath martensite revealed by rapid tempering and conventional tempering treatments of medium-carbon steel

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562 Deformation-Induced Microstructural Evolution in a High-Nitrogen Stainless Steel: A Detailed EBSD Study

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623 A New Carburizing Steel Grade for Aeronautical Transmission: Design and Modelling

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645 Design of QP heat treatments for plastically-deformed and undeformed austenite in medium-Mn steels alloyed with Mo and Cu

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648 Thermal Stability of Nanostructured Bainitic Steels: Investigating the Microstructural Changes and Mechanical Properties After Reheating

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649 An in-situ analysis of the kinetics of κ -carbide precipitation in Fe-Mn-Al-C low density steels

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692 Bimodal 316L austenitic steel: Enhancing mechanical performance through ODS strengthening

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715 Effects of silicon addition on the microstructure and mechanical properties of austenitic stainless steel

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728 Experimental and simulation study of the mechanical behaviour of high-strength steel processed by friction stir welding

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746 Phase transformation behaviour in a laser powder bed fusion produced maraging steel

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781 Microstructural constituents influencing toughness in maraging steels

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834 Decomposition of carbide-free bainite during prolonged holding at bainite transformation temperatures

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856 Advanced High-Strength Steels: Fundamental Insights and Industrial Applications

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890 Revealing the history of white etching layer formation by correlative multiphysical characterization

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897 High-throughput method for steel development using directed energy deposition

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948 Impurities in Recycling Steels - Challenge and Potential for the Fatigue Resistance of Steels

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953 Exploring G91 Steel in Laser Powder Bed Fusion: Powder, Parameters and Microstructure

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990 Making High Mn Steel by Sustainable Ferromanganese Pre-alloy for Cryogenic Applications

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996 Microstructural optimization and mechanical behavior of SS-QP treated 30CrNiMo8 steel

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1052 Effect of Mo and Cu on hot deformation behavior, recrystallization kinetics and thermomechanical processing of QP-treated medium-Mn steels

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1272 Understanding the effect of laser powder bed fusion thermal cycles on the microstructure of a tool steel

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1318 Optimizing Tool Steel Performance through Additive Manufacturing: Exploring PBF-EB and PBF-L Technologies

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1319 Additive Manufacturing of Fe-Mo-W-C high thermal conductivity steel by electron beam and laser powder bed fusion

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1334 Atom-scale insights on the influence of B in preventing liquid metal embrittlement (LME) of third-generation advanced high-strength steels (AHSS)

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1350 Calibrating a TRIP crystal plasticity material model from in-situ high-energy X-ray diffraction data considering the uniaxial load direction

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1390 Atom probe tomography investigation of the impact of tramp elements from steel scrap recycling on the embrittlement of 51CrV4 quenched and tempered steel

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1574 FATIGUE CRACK INITIATION AND GROWTH IN ADVANCED BAINITIC STEELS: NOTCH AND MICROSTRUCTURAL EFFECTS

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1600 The Influence of Mo and Cu on Microstructure and Mechanical Properties of Air-hardening Ductile Forging Steels

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1650 Microstructure development in case-carburized bearing steels for wind turbines

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1671 Habit plane induced anisotropy of lath martensite micro-plasticity in dual-phase steel

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1791 Advancing of mechanical and exploitation behaviors of steel grinding balls by industrial-scale “Quenching and Partitioning”-based processing

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1806 Iron oxidation simulation on IF-Ti steel: kinetics and diffusion mechanisms

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2123 Carburizability and transformation kinetics of new high silicon steel alloys for nanostructured bainitic surface layer in wind turbines applications

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2167 Quenched and Partitioned Steel for Advanced Engineering Applications: Insights into Microstructure and Properties

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217 Impact of the interparticle forces in the rheology and particle size of binary blended cements.

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256 Thermal treatment of beech wood under controlled conditions: Physico-chemical characterisation.

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286 Scalable Cement-Based Thermoelectric Systems for Sustainable Energy Harvesting in Outdoor Environments

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298 Mechanism of Alkali-Activated Cements Retardation by Zinc Addition

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348 Innovative Geopolymer Composite for Buildings Thermoregulation

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403 Investigating the micro-structure of calcium carbonate precipitated during bio-cementation of sand

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555 Machine Learning to Predict the Thermomechanical Properties of Reinforced Polymeric Composites Manufactured with Thermoplastic or Thermosetting Matrices – A Review for Civil Construction Applications

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590 Effect of PCE superplasticizers on the control of the rheology of low clinker cements

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659 Study on the Reinforcement of Eco-Friendly Basalt/Epoxy Composites with Varying CNT/Graphene Content

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701 Recycling of gypsum based binding materials

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785 Ceramic 3D printing of constructive systems of façades. Pros and Cons

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1130 FUNCTIONALIZED CARBON MATERIALS IN CEMENT BASED COMPOSITES, A MULTIVARIATE APPROACH

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1153 Development of new glass frits for melting via sustainable electrification systems

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1245 Cement-based sorption thermal energy storage materials for applications in the energy and construction sector

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1291 Sustainable Concretes Containing Red Mud And Slag: Mechanical Characterisation, Radioactivity and Heavy Metal Leaching

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1303 Mechanisms involved in the flow evolution in superplasticized limestone- blended cements

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1306 CaCl₂/MgCl₂/Silica Gel Sorbent Material for Thermal Energy Storage

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1313 Fresh and hardened properties of concrete formulated with enforced carbonated recycled aggregates

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1317 Competitive low-carbon cements prepared with low-grade kaolinitic clays as SCMs: enhancing strength through C-S-H gel nucleation seeding

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1323 Unveiling the Link: Correlation Between R3 Test Results and Compressive Strength in Five SCM Families

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1340 Carbon-negative concrete by using biochar

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1465 Alginate biopolymers for sorption technologies in building and industrial applications

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1499 Experimental analysis and optimization of sorption thermal energy storage systems

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1520 Microstructural Analysis of Fractures in Cementitious Materials: From the Matrix to the Concrete Scale

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1652 Preliminary Research on the Incorporation of Wind Turbine Blades Wastes into Clay Materials

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1668 Kinetic feature in Calcium Chloride-Impregnated Mesoporous Silica Gel Composites for Thermochemical Energy Storage

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1756 Recycling of oil bleaching earths and mine tailings as a precursors in alkaline one-part cements activated with a sodium silicate based on spent diatomaceous earth residues.

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1761 Incorporation of Mine Tailings into diverse industrial waste for the production of Alkali-Activated Cements in Sustainable Construction

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1794 Synthetic precursors as efficient SCMs

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2184 Valorization of phosphate mining waste: Dolomite sand application in durable self-compacting mortar systems

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55 Microstructural Investigation of β - and π -type Fe-rich phases in Al-Si cast alloys

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105 A new Al-Si casting alloy with high elastic modulus

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112 Simulation of the Extrusion of high purity aluminum wires

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366 Influence of cooling rate and Mo/Fe-ratio on solidification path in a secondary Al7Si-alloy with focus on structural appearance of phases.

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376 Recrystallization Mechanisms in an AA2024 Sheet Alloy

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399 Multi-scale microstructure characterization of ultrafine Ti-Fe-based eutectics for additive manufacturing

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445 Novel aluminium-carbon nanomaterials fabricated by means of friction stir processing and plasma welding

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450 A new approach on TWIP titanium alloys design: oxygen segregation through grain boundaries engineering

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499 Influence of Fe concentrations on the improvement of the recycling content of Al-Mg-Si wrought alloys.

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549 Tailored Nanocrystalline Aluminium Grain Size in a Nanolaminated Architecture: New Horizons

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561 Microalloying Strategy: How Small Additions of Alloying Elements Can Significantly Boost the Strength of Titanium Alloys

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575 Effects of Creep in Titanium at Room Temperature during Tensile and Profilometry-based Indentation Plastometry Testing

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665 The Effect of Si Additions to an Industrial 7xxx Aluminium Alloy in the Context of Recycling

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690 Grain size and texture effects on twinning in magnesium alloys

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717 Corrosion Behaviour in NaCl and PBS Solutions of the Magnesium Alloy ZK60 after High Pressure Torsion Extrusion

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748 Tensile instabilities in 6xxx series aluminium alloys

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754 Modeling Strain Hardening in Al Alloys: Effects of Solutes and Microstructure Across Binary and Technical Alloy Systems

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817 In-situ synthesis of Metal Matrix Composite (MMC) by Laser Powder Bed Fusion

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938 Laser-ultrasonic characterization of additively manufactured TiNb alloys with low elastic moduli
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1028 Investigation on the interactions between nucleation, grain growth, and particle dispersion in magnesium-SiC nanowhiskers composites

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1120 Aging of ZA63 alloy containing stable quasicrystal phase

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1191 Microalloying Al-Mg-Si alloy with indium as a new approach to control precipitation processes

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1593 Effect of iron on the crystallographic texture and mechanical properties of extruded 6xxx aluminium alloys

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1601 Microstructure evolution via 3D printing parameter development of Scamallo/SiC metals matrix composite

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1636 Tailoring strength, ductility and directionality in laser powder bed fusion processed Ti-6Al-2Sn-4Zr-2Mo-Si and Ti-6Al-4V via post-process heat treatments

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1664 The effect of deformation on Al-Mg-Si(-Cu) alloys

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1665 SiC nanowhisker reinforced lightweight metal composites: a detailed study of the interface

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1675 Impact of microstructure heterogeneities and casting defects on the very high cycle fatigue of Aluminium components

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1727 The effect of Zn on grain boundary segregation and IGC in Al-Mg-Si-Cu alloys

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1834 Elimination of stretcher strain marks in high-Mg Al-Mg alloys: deformation behavior and microstructural insights in H16 temper

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2045 Structural application focused characterization of Continuous Fibre based Aluminium MMCs

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165 Effect of rhenium on rotating bending fatigue properties of single crystal superalloys

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270 Research Progress in High-Temperature Titanium Matrix Composites and Their Precision Thermoforming Technology

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328 Hybrid Reinforced Ferritic Alloy Fabricated by Mechanical Alloying and Spark Plasma Sintering: Preparation and Selected Properties

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360 Influence of cobalt content on the grain growth and recrystallization kinetics of VDM Alloy 780

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391 Effect of withdrawal rate and wall thickness on the microstructure of LEKv – 94 single crystal nickel-based superalloy

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425 The influence of spark plasma sintering parameters on the structure and properties of NiAl based materials

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461 High temperature oxidation behaviour of Ti-nitrides and O or N-enriched Ti model materials

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500 A new model for particle pinning in 2d polycrystals

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527 Additive manufacturing of a high-temperature coating for aero-engine applications

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783 Precipitation and microstructure features affecting the mechanical properties of a newly developed Ni-Based Superalloy

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796 Stress relaxation and analysis of activation volumes in 9% Cr-steel: insights into dislocation glide
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798 Modeling of the thermodynamic and diffusivity properties of the Ti-N system

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803 Development of a novel Method for repairing Crack-like Structures in Ni-based Superalloys

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809 Misfit strains and deformation behavior of lamellar (alpha2+gamma) colonies in-Ti-42Al-8.5Nb

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820 Role of Intermetallic Phases in Fe-based Shape-Memory Alloys

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831 Corrosion mechanisms under phosphate-rich deposits during (co)-incineration of sewage sludge and mitigation strategies for sustainable waste management

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842 Enhancing Creep Strength of Co-based Superalloys Utilizing Local Phase Transformation Strengthening and CALPHAD Based Design

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872 Revealing the influence of temperature, stress and strain rate on deformation mechanisms of the Ni-based superalloy Udimet 720Li

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930 Effect of Laser Treatment on the High-Temperature Oxidation of Titanium Alloys Through Surface Nitrogen Enhancement

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957 Influence of the oxygen partial pressure on the oxidation mechanism of rutile-type oxide-forming refractory high entropy alloys

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973 Live presentation of CreeSo - Creep Software

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991 Data-driven study of the enthalpy of mixing in liquid alloys

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1013 In-Situ Precipitation of Secondary Phases for the Strengthening of AISI 316L Austenitic Steel

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1098 Bridging Alloy Design and Processing: Microstructure, Mechanics, and Additive Manufacturing of Hf-Mo-Nb-Ti RMPEAs

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1111 Microstructural characterization of GTA and EB welded Inconel 718®, subjected to prolonged high-temperature aging conditions.

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1139 Effect of long-term thermal aging on microstructure and tensile properties of a highly-molybdenum nickel alloy

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1148 Evolution of the microstructure and mechanical properties of TiNbAl (beta+O) alloys with additions of Ta, Mo or W

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1187 Control of impurity elements in molten Ni-based superalloy

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1456 Development of Ca-based coatings for vanadium alloys used in high temperature corrosive environments

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1585 Advanced Polycrystalline γ' -Strengthened CoNiCr-Based Superalloys

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1687 Evolution of deformation micro-mechanism in thermally exposed Superalloy 625: Tracing strain hardening characteristic using a physics-based model

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1692 Influence of the fabrication process on the oxidation behavior of a eutectic high-entropy alloy

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1744 High Temperature Intergranular Oxidation of Nickel Based Superalloy Inconel 718 and Stainless Steel 316L

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1815 Dynamic recrystallization during hot deformation of an oxide-dispersion-strengthened ferritic steel

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1860 Oxidation of additively manufactured Ni-base alloy IN625: mechanism of intergranular oxidation

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1973 Hot tensile behavior of cold worked XH43 superalloy at 650 °C - Role of η phase.

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2005 Evolution of microstructure and mechanical properties as a consequence of tensile creep strain of NNS-HIPped nickel-based superalloy

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2103 Isothermal Oxidation Behavior of Mo-Ti-Si-B Multiphase Intermetallic Alloys at 1200 °C

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115 Laser structuring of ceramic endoprosthesis and its influence on the strength, aging behavior and tribological properties of ATZ ceramics

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164 Characterization of the deformation and damage behavior of fiber-reinforced ceramics in bending test

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1660 Development and Integration of Novel Ultra-High Temperature Ceramics

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1666 High Entropy Ceramics with Improved Oxidation Resistance

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1822 Behavior of Ceramic Oxides in Durability Tests for High-Temperature Solar Receivers

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1839 Microstructural evolution and mechanical properties of ultra-high temperature binary carbides

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40 Hydrogen trap characterization in 200 and 1,000 bar charged CoCrNi medium entropy alloy compared to steel AISI 316L

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91 Dislocation mechanisms in MPEAs enable simultaneously high strength and ductility

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155 High-temperature in-situ investigation of refractory high entropy superalloys

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166 Investigation of Thermophysical Properties and Chemical Compatibility with Alumina of High-Entropy Zirconates

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169 Strong and tough high-entropy materials with excellent multifunctionality

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266 Martensitic islands in the AlCoNiV multicomponent alloy

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323 Deformation mechanisms in Refractory High Entropy Alloys comprising two-phase B2/bcc microstructures

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325 Stability and properties of BCC-B2 refractory “high entropy” alloys

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392 Fabrication and characterization of a Ni-based high-entropy alloy for the hydrogen industry

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529 Superb cold-drawn deformability of NiCoCrFeMo high-entropy alloys mediated via planar defect engineering

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541 Empowering high-entropy alloys with unique nanostructure for exceptional oxygen evolution performance through self-replenishment

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557 Mechanical properties of the quaternary high-entropy alloy Zr₄₅Ti_{31.5}Nb_{13.5}Al₁₀ after plasma nitriding or nitrogen ion implantation followed by heat treatment

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572 Notable local lattice distortions in BCC refractory high-entropy alloys probed by total scattering

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581 High temperature oxidation behavior of high entropy alloys elaborated by Spark Plasma Sintering and Hot Isostatic Pressing

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584 Chemically architected high-entropy alloys: exploring composition space to generalize the concept

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588 Phase stability and mechanical behaviour of oxygen-doped refractory high-entropy alloys.

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595 Interstitial solid solution high-entropy thin films

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600 Active learning prediction of the enthalpy of mixing of BCC, FCC and HCP solid solutions

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638 Experimental and computational analysis of nanoindentation-induced plasticity in arc-melted equiatomic Mo-Ta-W refractory bcc single-phase alloy

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667 Microstructure evolution and excellent mechanical properties of TiVNbHf refractory High Entropy Alloy fabricated by powder metallurgy

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686 Phase transformation and texture evolution in a metastable medium entropy alloy

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691 Optimizing oxide dispersoid content towards enhancing mechanical properties of ODS Ni-based high entropy alloy

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744 Development of High Specific Modulus Multicomponent Alloys with An FCC Structure

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853 TiVCr-based High Entropy Alloys for solid-state hydrogen storage

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857 Nitrogen Ion Implantation in Refractory High Entropy Metallic Glass HfMoNbTaTiVWZr: Structural and Mechanical Effects

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884 Size effects and strain rate sensitivity in nanocrystalline High-Entropy CuMoTaWV

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937 Influence of Carbon Content on the Microstructure and Mechanical Properties of High-Entropy (Mo Nb Ti V W)C Carbides

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993 Processing of Biphasic High-Entropy Alloys by Laser Powder Bed Fusion and Optimization of Heat Treatments: Enhancing Strength at High Temperatures via Precipitates Strengthening.

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1030 Oxygen-induced decomposition of the BCC HfNbTaTiZr high-entropy alloy

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1109 Development of layered Cu-Mo composites with tailored thermal properties

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1199 High-throughput screening of Al-Co-Cr-Fe-Ni-Ti compositionally complex alloys: from CALPHAD simulation to AM-generated component

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1215 Laser metal deposition of NbTaTiV Refractory High Entropy Alloy

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1216 Structural and mechanical properties of refractory alloy thin films: TiZrHfTa system

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1243 Spinodal Decomposition in FeMnNiCoCu High-Entropy Alloys: A Combined Theoretical and Experimental Study

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1261 High temperature corrosion resistance of HEA for application in hydrogen energy

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1269 Chromium effect on the behavior of NbTiZr refractory medium entropy alloys

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1368 Microstructural Evolution and Deformation Mechanism Analysis of AlTiVCr High-Entropy Alloy with Varying Al-Ti Ratios

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1579 Chemical short-range order and local lattice distortions in High-Entropy Alloys: state of the art
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1609 Hydrogen-assisted spinodal decomposition in a TiNbZrHfTa complex concentrated alloy

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1617 Investigation of phase content of TiZrAlNbMo high entropy alloys with compositional gradient

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1777 Micromechanical characterization of multimetal carbides

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1845 The phase transition of multi-component (TiZrVNb)C ceramics: The phase decomposition induced by carbon content

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1855 From binary to high-entropy : tailoring microstructure and mechanical properties of diboride-carbide composites through reactive sintering

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1863 Influence of Si on structure, mechanical properties, and thermal stability of reactively and non-reactively sputtered high-entropy (Hf,Ta,Ti,V,Zr) carbides

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1893 Elucidating the Equilibrium Vacancy Concentration and Diffusion Behaviour in Refractory High-Entropy Alloys from First-Principles

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2116 High-entropy MAX phase with high strength and large plasticity mediated by local chemical fluctuations

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2159 Radiofrequency plasma spheroidization of mechanically alloyed complex concentrated alloy NbTiVZr

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210 Effect of the residual stress induced by surface treatment processes on the mechanical behavior

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338 Fatigue Corrosion Performance of Cast- and Chip-Based Produced AA6060 under Varied Heat Treatments

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441 Fretting wear of a B4C-SiC composite spark-plasma-sintered at 1400°C from B4C+Si

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462 Assessment of early-stage degradation of coil coated steel

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472 Influence of the mesostructure on the cyclic fracture-mechanical behavior of Al/Cu-Laminates

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508 In-situ investigation of the influence of corrosion protection systems on microbially influenced corrosion inside offshore monopiles

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711 The enrichment behavior of Ni in austenitic stainless steel during the corrosion in liquid lead-bismuth eutectic at 550 °C

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733 Surface inspection to detect early fatigue crack initiation in low cycle fatigue regime of high carbon steel using a scattered light sensor

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885 Study of the tribological behavior of SnO₂ coatings under low atmospheric ethanol contamination
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888 Investigating the correlation between wear and fatigue properties of cryogenically treated high-alloyed tool steels using cyclic indentation testing

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916 Fatigue strength enhancement of welded steel through residual stress tailoring by electrodeposition of a Cu/Ni multilayer thin film

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940 Effect of Grain Size on Corrosion Behaviour of Rolled Pure Magnesium

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943 Type I-Pitting of Copper Tubes in Drinking Water Supply Networks - Recent Insights into Damage Patterns and Corrosion Mechanism

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960 Microcrack initiation of a second-generation nickel-based single crystal superalloy during thermal fatigue

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962 Corrosion behavior and mechanical properties of ER70S-6 Wire Arc Additively Manufactured Steel
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1027 Low Cycle Fatigue of High Manganese Steel with Variable Microstructure Processed by Laser Powder Bed Fusion

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1034 Premature Failure of a Coated Gas Turbine Compressor Rotor at SP Subang: A Synergistic Effect of Corrosion, Erosion, and Coating Degradation

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1047 A Case Study of Gas Turbine Failure: Unraveling the Impact of Soot Ingestion on NGV, Heat Shield, and Turbine Impeller Damage

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1048 Ground WC-Co hard metal grades evaluated under service-like working conditions: mechanical and microstructural evolution

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1059 Effect of dynamically reconstructed microstructure on the precipitation of secondary phases and their impact on corrosion properties in a cast UNS 32760 super duplex stainless steel

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1073 Effect of isothermal annealing on phase transformation and corrosion properties of UNS S32760 cast SDSS

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1082 Design and realization of a tribometer for journal bearing applications in non-lubricating fluids

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1258 Effect of air, vacuum, and liquid metal environment on fatigue crack growth in 316L stainless steel at 450 OC

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1266 THE MULTISCALE NATURE OF MATERIALS DEGRADATION: USE OF ION SELECTIVE SENSORS FOR HIGH RESOLUTION IMAGING AND CHEMICAL CHARACTERIZATION

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1312 Role of Chemical and Physical Conditions on Nitrogen Insertion During High-Temperature Oxidation of titanium in Air

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1332 Slurry and cavitation erosion behavior of HVOF sprayed Metallic and Cermet Coatings

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1415 Design and implementation of an in-situ electrochemical setup for fatigue testing under the influence of hydrogen charging

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1512 Advances in Cermets for harsh environments: Unlocking Wear and Corrosion Resistance Through Microstructure and Binder Optimization

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1516 Influence of Hybrid Silica-Based Sol-Gel Coatings on the Fatigue and Corrosion Behaviour of 16Mo3 Steel

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1553 “Hybrid” multi-component alloys: chemical composition optimization to enhance an abrasive wear resistance

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1672 Investigation of High-Temperature Fatigue and Microstructural Influences on Crack Propagation in Nickel-Based Superalloy IN718

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1892 Very high cycle fatigue behavior and failure mechanism of Fe-24Mn-10Al-1C lightweight steels

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2055 Damage nature in metallic material during very high cycle fatigue

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2178 New Thermal Barrier Coatings with Polymer Derived Ceramic Bond Coats for TiAl alloys

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106 Evaluation of Damage Models for Predicting Bending Failure in Advanced High-Strength Steels (AHSS)

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227 Analyses of UNSM treatment on mechanical properties and microstructures of Inconel 718 alloy

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240 Dynamic Strain Aging in CP-Titanium: Insights from Tensile and Cyclic Loading Tests

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250 X-ray diffraction for characterization of materials in nuclear industry

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252 Sample shape effects on the experimental characterization of compressive and shear moduli

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291 Dynamic Response and Challenges in High-Frequency Testing of Elastomeric Specimens

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305 Effect of humidity on the wear behaviour of a medium carbon high silicon nanostructured bainitic steel

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315 Microstructural Changes in Zr-4Nb-2Al Alloy During Hot Rotary Swaging

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336 Characterisation of a cast iron alloy produced with the addition of TiC nanoparticles

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356 Impact of different types of fillers into the UV-ageing behavior of rotomolded PE composites

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373 In-situ neutron microstructural and mechanical characterization of WL –DED 316L stainless steel

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419 Copper-Free, Eco-Friendly, Composite Brake Linings: Optimization of Manufacturing Parameters

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429 Aging-Induced Embrittlement in Short-Fiber Reinforced Thermoplastics: A Micromechanical Approach Using Numerical Homogenization

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434 Optimization of aluminum content in the zinc bath to improve wettability and galvanizing performance of AHSS

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436 Influence of microstructural features on Charpy impact toughness properties of low alloy steels.

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510 Investigation of recrystallization in high strength Ti-10-2-3 forged alloys: impact of the stored mechanical energy on active mechanisms

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513 Characterization of microstructure in bent Al-Mg-Si-Cu alloys and their correlation to crack development at high and low quench rate

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576 The use of High Temperature Profilometry-based Indentation Plastometry (HT-PIP) for the Rapid Characterisation of High Temperature Alloys

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591 Experimental and numerical study of the interaction of a Zinc based alloy with Stainless Steel 430

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641 In-situ synchrotron X-ray diffraction study on the deformation mechanisms of advanced steels under various load paths from cryogenic to high temperatures

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688 Evaluation of Springback Prediction of the 980MPa High Strength Steel Sheet Using a Yield Function with a Hardening Model

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694 Secondary Grain Boundary Dislocations Modulate Segregation Energy Spectra in Fe-W Alloys

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712 Characterization of the fracture toughness of material interfaces

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755 Kinetic degradation determination of the Ion Exchange Resins used as a solid-active media for dry-electropolishing applications

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768 DURABILITY TESTING OF NEXT-GENERATION MATERIALS FOR SOLAR REFLECTORS

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829 Influence of the Pt addition on the primary microstructure of heat-resistant Ni-based superalloy for aerospace applications

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830 Effects of specimen geometry and tensile testing system on the ductility and stability of ausferrite

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841 Residual Stress Analysis for Aluminum Cast Alloys

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878 Microstructure evolution of alloy 625 subjected to concentrated solar radiation at 600°C

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882 Damage and delamination behaviour of oxide scale layers

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919 Design and assessment of Si enriched innovative alloys resistant to liquid lead corrosion

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939 Microstructural and mechanical characterization of PBF-LB 316L by neutron and synchrotron diffraction

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951 Tensile deformation behavior of CoNi-based single crystal superalloys at different temperatures

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985 Influence of heat-treatment-induced microstructural evolution on the low-cycle fatigue behavior of 316L stainless steel fabricated by laser powder bed fusion

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1010 Effect of the tempering on microstructure development and mechanical properties of bainite in a 42CrMo4 steel

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1019 In-situ time resolved synchrotron X-ray imaging and tomography at Diamond I12-JEEP

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1046 Correlated Analysis with a Nanomechanical Microscope

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1060 High-Throughput Mapping of Dislocation Recovery in Low-Carbon Graded Alloys via In Situ HEXRD

Prof. Vuk Manojlovic^{1,2}, PhD Hugo Paul Van Landeghem², PhD Veijo Honkimäki¹, PhD Océane Buggenhoudt³, PhD Frédéric Bonnet³, PhD Benoît Denand⁴, PhD Guillaume Geandier⁴, PhD Alexis Deschamps²

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1105 Advanced Correlative Characterization of a Gas-Nitrided 42CrMo4 Steel: Insights into Gradient Microstructure and Mechanical Properties

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1160 Advancements and Challenges in Automated Non-Destructive Testing: AI- Driven Techniques, Emerging Trends and Future Directions

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1228 The potential of Scanning Microelectrochemical Techniques to monitor chemical activity across surface layers and coatings on metals

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1240 A case study of polymeric capsule failure in cold thermal energy storage applications

Dr. Maria Jesus Ariza Camacho¹, Mr. Pablo Godoy-Moreno¹, Mr. Álvaro Castro-Vizcaíno¹, Prof. Manuel Ángel Aguilar², Dr. Manuel Servando Romero-Cano¹, Dr. Juan Luis Bosch-Saldaña¹, Dr. Joaquín Alonso-Montesinos¹, Prof. Antonio Manuel Puertas¹, Dr. Bartosz Gil³, Dr. Sabina Rosiek³

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1244 Advanced Characterization of Coating Microstructure for CERN Future Circular Collider

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1249 Role of precipitates on deformation processes in Al alloys

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1300 Adhesion properties of carbide-rich nano-coatings produced by ion irradiation

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1314 Effect of selective laser remelting on microstructure and tensile properties of 304L stainless steel processed by laser powder bed fusion

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1336 Study on microscale strain localization and slip activity in ferrite-carbides steel: An integrated study of SEM-DIC and crystal plasticity modeling

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1342 Precipitation evolution in FeNbVC microalloyed steels during welding

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1343 Simulation of Steel Plate Response undergoing Differential Cooling with Air and Water Impinging Jets

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1370 In situ DSC of homogenization in 6xxx aluminium alloys

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1383 Wire-arc directed deposition of Ti-6Al-2Sn-4Zr-2Mo: insights on mechanical behavior and high temperature creep dynamics

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1405 Development of curve smoothing systems for a more accurate and automated Ball-on-Disc test analysis

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1479 Small-specimen methods for extreme temperature and plastic strain rate material characterisation

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1484 Uncertainty quantification of composite failure

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1492 Low temperature Peltier-based nanoindentation setup for in-situ measurements in SEM

Mr. Taulant Sinani¹, Mr Hendrik Holz¹, Prof. Gerhard Dehm¹, Prof. Baptiste Gault¹, Dr Rajaprakash Ramachandramoorthy¹, Dr James Best¹

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1501 Uncertainty quantification and validation for centre hole-drilling residual stress measurement: A combined finite element and experimental framework for enhanced reliability in advanced materials

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1539 Micromechanical study of the influence of ion irradiation on the mechanical properties of anodized Al6061-T6 alloy

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1558 The Microstructure Evolution and Mechanical Response of Cold-Worked and Heat-Treated Heterostructured Materials

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1640 Mechanical Testing at Elevated and Cryogenic Temperatures with Concurrent Acoustic Emission and Electrical Resistivity Monitoring

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1641 Texture Evolution in Transforming and Twinning Materials: A Comparison of Neutron Diffraction and MTEX-Based Simulations

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1740 Defect detection in composite materials with lab-based X-ray scattering

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1749 3D strain heterogeneity and fracture studied by absorption and diffraction contrast X-ray tomography and crystal plasticity in an aluminium alloy

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1804 Effect of Surface Defects and Oxide Layers from Different Stages during Hot Rolling on the Bendability of Martensitic Wear-resistant Steel

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1881 Temperature and Grain-Size Dependence of Deformation Behavior in Commercial-Purity Titanium

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1899 Influence of the crystallographic orientation on the crystal rotation under tribological load

Mrs. Bonita Beichert¹, Dr. Antje Dollmann¹, Mr. Malte Flachmann¹, Prof. Dr. Christian Greiner¹

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1902 As-built microstructure characterization of thin walled laser wire directed energy deposited (LW-DED) AISI 316L with different process parameters

Mr. Srinidhi Sampath¹, Dr. Erik Johansson¹, Mr. Oskar Karlsson², Dr. David Lindell¹

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1926 Influence of the annealing parameters on the development of microstructure and porosity due to the Kirkendall effect in diffusion couples of Ni/Ni-based Superalloy CMSX-4

Prof. Bettina Camin¹, Igor Nasonov¹, Dr. Julia Kundin², Dr. Ahmadreza Riyahi khorasgani², Prof. Dr. Ingo Steinbach²

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1961 Microstructural and Mechanical Characterization of Ultra-Pure Aluminum for Low-Vibration Cryogenic Applications

Ph.D. Mirko Pigato¹, Filippo Agresti⁵, Alberto Benato¹, Carlo Bucci², Irene Calliari¹, Serena D'Eramo^{2,3}, Fu Shihong², Simone Quitadamo^{4,2}, Luca Pezzato⁵, Andrea Zambon¹, Antonio D'Addabbo²

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2006 Advanced quenching of steels for controlled and improved properties

Prof. Mattias Calmunger¹, Dr. Pavel Romanov², MSc Getiye W. Gebeyaw², Prof. Bahram Moshfegh²

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2011 Exploring three dimensional orientation and residual stresses in railway steels

Dr. Louis Lesage¹, Dr. Can YILDIRIM¹, Dr. Yubin ZHANG², Prof. Fang LIU³, Dr. Erika STEYN⁴, Prof. Johan AHLSTRÖM³

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2016 Fatigue performance of steels for next generation electric heavy-duty vehicles leaf springs

MSc Yuan Tian¹, Prof. Mattias Calmunger¹, Dr Jinghao Xu¹, Prof. Ru Lin Peng¹, Prof. Johan Moverare¹

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2017 The formation of solid-state zinc thermal diffusion coatings on steel surfaces and their wear performance

Mr. Jorge santos¹, Mr. João Bastos², Mr. César Cardoso², Mr. Filipe Oliveira¹

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2019 Electrochemical diagnostics for molten salt corrosion

Ph.D. Maria Elena Gennaro¹, Mr Fabio Todesco¹, Ms Silvia Vicini¹, Mr Enrico Tognella¹, Mr Alberto Pontarollo¹

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2118 Detection using computer vision and analysis of the mechanical effect of fiber orientation degree in composite materials.

Prof. Juan Antonio Almazán-Lázaro¹, Eng. Juan Liébana-Cruz¹, Prof. Elías López-Alba¹, Prof. Giancarlo Gomez-González¹, Prof. Francisco Alberto Díaz-Garrido¹

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2130 Mechanical properties of 304L stainless steel at 4K

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212 Comparison of hydrogen embrittlement fractures of tempered martensitic steel obtained by various test methods

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483 Tritium-based micro-fracture experiments for mechanistic understanding of hydrogen embrittlement

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816 Hydrogen compatibility of internal combustion engine components

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869 Metallographic analysis of end-of-test metal components of hydrogen-fueled internal combustion engines

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1031 Simulation of hydrogen behavior at crystal defects in Fe-based alloys

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1069 Integrating in-situ performance tests, advanced materials characterization, and computational modelling to understand hydrogen-material interactions

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1131 Evaluation of the hydrogen embrittlement index for a martensitic advanced high strength steel using ex-situ tensile tests

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1190 Hydrogen Distribution in FCC and BCC Alloys: Impact of Electrochemical Charging Conditions

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1463 Hydrogen embrittlement of 316L stainless steel studied by synchrotron tomography.

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1543 Effect of hydrogen on the passivity of steel: investigating the role of the surface and interfaces

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1837 Hydrogen induced softening and deformation mechanisms in nanoparticle reinforced CoCrFeNi

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1891 Hydrogen-defect interaction in nanostructured iron samples

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1976 Hydrogen effects on the scratch-induced deformation of pearlitic steel

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2080 Boron segregation informed HE mitigation strategy in a two-phase lightweight steel

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2107 Hydrogen Effects in Pre-Strained 316L Austenitic Stainless Steel Sheets

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967 Alloy design of γ' -strengthened CoNi-based superalloys with low crack susceptibility suitable for additive manufacturing

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1982 Machine-learning the thermodynamics of multi-principal element structural alloys through chemically embedded cluster expansions

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59 Novel directed energy deposited WC-Fe/Ni based wear resistant coatings for tillage tools

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69 Development of Sustainable Fe-based Composite Powders for Highly Wear-Resistant Coatings

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95 Niobium alloy C-103 for high-performance space applications – first results with using Cold Spray Additive Manufacturing – CSAM

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184 Additive Manufacturing of CuCrZr Alloys for Nuclear Fusion Applications

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207 Grain growth and mechanical behaviour of a solid-state additively manufactured Mg-4Y-3RE alloy

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260 Application of Thermo-Calc's Additive Manufacturing Module for LPBF of Steel, Aluminium, and High-Entropy Alloys

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290 Influence of PBF-LB and in-situ alloying on the microstructural features of refractory-based complex concentrated alloys

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302 Effect of solidification mode on the resulting microstructure of 304L steel produced with L-PBF
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310 Powder Reuse in Additive Manufacturing of Titanium Alloy: Effects on Corrosion Performance

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335 Microstructure and Mechanical Properties Correlation of Additively Manufactured IN939 Superalloy

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358 Enhancing the Processability and Mechanical Properties of 2618 Al Alloy via Powder Functionalization for Additive Manufacturing

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411 Fatigue behavior of 316L stainless steel and polylactic acid joints fabricated exclusively via additive manufacturing

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454 Development and Additive Manufacturing of an Al-Ni-Mn Alloy using Laser Beam Powder Bed Fusion (LB-PBF)

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463 Development and processing of the Al 5356 aluminium alloy by additive manufacturing using wire laser-based DED technology (DED-LB/M)

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465 Study of Reciclability of Metal Powders, Debinding and Sintering in Binder Jetting

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468 Optimization of Binder Infiltration Mechanisms in Metal Jetting for High-Quality Stainless-Steel Components

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556 Operando X-ray Investigation of Cracking in Copper-Steel Multi-materials

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613 Microstructural characterization of aluminum samples fabricated by the Molten Metal Deposition additive manufacturing technology

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614 Blown-Powder Directed Energy Deposition (DED) of Inconel 625: process simulation and experimental validation

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620 Characterization of the effect of copper addition on 316L Stainless Steel samples manufactured by Laser Powder Bed Fusion (LPBF)

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650 Effect of build orientation on the microstructure and corrosion properties of additively manufactured SS316L

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668 Spatter Formation Behavior Induced by Machining Chips in Hybrid Additive Manufacturing

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756 Additive manufacturing of soft magnetic materials with Permalloy-80

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782 Effect of substrate preheating on repairing Inconel 718 parts by Cold Spray Additive Manufacturing

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793 ODS Steels Produced by Additive Manufacturing for Materials in Harsh Environments

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833 High-temperature profilometry-based indentation plastometry for nickel alloy development in additive manufacturing

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868 Effect of surface roughness, defects, and residual stresses on the fatigue behaviour of additively manufactured metals

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887 Laser powder bed fusion of AISI 4140 high strength low alloy steel: parameter optimization, microstructural and mechanical properties

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899 Tungsten alloyed with varying carbon contents manufactured by Powder Bed Fusion – Laser Beam

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914 Innovative chemically-assisted mass finishing processes for additively manufactured metallic components

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933 Additive Manufacturing of Hot Work Tool Steel Parts Using the L-PBF process

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988 Insights on Interface Features in 3D-Printed Multi-materials

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1020 PBF-LB of a non-weldable Ni-base superalloy CM247LC: from conventional to non-conventional parameters

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1043 EFFECT OF PRINTING PARAMETERS ON THE MICROSTRUCTURE OF BLUE LASER DIRECTED ENERGY DEPOSITION OF A CuCrZr ALLOY

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1068 XCT image analysis for characterizing 3D printed thermomagnetic materials in energy harvesting applications

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1074 Microstructure and Mechanical Properties of Laser Powder Bed Fusion Processed NiTi SMAs: A Comparative Study of Different Feedstock Powders

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1097 Tensile and Low-Cycle Fatigue Behavior of Laser Powder Bed Fused Inconel 718 at Room and High Temperature

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1106 Microstructural characterisation and thermophysical analysis of additively manufactured scrap aluminium alloys for circularity of material

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1113 DED-LB/Mp additive manufacturing of a G91 steel using atomized and mixed commodity powders

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1119 Effect of long annealing heat treatment on the microstructure evolution and mechanical behaviour of LPBD Ti-6Al-4V alloy

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1124 Dynamic Chemical Milling for Enhancing Internal Surface Quality of LPBF-Manufactured Scalmalloy Components

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1136 Probing the Influence of HfC Nanoparticles on the Crack-Free Fabrication of CMSX-486 Nickel-Based Superalloy via Laser Powder Bed Fusion

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1155 Strategies for enhancing TiNbTa alloys via laser powder bed fusion processing: Effects of layer thickness, scanning speed, and remelting

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1159 In-Situ Lamination during 3D Printing of High Silicon Steel

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1232 Real-Time Insights into Microstructure Evolution in Laser Powder Bed Fusion Using Operando Neutron and X-ray Diffraction

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1278 Accelerating Thermal History Predictions in Additive Manufacturing with Artificial Intelligence.

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1335 4D printing of buckling-induced architected Fe-based shape memory alloys, microstructure and mechanical behavior

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1421 Effect of Surface Finish and Heat Treatments on the Mechanical Behaviour of WE43 Alloy Lattice Structures Fabricated by Laser Powder Bed Fusion

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1467 Heat treatments of 17-4PH stainless steel produced by binder jetting: tailored cooling rates for performance repeatability

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1470 Sustainable processing of metal components by material extrusion additive manufacturing technique and concentrated solar energy

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1486 Solar reactive sintering applied in Additive Manufacturing and Powder Metallurgy to process multi-material components

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1530 Microstructure, mechanical and thermal properties of copper – steel multimaterials fabricated by laser direct energy deposition

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1544 Additively manufactured high-strength and heat-resistant eutectic aluminum alloys

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1576 A new stainless steel with microstructural and compositional gradient by selective laser melting

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1588 Influence of laser powder bed fusion on the microstructure and thermoelectric properties of CuNi

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1602 Microstructure Analysis and Micro-Mechanical Properties of Cu-based Metallic Glass between Different Scanning Strategies by Laser Powder Bed Fusion

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1611 Microstructural Evolution and Mechanical Performance of Heat-Treated LPBF 17-4PH Stainless Steel:

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1637 Design of thermal treatments and composition evaluation of bio-compatible HEA Ti 3DP alloys based on computational thermodynamic approach

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1725 Post-processing effects on surface integrity of C300 subjected to different finish machining conditions.

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1734 In-situ x-ray imaging of porosity control by power modulation during additive manufacturing by the directed energy deposition technique.

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1753 Innovative FeCr alloys SOFC/SOEC Interconnectors processed by advanced processing technologies leveraging master alloy concept

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1771 Effect of static recrystallization on the anisotropy of mechanical properties of Inconel 625 additively manufactured by LPBF process

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1827 High-temperature oxidation behavior of Inconel 625 superalloy processed by additive manufacturing

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1831 AM2C3 Twinning Project: Development of Al-based Metal Matrix Composites for Laser Powder Bed Fusion Additive Manufacturing

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1864 Microstructure and mechanical properties of additive manufactured 18Ni-maraging steel after two-step aging treatment

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1989 Altering microstructure and enhancing mechanical properties during additive manufacturing of Ti-6Al-4V via in-process laser heat treatments

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2077 Correlation between Process Parameters and Microstructure of Nano- to Micro-Particle-Reinforced 3D Printed Aluminum Matrix Composites

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2094 Coupling a continuous wave laser with a scanning electron microscope; use to improve mechanical behaviour of additive manufacturing 316L stainless steel

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2097 Manufacture of tailorable biodegradable Mg/Zn multimaterial by additive friction stir deposition; microstructural and interfacial characterisation

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2182 Laser Powder Bed Fusion of Crack-Susceptible AISI M2 Tool Steel: From Process Parameter Development to Industrial Validation — A Comparative Study of Additively and Conventionally Manufactured Components

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2 LOW- VELOCITY IMPACT PERFORMANCE OF 3D PRINTED CONTINUOUS FIBRE REINFORCED BIOINSPIRED COMPOSITES STRUCTURES

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134 Advances and challenges in direct additive manufacturing of Al₂O₃ and ZrO₂-based Eutectic Ceramic Oxide

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202 Advancing Sustainable Filtration: Integration of 3D Printing and Graphene Oxide-Based Composites

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204 Voxel-level control in stereolithography 3D printing: Achieving dual properties from a single material

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343 3D Printing of bio-based polymeric composites obtained by vat-photopolymerization technology containing biofillers

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390 Towards In-Situ Pre-Programming of Transformation Characteristics in Shape Memory Polymers During Fused Filament Fabrication

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474 Additive Manufacturing of Gradient Polymer Nanocomposite Structures Using SLA 3D Printing

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530 Tailoring the Microstructure of 3D printed pieces by incorporating Cellulose Nanofibers into the PLA-based formulations containing Inorganic Phases

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647 Development of physical vapour deposition coatings for weathering protection of additive-manufactured polymer substrates

Prof. Ramon Escobar Galindo¹, Dr. Jesus Hernández-Saz², Dra. Teresa Cristina Rojas³, Dr. Bertrand Lacroix¹, Dr. Daniel Moreno-Sánchez⁴, Dr. Juan Carlos Sánchez-López³, Prof. Sergio I. Molina⁴

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718 Fiber-Reinforced Photopolymers - Additive Manufacturing of High-Performance Composites

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720 Continuous fiber reinforcing lithography-based additive manufacturing

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1041 RHEOLOGICAL BEHAVIOR OF ZEOLITE PASTES REINFORCED WITH GRAPHENE FLAKES FOR 3D PRINTING OF MEMBRANES WITH POTENTIAL APPLICATION AS GAS SEPARATION

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1309 Advancing 3D Printing with Vacuum Technology: Process Optimization, Material Properties, and Hybrid Manufacturing

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1401 Characterization of highly filled PLA-based composite filaments with silica and alumina for desiccant applications

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1457 Interpenetrating phase composites with complex geometries: pressureless infiltration of alumina-based systems

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1473 APPLICATION OF 3D PRINTING TECHNOLOGY TO CERAMIC WASTE RECYCLING

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1552 Evaluation of properties of PA 12 used in the Multi Jet Fusion printing process after reprocessing in an extruder.

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1694 Thermal Shock-Resistant Cordierite Ceramics: A Breakthrough for Aerospace Optics

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1705 Inkjet printing of PVDF-TrFE thin films: influence of solvent and annealing conditions on piezoelectric properties

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1732 Influence of Printing and Bed Temperature on the Mechanical Strength of Simple PLA Filament Joints

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1963 4D-printing of nacre-inspired ceramic-polymeric composites

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589 Design of an innovative cathodic arc source with high deposition rate and low macroparticles generation

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795 Biocompatible multilayer system for the degradation control of an additively manufactured WE43 alloy

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905 Wetting properties of titanium surfaces tuned by duplex treatments combining nanosecond laser treatment and chemical functionalization

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1054 Hierarchically Structured Catalysts Via Additive Manufacturing For Emerging Applications

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1076 Design and Investigation of DC Magnetron Sputtered TiN/TaN superlattice structures

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1176 Innovative Cold Spray Solutions for Composite Substrate Metallization

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1196 Helium-assisted deposition of Cu-doped TiO₂ for Conductometric Hydrogen Sensing via DC Magnetron Sputtering

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1207 Low-temperature plasma-assisted carburizing of additively manufactured 316 L steel

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1223 Investigation of the nanostructure of TiSiN coatings using high resolution methods

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1274 Laser Surface Treating WSC Coatings to Optimize WS2 Crystallization-to-Carbon Phase Graphitization

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1295 Plasma etching-controlled microstructure and optical properties of ZrN Coatings on ABS for automotive applications

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1316 Assessing hydrogen diffusion in ceramic PVD coating materials

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1321 Correlation of ab initio methods with experimental phase exploration of TM-Al/Si-C thin film materials

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1341 The Role of Substrate Roughness and Chemical Composition in HiPIMS-Coated Cutting Tools

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1374 A Materials Science Approach to the Analysis of Ion Diffusion Effects in Barley Seed Surfaces Treated with an Air Plasma Discharge

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1375 Electrical insulation properties of reactive grown AlN thin films at high-temperatures

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1417 Characterization of antifouling efficiency, mechanical and chemical properties of polydimethylsiloxan Fouling Release coatings

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1435 Innovative Copper-Based Electrocatalysts: Harnessing 3D Printing for Sustainable Nitrate Management in Drinking Water

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1464 Concentrated Solar Energy for the elaboration of VC-reinforced steel as a sustainable alternative to conventional arc melting

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1469 High-Temperature Concentrating Solar Technologies for direct surface processing of metallic parts

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1517 Influence of Mo on the mechanical and tribological properties of DCMS and HiPIMS deposited TiB₂+z thin films

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1587 Functionally graded laser deposition to overcome fabrication challenges in Tribaloy™ T800 hardfacing on stainless steel

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1608 Influence of thermal treatments and UV irradiation on anisotropic TiO₂ architectures prepared by oblique angle deposition

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1709 Electrodeposition of nickel-matrix nano-composite coatings for tribological applications from REACH compliant electrolytes

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1840 Laser micro-textured aluminium metallic surfaces for self-cleaning and stickers anti-vandalism urban furniture applications.

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1880 SiZY-Coat: Silicon-Zirconium-Yttrium coatings for graphitic materials

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1887 Comparative Assessment of Plasma and Gas Nitriding on Air-Hardening Ductile Steels

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1903 Operational properties of Mn1.9CuFe0.104 protective coatings deposited on ferritic stainless steels of different Cr content for SOC application

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1917 Sintering Response of Columnar Thermal Barrier Coatings Deposited by Solution Precursor Plasma Spray (SPPS) Technique

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1948 Smart Coatings Through Sol Gel Microencapsulated Additives

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1950 DEVELOPMENT OF WEAR-RESISTANT SURFACES BY DEPOSITION OF SOL-GEL COATINGS DOPED WITH Co_Ni NANOPARTICLES

Ph.D. Pascal Sanchez¹, PhD MariFe Menéndez Suarez¹, PhD Ana L. Martinez Diez¹

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1980 Assessing the anticorrosion efficiency of functionalized hybrid sol-gel coatings for environmentally-friendly passivation of galvanized steel

Dr. Lucía Florentino¹, Mrs Verónica Maestre Peña¹, Mrs. Marta Prado García¹, Dr. Olga Conejero Iglesias¹

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1985 Hybrid Highly-Porous Photonic Structures for Photocatalysis Fabricated by Atomic Layer Deposition

Nithin Thonakkara James¹, Dr. Carina Hedrich², Laura Maragno², Prof. Robert Blick³, Dr. Robert Zierold³, Prof. Kaline Pagnan Furlan¹

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1986 Tribological testing and crystallographic analysis of high hardness, ultra-low friction Mo-S-C thin film coatings with self-assembling tribolayers

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2002 MECHANICAL AND WEAR PERFORMANCE OF HYBRID POWDER COATINGS: THE ROLE OF CURING CONDITIONS

Mrs. Nataly Elizabeth Calderón Perea¹, Mrs. Laura Gonzalez Mozzicato¹, Mr. Francisco Velasco¹, Mrs. Asunción Bautista¹, Mrs. María Fernández Álvarez²

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2066 The morphology of the INCONEL 686 alloy and WC powder mixtures after mechanical synthesis dedicated for the Cold Gas Spraying process

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2071 Multifunctional Coatings for Harsh Environments

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2072 From passive to active structurally controlled optical coatings for energy and eyewear applications

Dr. Bill Baloukas, Mr. Martin Crouan, Dr. Oleg Zabeida, Prof. Jolanta Klemberg-Sapieha, Prof. Ludvik Martinu

2114 Pulsed laser interference heating of FeSiB ribbons - Structure and properties characterization

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2117 Study of ceramic materials by magnetron sputtering for barrier properties in paper-based food packaging

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2143 Optimization of solution composition and parameters for electrophoretic deposition of SiO₂ coatings on NiTi alloy

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2153 Stress evolution during thin film growth: in situ studies of interface reactivity and structure formation at the nanoscale

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2172 Research on medical Ni-Ti alloy with ZrC coatings deposited by PVD technique

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C5 Advanced Ceramic Materials Processing

293 Ultrafast high-temperature sintering of B₄C with Si aids

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383 Straightforward design of 3D structured SiC objects via a granule-derived FDM technology of polycarbosilane-based formulations

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601 WC based cermets with low additions of Ni

Mrs. Aida Martínez Barja¹, Dr. Begoña Ferrari², Dr. Antonio Javier Sánchez-Herencia², Prof. Jose Ygnacio Pastor Caño¹

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734 Development of ceramic photocurable slurries with metal precursors for the fabrication of functional materials by Digital Light Processing

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913 2D materials-based nanostructured interfaces for advanced membranes and porous materials synthesis for application in energy and environment

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917 From the 1st order phase transition in cristobalite to a compact high-temperature stable chemically stabilized ceramic

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927 Effect of precursors properties and mixing on the development and final properties of dense boron carbide and B-rich boron carbide

Dr. Sébastien Lemonnier¹, Florence Moitrier¹, Julie Rossit¹, Laurine Tersigni¹, Thierry Bourre¹, Georg Guetter¹, Jérôme Christen¹, Dr. Anthony Bracq¹, Dr. Fabian Delorme¹

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1157 Sol-gel derived SiOC(H) particles as inorganic components of hybrid bigels based on polyelectrolyte complexes for HIV prevention

Mrs Silvia Gómez-Peral, Dr Araceli Martin-Illana, Dr Raul Cazorla-Luna, Dr Fernando Notario-Pérez, Dr. Aitana Tamayo¹

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1247 Novel multi-functional porous Si₃N₄-SiC composite for high-temperature applications

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1422 Establishing a processability window for laser processing of regolith simulants: Ex-situ analysis and in-situ monitoring

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1429 Thermo-Mechanical and Tribological Analysis of WC/Ti(C,N)-FeNi Ceramic-Metallic Compositions Obtained By Colloidal Processing

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1439 From the properties of ceramic slurries to sintered elements - shaping through aqueous-based ceramic suspensions.

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1471 Shaping of ceramic beads via UV curing assisted drop-casting method

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1488 Challenges and new solutions in manufacturing ceramic matrix composites

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1715 Colloidal processing of ceramic matrix composites

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1745 3D printing of ceramic materials reinforced with metallic nanoparticles

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1763 Effect of process parameters and feedstock composition on the functional properties of 3D-printed ceramic-based composites

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1766 Smart Ultraporous OD-Nanocarbon Containing Ceramic Composites for Environmental Remediation

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1823 Silicon-based ceramics: influence of sintering atmosphere

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1968 Sandwich Structured SiCf/Si3N4 Composite with Discontinuous Absorption Attenuating Layer for Temperature-Insensitive and Broadband Microwave Absorption

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1969 Interfacial Mechanics and Polarization Behavior of Structural-Functional-Integrated SiC/Si3N4 Composites in Different Fiber Preform

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1971 Multiscale synergistic design of SiCf/SiBCN-based metamaterial for high-performance electromagnetic wave absorption in a wide temperature domain

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1981 Achieving High-Temperature Stable Structural Color through Nanostructuring in Polymer-Derived Ceramics

Dr. Benedikt Winhard¹, Alberto Gomez-Gomez², Laura G. Maragno¹, Dr. Diego Ribas Gomes³, Prof. Kaline Pagnan Furlan³

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2008 Processing, microstructure development and mechanical properties of reactively sintered SiC ceramic composites reinforced with various NbC fillers

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2060 UV-Curing-Assisted Drop-Casting as a novel approach in the production of ceramic beads

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2092 SiOC-Based Strain Gauge with Ultrahigh Piezoresistivity at High Temperatures

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2150 Electron Paramagnetic Resonance Spectroscopy of Fast and Ultrafast Sintered 3YSZ Ceramics

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C6 Advanced Polymers and Composites Processing

15 Modeling the Extrusion Process of PPS Solar Collectors

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362 Advanced Finite Element Modeling of Reinforced PPS Extrusion for Solar Thermal Collectors: Integrating Crystallization Kinetics and Thermo-Mechanical Behaviour

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721 Experimental quantification of the uncertainty in the mechanical properties of short fiber reinforced thermoplastics

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805 Revalorization of Ion Exchange Resins in elastomeric matrix

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971 Potential of pultrusion for the production of C/C composites

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995 Enhancing Sustainability in Polymers: Gum Rosin as a Key Component for Green Solutions

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1279 Discrete Element Method Approach for Powder Flow Modelling in Rotational Moulding

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1353 Incorporation and Optimisation of Post-Consumer Recycled (PCR) Polyethylene for Advanced Rotomoulding Applications

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1437 Engineering Lignin/Recycled Polymer Composites as Precursors for Sustainable Carbon Fibers

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1821 Roll to Roll Manufacturing of Multifunctional High-Nanotube-Content Nanocomposite Fabrics
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2144 Enhancement of UV Resistance and Water Repellency in Aramid Nonwoven Fabrics via TiO₂ and HDTMS Coating

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2145 Beeswax Content Effects on Mechanical Properties and Antioxidant Activity of Beekeeping Foundation Sheets

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2147 Preparation and characterization of eco-friendly composites utilizing waste leather and water-dispersed polyurethane

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2149 HYBRID BALLISTIC HELMET MADE IN A ONE-STEP PRESSING PROCESS

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222 Direct Laser Writing of hybrid biocompatible 3D scaffolds for tissue engineering

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889 Laser Beam Welding of IN625: optimization of process parameters

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1158 Porous ceramics from laser surface melting of eutectic mixtures: Mg-stabilized zirconia

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1183 On synergy of theory and experiment in ultrashort laser irradiation of bandgap materials

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1376 Fabrication of Raman-Nath and Bragg diffraction gratings on ophthalmic polymers by ultrashort laser pulses

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1387 Ultrashort pulsed laser-assisted biomineral coating on an additive manufactured Ti64 implant for enhancing osseointegration

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1394 Effect of doping on the formation and coherent propagation of LIPSS in zinc oxide films induced by fs-laser irradiation

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1627 Ultrafast structural transformations of Fe under sub-ps pulsed laser annealing

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1788 Laser surface alloying of 316L stainless steel with 316L+20wt% Cu alloy

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1846 Femtosecond Laser 3D Printing of Nanocrystals via Two-Photon Absorption for Enhanced Biomedical Chiral Sensing

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1858 The influence of laser surface treatment on the microstructure and friction-wear properties of Ti
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743 Deformations in large aluminium automotive subframes

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931 Experimental Study of Dissimilar Yb: YAG Laser Beam Welded Inconel 718 to Ti-6Al-4V

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983 Analysis of Austempered Ductile Iron Castings Reinforced with Titanium Carbides

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1118 Solidification and structure of thin-walled austenitic ductile iron castings

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1178 Investigation of medieval arquebuses made from malleable iron

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1198 Additively Manufactured short carbon fibre reinforced Polymer and Aluminium alloy Multi-Material joints using Friction Stir Welding (FSW) for light and thermal management applications in the transport sector.

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1513 Optimization of A-TIG welding for X5CrNi18-10 stainless steel

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1522 Influence of brazing parameters on the microstructure and mechanical properties of nickel-based superalloys joints

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1638 Influence of weld-related thermal cycles on the sensitization of AA5XXX

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1720 Microstructure comparison of welded Nitinol thin foils with linear, oscillating and pulsed laser beam

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1738 Experimental evaluation of TIG lap welds made from 316L sheets for use in liquid hydrogen storage tanks.

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1782 Identification of the dissipative micro-mechanisms during mixed-mode fracture of pressureless silver sintered joints in power packages

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1983 High-temperature interactions of amorphous alloys TiCuZrPd with a Kovar substrate

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2112 Component-test for determination of welding residual stresses and their effect on stress relief cracking in thick-walled welds

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C9 Thermomechanical Processing, Severe Plastic Deformation & Nanostructuring

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16 Recrystallization mechanisms activated during multi-pass forging of austenitic stainless steels

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20 Textural evolutions in aluminum alloys building by multi-layer friction surfacing (MLFS) deposition

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178 Microalloyed steel wires reinforced with a titanium core

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267 Application of the stochastic model of thermomechanical processing to simulation of the evolution of heterogenous microstructures and evaluation of the uncertainty of the product properties

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311 Enhancing mechanical properties of NbTi alloys by thermomechanical processing

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377 Cooling Effect of Remaining Water Layer on Various Steel Surfaces

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607 HPT processing of Cu-Mo composites with tailored properties for thermal management

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673 Effect of Stacking Fault Energy Regulation on the Microstructure and Mechanical Properties of Cu-Al-Zn-Sn Alloys

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708 Carbon Nanomaterials Reinforcements in Inconel 718: Enhanced Strength, Thermal Stability, and Tribological Characteristics

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747 The influence of thermal interference fit value on the stress and strain distribution in the area of divided tools used in the dynamic hot hammer forging process

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894 Severe Plastic Deformation for Processing of Additive-Manufactured Alloys

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1939 Grain boundary engineering in nanostructured metals

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1959 Microstructural aspects of plastic deformed martensite decomposition in the Ti-6Al-4V alloy

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1974 Mechanical and electrochemical analysis of AA5083- AA7075 dissimilar alloy joints fabricated by friction stir welding

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2061 Evidence for a new work hardening stage at colossal strains

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2070 Effects of Severe Plastic Deformation under the particular conditions of the KoBo Extrusion Process of Various Metallic Materials

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606 Accurate nanoscale temperature determination in in-situ TEM heating using PEET

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760 THICKNESS-DEPENDENT INTERFACE AND SURFACE POLARITY IN INFINITE-LAYER NICKELATE FILMS AND SUPERLATTICES

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761 In-situ insights into interfacial processes at reactive liquid-solid interface during magnesium corrosion using cryo-atom probe tomography

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1050 Multi-modal in-situ electron microscopy and spectroscopy of high-temperature structural evolution in phase-change and nanostructured materials

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1077 4DSTEM-in-SEM in event driven mode to characterize metallic materials

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1149 Enhancing the photocatalytic performance of carbon nitrides through controlled local structure modification

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1268 Towards Single-Pattern Absolute HR-EBSD without using Simulated Patterns as Reference

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1328 Resolving Overlapping EBSD Patterns Using Iterative Dynamic Template Matching

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1404 Development of a High-Throughput method for Microstructure Analysis of Aluminum HPDC components

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1460 New insights into luminance quantification via correlated photoluminescence and confocal Raman microscopy

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1594 Detection of magnetic circular dichroism from individual atomic planes in a scanning transmission electron microscope

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1612 High sensitivity electron holography combined with in situ biasing for studying dielectric and ferroelectric nanocapacitors.

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1730 Correlation of feldspar crystalline phases with measurement artifacts in confocal Raman microscopy

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1779 Atomic resolution DPC-STEM imaging of magnetic signal in antiferromagnets

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1808 EDS and EELS of Lithium in a 0.5 to 30 keV Electron Microscope

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2186 Advanced Microstructure Characterization to Decode Solidification and Phase Transformation Induced in Additively Manufactured Tool Steel

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90 Development of an Integrated UTM and PIXE System with Proton Beam Irradiation for Real-time Material Testing

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108 Development of a PIXE Analysis System Using the MC50 Cyclotron Beamline

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299 Resolving the limits of the J-integral in a nanocrystalline Cantor alloy using multi-method stress-strain mapping

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324 Advancing 3D/4D Diffraction Imaging: ESRF's New ID03 DFXM Beamline

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515 Nanoscale examination of degradation in copper metallization layers using lab-based nanoTXM and DFXM

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539 Dual Synchrotron X ray diffraction approach to strain imaging: application to quantum devices.
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563 In situ study of precipitation kinetics in friction extrusion and consolidation of Al alloys using FlexiStir

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592 Operando Neutron and X-ray Diffraction: A Window into Microstructure Evolution in Laser Powder Bed Fusion

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617 Structure-Property Relationships across Gradient Thin Films on Non-Planar Substrate Geometries

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672 Local Lattice Distortion Analysis of TiVZrNb Lightweight High Entropy Alloys Using Pair Distribution Function (PDF)

Mrs. Juree Jung^{1,2}, Mr. Jongtae Kim^{1,2}, Dr. Leeseung Kang¹, Prof. Jiwoon Lee³, Mrs. Mihye Lee¹, Dr. Konrad Kosiba⁴, Prof. Donghyun Bae², Dr. Junhee Han¹

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819 3D Mapping of Intragranular Strain and Microstructure in Recrystallized Iron Using Dark-Field X-ray Microscopy

Mrs. Virginia Sanna¹, Dr. Yubin Zhang, Prof. Wolfgang Ludwig, Dr. James Ball, Mr. Abderrahmane Benhadjira, Dr. Marilyn Sarkis, Dr. Carsten Detlefs, Dr. Can Yildirim

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848 X-ray diffraction mapping at the DanMAX beamline - Large areas, texture, and tomography

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849 Using Small-Angle Scattering to Investigate the Structure of Mesoporous Silica and the Spatial Arrangement of Ionic Liquid Films at the Pore Surface

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879 Synergetic use of powder diffraction and electron backscatter diffraction

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1071 3D Intragranular Orientation Mapping in Cold-Rolled Ferrite at Industrially Relevant Deformation Levels

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1092 In Situ Deformation Experiment at the Swedish Materials Science Beamline at PETRA III

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1163 Analytical characterisation of nuclear material by multiscale approach

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1386 Ultrafast melting of polycrystalline Palladium: bridging experiment and simulation with X-ray free-electron laser probing

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1412 Advanced operando X-ray diffraction to explore power electronics in space and time

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1502 Influence of trace and tramp elements on the phase transformation behavior of low-carbon steel analyzed by in-situ high-energy X-ray diffraction

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1523 Advancing Laboratory-Based 3D X-ray micro-beam Diffraction for Multiscale Materials Characterization

Dr. Yubin Zhang¹, Dr. Jette Oddershede², Dr. Anthony Seret³, Dr. Azat Slyamov², Dr. Jan Kehres⁴, Dr. Florian Bachmann², Dr. Carsten Gundlach⁴, Dr. Ulrik Olsen⁴, Dr. Jacob Bowen², Prof. Henning Poulsen⁴, Dr. Erik Lauridsen², Prof. Dorte Juul Jensen¹

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1615 High-energy synchrotron X-ray diffraction and its applicability for depth-resolved residual stress analysis

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1680 Welding at the Beamline, the Beamline P61A and it's use for Materials Manufacturing Research

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1693 X-Ray Stress Tensor Tomography

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1781 xrd_simulator: Towards a PyTorch-based framework for FEM simulation of crystalline materials and diffraction experiments

Dr. Marc Raventós¹, Dr. Axel Hennigsson², Dr. Catalin Popescu¹, Dr. Leila Panahi¹, Dr. Oleg Usoltsev¹, Antonio Camps¹, Dr. Lucía Aballe¹, Dr. Klaus Attenkofer¹, Dr. Joaquín Otón¹

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18 Influence of the interfacial strength on wear resistance in Ni-SiC composite

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29 Defects in glass to metal bonds of electric terminals for hermetic seals

Mrs. Julia Puntigam¹, Mr. Markus Spoerk², Mr. Michael Gartner², Dr. Andreas Egger², Dr. Fabio Eduardo Machado Charry³, Assoc.Prof. Dipl.-Ing. Dr.techn. Norbert Enzinger¹

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53 Elastic Microstructures in Bulk Metallic Glasses — Are They Real?

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84 Nanoindentation and Defect Dynamics in Irradiated Fcc NiFe_{1-x} Alloys: Insights from Experiments and Atomistic Modeling

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275 Residual stress and machining path optimization based on artificial intelligence

Ph.D. Hyunsung Choi, Mr. Min Jae Baek, Mr. Shin Youn Woo, Mrs. Yunji Cho, Ph.D. Hyeonil Park, Ph.D. Moo-Young Seok, Ph.D. Dong Jun Lee, Ph.D. Yong Nam Kwon, Mr. Chan-Uk Jeong

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347 High Strain Rate Mechanical Behavior of Structurally Graded Materials Processed by Surface Mechanical Attrition Treatment (SMAT)

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350 Enhanced mechanical and tribological properties of nitrogen-doped PVD MoS₂ coatings in rolling-sliding contact

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357 Orientation dependence of serrated flow: insights from microcompressed Mg-Gd single crystals

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378 In-situ SEM micro-shear experiments to evaluate the failure modes of metallization interfaces in electronics

Mr. Christoph Sander¹, Juliane Posseckardt¹, Sylvia Conzendorf¹, Emanuele Cattarinuzzi², Francesco Somaini², Samuele Sciarillo², Irene Baldi², Vincent Coutellier³, Simona Spadoni², André Clausner¹

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384 High-Temperature Nanoindentation Behavior of Single-Crystalline Titanium: A Molecular Dynamics Study

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389 Investigating humidity-driven variations in fracture toughness of alumina using microcantilever testing and Gaussian regression approach

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405 Multiscale Modeling of Creep Deformation in 30CrMoNiV11-5 Steel: Integrating Mean-Field Theory, Dislocation Dynamics, and Experimental Validation

Dr. Fan Chen¹, Mr Rojas Ulloa Carlos Eduardo, Olivier Dedry, Prof. Jérôme Tchoufang Tchuindjang, Rishabh Bharadwaj, Prof Aarne Pohjonen, Anne Mertens, Prof Anne Marie Habraken

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430 Atomic scale simulations of plasticity in Cu/Ag nanolamellar systems

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431 Atomistic Mechanisms of Dislocation Motion and Reaction in Laves phases

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432 Molecular dynamics study of nanotwinned gold thin films deformation

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446 In-Situ TKD Tensile Testing Reveals Complex Nanoscale Deformation Twinning in Rhenium

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451 Tensile Twinning in Magnesium: A Correlative Nanomechanical and Atomistic Study

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473 Effect of polishing on near-surface residual stresses in commercially pure titanium

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522 Strain rate dependence of slip vs. twinning in c-axis compression of α -titanium

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554 Plasticity beyond Fundamental Building Blocks: A Case Study of Sm-Co Intermetallics

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580 Multiscale Modelling of Superplasticity of Ti-6242

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612 Micro-texture dependent variation of microscale residual stresses in Ti-6Al-4V

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632 Lattice strain distribution in BCC polycrystals - How does the local grain neighbourhood influence microstructural strain level

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745 Accelerated discovery of novel materials: The need for high-throughput analysis of crystal structure, chemical composition, mechanical and functional properties integrated into a single instrument combined with machine learning

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775 Modeling of single crystals and polycrystals of NiAl using the Deformable Discrete Element Method

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784 Mechanical properties of RE-Ni₂ Laves phases and effect of vacancy on partial dislocation motions

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814 The origin of interface stress transition in Cu/W nanomultilayers

Dr. Yang Hu¹, Dr. Giacomo Lorenzin¹, Dr. Jeyun Yeom¹, Dr. Manura Liyanage², Prof. Dr. William Curtin², Dr. Lars Jeurgens¹, Dr. Jolanta Janczak-Rusch¹, Dr. Claudia Cancellieri¹, Dr. Vladyslav Turlo¹

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827 DVC-Driven Analysis of Mechanical Deformation in SLM WE43 Scaffolds with In Situ X-ray Characterization

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875 Finite element modeling of effective mechanical properties of multiphase metal matrix composites with various interphase zone

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1000 Separation of humidity, strain rate and temperature effect on the orientation dependent micromechanical properties of cortical ovine bone

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1032 Ab initio simulations of small nanoparticles mechanical properties

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1087 Mechanistic Insights into Strengthening via Precipitate Assemblies Using In Situ Micropillar Compression of Ni-Cr-Al-Nb Alloys

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1145 Micromechanical Assessment of Electrodeposited Zinc Coatings: A Comparative Study of Spherical Nanoindentation and Micropillar Compression

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1154 Evaluation of Strain Rate Sensitivity in a Superplastic Zn-1Cu Alloy: A Comparative Study of Nanoindentation Instrumental Effect

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1167 Stress-strain Relationship of Metals by Indentation Tests

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1182 Insights into the Origins of Friction in Hard Materials from Two-Axis Nanoindentation

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1188 Toward High Strain Rate Nanoindentation Testing

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1264 In situ Transmission Kikuchi Diffraction (TKD) Tensile Testing

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1297 High-strength and non-brittle crystalline-amorphous PVD-ALD nanolaminates of amorphous alumina and AlCoCrFeNi high-entropy alloy

Mr. Samuel Bojarski^{1,2}, Dr. Simon Tsianikas^{1,3}, Dr. Amit Sharma^{1,4}, Dr. Chunhua Tian^{1,5}, Dr. Tijmen Vermeij¹, Dr. Johann Michler¹, Dr. Xavier Maeder¹

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1299 How experimental micromechanics can help in the design of High Temperature Superconducting magnets

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1308 Metal-Ceramic Nanolaminate Design for Enhanced Mechanical Properties

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1326 High-Speed nanoindentation mapping for a deeper understanding of microstructures

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1352 The impact of grain boundary states on mechanical failure in nanocrystalline materials

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1389 A novel approach to determine the brittle-to-ductile transition temperature via dynamic nanoindentation

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1414 In situ TEM tensile testing of small-scale model systems to study the effect of ordering and interfaces

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1449 A novel 3-electrode-based backside H-charging setup for in-situ micromechanical study: Development and demonstration

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1475 Dynamic Nanoindentation – A Key to Advanced Materials Understanding Under Extreme Conditions

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1534 Creep Dominated High Cycle Fatigue of Freestanding Gold Thin Films: Microstructure and Temperature Dependent Deformation Mechanisms

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1541 MecaNano COST Action - European Network for the Mechanics of Matter at the Nano-Scale

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1547 A combined experimental-computational study of the compression of hemispherical nanoporous gold nanoparticles

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1575 Impurities Affecting Grain Boundary Cohesion in Nanostructured Tungsten: A Micromechanical Study

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1580 Multi scale micromechanical testing for new Polymer Core Solder Ball (PCSB) interconnections reliability in operating conditions

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1633 Identification of material parameters by analyzing indentation test data using neural networks

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1646 Hot-Working Characteristics and Microstructural Evolution of INCONEL 625 Multiphase Superalloy

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1686 Micro scale fracture and fatigue of electrolytes for solid state lithium ion batteries

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1688 Unsupervised learning of nanoindentation data of complex materials

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1716 Deformation twinning induced mechanical properties of layered twin-matrix FCC metallic materials

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1767 Statistics of micro-deformation mechanisms of HCP zinc coatings quantified by SSLIP analysis of in-situ EBSD-SEM-DIC testing

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1770 Indentation stress relaxation tests for studying transient plasticity in metals

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1838 In situ TEM investigation of fracture growth in novel nanolaminate thin films

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1848 Plasticity of olivine at high strain rates: an experimental micromechanics study on meteorite impact dynamics

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1912 Effect of temperature, strain rate and grain size on the strain partitioning in the Alloy 718 up to 650 °C: A HR-DIC investigation

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1955 INNOBIO Project – Predicting the behavior of casted bioceramics

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1988 Crystallinity and mechanical properties in glass-ceramic glazes by Raman Spectroscopy

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2034 Delineating thin-film microstructure contributions during ultrafast laser irradiation using atomistic simulations

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2038 Influence of material properties on the mechanical behavior of architected structures

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2104 Exploring Mechanical Properties of Soft Materials at the Nanoscale Using Indentation Methods

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2122 A High-Throughput Framework For Pile-Up Correction In High-Speed Nanoindentation Maps

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22 Layered nanostructured magnesium alloys for hydrogen storage synthesized by accumulative fold-forging (AFF)

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39 Component test for the assessment of in-service welding on/onto pressurized hydrogen pipelines

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424 Tracking hydrogen in metals: permeation and thermal desorption study using a deuterium tracer

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493 Hydride-Driven Formation of Zirconium Islands in Irradiated Fuel Claddings: Alloying Element Segregation and Implications for Structural Nuclear Materials

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543 Multi-Scale Computational Study of Hydrogen Adsorption and Phase Transitions in Metal-Hydrides for Energy Storage

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599 Characterizing hydrogen in amorphous alumina thin films through integration of modeling, theory, and experiment

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759 OPTIMIZATION OF ALPHA AND GAMMA ALUMINA CATALYSTS VIA ADDITIVE MANUFACTURING

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772 Effect of gaseous hydrogen on polyethylene pipe materials

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1012 Digital material design guidelines for mitigation of hydrogen embrittlement

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1045 Hydrogen embrittlement of precipitation hardened austenitic alloys at liquid helium temperature – The role of hydrogen diffusivity and serrated flow

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1327 Characterization of the H₂-rich fuel combustion process - model and experimental approach

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1385 The impact of hydrogen on mechanical properties of nickel: a hybrid grand canonical Monte-Carlo/molecular dynamics study

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1388 Multi-species diffusion model for hydrogen within actual steel microstructure

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1431 The influence of copper on the distribution and trapping of hydrogen in steels

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1447 Hydrogen embrittlement mechanism in additively manufactured stainless steel

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1504 Numerical simulation of pressurized microtubular reversible solid oxide cells for hydrogen production

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1550 Influence of ceramic additive in thermoplastic polymers for liners in Type IV hydrogen tanks

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1584 Investigating Hydrogen Embrittlement in Superalloys: The Role of Intermetallic Phases

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1696 Ab initio and atomistic simulations of defect induced hydride formation

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1972 Multiscale Modelling of Hydrogen Diffusion in Polycrystalline Metals

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2023 LOW TEMPERATURE CATALYTIC SUPERCRITICAL WATER GASIFICATION FOR CONTINUOUS HYDROGEN GENERATION FROM BIOMASS WASTEWATER

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2030 Hydrogen risk mitigation using high-porosity autocatalytic materials

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2108 Atom probe tomography and advanced thermal desorption spectroscopy for atomic scale characterisation of hydrogen in materials

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D5 Advanced Biomaterials - Characterization and Modelling

203 Influence of Synthesis Parameters on the Microstructure and Porosity of Hydroxyapatite

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304 Restoration of physiological conditions in the assessment of the biocompatibility of SiO₂ coatings deposited on Nitinol cardiovascular implants through electrophoretic deposition

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494 Biomechanical and Microstructural Characterization of Biocompatible Metamaterials for Surgical Applications

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640 Advanced biomaterials for pediatric miniaturized heart pumps – characterization and modelling
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807 Modelling and Experimental Verification of the Freezing Process in Ice Templating
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1067 Microbiological techniques assessing the infection risk associated with materials designed for laparoscopic instruments

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1220 Tunable nano-Rare Earth oxides for pAthogen mitigation (TREAT)

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1292 Advanced multifunctional biomaterials supporting bone tissue regeneration and healing

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1382 Bridging In Vitro and In Vivo Degradation of Biodegradable Implants: An ODE-Driven DoE and Uncertainty Quantification Approach

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1510 Engineering Biocompatible Surfaces with Oligoproline: A Powerful Anti-Biofouling Peptide

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1557 Characterization of osteoarthritis bone changes with nano-CT observation

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1571 New generation copper-based coatings of improved antimicrobial resistance to pathogens

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1631 Biodegradable polymer coatings release active ingredients in implantology

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1632 Influence of UV polymerization conditions on the physicochemical properties of temporary dentures fabricated by the Digital Light Processing additive manufacturing

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1707 Effect of Post-Processing Parameters on the Surface Properties of Ti6Al4V Scaffolds Manufactured by SLM

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1708 Artificial staining of 3D X-ray virtual histology of bone implants through deep learning

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1211 First principles modeling of short-range order in Fe-Si-Al alloys

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1311 Investigation of Carbide Effects on the Mechanical Properties of AISI 420 Steel by Crystal Plasticity Simulation

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1527 Machine learning-enhanced modeling of interactions between diamond surfaces and protein sequences

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1629 Modeling complex diffusion phenomena in compositionally-graded single-crystal Ni-based superalloys

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1701 Metastable defect phase diagrams as roadmap to tailor chemically driven defect formation

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1722 Unraveling Atomistic Mechanisms of Pressure-Induced Phase Transitions in Silicon and Germanium

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1876 Foundation Models For Aluminium Alloys

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258 A unique authenticator for additively manufactured parts derived from their microstructure

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1055 ML-driven optimization of corrosion inhibitor mixtures with an automated platform

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1197 Digital representation of physical metallurgical knowledge

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1271 Enhancing FAIR Data Management in Materials Science and Engineering (MSE): Integrating FAIR Digital Objects into the MSE Knowledge Graph

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1833 Building a Legacy Lab for Advanced Functional Materials: Integrating Synthesis and Characterization Capabilities

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1937 A seamless dataflow combining material, virtual engineering workflows and production data in the project lifecycle

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2003 Accelerated steel development on the ALPmat platform

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2032 Automating Knowledge Graph Composition for Multi-Scale and Interdisciplinary Research

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2171 Representing MSE Research Metadata Using the NFDI MatWerk Ontology: Patterns and Use cases

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639 High-throughput hard X-ray reflectometry to investigate interfaces in materials

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763 High-Throughput Materials Informatics Integrating Ab Initio, Machine Learning, and CALPHAD Data

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860 Optimized Electrodeposition of Multi-Principal Element Alloys through Automation by Material Acceleration Platform

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984 Phase transformations during post-processing of metastable β titanium alloys fabricated through additive manufacturing

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1351 Gas adsorption meets deep learning

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1772 Combined high-throughput computational and experimental screening of aluminum alloys suitable for additive manufacturing from scraps

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635 Deep learning based strategies for noise reduction of synchrotron X-ray nano-tomography images of light alloys: investigation on experimental extensive dataset.

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867 Machine learning approaches for the determination of liquidus and eutectics

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977 Multiscale modeling of microstructure formation in re-heating and quenching process for understanding creep related properties of large shaft

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1016 Machine Learning-Driven Prediction of Mechanical Properties in Resorbable Magnesium Alloys for Biomedical Applications

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1173 Using Computer Vision and Microstructure Informatics to Characterize Dendrite Growth in Ni-base Single Crystal Superalloys

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1229 Optimal Discovery of multi-dimensional Pareto Sets in High Entropy Alloys

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1288 MicrostructureDB: An AI-Powered Open Data Platform for Materials Characterization

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1304 Effect of microsegregation on phase transformation behaviour and microstructural evolution in a continuously cooled 1CrMoV bainitic steel

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1337 Materials Design and High-throughput Screening of Multicomponent High-temperature Coatings Accelerated by Artificial Intelligence

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1378 Can AI Clean Up Your Characterization Data? Modern Approaches to Historical Dataset Curation

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1380 AI for Materials Industry: An Open Online Course

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1381 Real or Fake? Evaluating synthetic Electron Microscopy Data in Materials Science

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1538 A common workflow description for experimental and computational materials science

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1561 EMMO Ontology enabling AI-based innovative advanced materials development: the CoBRAIN Knowledge Base for Hardmetal Thermal Spraying Coatings

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1567 Effects of cooling rate and tempering on the microscale mechanical properties of heat resistant steel (30CrMoNiV5-11)

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1583 Bayesian Active Learning for Physics-Informed, Multi-Constraint, Multi-Objective Alloy Design: A Probabilistic Approach

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1667 Leveraging AI and Genetic Algorithms for Self-Healing Alloy Design

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1758 Advancing Interoperability and Digitalization in Materials Science and Manufacturing: A Semantic Workflow Module for Standardized Data Management

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1765 Multiscale mean-field framework for process-structure-property prediction in large-scale component manufacturing: A case study of turbine shaft forging

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1967 Machine Learning Approaches for Predicting Engineering-relevant Material Properties

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2044 Advanced Correlation Analysis of Process-Microstructure-Property Relationships in LPBF AlSi10Mg: Beyond Traditional Metrics

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354 Effects of different surface treatments on the fatigue behaviour of AlSi10Mg alloy produced by Powder Bed Fusion-Laser Beam: a comparison between machining, sandblasting and Ni-9%P+(a:C-H)DLC multilayer coating

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1091 Environmental impact assessment of battery module lifecycle: a comparative evaluation of components replacement in the circular economy concept

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1391 Sustainable Recovery of Critical Raw Materials through Advanced Hydrometallurgical Recycling

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1418 Additive manufactured complex cooling channels for High Pressure Die Cast (HPDC) electric power train components for automotive applications

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1432 Advanced Laser welding processes for joining of High Pressure Die Casting (HPDC) components made from secondary aluminum alloys

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1476 Multiscale models combined with LCA design framework to conceive sustainable and circular energy storage systems

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1657 Sustainability Assessment of Hydrometallurgical Recovery of Platinum Group Metals from End-of-Life Hydrogen Fuel Cells and Electrolyzers

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1830 Multi-material Lightweight Design with Aluminum-Steel Hybrid-Casting: Process Parameters and Influencing Factors

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1894 3D-Printed integrated circuits for adhesive joints disassembly and locally thermal curing

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1908 Aluminium matrix composites with recycled alloys for lightweight automotive brake discs

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1975 Fe, Cu and Zn modification strategies in recycled AlSi10MnMg alloy: insights from high-pressure die casting (HPDC) and gravity casting processes.

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540 Enhancing thermal performance of micro-nano Al/SiC/cBN hybrid composites made for satellite applications via nitride-induced self-forming method

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838 Gravity independent Additive Manufacturing of an Al-Si alloy by Molten Metal Deposition (MMD)
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876 Influence of Interfacial Characteristics on the Strengthening Mechanisms of B₄C-Reinforced Aluminum Matrix Composites

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1283 High-Throughput Screening of Precipitates in Al-Cu Alloys Using Compound Big Data for Aerospace Applications

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1310 Thermal conductivity and dynamic oxidation resistance of additive-free silicon carbide ceramics

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1354 In-space 3D printing of Li-ion batteries by Fused Filament Fabrication

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1359 Unveiling δ Phase Strengthening Mechanisms in LPBF-Processed Inconel 718 at Elevated Temperatures

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1503 PEEK composites with carbon nanoparticles for high performance applications

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1532 TEMPUS - A microgravity electromagnetic levitation facility for parabolic flights

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1679 EML – Electromagnetic levitator onboard the ISS: investigation of thermophysical properties & solidification of liquid metals

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1817 Alloy Design for Magnesium Alloys in Aerospace Applications: Optimizing Strength and Thermal Conductivity

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1828 Effect of the use of new aviation fuels on polymeric materials for use in aircraft

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1897 Advanced Sustainable Composite Materials Based on Renewable Resources for Space Applications

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1938 Pt nanonetwork coatings for spacecraft charging mitigation in photovoltaic solar arrays

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1947 Fully-recyclable CNT sheets for multifunctional thermoset and thermoplastic composites

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1951 Space experiments on High-Temperature Molten Oxides, Metals and Alloys Using an Electrostatic Levitation Furnace on the International Space Station

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2009 Shaping the future of space exploitation with advanced materials and processes

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2029 ISRU-approach on designing and fabricating successfully composite materials on the lunar soil

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E4 Energy Storage

85 Dendrite Growth on Aluminum Anodes in Non-Aqueous Aluminum Batteries: Influence of Alloying and Electrolyte Chemistry

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195 Thermophysical and surface properties of Al-Sn miscibility gap alloys (MGA) phase change materials for Thermal Energy Storage applications

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248 Development and characterization of solid-liquid metal alloys phase change materials for high temperature thermal energy storage

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443 Melt-spun Cu-Al based ribbons as current collectors for Anode-Free cells in ASSBs

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460 Containment of metallic phase change materials for latent heat thermal energy storage solutions
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511 Electrifying foil characterization – Mechanical characterization of electrode materials for simulation purposes

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534 Development of Additively Manufactured Anodes for Aluminum-Air Batteries: Influence of Microstructure on Performance

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583 Study of the degradation mechanisms of a thermal energy storage system based on molten metal
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596 Electrochemical Charging of MAX Phases and MXenes as Candidates for Hydrogen Storage Materials

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634 Development of a Machine Learning Model for Estimating Microstructural Phase Fractions in Compacted Graphite Iron (CGI)

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678 Investigation of Processing and Microstructure on Electrode Materials for Fe-Air Battery Performance

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924 Polymeric waste shells for developing new microencapsulated phase change materials (MPCM)

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945 Multimodal Microscopy and Spectroscopy for Battery Characterization: Understanding Degradation Mechanisms

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974 Mechanistic Insights into the Impact of Sulfide-Based Surface Treatments on Iron–Air Anodes

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976 Shape-stabilized phase change materials based on natural rubber

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1029 Uncovering CSP-TES Synergies Aligned with Global and European Roadmaps in the COOPERANT Project

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1168 Negative charged covalent organic framework (N-COF)-based Li ion filtering protective layer for stable Li metal anodes

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1298 Self-healable polymer electrolyte for lithium batteries, targeting light-mediated and 3D-printable processes

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1347 3D Simulations of Ultra-High Temperature Phase-Change Material Storage for Thermophotovoltaic Conversion: The SUNSON-BOX Approach

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1360 Hybrid Sensible-Latent Heat Thermal Energy Storage for Concentrated Solar Power Applications

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1489 Iron oxide-based catalytic structures as enablers of a thermochemical cycle based on solid sulphur for long-term storage of solar thermal energy

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1490 Efficient perovskite-based high-temperature hybrid sensible-thermochemical heat storage systems for integration with renewable energy sources

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1505 A re-investigation of the phase diagram of the disodium hydrogen phosphate/water system and its consequences for latent heat storage applications

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1514 Back to Basics: using conventional techniques to characterize graphite blends components for applications as anode in batteries

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1577 Environmentally sustainable alternatives to Portland cement optimized with phase change materials (PCMs) for low temperature thermal energy storage

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1697 Characterization of microencapsulated phase change materials developed from waste for sustainable constructive materials.

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1872 NEWIRONAGE: IRON AS A FUEL IN NEW ENERGY STORAGE CYCLES

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1936 Improvement in Performance of Energy Storage Technologies through Online Acoustic Emission Sensor-Based Battery Mixing

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2014 Joule-Heated Perovskite Metal Oxides for Thermal Energy Storage

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2024 Processing Al-based MGA systems as phase change materials

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E5 Renewable Energy and Hydrogen Technology

67 PRODUCTION AND CHARACTERIZATION OF NEW MEMBRANES FOR HYDROGEN PURIFICATION BASED ON THE Nb-V-Pd SYSTEM

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174 Study of RF Co-Sputtered ZnS_{1-x}Se_x Alloys for Potential Photoelectrochemical Cell Applications

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182 SAN and ABS polymers as binders for metal hydride pellets for hydrogen storage at the solid state

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183 Role of Co, Cu, Cr, and Al in Recycled TiFe Alloys for Hydrogen Storage

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205 Molecular simulations of nanoporous carbon-based electrocatalyst for H₂ production

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231 Fraunhofer High Performance Center Green Materials for Hydrogen – GreenMat4H2

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262 Effect of Different Dynamic Operating Conditions on the Materials of a PEM Electrolyzer

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268 BiOCl microsphere-based photoanodes and the effect on DSSC performance

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466 Metal-oxide ALD-coated electrospun nanofibers for fluorine-free and freestanding bipolar membranes

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551 Modeling of the hydrophobic treatment of Gas Diffusion Layers to predict PTFE distribution after the drying step

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704 Polymer-derived micro/macroporous Si-C-O-N-based ceramics with integrated catalytically active metal sites to stimulate superior oxygen and hydrogen evolution reaction activities

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732 Modified cryptomelane catalysts for OER

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778 The role of precipitates in hydrogen embrittlement of precipitation hardened Al_{0.35}CoCrFeNi complex concentrated alloy

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792 A joint experimental and computational investigation of Sr_{n+1}(Fe, Ta)O_{3n+1} (1 < n < ∞) catalysts for the Oxygen Evolution Reaction

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858 Optimisation and scale-up of solid oxide fuel cells employing aqueous-based tape casting of anodes and spray pyrolysed active layers

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859 Alkali Metal-Promoted Ru/Al₂O₃ for Optimized NH₃ Decomposition and Electron Density Control

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1137 Atomistic Modelling of Hydrogen Storage in Graphene Using LAMMPS Molecular Dynamics

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1217 Advanced Transition Metal Vanadate Catalysts for Efficient Aqueous Electrochemical NRR

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1218 Selective Dinitrogen Electroreduction to Ammonia on Zn₂V₂O₇ Pyrochlore

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1219 Catalysts of Change: Advanced Ceramic Materials Steering Energy Transition

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1307 Optimising NiCoMn Electrocatalysts for Efficient Hydrogen Production

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1348 Exploring a smart catalysts platform for the electroreduction of nitrogen species into ammonia: materials/performance correlation

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1426 Parametric investigation of the operation of an SO₂ depolarised electrolyser for hydrogen production

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1614 Strategic Needs, Market Opportunities and Technical Advancements in Large-Scale Manufacturing for Wind Turbine Components and Hydrogen Storage.

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1673 Fe/Mo bimetallic phases supported on TiO₂ for N₂ reduction into NH₃ by photo-processes

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1731 Effect of bimetallic Fe-Co catalysts deposited on neodymium oxide on the properties and activity in ammonia synthesis

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1746 Composite electrodes and membranes for energy storage and conversion devices

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1913 Luminescent Solar Concentrators for Efficient and Sustainable Use of Solar Energy

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2091 Compositional Complexity and Structural Disorder as Enablers for the Circular Economy

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2189 Vacuum Insulation Panels for Liquid Hydrogen Storage and Transportation Applications

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E6 Energy Harvesting

280 Multiscale strategies for modelling the working mechanisms of triboelectric nanogenerators for drop energy harvesting

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571 Mechano-Responsive Bio-Piezoelectric Nanofibers for intelligent drug delivery

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627 Energy Harvesting from Post-Consumer Plastic Waste: A Sustainable Approach to Electricity Generation

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1138 Harnessing magnetoelectric coupling at the nanoscale for advanced spintronics

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1230 Exploring multifunctional properties of BaTiO₃ –based ceramics by addition of multi-walled carbon nanotubes

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1236 Material design and development of Pb-free ceramics with improved piezoelectric Figure of Merits for energy harvesting applications

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1238 Exploring the effect of phase superposition in BaTiO₃- solid solution ceramics for enhanced functional properties

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1548 Computational analysis of inverse opal photonic crystals using the RCWA method for photocatalysis applications

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1706 Local vs. macroscopic dielectric and ferro/piezoelectric responses in porous BaTiO₃ ceramics determined on the basis of 3D reconstructed ceramic microstructures

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1768 Design of metallic Phase Change Materials: Surface properties of liquid Al-Si-Sn alloys

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1919 Adamantane plasma polymers as versatile vacuum processable triboelectric thin films for mechanical and droplet energy harvesting

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2010 Preparation of flexible PVDF-BT piezoelectric composite films for energy harvesting

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2059 PLLA-based piezoelectric and magnetoelectric composites for flexible energy harvesting devices

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E7 Thermal Energy Management

127 Advancing Elastocaloric Cooling Solutions through 3D Printing of Superelastic NiTi shape memory alloy

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326 Additive Manufacturing of An Sn-Based Alloy on Silicon Wafer by Laser Powder Bed Fusion for Advanced Cooling of Electronic Circuits

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752 Magneto-mechanical coupling in NiMnGaCu multicaloric alloys: functional experimental investigation under magnetic field

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808 Development and Optimization of Polymer-Metal Composites for Superior Thermal Management

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870 Thermal Optimization for Sustainable Data Center Cooling Using Thermochemical Heat Systems

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928 Novel material development for Ammonia based Thermochemical Heat valorization from Data Centers

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929 Enhancing thermochemical heat storage performance with additively manufactured aluminum alloys: A study on porous matrix design and heat transfer

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964 Kirkendall Effect guided Void Formation in PVD Manufactured Cu-Au Thin Films for low Thermal Conductivity Coatings

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1024 Thermal Characterization of combined Al-Based and Sn-Based Alloys as Composite Phase Change Materials for Thermal Energy Management

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1081 Exploring the potentialities of TPMS-based composite Phase Change Materials

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1090 Innovative and sustainable materials for high temperature Thermal Energy Storage (TES) systems

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1125 Interrelation between Microstructure and Thermal Conductivity of Metal-Graphene Material Systems

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1180 Development of Grcop42/Copper-Inconel 718 multi material structure through laser powder bed usion for heat transfer applications

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1222 Suitability of plasma sprayed AlSi10Mg+Sn coatings for Thermal Energy Management

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1407 Optimization of Heat Transfer Between Phase Change Materials and Thermal Loads Using Thermal Conductivity Enhancers

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1481 Elastocaloric effect in polycrystalline NiMnTi alloys produced through suction casting and melt-spinning processes

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1573 Bio-Waste Derived Activated Carbon for Sustainable Energy Storage Applications

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1616 Hybrid foamed concrete as a porous material for thermal energy management applications.

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1618 Green processes using 3D waste materials- water purification in Energy sector.

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1622 Advancements In Sustainable Concrete for Global Challenges

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1651 Shielding properties of a novel porous concrete towards Electromagnetic Interference

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1655 Exploring the microstructural and electrochemical behavior of the CuMnNiSn alloy for thermomagnetic applications

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1778 Metallic-Phase Change Materials casting: comparison of experimental results with theoretical consideration.

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2196 Non-vanadium aqueous redox flow batteries

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E8 Nuclear Energy: Fission & Fusion

17 Insight into He trapping mechanisms in implanted 9Cr and 14Cr ODS steel for fusion reactor applications

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66 Joining, Coating and Characterization of SiC/SiC and SiC-based cladding materials for safe Nuclear Energy Applications

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96 Thermo-mechanical, lead corrosion and thermal stability assessment of innovative Alumina Forming Austenitic Alloys for LFRs

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186 Accelerated Oxidation of Stainless Steels in Heavy-Water Reactor Spent Fuel Pool Accidents

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187 High-Temperature Oxidation Behavior of Zirconium Alloys in Simulated Spent Fuel Pool Accident Conditions

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234 Overview and status of the IFMIF-DONES Facility

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567 Characterization of cyclic softening effect on EUROFER-97 mechanical properties through combined LCF + tensile tests

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593 Qualification of Materials for Lead-cooled Fast Reactors: Testing standardization and experimental results

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642 Irradiation and corrosion behavior of oxide-forming FeCrAlNi coatings deposited by HiPIMS

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705 Impact of vanadium addition on the mechanical properties and irradiation resistance of FeCrAl-Y2O3-Ti ODS alloys for components of Generation IV nuclear reactors

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773 Solid-State Ionic Characterization of Oxygen and Metals in Lead Nuclear Coolant for the Development of Corrosion Resistance Materials

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802 Plastic deformation in CrMnFeCoNi HEA: Linking 3D EBSD and Molecular Dynamics simulations

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850 Evolution of the microstructure of neutron irradiated RPV model steels with different content of Ni, Mn and Si

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975 Durability of W/WC coating on inner surface of 316L steel Venturi tube in contact with high velocity flow of liquid Pb-Bi eutectic at 350 °C after one year of operation

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1102 Liquid metal embrittlement occurrence by lead and Pb-Bi eutectic of Face-Centered Cubic metallic alloys: austenitic steels and Complex Concentrated Alloys

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1114 Advanced investigations to understand the damage of a Face-Centered Cubic metallic alloy in presence of liquid lead and Pb-Bi eutectic and under mechanical loading

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1259 Mechanical properties of neutron irradiated 316L stainless steel additively manufactured by laser powder bed fusion: effect of post-manufacturing heat treatments

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1284 Harmonization of materials testing for LFR: R&D proposal on guidelines for corrosion tests in molten Pb/LBE

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1285 Corrosion mitigation strategies in molten lead: coatings and advanced alloys for nuclear LFR systems

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1330 Correlation between creep and stress relaxation properties in a martensitic steel

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1338 Three new high alloyed AFA steels for LFRs

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1361 Development of physics-based models for volatile fission products in minor actinide-bearing fuels for generation IV reactors

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1362 On a physics-based model of HBS pores overpressurization and its effects on high burn-up fuel fragmentation

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1515 Microstructural characterization of advanced doped UO₂ fuels

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1555 Development, Qualification and Industrialization of materials for Lead Cooled fast Reactors – The INNUMAT approach

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1610 Investigating Water Radiolysis and Iron Speciation in Water-Cooled Breeding Blanket for DEMO: Implications for Corrosion Mitigation and Surface Effects

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2012 High velocity impact on tungsten: molecular dynamics study

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50 High-Entropy Zirconates as future Thermal Barrier Coatings: Resistance to Corrosion by Volcanic Ashes and Sands

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98 Design and properties of novel innovative insulating materials for high-performance motors of electric vehicles

Prof. Takashi Yamashita¹, Dr. Ayumi Kobayashi¹, Dr. Ryoma Amanuma¹, Dr. Professor Kohei Iritani¹

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955 Computational design of new electrolytes for supercapacitors

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1448 Optimizing press-fit diodes reliability through manufacturing process modifications

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1582 Titanium Production Through Carbon Free Methods - The UAT Process

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1586 Sustainable Synthesis of High-Performance Lithium Nickel Manganese Oxide Cathodes: A Study of Mn-Based Precursors and Calcination Effects

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1877 Development of new equations for unsaturated infiltration.

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1878 Composite materials obtained by reactive infiltration: The Si-Ti-C system

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2193 Sustainable Aviation Fuels from CO₂ and H₂: Additive Manufacturing-Enabled Catalyst Systems

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F1 Biofabrication and 3D printing of biomaterials

235 3D in vitro skin model as broadly available and comprehensive platform for antibacterial therapies

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506 ADDITIVE MANUFACTURING OF BIOABSORBABLE CONTINUOUS WIRE-REINFORCED COMPOSITES FOR TISSUE ENGINEERING

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514 Gelatin Methacryloyl as an effective alternative to conventional matrices for patient-derived 3D models of metastatic colorectal cancer (mCRC).

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658 Advanced composite nano-structured bioactive scaffolds for bone tissue engineering

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815 Macrophage Immune Response to a Skin-Mimicking Biocompatible Matrix: A Functional Insight
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932 Advanced Hydrogel Bioinks composed of Natural Nanofibers and Polysaccharides for 3D Bioprinting applications

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969 Improving Fatigue Resistance in Organic-Inorganic PCL-Based Melt Electrowritten Scaffolds for Biomedical Applications

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1035 Fabrication and Optimization of GelMA Hydroxyapatite Scaffolds for 3D Printing via Digital Light Processing

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1039 Volumetric 3D Printing toward 3D printing complex structures for biomedical application

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1096 Polysaccharides chemical modification for biomedical additive manufacturing

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1208 Cell-Derived Extracellular Matrices for 3D in vitro Tumor Models for Breast Cancer Research

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1255 Smart polymer materials based on fiber spinning and additive manufacturing

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1262 3D Bioprinted Cell-Laden Gel for Autologous Chondrocyte Implantation (ACI) Procedures

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1263 Reactive jet impingement bioprinting with fibre, metal and ceramic substrates for enhanced composite cell cultures

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1364 3D constructs enhanced with nano(bio)materials for functional regeneration of both hard and soft tissues.

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1366 Bilayer electrospun membrane enabling the stimulation of angiogenesis in advanced 3D skin model

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1372 Advanced biofabrication technologies to design in vitro central nervous system models

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1411 Biofabrication of a piezoelectric cardiac patch for the regeneration of the infarcted heart tissue

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1416 Novel biomaterial ink formulations and approaches for in situ bioprinting and regeneration of colorectal mucosa and submucosa

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1419 Bioprinting and electrophysiological evaluation of a 3D cardiomyocyte culture

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1420 Multiscale Perfusable Cardiac Tissue Model Using Electrospun PCL Fibres and a Bioprinted Cardiac Co-Culture

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1480 Coaxial Electrospinning of an Anisotropic Piezoelectric PVDF-based patch for Modulated Drug Delivery in Myocardial Infarction Therapy

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1483 Spray-dried polymeric carriers for in-situ mucosal and submucosal regeneration in colorectal disease

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1674 A Functional AM approach for Biofabricating Micro-Optofluidic Devices for Medical Non-invasive Diagnosis-related Bioapplications

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F2 Smart biomaterials and bioresponsive systems

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340 Solvothermal production of a piezoelectric layer on titanium implant materials

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369 Tailored-magnetic nanoparticles for theranostics in osteosarcoma

Mrs. Ana Laura Coria Gutiérrez¹, Pr. Anna Piperno¹, Pr. Angela Scala¹, Dr. István Puskás², MSc. Sunčica Sukur³, Dr. RNDr. Václav Ranc³, MSc. Mohamed Saqawa⁴, Dr. Monica Montesi⁴

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444 Controlling release kinetics from nanotube drug containers - modulated diameters, capped and multi-molecule filled nanotubes

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481 Characterization of Oxidized Alginate-Gelatin Nanocomposite Hydrogels Incorporating MXene Nanosheets for 3D Bioprinting

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524 Magnetoelectric, bio-hybrid nanointerfaces as enablers of wireless tissue stimulation and drug management

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801 Hydrogels based on natural polymers for the magneto-mechanical stimulation of cells

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837 Magnetic Nanostructured Complex with DFO for Dual Imaging Applications

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1009 Microfluidic Synthesis of Targeted Lipid-Coated ZnO Nanoparticles for Advanced Cancer Immunotherapy

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1066 Stimuli-responsive, drug-loaded nanoconstruct for multiple myeloma treatment: therapy and diagnosis

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1214 New insights into the molecular organization of fluorescent nanovesicle-based bioimaging probes from Molecular Dynamics simulations

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1436 Next-Gen Radioprotection: Thermo-Sensitive Hydrogels for Localized Amifostine Release

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1454 A dual light and magnetic responsive mesoporous silica nanosystem for cancer therapy

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1810 Neuroprotective profile of carbosilane dendrimers as nanocarriers of Memantine against Alzheimer's disease

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F3 Biomaterials for infection control

228 Thymol-Zinc Combinations for the Prevention of Biofilm Formation on 3D Printed Polysaccharide-based Scaffolds

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375 Laser Surface Texturing of Titanium-Based Implant Alloys

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395 Metal Ion-Enhanced Titanium Abutments for Optimized Soft Tissue Attachment

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845 Dendritic zeolites as drug delivery systems to face antimicrobial resistance

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987 Functionalization with an Amino Acid and Silver of Titanium Surfaces for Balancing Cytocompatibility and Infection Control

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1141 Engineering exosome-functionalized electrospun fibres: a new strategy for modulating cellular responses in soft tissue

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1379 Surface modification of bioactive glasses through plasma technology to impart antiadhesive properties

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1398 Functional starch/porphyrin-based materials for wound healing

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1643 3D-printed PEEK with Antimicrobial and Bioactive Coatings Using Vacuum Arc Plasma Deposition
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1795 Surface Design of Faceted Oxide Particles: Boosting Antimicrobial Properties

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1904 Development of a novel antibiotic-doped calcium-phosphate cement for bone infection treatment

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2111 An innovative heparinization strategy for blood-contacting biomaterials: Alternating current electrophoretic deposition for enhanced hemocompatibility and antibacterial properties

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359 Innovative PLA Nanocomposites with MWCNTs and MWCNTs-COOH for Printed Electronics (PE)
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414 ENHANCING THE SENSITIVITY AND REPRODUCIBILITY OF GRAPHENE FIELD-EFFECT TRANSISTOR BIOSENSORS FOR PRECISE LABEL-FREE SARS-COV-2 DETECTION THROUGH OPTIMIZED SURFACE BIOFUNCTIONALIZATION

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1237 Novel nano- and submicron carriers with controlled high enzyme loading for electrochemical sensing

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1333 Laser-induced graphene on synthesized polyimides

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1344 SERS based biosensing: leveraging the ex-vivo potential of a plasmonic sensor for the classification and prediction of cancer patterns

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1403 Tuning the chiroptical response of discrete gold nanoparticles

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1406 Wearable Heart Rate Sensors Based on Laser-Induced Graphene on Alginate and Novel Polyurethanes

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1408 Enhanced Electrochemical Sensing of Doxorubicin Using a Polymer Nanocomposite-Modified Screen-Printed Carbon Electrode

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1525 Optimization of Liquid-Gate Graphene Field-Effect Transistors for Enhanced Sensing Reliability and Portable Characterization

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1569 Microbial production of silver nanoparticles: characterization and applications

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1645 Engineering Fluorescence Resonant Energy Transfer (FRET) via plasmonic systems for ultra-sensitive biosensing

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1737 SERS-based platform for mutation analysis in acute myeloid leukemia

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1750 Microfluidic based LC sensor and antennas with tuned performances using liquid conductors

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1853 High-Sensitivity Graphene Liquid-Gate Transistors for Next-Generation Biosensing Applications

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1928 SERS-on-a-chip as an excellent tool for the One Health approach of AMR monitoring

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2025 Electrically Controlled Molecular Motions Tracked by Graphene-Enhanced Fluorescence Lifetime Microscopy

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372 Combining In Ovo Testing and MicroCT Imaging to Assess Tissue Integration and Angiogenesis in Porous Scaffolds

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495 Protein adsorption on biomaterials for tissue integration: a predictive way and a surface modification strategy

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1156 Self-Healing polysaccharide-based hydrogel as three-dimensional carrier for tissue repair

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1320 A Microfluidic Model to Evaluate the Proangiogenic Effects of Biomaterials

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1339 Bone-on-a-chip with biomimetic scaffolds

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1451 Photocrosslinked 3D Foamed Scaffolds Based on GELMA/HEMA copolymers and MBGs: Potential Application in Bone Tissue Engineering

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1452 Omics technologies to identify key biochemical pathways involved in the antitumor activity of a mesoporous silica nanosystem containing selenium nanoparticles

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1453 Biofunctional magnetic scaffolds that enhance osteogenic differentiation of mesenchymal stem cells through mechanotransduction

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1459 Multifunctional copper-containing mesoporous glass nanoparticles for wound healing in bone infection treatment

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1478 Impact of synthesis method, coating, and functionalisation on the cellular internalisation and efficacy of superparamagnetic iron oxide nanoparticles for bone tissue engineering

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1630 Enhanced osteogenic differentiation and extracellular matrix formation by mechanically stimulated electroactive scaffolds

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1635 Dynamic stimulation using uniaxial compression promotes the osteogenic and anti-osteoclastogenic responses of cellular co-cultures within composite scaffolds

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1662 Bioprinted bioactive complex constructs under mechanical stimulation promote vascularized bone formation

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1747 Agarose as a tissue mimic for porcine kidney at the macro and micro-length scale

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365 Bio-Based NIPU Nanoemulsion Sponges for Sustained Drug Delivery in Topical Wound Delivery
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386 Synthesis of eugenol derived biobased polymers as Green alternative to plastics

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459 Synergistic effects of arginine and tannic acid on chitosan matrices: A green approach for hemostatic sponge development

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622 Numerical analysis for a PEGDA microfluidic-device featuring a Y-shape for hydrogel microspheres synthesis

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655 Engineering bacterial nanocellulose membranes for skin applications

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810 Bacterial nanocellulose membranes containing flavonoid-based metal complexes with potential for wound healing

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832 Additive Manufacturing and Optimization of Magnetoactive Polymer Composites Based on Cobalt Iron Oxide

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1051 Olive oil waste as basis for polyurethane coatings

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1078 Bioactive release profile of electrospun alginate nanofibers loaded with nitric oxide

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1089 Dissolvable pullulan microneedles for transdermal lidocaine delivery

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1275 Development of a hydrogel composed of alginate and lysozyme amyloid nanofibrils for the administration of a novel chemotherapeutic chrysin-based metallodrug

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1581 Predicting Printability of Bio-inks by Capillary Rheology

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1599 First-Principles Insights into the Enhanced Catalytic Activity of Mg-Doped Prussian Blue for Hydrogen Peroxide Decomposition

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1816 Dielectric Properties of Chitosan-Based Bionanocomposites

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1900 Tubular polyester-based electrospun constructs with anti-adhesive and anti-inflammatory potential to repair ruptured deep flexor tendons

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2031 The versatile role of tannic acid as green crosslinker and bioactive compound in the development of Gellan Gum-based hydrogels for in situ cartilage repair

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2068 Synthesis of P3HB/Chitosan Blends with Enhanced Properties for Biomedical Applications

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2069 Synthesis and characterization of electrospun fibers based on piezoelectric bioplastics

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498 Mn-Doped Ti Coatings for Dental Implants: Effects on HOI differentiation, Immune Modulation, and Protein Binding

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586 Development and characterisation of geopolymer and Mg doped hydroxyapatite-based coatings on Ti6Al4V substrate for orthopaedic applications

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700 Modification of microemulsion-assisted sol–gel method to control the composition of multi-ion-doped mesoporous bioactive glass particles

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757 CNC-manufacturing versus ceramic injection moulding for ATZ shoulder resurfacing

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777 Alternative sintering process of biomaterials for prostheses: microstructural control using electromagnetic field

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1267 Enhancing Patient Comfort in Cranioplasty: Coated Titanium Implants for Better Thermal Regulation

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1363 Mesoporous silica nanoparticles carrying an iron chelator for the treatment of iron overload diseases. Proof of concept.

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1443 Design, synthesis and optimization of ion-doped mesoporous bioactive glass nanoparticles with large pore size: A promising platform in bone tissue regeneration

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1117 The influence of the surface pre-treatments on the chitosan/bioglass coatings deposited on the titanium substrate

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1126 Enhancing the Mechanical Properties of Zn-Based Biodegradable Alloys Through Harmonic Structure Design

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1193 Exploring the deformation mechanisms and degradation in Mg10Gd using acoustic emission and in situ SR μ CT

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1487 Processing of Ti-10Nb-10Ta alloy foams via powder metallurgy with solar sintering

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1885 Additive manufacturing of metallic bioresorbable stents

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2041 New generation of porous composites titanium/ Hap biomaterials.

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1736 Pioneering Women in Materials Science

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1943 AI Explainability by Transparency for Surrogate Computation, Inference and Data Exploration in Material Informatics

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176 Sustainable battery recycling using electrodialysis with X-ray fluorescence process control

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277 Thermal drying for safe, high-quality and high-yield recycling of battery cells with liquid electrolyte

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371 Ink formulation from spent NiMH batteries

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677 Recycling and Calcination Behavior of Leaching Sludge from Secondary Batteries

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767 Black mass recovery from lithium-ion battery recycling: interplay of efficiency and chemical composition

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925 Optimization of parameters to obtain metallic cobalt from lithium-ion batteries with microwaves irradiation process

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1115 Reduced graphene oxide supported on polyurethane foams for metal recovery from e-waste

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1497 BATCycle: green chemistry for recycling Li-ion NMC-111 Cathode material.

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1528 Eco-friendly electrospun lignin membranes for sustainable precious metal recovery from e-waste
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1566 Enhanced Metal Recovery from spent Lithium-Ion Batteries Using ChCl:PTSA Deep Eutectic Solvents: A Study on Conventional and Microwave-Assisted Leaching Process

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1598 Sustainable Recovery of Rare Earth Elements from Nd-Fe-B Swarf via Hydrogen Plasma Reduction
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1607 Electrochemical leaching of CIGS PV panels for recovery of CRMs

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1874 Hydrogen Processing of Recycled NdFeB Powders via HPMS and Production of New Magnets

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1942 Thermodynamic Approach for Metal Recovery from Black Powder of Used Secondary Batteries through Pyrometallurgical Process

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2056 Electrochemical recovery of metals and silicon from c-Si photovoltaic module

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2126 Optimization of thermal pretreatment parameters to enhance black mass recovery in lithium-ion battery recycling

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H2 Circular economy in the construction and ceramic industry

247 Sustainable ceramics: Circular economy implementation and prospects

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297 Rigid polyurethane foams with a reduced petrochemical content

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319 Assessment of earthen soil binder for 3DP

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353 Investigation of the impact of reducing the albedo of the coloured wall tiles of an Italian building heritage of the Second Twentieth Century for sustainable restoration purposes

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374 Building with Rammed Earth: Characterization and Optimization of Earth Mixes from a Monticello d'Alba Case Study

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697 Development of Hemp insulation Biopanel with Tannin-Based Adhesives: A Sustainable Solution for Green Construction

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920 Recent advances in microencapsulated phase change materials for energy-efficient buildings

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949 Use of cement paste containing foundry wastes as anodes for electrochemical chloride extraction in concrete

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1023 Overview of agricultural waste-based SCMs from Kenya for climate care and a circular economy

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1100 Recycling of Rigid Polyurethane Foam with Solid Filler: Flammability and Thermal Conductivity Analysis of Newly Synthesized Materials

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1521 Utilization of Wind Turbine Waste in Cementitious Materials: Circularity and Sustainability

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1754 Sustainable Geopolymer Catalytic Supports from Construction and Demolition Waste and Metakaolin Activated with Alternative Siliceous Waste-Derived Activators

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1775 Thermochemical Synthesis of a Sodium Silicate Activator from Refractory Casting Bag Residues for Sustainable Geopolymer Production

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H3 Carbon-Capture technologies, polymeric and bio-based materials in circular economy

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45 Advancing the Future of High-Performance Materials: Bio-Based Epoxy Resins for Sustainable Innovations

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51 Ionic liquids for biopolymer dissolution and regenerated fiber spinning

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60 Positron Annihilation Spectroscopy: Unlocking Atomic Insights for Next-Gen Energy Materials

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520 High-cell-density strategies to maximise bacterial production of biopolymers from real by-products

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523 Development of mycelium-based composite materials through valorization of agro-industrial wastes

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537 Vegetable oils as source of building blocks for high added value materials

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569 Biobased Antioxidants: A sustainable solution to thermomechanical degradation of recycled polypropylene

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961 A semi-industrial prototype bearing ceramic materials for Carbon Capture and Storage

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1121 COPPER AND ZINC REMOVAL BY BIOCHAR-BASED MATERIALS

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1129 Synthesis of lignin-based resin using epoxidized cross-linkers from bio-sources.

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1225 Direct chemical conversion of *Pleurotus ostreatus* whole mycelium into biodegradable films

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1242 Influence of processing methods on the crack resistance for a polypropylene/recyclate blend and the virgin material

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1554 Ecotechnology applied to the manufacturing of ecological material by biomineralization processes with the *Sporosarcina pasteurii* bacteria

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2013 The scaling and use of solid sorbents for decarbonisation of industrial CO₂ emitters

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H4 Sustainable Production and Processing of Metals

253 Modelling microstructure evolution during reduction of iron oxide pellets

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281 Theoretical predictions and high-resolution experimental observations of lenticular hematite formations in partially oxidised magnetite powder

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282 Thermodynamic-guided sustainable alloy design via hydrogen-based direct reduction of metal oxide mixtures

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312 Scope 3 emissions in secondary steelmaking: relevance and impact on CFP

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344 Direct reduction of iron oxides by hydrogen: Elucidating microstructure effects in single crystal and polycrystalline hematite

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370 Solid-state recycling of aluminium AA6060: effect of thermomechanical coupling on oxidation during extrusion

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388 Computational prediction of the effect of process parameters and pellet properties on the hydrogen direct reduction of iron oxide pellets

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546 Heating and melting behavior of hot briquetted iron (HBI) under isothermal conditions for sustainable electric steelmaking

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679 Sustainable manufacturing of FeCrCoMnNi high-entropy alloy (HEA) using ferroalloys feedstock via slagging methods

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696 Life cycle assessment for a holistic approach to sustainable steel design

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740 One step alloy-making from oxides: From thermodynamic design maps to atomic-scale chemistry
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771 Science of Dirty Alloys: improving the recyclability of Al alloys

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800 UTILIZATION OF MICROWAVE ENERGY IN ZINC WASTE PROCESSING

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911 Methodology to design a new high performance HPDC aluminium alloy with a high recycled content

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947 Circular economy of aluminium alloy to extrusion process: From dismantled batteries to batteries.

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980 Evaluating sustainable steam shaft production strategies through Life Cycle Assessment

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1004 Interplay of scrap introduced tramp elements and non-metallic inclusions in steels on wetting conditions and deformation behavior of inclusions

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1044 Solid-state recycling of AA6006 via chips compaction and hot rolling

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1184 Solvometallurgical process for copper and cobalt extraction from DRC oxide ores using Di-(2-ethyl hexyl)phosphoric acid

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1324 UTILIZATION OF MICROWAVE ENERGY IN OBTAINING METALS FROM SULPHIDIC ORES

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1409 Unravelling the copper precipitation mechanism at the grain boundaries and intergranular cementite in copper alloyed ferritic steels: steps towards enhanced understanding and use of copper in steel scrap.

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1427 Hydrogen-based direct reduction and decomposition of mill scale at 400°C-700°C

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1509 Sustainable production of iron and steel via electric steelmaking routes for mitigation of CO₂ emissions

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1531 Thermochemical aspects of the substitution of natural gas by hydrogen in blister copper deoxidation during fire refining

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1563 TiC-Containing Ferritic Steels: A Path Toward Lightweight, High-Performance, and Sustainable Vehicles

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1682 Iron recovery from EAF slags through hydrogen-based reduction

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1798 Hydrogen use in valorization of bauxite residue to extract iron and alumina

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1820 Sustainable metal production via hydrogen- and ammonia-based direct reduction of metal oxides

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1836 Effect of Surface and Thermal Reconditioning on the Re-Use Potential of Quenched and Tempered Martensitic Steel in a Circular Steel Economy

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1940 Effect of Tramp Elements on Hot Shortness in Steel Products

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1970 Graduate School Circular E-Cars: Development and establishment of a circular economy for e-cars in the Rhenish Mining Area

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H6 Materials Circularity for Sustainability

76 Circular materials characterisation with synchrotron X-rays: an update on the European project ReMade@ARI

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81 A Digital Platform for Circular Management of Critical Raw Material: Emission Estimation Module

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491 Everglass: The new role of glass in a sustainable society. Technology for the integral recycling of glass

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504 SUSTAINABLE USE OF ELECTRIC ARC AND LADLE FURNACE SLAGS AS CONVENTIONAL FILLER REPLACEMENT FOR NITRILE BUTADIENE RUBBER

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548 Porous glass-derived products using vitrified ashes from municipal solid waste incinerators

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574 Enhancing the Wear Properties of CoCrMo Alloy for Orthopedic Application by High-Power Impulse Magnetron Sputtering Nitriding Treatment: Life Cycle Assessment and Critical Raw Material Analysis

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582 Cost-Effective Approach to Managing Steel Development Using Mixes of Commodity Alloys

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624 Thermomechanical analysis of biochar-containing polymer-based composites by Dynamic Mechanical Analysis

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625 Investigation of the Tensile Strength of Biochar-containing Thermoplastics

Mrs. Viktoria Theodorou¹, Mr. Paraskevas Kyriacou¹, Dr. Ioannis Ioannou¹, Mr. Spyridon Rallis², Mrs. Nikoletta Karydi², Mr. Charalampos Botsas², Mr. Panagiotis Katsikakis², Mr. David Stephen Garnett³, Mr. Nicos Larkos^{4,5}, Dr. Andreas Grigoriou⁶, Mr. Charis Mikkides⁶, Prof. Theodorou Krasia-Christoforou¹

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Maialen Uribarrena¹, Prof. Koro de la Caba¹, Prof. Pedro Guerrero¹

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Mr. Daniel Obregon¹, PhD María R. Sun-Kou², Ms. Fabiola Bravo², PhD Lorena Vidal³, PhD Maria del Pilar Taboada-Sotomayor⁴, PhD Gino Picasso¹

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Dr. Ana Luísa Alves¹, Dr Joana Moreira¹, Dr Tiago Macedo¹, Lisandra Vilaça¹, Luís Gonçalves¹, Dr Juliana Oliveira¹, Regina Malgueiro¹, Dr Cláudia S. Oliveira², Freni K. Tavaría²

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Dr. Ilija Rašović¹, Dr. Kylee Goode¹

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Prof. Roberto Scotti¹, Dr. Daniele Montini¹, Dr. Silvia Mostoni¹, Prof. Massimiliano D'Arienzo¹, Prof. Barbara Di Credico¹, Prof. Roberto Nisticò¹, Dr. Claudio Cara², Dr. Luca Pala², Dr. Sergio Molina⁴, Prof. Elisabetta Finocchio³

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1195 Mapping Circularity, Responsibility and Sustainability in Power Electronics Research: A Bibliometric Analysis

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1373 Upcycling bio-based side streams for 3D printing of sustainable bioplastic filaments

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1542 Hybrid nanomaterials from biowastes for sustainable agriculture

Dr. Sebastiano Marra², Dr Virginia Venezia¹, Dr Maria Vittoria Verrillo³, Dr Antonia Puzone¹, Dr Simone Serrecchia^{1,4}, Prof. Fabrizio De Cesare⁵, Prof. Brigida Silvestri², Dr. Antonella Macagnano⁴, Prof. Giuseppina Luciani¹

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1653 Reuse of Plastic Waste in the Agricultural Sector: Another Step Towards Sustainability

Mrs. Victoria Santos Romero¹, Mr. José Carlos Rebollo Alburquerque¹, Dr. Natividad Antón Iglesias

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1711 Replacing boric acid in industrial nickel electroplating: toward REACH compliant electrolytes
Dr. Filippo Zoia¹, Dr. Roberto Bernasconi¹, Dr. Fabio Buttafava², Dr. Emanuele Grillo², Prof. Luca Magagnin¹

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Mrs. Sonia Marín-Cortés¹, Víctor Fuertes¹, Aida Serrano¹, Jesús López-Sánchez¹, María Fernández-Álvarez¹, Sara Román-Sánchez¹, Marina París Ogáyar², David Muñoz³, María José Cabrera³, José F. Fernández¹, Esther Enríquez¹

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1774 Development of a thermoplastic starch-based compound for extrusion of biodegradable foams

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1873 Circularity for Metal Additive Manufacturing: a review

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Dr. Hossein Rajaeinajafabadi¹, Prof. Cinzia Menapace¹, Dr. Lorenzo Romanelli², Prof. Giuseppe Macoretta², Prof. Ciro Santus², Prof. Bernardo Disma Monelli², Dr. Ivan Senegaglia², Prof. Matteo Benedetti¹

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1997 Safe and Sustainable by Design Framework: An Exploratory Case Study in Additive Manufacturing with a Focus on Surface Functionalization of Parts with Complex Geometry

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Khadija Sarquah^{1,2,3}, Prof. Dr. Satyanarayana Narra², Prof. Dr. Gesa Beck^{1,3}, Nana Sarfo Agyemang Derkyi⁴, Dr. Edward Awafo⁴, Prof. Dr. Michael Nelles², Prof. Dr. Michael Hartmann¹

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2086 Advanced Thermal Insulation Composite Material for Sustainable Construction Using Palm Fiber and Basalt Waste

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2127 Magnets in Resilient Supply Chains

Ph.D. Ane Jimenez¹, Mr. David Eguizabal¹, Mr. Marko Etxabeguren¹

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2190 Measuring Circularity in Practice: Insights from Repairability Assessment

Mrs. Setenay Saglam¹, Dr. Joana Francisco Morgado¹, Mrs. Smriti Anand Jha¹, Dr. Patrick Wäger¹, Dr. Kirsten Remmen¹, Prof. Dr. -Ing. Vera Susanne Rotter², Mr. Valentin Wewer², Mrs. Hannah Schlicht²

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ABSTRACTS

Vacancy-Confined Single-Atom Catalysts on MXenes for Enhanced CO₂ Reduction

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

MXenes, a versatile class of two-dimensional (2D) materials, exhibit exceptional electronic conductivity, tunable surface chemistry, and catalytic properties, making them promising candidates for sustainable energy applications. This study investigates vacancy-confined single-atom catalysts (SACs) supported on MXenes to enhance CO₂ reduction performance. Using density functional theory (DFT) and experimental techniques, we uncover the role of vacancies and single-atom configurations in optimizing catalytic activity and selectivity.

Our computational analysis reveals that introducing vacancy-confined SACs on Ti₃C₂T_x MXenes functionalized with oxygen, hydroxyl, and fluorine groups tailors the electronic structure and adsorption properties of key intermediates, such as *CO and *CHO. The vacancy sites effectively anchor single atoms, enhancing charge transfer and stabilizing intermediates. This enables selective reaction pathways toward CO and CH₄ production, with proton-coupled electron transfer mechanisms elucidated through transition state calculations. Notably, oxygen-functionalized MXenes demonstrate near-zero Gibbs free energy for intermediate adsorption, ensuring high catalytic efficiency.

Experimental validation through scalable synthesis of functionalized Ti₃C₂T_x MXenes confirms the presence of vacancy-confined SACs. Characterization techniques, including X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, and electrochemical analysis, reveal the active site formation and their role in CO₂ reduction. The combination of high surface area, vacancy engineering, and synergistic electronic properties positions MXenes as superior catalysts compared to conventional materials.

This work highlights the transformative potential of vacancy-confined single-atom catalysts on MXenes for enhanced CO₂ reduction, providing a pathway for the rational design of advanced materials in renewable energy and carbon capture technologies.

Increasing the functionality of graphene-based materials: pathways to carboxyl enrichment of Graphene Oxide

Dr. Leonardo Giaccari¹, Ph.D. Francesco Amato¹, Dr. Sara Colecchia¹, Ph.D. Yury Kolyagin², Prof. Alessandro Motta¹, Ph.D. Laurent Delevoye², Prof. Andrea Giacomo Marrani¹

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A1_1, Z4 Room (Level -3), septiembre 16, 2025, 10:30 - 13:30

In the last two decades, the interest in graphene oxide (GO) has grown significantly due to the discovery of the wet chemical route to graphene. GO is a non-stoichiometric, 2D, carbon-based nanomaterials with outstanding properties and quivering chemistry. It is usually produced via the Hummers method, a wet chemical synthesis from bulk graphite [1]. GO can be described as a graphene layer decorated with islands of various oxygen-based functional groups (OFGs) such as: hydroxyls and epoxides in the basal plane and carbonyls, carboxyls, and phenols on the edges and defects [2]. Since the coexistence of these two domains, graphene oxide can be functionalized either covalently or non-covalently through a plethora of different reactions. Additionally, GO and functionalized GO can be reduced to partially restore the π -aromatic network and obtain properties similar to graphene. These unique assets make GO the perfect starting point for the synthesis of new functional materials [3].

Due to the very low abundance of carboxyl groups in graphene oxide, various attempts have been made in order to increase their quantity. In this work, two different functionalization reactions to obtain carboxyl-rich graphene oxide are presented. The first reaction is an O-acylation reaction with succinic anhydride in N,N-dimethylformamide (DMF) which involves alcohol and phenols-like groups [4]. An alternative approach is a nucleophilic substitution on the epoxide rings with γ -aminobutyric acid (GABA) in water. All the nanomaterials submitted have been fully characterized via various spectroscopic techniques such as: x-ray photoelectron spectroscopy (XPS), Raman spectroscopy, UV-Vis spectroscopy, solid-state nuclear magnetic resonance (SS-NMR), and cyclic voltammetry (CV). The obtainment of a carboxyl-rich GO points to fostering the implementation of graphene-based materials in various fields such as: proton exchange membranes (PEM) in low-temperature fuel cells (LTFCs), removal of heavy metal ions from wastewaters, and amide-coupling with various amine-rich nanomaterials [4].

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Ion-matter interactions for material modification and functionalization: insights from atomistic modeling

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A1_1, Z4 Room (Level -3), septiembre 16, 2025, 10:30 - 13:30

Ion beams are a very useful tool in multiple fields and applications, from material characterization and material synthesis to material modification and introduction of specific functionalities. Achieving exceptional material properties through material modification with the use of ions requires fundamental understanding of the multiscale processes that take place in ion-matter interactions. In this talk, I will discuss atomistic modeling approaches for understanding the underlying mechanisms in ion-matter interactions in 2D materials for controlled functionalization and efficient synthesis, where minimization of the induced damage and controlling the material's response are key challenges. I will present insights from modeling and compare with experimental observations, highlighting the importance of combining the two for the development of predictive capabilities.

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New insights into the mechanism of direct amination of unsaturated carbon with hydroxylamine derived reagents: possible application toward graphene oxide functionalization.

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Amines are organic compounds of fundamental importance due to their application in several fields. They represent the core structure of numerous biologically active compounds, dyes, pharmaceuticals and are vital in producing functionalized organic materials¹. Various synthetic methods for amines have been devised: for example, the synthesis of aromatic amines often involves reduction of nitroarenes, copper-catalyzed substitution reactions, or palladium-catalyzed cross-coupling reactions². The efficient synthesis of amines remains an active area of research, with continuous progresses in achieving high chemoselectivity and yields. In this perspective, we introduce a novel reaction mechanism for the amination of unsaturated carbons with hydroxylamine derivatives (O-(methylsulfonyl)hydroxylammonium ([MsONH₃]⁺) and O-(pivaloyl)hydroxylammonium ([PivONH₃]⁺) in the presence of ferrocene. This mechanism, deeply investigated by DFT calculations, has clarified the interaction that occurs between the ammine reagent, the iron-based species, and the substrate, defining the formation of the nitrogen-based radical species responsible for the addition to the unsaturated carbon.

This approach holds potential for the functionalization of graphene oxide (GO): compared to methods that rely on epoxide ring-opening³ or those that attach the amino group to the material via a molecular spacer, the use of hydroxylamine derivatives as aminating agents allows the formation of primary amines directly bound to the nanomaterial's layer, thus enabling the obtainment of both aliphatic and aromatic amines. Moving from the molecular scale of benzene to that of graphene oxide, DFT calculations are performed on carbon clusters of varying sizes, allowing the study of reactivity both at the edges and on the basal plane.

GO with aromatic amine domains would allow access to a previously unexplored chemistry of this nanomaterial. By exploiting the functionalizations made possible by the presence of this new functional group, it would be possible to control the nanomaterial's bottom-up lateral growth. Such a functionalized graphene oxide could then pave the way to advanced materials, such as innovative membranes with anticorrosion and electrical conductivity properties⁴.

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Pulsed electrochemical exfoliation for an HF-free sustainable MXene Synthesis

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A1_2, Z4 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

MXenes are a two-dimensional materials (2DM) class with high industrialisation potential, owing to their superb properties and compositional variety which brought to their vast application in different fields ranging from energy conversion and storage to medicine and diagnostics, sensing and tribology. One of the big questions in MXenes is how to produce them in high amount and without involving hazardous chemicals. We have recently demonstrated a novel method to produce high quality MXenes in a sustainable manner, using pulsed voltammetry electrochemical synthesis. In a nutshell, we precisely control the potential applied on the anodic working electrode (MAX phase) at the Al etching potential and apply reverse cathodic pulses to foster surface reactivation and improve intercalant diffusion. This novel protocol led to a final product (EC-MXenes) with great physical and chemical properties and a production yield to 60% with no byproducts counted and out of a single exfoliation cycle.

In the talk I will present the details of the methodology and how synthesis of MXenes is related to the formation and control of electrochemically formed bubbles at the cathode's interface. Moreover, I will detail the extensive surface analysis performed on our product, which includes SEM, EDX, LEIS, Raman, AFM, TEM, XRD, and XPS.

Finally, I will present the follow up steps we are currently investigating, which include for instance the tribological application of this material and surface termination's post modification (e.g., amino acid) for high tuning of final physical/chemical properties.

To conclude, the work is setting the bases for a facile synthesis of MXenes in any labs and industries, where no specific infrastructure (for management of HF) is required.

From solution to surface: applying supramolecular chemistry principles for device manufacturing through molecular self-assembly

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The application of supramolecular chemistry principles to the assembly of active layers for devices is challenging because molecule-substrate interactions are added to the molecule-molecule interactions present in solution. In this talk I shall illustrate what this implies for building an ordered array of fluorescent molecules at a specific distance from each other, while preserving their functionality by decoupling them from the surface. The approach was to make use of pedestals to which the fluorophore was attached by metal-ligand coordination. Zinc phthalocyanine or zinc diphenylporphyrin were chosen as pedestal, perylene as the functional unit, and a pyridyl group as linker. The successful assembly of the three building blocks on a graphene surface was verified with the help of scanning tunneling microscopy and X-ray photoelectron spectroscopy, while near-edge X-ray absorption fine structure spectroscopy was used to determine the precise orientation of the fluorescent unit with respect to the pedestal, and hence the surface. We demonstrate that supramolecular chemistry principles can indeed be applied to build ordered 3D arrays of functional molecules on surfaces and show that it is even possible to exploit the molecule- surface interaction to achieve an arrangement that is not necessarily favoured in solution.

Synthesis and Characterization of MoS₂ by using a Hydrothermal method: Influence of Reactive Volume and Addition Rates.

Mrs. Andrea Carolina Villalvazo-Hidalgo¹, Mrs. Anayancy Itzel Villatoro-Guillén¹, Dr. Miguel Ángel López-Álvarez¹, Dr. Gregorio Guadalupe Carbajal-Arizaga¹, Dr. Orfil González-Reynoso¹, Prof. Mario Alberto García-Ramírez¹

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A1_2, Z4 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

In this study, molybdenum disulfide (MoS₂) was synthesized via a hydrothermal method. The structural impact and morphological properties of MoS₂ were tested by adding different reactive volumes and two rates of addition. The final structures were systematically investigated by X-ray diffraction (XRD), Energy Dispersive Spectroscopy (EDS), Scanning electron microscopy (SEM), and transmission electron microscopy (TEM). Experimental results demonstrate that variations in reactive volumes and addition rates significantly influence the reaction development. A smaller reactive volume leads to MoS₂ formation. On the other hand, a large volume forms sulfur. Effects on the synthesized MoS₂ morphology were also observed. By adding a lower reactive volume, it was possible to get MoS₂-2H. By featuring a larger volume, a heterojunction between MoS₂-3R and Sulfur is formed. In contrast, undesirable byproduct formation is generated due to lower addition velocities. The study contributes to the fundamental MoS₂ hydrothermal synthesis understanding and it provides valuable insights for tailoring the key properties of MoS₂-based applications such as catalysis, energy storage, biosensors and electronic devices.

Synthesis and characterization of biographene oxide@carbon dots derived from agricultural wastes (pomegranate peels and cotton stems): Application for Cr(VI) removal from aqueous solutions

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Increased industrialisation has resulted in the release of immense quantities of wastewater containing heavy metals into the environment. Cr exists as both Cr(III) and Cr(VI), with Cr(VI) being more poisonous causing developmental abnormalities, DNA damage, and cancer in all creatures. As a result, WHO claims that Cr(VI) is one of the heavy metals that pose a major risk to human health, with the maximum allowed concentrations in surface water and drinking water being less than 0.1 and 0.05 mg/L, respectively. Among the methods used for water purification, adsorption is considered an advantageous candidate because its easy operation and high efficiency. In the present work graphene oxide (GO) decorated with carbon dots (CDots, both derived from the same biomass is suggested). Agricultural wastes used are pomegranate peels and cotton stems and are carbon-rich biomass resources that can be transformed into products that work well as heavy metal adsorbents. Here we present a unique approach for synthesising GO from biomass using ferrocene as a catalyst. This method can be used to create high-quality nanostructured materials. GO has a vast surface area and functional groups that bind heavy metals through various mechanisms. CDots have functional groups, such as hydroxyl and carboxyl groups, that enhance adsorption capabilities.

Factors affecting the adsorption, such as the pH solution, initial concentration of Cr(VI), contact time, and temperature, were investigated. The composites' morphology and structure were characterized by FT-IR, SEM, BET and XRD analysis. Overall, the results indicate that GO@Cdots can be effectively employed for removal of Cr(VI) from aqueous solutions.

Acknowledgment

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An Effective Strategy for the Valorization of Industrial Waste Graphite Fines through the Preparation of Graphene Oxide-based Nanohybrids

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A1_1, Z4 Room (Level -3), septiembre 16, 2025, 10:30 - 13:30

Graphite is classified as a “strategic and critical mineral” by the US and EU, with a market value that is expected to reach \$28.33 billion by 2026. The growth of the graphite market is predicted to be primarily driven by the increasing demand for Li-ion grade graphite from the electric vehicle industry. Graphite is mainly produced in two forms: natural, which is obtained through mining; and synthetic, which is obtained by thermal annealing of highly pure graphitizable carbon materials at ultra-high temperatures (up to 3000 °C). In either form, graphite flakes need to undergo the micronization and spheroidization processes in order to be applicable as an anode material for Li-ion batteries. Consequently, these processes result in significant losses of the graphitic material of up to 70% in the form of ‘graphite fines’, which are regarded industrially as waste material or undesirable byproduct. Herein, we report for the first time an effective strategy to utilize industrial waste graphite fines through the development of graphene oxide-based nanohybrids as non-toxic and efficient antibacterial agents. To achieve this, graphene oxide (GO) was initially synthesized using industrial waste graphite fines as a graphitic precursor. Subsequently, hyperbranched polyethyleneimine (PEI), or either of its guanidinylated (GPEI) and N-sulfopropylated (SPEI) derivatives were successfully and homogeneously attached onto GO, as confirmed by various characterization techniques, yielding GO-PEI, and novel GO-GPEI and GO-SPEI nanohybrids. The antibacterial activity of these nanohybrids was assessed against Gram (–) *Escherichia coli* and Gram (+) *Staphylococcus aureus* bacteria. Both GO-GPEI and GO-SPEI were found to exhibit higher antibacterial activity, specifically against *E. coli* bacteria, compared to the pristine GO and GO-PEI nanohybrid, with GO-SPEI being more active than GO-GPEI. Moreover, GO-GPEI and GO-SPEI were found to exhibit low cytotoxicity against mammalian cells, signifying that they can be used as potential antibacterial agents in various applications, including those in the disinfection industry.

Carbon nanodisks decorated with triphenylphosphonium-functionalized hyperbranched poly(ethyleneimine) with enhanced antibacterial performance

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It is known that nanostructured carbon-based nanomaterials as well as polymers bearing suitable positively charged groups, such as triphenylphosphonium groups, guanidine groups, quaternary ammonium groups, etc., exhibit enhanced antibacterial properties [1,2]. Combining the above-mentioned categories, new nanomaterials with excellent antibacterial activities have been obtained [3-5]. Carbon nanodisks represent an interesting alternative to bulk graphite, produced through the so-called pyrolytic Kvaerner Carbon Black & H₂ (CB&H) process [6].

In this study, hyperbranched poly(ethyleneimine) of two different molecular weights (i.e. 1300 Da and 5000 Da) functionalized with decyl-triphenylphosphonium groups were developed and subsequently interacted through both covalent and non-covalent bonds with the acid-treated carbon nanodisks (oxCNDs), affording two nanohybrid materials i.e. oxCNDs@PEI(1300)-TPP(C10) and oxCNDs@PEI(5000)-TPP(C10). The successful attachment of polymers onto oxCNDs, was confirmed using various physicochemical techniques, while the polymer content in the hybrids oxCNDs@PEI(1300)-TPP(C10) and oxCNDs@PEI(5000)-TPP(C10) were found to be 20.45 and 24.04 %w/w, respectively. Also, the homogenous attachment of polymers on oxCNDs were confirmed by SEM and TEM microscopies. Subsequently, the antibacterial activity of the as-prepared nanohybrids were evaluated against Gram (-) *Escherichia coli* and Gram (+) *Staphylococcus Aureus*. From the obtained results, it can be concluded that all nanohybrids exhibit improved antibacterial properties compared to oxCNDs, especially against Gram (+) *S. aureus* bacteria, with oxCND@PEI(1300)-TPP(C10) being more efficient. Finally, their cytotoxicity was evaluated against mammalian cells and it was found that the hybrid materials do not exhibit any significant toxicity. These findings indicate that these nanohybrids have great potential to be used as safe and efficient antibacterial agents in various applications, including those in the disinfection industry.

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Multifunctional metal-graphene composites for tribological applications

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A1_1, Z4 Room (Level -3), septiembre 16, 2025, 10:30 - 13:30

Sliding metal-to-metal contacts frequently occur in switching devices (e.g. circuit breakers, contactors, disconnectors, and switches), used for electrical power distribution grid protection. These sliding mechanisms can both be electric-load carrying (e.g. Ag-to-Ag and Ag-to-Cu electric contacts) or be purely mechanical as part of the drive train (e.g. steel-to-steel contacts), and they are typically grease- or oil-lubricated to facilitate the switching actuation and to reduce friction and wear. However, lubricant aging and depletion constitute significant issues in these devices. In addition, metal oxidation is always a problem, especially in tough ambient conditions. Therefore, the development of robust and resilient metal contacts preferably providing solid-state lubrication to replace “wet” lubrication is of great interest for a broad range of applications.

Graphene (including bi-layer and few-layer graphene, and graphene nanoplatelets (GNP)) has in recent years been highlighted as an efficient solid-state lubricant. Adding a small amount of graphene (typically 0.05-0.5wt%) into a metal matrix can provide self-lubricating properties while maintaining favorable metal properties. Benefits of using graphene compared to other lubricating additives, e.g. graphite, MoS₂, and WS₂, include high electric and thermal conductivity, insensitivity to ambient conditions, and oxidation resistance.

This paper summarizes an extensive work conducted on silver-graphene- and copper-graphene composite systems optimized for use in electro-mechanical or mechanical sliding contact systems in electrical switches. Both metallurgical (sintering) and coating (electroplating) synthesis routes have been explored. By material design and optimized processing, composite systems with a combination of valuable electrical, tribological, mechanical, and anti-oxidation properties have been obtained, taking full advantage of the multifunctional properties of graphene. The choice of graphene, extent of dispersion, and graphene/matrix morphology are shown to be critical factors for beneficial tribological effects. For well-performing, optimized systems, a carbon-rich, low friction ($\mu < 0.2$) tribofilm is formed in the wear track. During long-term operation, the film will continuously regenerate from the reservoir of graphene within the composite. A well-dispersed system can also enable nano-effects like dispersion-hardening of the composite, improving wear resistance and durability. For electrical applications, the choice of graphene is a critical factor for providing a low and stable contact resistance over time, as graphene may offer conductive pathways through the contact area even as surface oxides of the metal (especially copper) grow over time.

An overview of the work and the main findings and achievements, including product demonstration, will be presented. The commercial applicability and sustainability of the processing methods will also be discussed and highlighted.

New heterogeneous photocatalysts based on novel 2D materials for photochemical upcycling of plastic wastes

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Much of the research effort on 2D materials focuses on its use as building block for the development of novel hybrid structures with well-defined dimensions and behavior suitable for applications among else in gas storage, heterogeneous catalysis, gas/liquid separations, nanosensing and biology. Towards this aim, here we demonstrate the development of green and sustainable processes using novel 2D heterogeneous catalysts for the photochemical upcycling of plastic wastes, such as polystyrene (PS). Various photocatalytic anthraquinone and thioxanthone derivatives were successfully synthesized and immobilized in different types of 2D matrices to produce novel heterogeneous photocatalysts. 2D Xanes of group-14 [germanane (GeH) and silicane (siloxane)], anionic layered double hydroxides (LDHs), cationic clay minerals and synthetic clay analogues (SCA) with high surface area, tunable pore size and functionalities were prepared using top-down synthetic approaches and applied as supports of the photocatalytic molecules. All materials were characterized by a combination of analytical techniques. Finally, the heterogeneous photocatalysts were tested in the aerobic photochemical upcycling of PS but also in other demanding plastics, such as PET, PE and PP.

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2D Nanostructures from bulk solids. A sustainable treatment based on sonication in aqueous solution.

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Ultrasonic processing has become an important tool for the development of environmentally friendly methods for the construction of low-dimensional structures. In recent years the interest has been focused on two-dimensional materials or even better on monolayer nanostructures which are usually characterized by the -ene suffix. In the present work, emphasis is placed on the use of aqueous dispersions to assist the exfoliation of monolayer structures from groups IIIA - VIA of the periodic table and their derivatives. The low-dimensional materials produced in this way can be exploited in biological applications as well as in energy applications depending on their individual properties. The systematic study of the treatment of such materials shows that ultrasonic treatment can be applied to many classes of materials with positive results. However, oxygen groups often appear in the products depending on the chemical activity of the materials.

We have so far studied elements such as tellurium, antimony, bismuth, tin, silicon, aluminum, and minerals such as hematite, magnetite, or solids like tungsten and molybdenum sulfides. The derivatives resulting from the exfoliation are often 2D and have interesting chemical and optoelectronic properties.

The aim of this work is to identify suitable natural extracts that, in combination with ultrasonic treatment, yield sufficient quantities of nanomaterials without affecting their basic properties. Also, often the functionalization of nanomaterials with natural products that have biological activities such as curcumin can act synergistically to increase the therapeutic properties of the materials.

Sertraline adsorption on graphite oxide: Kinetic and thermodynamic study

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Sertraline is a commonly prescribed medication for the treatment of depression and obsessive-compulsive disorder. It is often released into raw wastewater and subsequently into the environment from wastewater treatment plants (WWTPs) due to insufficient removal. Therefore, it is crucial to eliminate sertraline from aquatic environments. In this study, graphite oxide was used to remove sertraline. Graphite oxide was synthesized using a modified Hummers method. Various characterization techniques, including BET, XRD, XPS, Raman spectroscopy, FTIR, and elemental analysis, were employed to examine the physicochemical and structural properties of the composite material. Graphite oxide exhibited a high adsorption capacity, compared to -commercially available-activated carbon, achieving an adsorption value of $245.1 \mu\text{mol}\cdot\text{g}^{-1}$ for sertraline at 25°C after 6 hours of contact time. The kinetic study revealed that the non-linear form of the pseudo-second-order model best represented the adsorption behavior of sertraline on graphite oxide. The adsorption isotherms were analyzed using the Langmuir and Freundlich models, in both linear and non-linear forms, at temperatures of 10, 25, and 40°C . The results indicated that the non-linear form of the Langmuir model effectively described the adsorption isotherms of sertraline.

Additionally, a thermodynamic study was conducted to calculate the free energy, enthalpy, and entropy parameters (ΔG° , ΔH° , and ΔS°). The thermodynamic parameters suggested that the adsorption process of antidepressants was spontaneous and endothermic within the temperature range of $10\text{--}40^\circ\text{C}$. Moreover, equilibrium experiments were carried out to investigate the effects of various factors, such as the pH, the composition of the water matrix, and the ionic strength. It was found that ionic strength and aqueous medium composition significantly reduce graphite oxide's adsorption capacity. Excess ions, like Na^+ , and the components of the aqueous matrix, respectively, compete with sertraline for active sites on graphite oxide, limiting its effectiveness in water treatment.

Atomic-level insight into graphene-enhanced anticorrosive coatings deposited on aluminum alloy surfaces

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A1_1, Z4 Room (Level -3), septiembre 16, 2025, 10:30 - 13:30

Metal corrosion causes heavy losses on human life and economy [1]. Anti-corrosion polymer coatings undergo self-decomposition under exposure to harsh conditions, which leads to their short-term loss of functionality [2]. Excellent chemical inertness, thermal stability and diffusion barrier properties of graphene have attracted growing interests in designing graphene-based composite (GC) coatings for anticorrosion purposes. The size of graphene flakes, structure, chemical composition, and roughness are important for obtaining adhesive, tightly covering layer of GC coating on metal surfaces with improved anticorrosion properties [3].

In line with recent literature data, herein we provide an atom-level picture of structure and properties of functionalized graphene oxide (fGO) coatings deposited on aluminum alloy surfaces exposed to corrosive media. Atomistic calculations, DFT and reactive molecular dynamics methods, are combined with experimental studies. fGO flakes varying in size and oxidation degree on metal surfaces were considered and discussed in view of the experimental knowledge of different properties of graphene materials[4]. Structural, morphological, chemical, and topological aspects of fGO deposited on Al-based alloy surfaces are discussed. The oxidation state of fGO on an Al alloy surface was characterized using Raman spectroscopy and X-ray photoelectron spectroscopy (XPS). Roughness and surface topography of fGO layer on Al alloy surfaces were determined experimentally and computationally. Electrochemical performance of fGO-covered Al alloy surfaces were established and discussed with available literature data.

Acknowledgment: The presented results were obtained using computational resources provided through PLGrid Infrastructure at Academic Computer Centre Cyfronet AGH (no. PLG/2024/017514).

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Defect Engineering in MoS₂ Nanomaterials via Low-Energy Ion Implantation for Next-Generation 2D Functional Devices

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The exploration of two-dimensional(2D) materials, such as molybdenum disulfide(MoS₂) and other transition metal dichalcogenide(TMDs), has gained significant attention due to their extraordinary electronic, optical, and mechanical properties. These materials hold immense potential for applications in electronics, optoelectronics, catalysis, and energy storage.

Ion implantation has emerged as a promising technique for modifying the structure and properties of 2D materials by introducing dopants and defects into the atomic lattice. This enables precise control over substitutional dopants, vacancies, and interstitials, allowing for tailored modifications in electronic, optical, and mechanical characteristics. This study explores how low-energy ion implantation can modify MoS₂, unlocking applications in catalysis, optoelectronics, and other advanced fields.

Existing research primarily focuses on the effects of high-energy ions on 2D materials. In contrast, the impact of ultra-low-energy ions, such as argon(Ar) and xenon(Xe), on MoS₂ has not been as thoroughly investigated. This research aims to fill this gap by studying the effects of ultra-low-energy ion implantation on MoS₂ at varying ion energies by experimental (Scanning Transmission Electron Microscopy STEM and Raman Spectroscopy) and computational(Molecular Dynamics MD) approaches. By combining these approaches, this research aims to deepen the understanding of how ultra-low-energy ion implantation influences the properties of MoS₂.

Employing the KIIA ion accelerator at the University of Helsinki, mechanically exfoliated MoS₂ samples were irradiated at controlled doses(1×10^{14} – 1×10^{15} ions/cm²) and energies ranging from 15-200 eV. STEM analysis revealed significant structural alterations, including defect formation at energies 40, 45, 50, 55, 80, and 200 eV. A clear indication of trapping the ions in the van der Waals gap is seen in the simulation at 40, 45, 50, and 55 eV, but the experimental confirmation is still underway. The transition from AB stacking to mixed AB/AA/AC stacking was observed, with stacking transformations occurring at the sub-nanometer scale.

MD simulation results showed that at 20 and 30 eV, no defects were introduced in the MoS₂ lattice. However, at 35–40 eV, defect generation in the top MoS₂ layer began. When the energy increased to 40–50 eV, Ar ions penetrated the first MoS₂ layer, leading to interlayer trapping, nanoscale pore formation, and stacking disorder.

A key finding is that 15 eV Ar implantation achieves clean and well-preserved MoS₂ surfaces, presenting a promising method for surface cleaning before property engineering. This study provides critical insights into how ultra-low-energy ion implantation enables precise defect engineering in MoS₂, fine-tuning its properties for nanoelectronics, optoelectronics, and catalytic applications. Future research will focus on refining implantation techniques, optimizing defect configurations, and further expanding MoS₂'s applicability in nanoelectronics and sustainable energy solutions.

High-Performance MoSe₂xTe_{2-2x} Alloy for Hydrogen Gas Sensing

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A1_2, Z4 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

This study provides one of the first comprehensive investigations into the out-of-plane growth of two-dimensional MoSe₂xTe_{2-2x} for three different Se:Te compositions, resulting in the samples MoSe_{0.46}Te_{1.55}, MoSe_{0.55}Te_{1.45}, and MoSe_{0.64}Te_{1.35}. Scanning electron microscopy (SEM) captures the morphological evolution, displaying nanoflakes primarily grown in a random out-of-plane orientation. Raman spectroscopy confirms the crystal structure of the MoSe₂xTe_{2-2x} samples, with no detectable MoO₃ or MoO₂ precursor residues. Characteristic peaks validate the presence of MoSe₂xTe_{2-2x}, and spectral shifts indicate compositional variations. Conductive Atomic Force Microscopy (C-AFM) was employed to measure the current flow between a diamond-doped AFM tip and the sample. Furthermore, the resistances of MoSe_{0.46}Te_{1.55}, MoSe_{0.55}Te_{1.45}, and MoSe_{0.64}Te_{1.35} compositions were characterized, yielding median resistance values of 108.0 Ω, 25.4 kΩ, and 240.0 kΩ, respectively. These values highlight the diverse electrical properties linked to Se content. Notably, the sample with the highest Se content shows increased resistivity, which aligns with the XRD spectra results. Finally, evaluation of the H₂ gas sensor revealed a decrease in electrical resistance of the samples upon exposure to hydrogen, particularly pronounced at higher temperatures. However, a complex relationship between sensor response and Se content was observed, with higher Se content samples exhibiting relatively lower response despite their potentially higher hydrogen absorption capability based on the morphology of the flakes.

Hydrogen Storage and Detection in MoSeTe-based Two-Dimensional Structures

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This study explores the potential of two-dimensional MoSeTe (with a composition of 25% Se and 75% Te) structures for hydrogen storage and detection. The material is grown out-of-plane on sapphire substrates using Chemical Vapor Deposition (CVD).

The sensor's properties are characterized through Raman spectroscopy, X-ray diffraction (XRD), and scanning electron microscopy (SEM) to analyze the crystal structure, morphology, and material quality. Resistance variations under hydrogen exposure are studied to assess the sensor's sensitivity and response time to changes in hydrogen concentration. MoSeTe's unique properties, along with its high surface-to-volume ratio in its two-dimensional form, make it a promising candidate for hydrogen detection applications.

Additionally, hydrogen uptake is evaluated using ERDA-TOF (Elastic Recoil Detection Analysis-Time of Flight) at the Particle Accelerator located at the Microanalysis Center (Cantoblanco).

How to measure properly fracture properties of brittle materials using molecular simulations? Application to mode I and mode III in silica glass.

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A2_4, Machuca Room (Level -2), septembre 15, 2025, 17:00 - 19:00

The fundamental understanding of the root causes of failure requires information on atomic-scale processes. Molecular dynamics (MD) simulations are widely used to provide these insights while maintaining chemical specificity. However, the boundary conditions that can be applied in MD fracture simulations are limited to the linear-elastic fracture mechanics far-field solution, which makes it difficult to apply bending or shearing deformations as they occur in classical experimental setups. This has to date prevented the accurate and precise prediction of key fracture quantities such as critical stress intensity factors. We here apply the domain-decomposition Capriccio method to couple a molecular model representing silica glass simulated using MD with the finite element method (FEM) and perform both mode I (tension, three- and four-point bending) and mode III simulations. We investigate multiple criteria to best identify the point of critical crack propagation: decrease in stress, decrease in the number of interatomic interactions, and increase in kinetic energy/temperature. We propose a novel protocol that allows us to determine the critical stress intensity factor of silica glass under mode I and mode III conditions from atomistic data with increased fidelity. Overall, our contribution demonstrates how more than ever MD simulations enable chemically specific quantitative predictions of the fracture behaviour of oxide glasses.

Nanostructured Polymeric Matrices for Enhanced Ablative Thermal Protection Systems in Space Exploration

Dr. Rita Bottacchiari¹, Dr. Giulia Pedrizzetti¹, Dr. Laura Paglia¹, Prof. Francesco Marra¹, Prof. Giovanni Pulci¹

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A2_3, Machuca Room (Level -2), settembre 15, 2025, 14:30 - 16:30

The continuous evolution of space exploration missions necessitates the development of advanced Thermal Protection Systems (TPS). Ablative TPSs (A-TPS) are essential for planetary entry missions as they are capable of withstanding the intense aerodynamic heating encountered by the vehicles. Phenolic-Impregnated Carbon Ablators (PICA) have long been the standard for A-TPS in space missions due to their effective thermal insulation and ablation resistance. PICA-like ablators comprise a carbon fiber reinforcement impregnated by a phenolic resin which, when invested by high heat fluxes, undergoes pyrolysis reactions bringing to the consumption of a considerable amount of the incident heat. Phenolic resin is widely used as matrix because of its excellent thermal stability, low thermal conductivity, and ability to form a protective char layer during pyrolysis. Traditional carbon-phenolic ablators, though effective, face performance limitations under the increasingly severe conditions of future missions. Therefore, it is of utmost importance to either improve PICA-like materials, by for example tailoring the microstructure and porosities, or design new A-TPSs exploring different polymeric matrices with higher thermo-mechanical properties.

This study focuses on the exploration of novel, nanostructured A-TPSs with two polymeric matrices: phenolic resin and cyanate ester. The alternative cyanate ester resin offers advantages such as higher char yield, higher decomposition onset temperature, and increased glass transition temperature compared to state-of-the-art phenolic resin. To obtain the nanostructuration of the resin matrix it is possible to use either a cross-linker or a polymeric additive which can alter the length of the polymeric domains formed during cross-linking and gelation. In this work different additives have been tested: hexamethyltetramine (HMTA), polyvinylpyrrolidone (PVP) and polyethylene glycol (PEG) were incorporated into the solutions to tailor the matrices' microstructure. Scanning Electron Microscopy (SEM) was employed to investigate the resin morphology and distribution within the carbon felt: the optimization of the manufacturing was conducted to obtain a homogeneous distribution of the matrix throughout the felt, the formation of micro-nano domains of the polymer structure and the presence of open and interconnected porosities. The as-designed ablators were characterized and compared to non-nanostructured ones. Thermo-ablative performances were assessed with oxyacetylene flame tests, exposing samples to a heat flux of 4MW/m² for 60 seconds. Surface and back-side temperatures were recorded, along with measurements of mass loss and surface recession. The exposed samples were further analysed with SEM equipped with an EDS system to compare the oxidation of the exposed carbon fibers and the in-depth formation of a char layer.

Dispersion and Self-assembly of Nanoparticles in Polymers for Multifunctional Applications

Prof. Hungjue Sue¹

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A2_2, Machuca Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Challenge to commercial implementation of many nanotechnology-inspired products are the lacking of robust approaches to decorate, disperse, and assemble nanoparticles in polymer matrices for specific targeted applications. To achieve desirable multi-functional properties, it is necessary to successfully manipulate nanoparticle dispersion and assembly in polymer matrices without compromising intrinsic nanoparticle properties and their intended purposes. In this talk, several successful examples of approaches in achieving dispersion and assembly of nanoparticles in polymer matrices for desired functionalities and mechanical properties are presented. These examples include dispersion and self-assembly of α -zirconium phosphate (ZrP) in epoxy, dispersion of carbon nanotubes in epoxy, and dispersion of ZnO quantum dots in epoxy. Fundamental principles responsible for manipulation of nanoparticle dispersion and assembly are described. Usefulness of the above research for functional and structural applications, especially for electrical conductivity and barrier properties, is also discussed.

Multi-functional Smart Soft Materials

Prof. Luyi Sun¹

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A2_3, Machuca Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Smart soft materials have one or more characteristics that can be significantly altered in convertible fashions by external stimuli. Inspired by the fascinating visual display strategies and adaptive mechanisms in animals and plants, we have fabricated a series of smart soft material-based devices that can respond to external stimuli with instantaneous and reversible fashions in optical, electrical, mechanical, and/or shape deformation signals. The key to successfully achieving those intriguing characteristics in these smart material systems lies in the function-orientated structural design, which integrates bioinspired design and surface engineering with multiscale architecture as the crucial elements. These materials are characterized by convertible topographies like dynamic cracks, folds, stimuli-responsive wrinkles, and other analogous structures. These systems demonstrate high design flexibility, excellent reversibility, and wide applicability.

Slide-Ring Materials for Circular Economy

Prof. Kohzo Ito¹

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A2_1, Machuca Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

We have developed the SR materials with polyrotaxane (PR), in which polymer chains are topologically interlocked by figure-of-eight cross-links.1) SR materials show active and smart multi-functional properties responsive to various external stimuli. Recently, we have reported the stretch induced crystallization of the SR gel, which leads to extremely high toughness and recoverability.2) When the SR gel is largely stretched, the movable crosslinks uncover and orient PEG axis chains, followed by the stretch induced crystallization of PEG chains: PEG chains drastically change the structure from amorphous to crystal. The nano-size PEG crystals prevent SR gels from fracture and yields the extremely high toughness.

On the other hand, we have found that PR drastically improved the mechanical properties, self-healing, chemical decomposition, and marine biodegradability of vitrimers.3) The optimal epoxy resin vitrimer incorporated with PR exhibited enhanced toughness, with an elongation at break 5.3 times greater than that of a vitrimer devoid of PR; it also showed self-healing properties, was chemically recycled 10 times faster, and was recovered twice as fast. These results are ascribable to the sliding diffusion motion of the PR, which lowers the energy required for transesterification. Furthermore, vitrimer-containing PR showed 25 wt.% biodegradation following exposure to seawater for 30 d. These findings may lead to the development of environment-friendly plastics that exhibit most of the properties required for a circular economy.

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Deformation Behaviors of High-Density Polyethylene Characterized by In-Situ Nanodiffraction Imaging

Prof. Hiroshi Jinnai¹, Dr. Shusuke Kanomi¹

¹Tohoku University, Sendai, Japan

A2_4, Machuca Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Semicrystalline polymers possess a hierarchical structure that consists of both crystalline and amorphous regions. During the stretching process of these polymers, their internal structures undergo various changes, including the rotation and fragmentation of crystals, elongation of amorphous areas, and the formation of voids. Although these deformation behaviors are closely related to mechanical properties, analyzing their relationship has proven challenging due to nanometer-scale heterogeneity. Nanodiffraction imaging (NDI), an advanced electron microscope imaging technique based on electron diffraction, allows us to observe polymer crystals and map chain orientation with nanometer-scale spatial resolution.

In this study, a high-density polyethylene (HDPE) specimen with well-oriented molecular chains was prepared and subsequently stretched within an electron microscope to investigate its deformation behavior.

We observed many voids generated within the specimen. The TEM image at a certain strain reveals a craze. Because crazes represent a unique form of plastic deformation in polymers, it is essential to clarify the generation and growth mechanisms to understand their mechanical properties. A fibrous region was observed just before the fracture. NDI was performed on the craze and fibrous regions. At the conference, we will present TEM images that illustrate the deformation behavior, along with NDI maps showing relative crystallinity and molecular chain orientation. Additionally, we will discuss the mechanisms of deformation and fracture of HDPE based on the shape of voids and fibrils, the spatial distribution of crystals, and the orientation of molecular chains.

The phase diagram of colloidal nanostructures sensitizing rare-earth photoluminescence

Dr. Guillaume Gouget¹, Dr Emanuele Marino¹, Dr Alexandre C. Foucher¹, Dr Morgane Pellerin², Dr Lauriane Pautrot-D'Alençon², Dr Thierry Le Mercier², Pr Eric A. Stach¹, Pr Christopher B. Murray¹

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A2_8, Machuca Room (Level -2), septembre 17, 2025, 10:30 - 13:10

To improve photoemission conversion yield of rare-earth (RE) emitters, one strategy is to host them in semiconducting nanocrystals. From the pioneering work of the field in 2005, innovative reaction pathways toward colloidal nanocrystals have increased emitter loading content from 0.6% in 2013 to 5% in 2021. Improvements were incremental, by choosing pertinent RE cationic sites and anionic environments, following the hard-soft acids and bases rule proposed by Ralph Pearson in the 60s. The most recent results consist of 5% Er-doped La_2S_3 nanophosphors we obtained in oleylamine at 220°C during 1h. They display near-spherical shapes, $3.9 \pm 0.7 \text{ nm}$ diameters, and so-called “ γ ” cubic phase. In the bulk, γ RE sulfides are stabilized only at 2000°C or by mechanical milling. We investigate erbium solubility in the cation network of nanocrystalline La_2S_3 , (i) looking for the best E(3+) content for Er(3+) photoluminescence, and (ii) with special care on phase identification.

Probing several $x = \text{Er}/(\text{Er} + \text{La})$ molar ratios, we combine pXRD, SAXS, TEM, HRTEM, HAADF-STEM and TEM-EDX mapping with sub-nanometer scale resolution to identify nanocrystals' structure, morphology and RE content. As x increases, three domains are observed, with only partial solubility of Er(3+) in La_2S_3 , up to $x = 0.25$. A second population of $\text{La}(3+)\text{:Er}_2\text{S}_3$ nanocrystals appears for $x \geq 0.25$. Both populations display the same γ -phase, but with distinct morphologies: cubic-like shapes for Er-poor nanocrystals versus plate shapes for Er-rich ones. Er(3+) photoemission is detected only for $x = 0.05$.

The oral presentation will discuss the peculiar behaviors of colloidal nanocrystals $\text{Er}(2x)\text{La}(2-2x)\text{S}_3$ ($0 \leq x \leq 1$) obtained by wet colloidal synthesis. First, we identify a limit of solubility for Er(3+) insertion in La_2S_3 . Still, the 25% solubility represents a 5-fold increase compared to our previous work. Considering photoluminescence of $\text{Er}(2x)\text{La}(2-2x)\text{S}_3$ nanocolloids, $x = 0.25$ shall not be exceeded for future studies. Second, higher loadings ($0.25 \leq x \leq 0.75$) lead to two populations with distinct shapes, and same crystal structure. Motivations for the system to favor such an atypical shape segregation will be discussed, in regard of the elemental environments and morphological differences.

Completing the $\text{Er}(2x)\text{La}(2-2x)\text{S}_3$ ($0 \leq x \leq 1$) series with a single-phase domain of nanoplates for $x > 0.75$, we propose a methodology to study full series of ternary, mixed RE chalcogenide nanocrystals. The methodology is inspired from phase diagram studies historically ran for compositions from the bulk. Additional examples will be provided for europium and lanthanum sulfides. The study emphasizes the need for in-depth, adapted characterizations to combine the structural, morphological, compositional and surface characteristics of nanocrystalline colloids.

Site determination and refinement in nanocrystalline thermoelectrics by electron channeling

Dr. Andreas Delimitis¹

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A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Electron microscopy-based spectroscopic techniques, such as energy dispersive X-ray analysis (EDX/EDS), or Electron Energy Loss Spectroscopy (EELS) have been widely exploited for structure determination and refinement since the 1960's. These methods take advantage of the electron channeling effect, where the yield of element characteristic X-ray emission, or electron energy loss is modified, dependent upon the direction of the incident electron beam with respect to the crystal structure and the kind of ions in the lattice. These channeling effects are powerful in determining atomic site locations; hence, techniques such as ALCHEMI (Atom Location by CHanneling Enhanced Microanalysis) have been developed and widely applied since then.

Structural analyses are particularly focused in materials for renewable technologies and energy harvesting, such as mixed magnesium silicides ($\text{Mg}_2\text{Si}_{0.38}\text{Sn}_{0.6}\text{Bi}_{0.02}$) or n-type ($\text{Ti}_{0.4}\text{Zr}_{0.6}$) $\text{O}_{0.7}\text{Hf}_{0.3}\text{NiSn}_{0.98}\text{Sb}_{0.02}$ half-Heusler (HH) thermoelectrics (TE), for medium to high temperature range applications. Synthesis of nanocrystalline TEs often comes along with a complexity of phases, so that host or dopant site kind and location remain controversial. Application, therefore, of electron channeling is highly desirable in order to accurately determine and refine their structural characteristics. Planar electron channeling experiments were performed using the {111} rows of reflections, as this enables to distinguish among different lattice sites in the unit cell. EDS spectra were acquired after small tilting increments of the sample, so the incident electron beam forms small angles with the {111}-types of planes.

The variations of the normalized X-ray emission revealed a strong channeling effect for both mixed Mg silicides and HH nanomaterials. In general, the X-ray intensities' profiles are asymmetrical, demonstrating a modification of their nominal structures. Furthermore, Mg or Ni normalized counts are always distinct and complementary with all other ones, which confirms that Mg or Ni ions predominately occupy the tetrahedral T sites in silicides or HH, respectively. Variations in the X-ray intensities' profiles, as well as the specific ion kind for tetrahedral or octahedral positions will be further analyzed and discussed.

Selective laser processing of particle accelerator beam-screen inner surfaces for electron cloud mitigation

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¹CERN, Geneva, Switzerland, ²University Dundee, Dundee, Great Britain

A2_9, Machuca Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Laser-induced surface roughening facilitates the reduction of secondary electron emission (SEE) from materials [1], which is crucial for mitigating electron cloud (EC) formation in particle accelerators operating with positively charged species, such as the Large Hadron Collider (LHC). The laser-induced material transformation also enables other functionalities such as surface blackening or wetting behaviour variation with a wide parameter tuning range. This study focuses on the development of a selective laser surface treatment of the copper inner surface of beam-screen (BS) pipes, which have a length of up to 15 meters, a cross section of about 50 mm, and are installed in LHC superconducting (SC) magnets. The main technical challenges for the laser processing are the reduction of treatment time, the control of ablation depth, and the minimisation of particulate dust creation. Based on the found correlations between processing parameters using ultrashort-pulsed lasers and the resulting materials properties [2], and considering all technical constraints given by SC magnets with BS of several meters of length and small apertures, a tailored laser processing strategy was developed [3]. It includes the creation of a rough copper surface with nanoparticle-covered trenches of 15-20 μm depth, and an initial secondary electron yield maximum of 1.4-1.5. This treatment is selectively applied to the most relevant regions inside the BS. The resulting material properties are characterized including the surface topography and resistance as well as the SEE at both room temperature and cryogenic conditions. The efficiency to mitigate EC formation and thus improve beam quality is demonstrated via EC simulations and electron-induced conditioning experiments. This study also explores under which treatment conditions the risk of particulate detachment from the surface, which could lead to critical beam interaction, can be minimized. Furthermore, the presentation will describe the technology needed for fibre-based laser light distribution [4] as well as the optimisation of the robot-based laser spot scanning, the required synchronisation between laser scanning in the tube and cable/fibre transportation system, and the strategy for the extraction of ablated particulates.

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High performance supported Fe nanoparticles as CO₂ activation catalysts that can self-heat by magnetic induction

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A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Introduction.

We investigated Fe-based catalysts for CO₂ utilisation via RWGS. Fe nanoparticles are ferromagnetic and can be inductively heated to the reaction temperature by a relatively small, alternating magnetic field with intensities in the order of 10⁻² T. The approach of using Fe nanoparticles both for catalysis and inductive heating is expected to bring advantages such as the elimination of heat transfer limitations, fast response and the possibility of directly using electricity from renewable sources [1]. This work studies the magnetic and catalytic properties of Fe and Fe-Co supported nanoparticles and their stability as catalysts and inductive heaters under RWGS reaction conditions.

Methodology.

Supported Fe and FeCo nanoparticles were prepared by wet impregnation on γ -Al₂O₃ and CeO₂ supports. Structure and redox properties of the catalysts were studied by in-situ XRD, H₂ temperature-programmed reduction and operando XAS. The catalysts were tested in a lab scale 9 mm ID fixed bed reactor, equipped with a coil generating an alternating magnetic field (B_{app}= 47 mT, f= 323 kHz) and online GC analysis. Catalysts were activated in a conventional oven at 550°C for 1h in 10% H₂ in Ar.

Results and discussion.

Our materials containing supported Fe and Fe(Co) nanoparticles on Ce-based supports inductively self-heat up to 500-600°C and under CO₂/H₂ /Ar gas flow (100 mL/min 1:1:2) and, under such conditions, they catalyse the RWGS reaction with 100% selectivity towards CO. It was determined that only materials with average nanoparticle size > 11 nm are able to heat sufficiently. Operando XAS combined with XRD revealed that about 50% of metal Fe forms Fe₃C under reaction conditions. This translates into a lower induction temperature due to its lower Curie temperature. Conversely, the addition of small amounts of Co leads to an alloy, which stabilises the metal particles against carbide formation, ensuring stable induction heating at 600°C for at least 2h. Alternatively, a pretreatment in CO₂ at 550 °C generates Fe₃O₄ phase that can be inductively heated up to 500°C and was found to perform stably as RWGS catalyst. Combining operando XRD-XAS with the characterisation of spent catalysts after induction shows the unique effects of induction heating of nanoparticles embedded in a non-magnetic support. Investigation of temperature nanogradients and their effects on catalytic activity and stability is on-going.

Acknowledgments.

The authors thank ALBA Synchrotron for the beamtime at NOTOS beamline (experiment 2023097875).

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Efficient Microwave-Assisted Synthesis of Copper Chromite Spinel: Structural and Thermal Properties Analysis

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Microwave-assisted synthesis has gained attention for its ability to accelerate reaction kinetics and enhance phase selectivity in complex oxides. In this study, we demonstrate that microwave processing not only reduces synthesis time for CuCr_2O_4 spinel but also alters the phase transformation pathway, providing an alternative route to achieve phase-pure materials with improved structural control. By tuning reaction temperature (180–200 °C) and synthesis time (15–30 min), followed by calcination at 400–700 °C, we elucidate the critical role of microwave irradiation in phase development. X-ray diffraction (XRD) confirmed that at 200 °C for 30 min, the tetragonal CuCr_2O_4 phase formed with high purity, while at 180 °C for 15 min, a biphasic mixture of tetragonal and orthorhombic phases persisted, indicating an incomplete transformation. Thermal analysis (DTA/TG) revealed that the 180 °C sample exhibited a sharp exothermic peak with mass loss, associated with oxidation-reduction processes and NO_x exchange, suggesting that phase transformation is chemically driven rather than purely thermal. In contrast, the 200 °C sample displayed a more gradual exothermic response with lower structural water loss, indicating a kinetically favored and more controlled transition. These findings provide compelling evidence that microwave-assisted synthesis not only accelerates phase formation but also influences the underlying redox chemistry, potentially bypassing intermediate states observed in conventional solid-state routes. The ability to tailor the oxidation state and structural evolution through microwave parameters opens new opportunities for designing copper chromite materials with enhanced functional properties for catalytic, electronic, and magnetic applications.

Highly dispersed iron sites on silica nanoparticles as sustainable curing activator for elastomeric nanocomposites

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A2_1, Machuca Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

Rubber vulcanization is a key process for crosslinking rubber polymers by polysulfide chains and producing nanocomposites with high mechanical properties for many applications, e.g., tyres. The industrial vulcanization process commonly employs ZnO as curing activator; however, its low affinity for rubber requires a high consumption, causing possible environmental concerns due to zinc leaching from the final material.

This work proposes Fe@SiO₂, featuring Fe(III) sites on silane-functionalized SiO₂ nanoparticles, as a sustainable alternative to ZnO. Fe@SiO₂ is a double-function filler as SiO₂ nanoparticles act simultaneously as substrate for single-site iron activator and as reinforcing agent for the rubber nanocomposite.

Fe@SiO₂ was produced through a two-step synthesis: i) SiO₂ nanoparticles were functionalized with (3-aminopropyl)triethoxysilane in toluene; ii) functionalized SiO₂ was dispersed in a Fe(III) salt containing ethanol solution, to anchor Fe(III) on the surface. Fe@SiO₂ activators with amount of Fe(III) ranging from 0.25% to 5.5% were prepared.

Fe@SiO₂ was characterized through a multi-technique approach. First, the presence of Fe on silica surface was confirmed by mapping in Scanning Electron Microscopy (SEM-EDX). Besides, Electron paramagnetic resonance (EPR) showed signals at $g \sim 4.3$ and at $g \sim 2.0$, corresponding to isolated Fe(III) centers and coupled Fe(III) centers, respectively. The latter is likely due to electrostatic or chemical interactions, e.g., oxygen bridging, and becomes predominant when Fe loading is increased.

Fe@SiO₂ was tested as vulcanization activator in isoprene rubber (IR) nanocomposites, prepared in a Brabender mixer and cured at 170°C. Dynamic mechanical tests were performed in a Rubber Process Analyzer (RPA). Generally, Fe@SiO₂ exhibited a faster kinetics and a more efficient vulcanization process respect to ZnO, with equal amount of Fe and Zn, while maintaining comparable reinforcement and mechanical properties. Fast kinetics is likely a consequence of the immediate availability of Fe(III) centers on silica surface to react with curatives. In fact, both the effective interaction of the surface Fe(III) centers with sulfur and curatives, as well as their stability during the curing reaction, were confirmed by studying Fe@SiO₂ by XPS in a Model Compound Vulcanization. No difference in reactivity was detected between isolated and coupled Fe species, as RPA tests demonstrated that vulcanization performances depend solely on the total amount of Fe.

Concluding, the activator Fe@SiO₂ was characterized in its structure and reactivity, showing high availability of the active center, good interaction with the curatives, outperforming ZnO in terms of vulcanization degree, and therefore demonstrating to be a valid and sustainable alternative to ZnO for rubber vulcanization.

Consolidation by Spark Plasma Sintering of β -Eucryptite/ Al_2O_3 composites obtained by colloidal route

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A2_9, Machuca Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Thermal expansion of materials has been regarded as a challenge for many precision applications due to the internal stress caused by high thermal gradients. In this context, ultrastable materials are essential for numerous industrial applications [1]. β -Eucryptite, which belongs to the hexagonal LAS family, has garnered significant interest for the development of low-CTE ceramic composites. The primary issue with this material lies in obtaining dense ceramic bodies without forming a vitreous phase, as this can lead to relatively poor mechanical properties. One potential solution to this problem is to employ unconventional sintering methods, such as Spark Plasma Sintering (SPS) [2], combined with the addition of secondary phases [3, 4].

In this study, the influence of incorporating alumina nanoparticles on the mechanical and thermal properties of β -Eucryptite–alumina composites, prepared via a colloidal route and sintered using SPS, has been investigated. The composites were characterized in terms of microstructure, hardness, toughness, Young's modulus, and mechanical strength. The presence of alumina nanoparticles helps control the grain growth of β -Eucryptite and enhances the mechanical properties: hardness is increased by at least 25%, fracture toughness by 30%, and mechanical strength by more than 40% in the composites compared to monolithic β -Eucryptite. Additionally, the composites exhibit a very low thermal expansion coefficient, making them promising materials for various industrial applications.

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Integrating SSbD Principles in the Synthesis of Bio-SiO₂ Functionalized with TiO₂ for Sustainable Solutions

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Nanomaterials (NMs) have garnered significant attention in recent years due to their unique properties and extensive applicability across diverse industries. However, concerns regarding the potential adverse effects of NMs on human health and the environment have driven the development of the Safe and Sustainable-by-Design (SSbD) framework. This concept emphasizes the intrinsic design of safer NMs while ensuring their sustainability across their Life Cycle (LC). The integration of SSbD principles is paramount for advancing nanotechnology in a manner that aligns with societal and environmental priorities.

In this work, we present the development of bio-inspired silica (bio-SiO₂) nanomaterial functionalized with titanium dioxide (TiO₂) using a hydrothermal synthesis method. This approach aligns with SSbD guidelines by emphasizing environmentally benign synthesis pathways and the production of nanomaterials with tailored functionalities for specific applications. The functionalized bio-SiO₂/TiO₂ materials exhibit a range of desirable properties, including antibacterial, adsorbent, and photocatalytic activities, making them suitable for applications in water purification, antimicrobial coatings, and air quality improvement.

The hydrothermal synthesis process enables precise control over the material's structural and functional attributes, ensuring reproducibility and scalability. Key performance indicators were evaluated, including:

1. **Antibacterial Properties:** The nanomaterial demonstrated antibacterial activity against common pathogens, showcasing their potential for healthcare and environmental remediation applications.
2. **Adsorption Efficiency:** The bio-SiO₂/TiO₂ composites exhibited high adsorption capacities for methylene blue (MB) as a pollutant probe, underscoring their utility in environmental remediation.
3. **Photocatalytic Activity:** Under ultra-violet (UV) and visible light irradiation, the materials achieved effective degradation of MB, highlighting their role in photocatalytic processes for water purification.

A comprehensive characterization of the synthesized materials was performed using advanced techniques, including scanning electron microscopy (SEM), X-ray diffraction (XRD), and surface area analysis, to correlate structural properties with functional performance. Additionally, life cycle assessment (LCA) methodologies were employed to evaluate the environmental impact of the synthesis and application stages, ensuring adherence to SSbD principles.

This study not only advances the design of multifunctional nanomaterials but also provides a roadmap for integrating SSbD principles into the development of nano-enabled products (NEPs). The results contribute to the growing body of knowledge required to achieve a balance between innovation, safety, and sustainability in nanotechnology. Future work will focus on scaling production, validating performance in real-world scenarios, and expanding the applicability of these materials to additional use cases.

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Theoretical probe into the kinetics of phase transitions and magnetization reversal in magnetite nanoparticles

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A2_7, Machuca Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

We examine the phase transition kinetics in 23 nm nanocubes using time-resolved X-ray diffraction (XRD), with phase fractions determined through Rietveld refinement. The process is modeled using three coupled reaction - diffusion master equations that describe the concentrations of oxygen, wüstite, and magnetite, incorporating thermally activated oxygen diffusion and its reaction with wüstite. Model parameters were optimized to match XRD data at 298 K and 353 K, while its predictive accuracy was evaluated by comparing predictions to experimental data at 403 K. Understanding how magnetic moments in single-domain magnetite nanoparticles reorient is essential for optimizing these nanoparticles for biomedical applications, such as magnetic particle imaging and magnetic hyperthermia. To explore this, we employ the geodesic nudged elastic band method to determine the atomic-level minimum energy path for field-free magnetization reversal in bulk magnetite and single-domain cuboidal magnetite nanoparticles with {100} surface termination. Our results reveal that this reversal occurs through three successive elementary rotations of magnetic moments within distinct {110} planes. For iron-rich surface terminations, the energy barrier for this process is influenced by surface spin anisotropy, particularly in nanoparticles with a high surface-to-volume ratio, while no such dependence is observed in oxygen-rich terminations. This effect weakens as the particle size increases.

Modeling and Simulations of Polymeric Nanostructured Materials Across Scales: From Atoms to Macroscopic Behavior

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A2_3, Machuca Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

The computational study of complex polymeric materials is a very challenging field, due to the broad spectrum of the underlying length and time scales. We present a hierarchical multi-scale methodology for predicting the macroscopic properties of polymer-based nanostructured systems, which involves atomistic and coarse-grained (CG) simulations, as well as homogenization approaches and continuum models. The CG models are derived through a systematic “bottom-up” data-driven strategy, using information from the atomistic scale without any adjustable parameter [1]. Moreover, Deep Learning algorithms are developed to reintroduce atomic detail on the CG scale, and obtaining atomistic configurations of long polymer chains [1]. Here, we first provide an overview of the above hierarchical approach that allows the study of macromolecular systems over a broad range of time scales, from a few fs up to ms and the prediction of their properties (structural, dynamical, rheological, etc.) [2].

Next, the proposed computational methodology is applied to provide a fundamental understanding of the mechanism of mechanical reinforcement in glassy polymer nanocomposites, which is of paramount importance for their tailored design. We present a detailed investigation of the coupling between density, structure, and conformations of polymer chains with respect to their role in mechanical reinforcement [3]. We found that the effective mass density and rigidity of the matrix region change with filler volume fraction, while that of the interphase remains constant. The origin of mechanical reinforcement is attributed to the heterogeneous chain conformations in the vicinity of the nanoparticles, which involves a twofold mechanism. In the low-loading regime, the reinforcement comes mainly from a thin, single-molecule, 2D-like layer of adsorbed polymer segments on the nanoparticle, whereas in the high-loading regime, the reinforcement is dominated by the coupling between train and bridge conformations; the latter involves segments connecting neighboring nanoparticles.

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Extraction of Reactive Dyes from Wastewaters with Metal-Organic Framework MIL-101(Fe)

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A2_6, Machuca Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Each year, textile wastewater grows richer with dyes, as sustainable practices like clothes recycling unintentionally amplify the issue by extracting dyes that end up in nature. These persistent or decomposed dyes infiltrate the water cycle, making their way into drinking water and posing significant risks to human health.

To address this pressing concern, researchers have explored numerous wastewater treatment methods. Among them, adsorption has stood out as a particularly cost-effective and efficient approach. One class of materials gaining attention for their adsorption capabilities is metal-organic frameworks (MOFs). Renowned for their exceptionally high surface area, customizable pore size, and structural versatility, MOFs have shown promise in removing dyes.

Most studies on MOF applications for dye removal focus on ionic dyes, such as methylene blue or methyl orange, which often have comparatively small molecule sizes and charge. At the same time, the processes of reactive dyes removal remain underexplored. Nevertheless, reactive dyes are particularly problematic due to their widespread use in dyeing natural fibers like cotton and linen. In this research we focus on solvothermal synthesis of iron-based MIL-101 for the application for removal of Reactive Blue 4 (RB4) dye.

A series of MIL-101(Fe) was synthesized with different $\text{FeCl}_3 \cdot \text{H}_2\text{O} : \text{H}_2\text{BDC}$ (terephthalic acid) molar ratios from 0.5 to 3.5 (MIL-101(Fe)-0.5 to MIL-101(Fe)-3.5). The SEM analysis of synthesized powders reveals that MIL-101(Fe)-0.5 has homogeneous particles size, whereas at higher precursors ratios, particles sizes are heterogeneous, and side compounds are produced. The FTIR analysis suggests that the structures of MOF with different ratios are similar, and that at a higher precursor ratio, the peak corresponding to Fe—O bond at 555 cm^{-1} is more pronounced because an iron-based side compound is produced due to the higher initial concentration of ferric chloride in the synthesis. This has its effect on RB4 dye adsorption. Removal of RB4 was two times greater in the case of MIL-101(Fe)-0.5 compared to MIL-101(Fe)-3.5. That is apparently due to the homogeneity of particles and their smaller size, exposing a higher surface area, which is one of the most important characteristics of an effective adsorbent.

Electrochemical synthesis of reactive Al/CuO nanocomposites at ambient temperature without surfactants

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A2_10, Machuca Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Reactive metal-oxide nanocomposites (or nanothermites) have gained significant attention in fields like propulsion, sterilization, energy storage, and advanced joining technologies. Among them, Al/CuO nanothermites stand out for their potential in applications such as soldering, welding, micro-actuators, and microelectromechanical systems (MEMS). The thermite reaction between aluminium metal (fuel) and copper(II)-oxide (oxidizer) is highly exothermic ($\Delta H_f^0 = -1'193 \text{ kJ/cm}^3$) and can thus provide enough heat to produce a molten Cu phase for e.g. reactive soldering. This study presents a two-step electrochemical synthesis route for fabricating Al/CuO nanocomposites with a very high density of pristine (i.e. unreacted and uncontaminated) Al/CuO interfaces, as required to obtain a self-propagating high-temperature synthesis (SHS) reaction upon ignition. In a first step, a nanoporous CuO framework is produced by electrophoretic deposition (EPD) of CuO nanoparticles (NPs) dispersed in ethanol. The resulting nanoporous CuO scaffold is then electrochemically infiltrated with Al using an ionic liquid as electrolyte (carried out in a protective Ar atmosphere to prevent oxidation of Al). Specific additive-free surface treatments, such as ozonation and thermal oxidation, were developed (as guided by XPS) to tune the chemical surface state of the CuO NPs to obtain stable highly-concentrated CuO NP dispersions and reproducible EPD processes without the use of any organic additives, like surfactants. An empirical correlation between the chemical surface state of aged and surface-treated CuO NPs (determined by XPS) and the ζ -potential of the dispersed NPs in ethanol (determined by the electroacoustic method) could thus be established. The nanoporous CuO thin-films with tunable thickness and porosity were characterized by a combined analytical approach using XPS, positron annihilation lifetime spectroscopy (PALS), BET (Kr adsorption), and HR-SEM with FIB. Successful electrochemical infiltration of Al into the nanoporous CuO scaffold could be demonstrated. The proposed 2-step electrochemical synthesis route is scalable, cost-effective, and environmentally friendly and, moreover, can be performed at ambient temperature, thus preventing premature reactions between Al and CuO.

NEW ELECTROACTIVE AND THERMO-REVERSIBLE DIELS-ALDER EPOXY NANOCOMPOSITES DOPED WITH CARBON NANOTUBES

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The manufacturing of reversible matrix epoxy nanocomposites with Diels-Alder bonds is highly complex and, therefore, constitutes a topic that is practically not treated in the state of the art. Diels-Alder epoxies need the addition of solid reagents, such as bismaleimide, that increase notably the viscosity and hinder the mixing and dispersion of nanofillers. Thus, the combination of network reversibility and self-healing with other smart functionalities such as electrical conductivity and Joule heating is hard to achieve. In this way, the state-of-the-art shows reversible epoxy nanocomposites that need contents of carbon nanotubes near or higher than 1 wt.%, which implies deep handling and economic drawbacks.

In the present work, a new manufacturing route is proposed to manufacture new electroactive Diels-Alder epoxy nanocomposites whose percolation thresholds are below 0.3 wt.%. The target is achieved by an optimized mixing methodology, and the materials show efficient thermo-electric behaviors, compared with previous attempts, that are close to conventional nanocomposites.

Composite ZnO/CeO₂ electrospun nanofibers as efficient antibacterial materials

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Infectious diseases from microbial pathogens constitute a major global health problem,^{1,2} which is further intensified by the escalation of the antibiotic resistance rendering the traditional treatments ineffective. Therefore, in quest of new strategies to fight against bacterial infection, metal or metal oxide nanoparticles have emerged as very powerful tool.³ Amongst them, ZnO and CeO₂ stand out on account of their natural abundance, low cost, low toxicity, good biocompatibility and high bactericidal effect.^{4,5} To this end, in the present study highly active composite ZnO/CeO₂ antimicrobial nanoformulations are fabricated through a facile water-based electrospinning method. The composite ZnO/CeO₂ electrospun nanofibers are produced from an initial sol-gel solution employing water as the only solvent, PVA as a carrier polymer and Zn, Ce nitrates as metal precursors. After calcination, according to SEM analysis, the produced materials present a highly homogeneous nanofibrous morphology with small diameters not exceeding 200nm. In addition, elemental mapping measurements reveal a high compositional uniformity with even distribution of both Zn and Ce species, while the ratio of Zn/Ce was 1.2:1. After the structural characterization of the synthesized nanomaterials, their antibacterial activity was evaluated against Gram-negative *Escherichia coli* and Gram-positive *Staphylococcus Aureus* bacteria, while their biocompatibility was investigated through cytotoxicity on mammalian cell lines. It was found that these composite ZnO/CeO₂ electrospun nanofibers exhibited an enhanced, dose-dependent antibacterial activity against both test organisms. Additionally, due to their low toxicity, these nanofibers can be considered as very attractive antibacterial materials.

Acknowledgements

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Some recent progress on filler structure and interfacial layer dynamics of polymer nanocomposites

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A2_2, Machuca Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

The macroscopic properties of polymer nanocomposites (PNCs) depend in a crucial way on the microscopic state of the filler nanoparticles (NPs) and the polymer. In particular mechanical properties are strongly affected by percolation of hard phases, which may be NP networks, or dynamically modified (i.e. hardened) polymer regions. In this talk, we will review some recent progress in small-angle scattering associated with simulations to study nanoparticle dispersions, and broadband dielectric spectroscopy (BDS) to investigate polymer dynamics at the NP interface.

Nanoparticles used in industrial applications may be very polydisperse, and form agglomerates of complex geometry. The conceptual difficulty of their analysis goes hand in hand with their superior performances. We will present one of the first self-consistent models of their structure based on a combination of electron microscopy with scattering [1]. We did not realize it back then, but this approach was the first based on a correlation hole analysis [2], which is a measure of the strength of interaction between particles or small aggregates, and thus the local concentration. In collaboration with Vera Bocharova and Alexei Sokolov [3,4], we then moved to an in-depth characterization of the dynamic state of the polymer using BDS in strongly attractive model systems. Here the combination of structural analysis based on scattering, with a careful look on interparticle distances, with BDS turned out to allow for a better quantitative determination of the thickness of the interfacial layer. The experimental system under scrutiny is a surface-modified PNC (C8 or C18 silane grafting), where the NP structure and the interfacial layer dynamics can be followed simultaneously as a function of grafting density and particle content. The strongest dynamical slow-down in the polymer is found for unmodified NPs, while grafting weakens this effect progressively. The combination of all three techniques enables a unique measurement of the true thickness of the interfacial layer, which is ca. 5 nm. Finally, the comparison between longer (C18) and shorter (C8) grafts provides unprecedented insight into the efficacy and tunability of surface modification. It is shown that C8-grafting allows for a more progressive tuning, which goes beyond a pure mass effect.

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Full-Stokes analyzer using near-field dielectric metasurfaces

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A2_7, Machuca Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

The polarization state of a light beam, that describes the path along with its electric field oscillates, is a relevant parameter in almost every area of science like astrophysics, medicine or biology, among others. Dielectric metasurfaces are ultrathin optical structures that modulate locally the phase or polarization of a light beam by modifying the field in the subwavelength scale. A phase change is introduced by a phase discontinuity under the general Snell's law rather than by optical path accumulations as the traditional optical components.

In this work, we propose an algorithm for designing metasurfaces that modulate the phase or polarization in the near field, along with their manufacturing process by electron beam lithography. The design method is based on the polar decomposition of a Jones matrix, which claims that any Jones matrix can be expressed as the product of a retarder (lossless) and a diattenuator (lossy). Given a desired polarization distribution in the image plane, we determine the Jones matrix of the metasurface, which corresponds to a pure retarder matrix as we aim to avoid any diattenuation. Since we are working in the near-field range, we apply the Vector Rayleigh-Sommerfeld (VRS) propagation method to iterate between the image and object planes and determine the final metasurface Jones matrix. Then, using Comsol software we relate the phase shifts given by the Jones matrix to the dimensions of the pillars for further fabrication. We have developed a full-Stokes analyzer that forms six light spots at the focal plane with 0°, 90°, 45°, 135° linear polarization states, right and left circular polarization states. By measuring the intensity of these focuses, we reconstruct the polarization state of the input light. We manufactured the device by electron beam lithography technique. In particular, we have patterned our metasurface design on a 1.2 μm GaN layer over a sapphire substrate. In this way, we developed a full-Stokes analyzer with which we are able to modulate the polarization at the nanometric scale.

Non linear mechanical and thermal properties of polymer nanocomposites : an atomistic point of view

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A2_2, Machuca Room (Level -2), septembre 15, 2025, 10:50 - 13:10

The first part of the talk will be devoted to the modelling of the non linear mechanical properties of polymer nanocomposites (PNCs). One of the most studied phenomenon is the so-called Payne effect, a drop in storage modulus with increasing amplitude, which occurs for deformation amplitude as low as a few percent. Several mechanisms have been put forward to rationalize such effect, including filler network breaking, polymer chain desorption and yielding of the polymer confined between the nanofillers [1]. In this contribution, we demonstrate that for PNCs involving fractal-like aggregates, the Payne effect may originate from the shear-induced alignment of the aggregates. We reach this conclusion by using a coarse-grained model, which combines an explicit representation of fillers with an implicit description of the polymer matrix [2]. We systematically characterize the effects of aggregate size and polydispersity in the amplitude of the Payne effect [3]. Moreover, we probe the mechanical response of the model PNCs after a first cycle of deformation. We observe slow recovery kinetics of the original storage modulus of the PNCs and relate this memory effect to the alignment of the aggregates. Our findings should contribute to clarify the relation between the macroscopic mechanical response of the PNCs and the mesoscopic state of the filler.

The second part of the talk will be devoted to the thermal transport properties of polymer nanocomposites. Polymeric materials generally display relatively low thermal conductivity, which restricts their use in microelectronics and more generally in thermal management applications. Dispersing conductive nanoparticles in a polymeric material is a common strategy to enhance the thermal conductivity of the nanocomposite, but the resulting conductivity hardly increases due to the existence of a thermal resistance at the interface between the nanofiller and the matrix. Here we investigate the thermal transport properties of grafted silica based polystyrene nanocomposites using non-equilibrium molecular dynamics simulations. We first show that grafting silica with polystyrene chains reduces significantly the thermal resistance between at the nanoparticle/matrix interface. We further demonstrate that this reduced resistance helps increase the total conductivity of the nanocomposite and discuss the effect of the silica nanoparticle diameter.

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Green Synthesis of Magnetic Iron Oxide Nanoparticles Using Agave tequilana bagasse extract and its Application for Toxic Dyes and Cr (VI) removal in aqueous solution

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Magnetic iron oxide nanoparticles (MIONPs) were synthesized using a novel green method consisting of a water-based extract from bagasse of Agave tequilana Weber var. azul (residual from the Tequila industries) used as the reducing agent and iron nitrate nonahydrate as the precursor during the microwave-assisted synthesis. The physical and chemical properties of the MIONPs, along with the ease of magnetic separation after reactions, make them a good candidate for removal of water contaminants. For the MIONPs syntheses, we used different percentages of bagasse extract (from 5 to 10% w/w), and we varied the concentrations of iron nitrate nonahydrate from 0.08 to 0.24 M. The nanoparticles were characterized using UV-Vis, FTIR, and Raman spectroscopies, as well as TGA, XRD, SEM, VSM, and TEM techniques. UV-Vis, FTIR, and Raman spectroscopies confirmed different iron oxide and hydroxide phases of the nanoparticles along with different sizes (10 nm to 36 nm) and shapes as confirmed by the TEM micrographs. The XRD confirmed crystalline and amorphous phases of iron oxide and hydroxide nanoparticles. The VSM technique showed paramagnetic and ferromagnetic-like behaviors of the nanoparticles. The color removal capacity of the nanoparticles was tested for the toxic dyes Maxilon red (MR), methylene blue (MB) brilliant green (BG) and, also for adsorption of Cr (VI) from aqueous solutions. The nanoparticles achieved good performance for Cr (VI) adsorption and color removal of toxic dyes in batch reaction experiments, with complete removal for BG and 90% removal of MB. The performance of the nanoparticles for Cr (VI) adsorption and color removal of toxic dyes was related to the crystallinity of the iron and iron hydroxide phases. The environmental impact of the wasted bagasse is huge in the area, and we are providing here an option to use it with a beneficial purpose.

Optimization methods for advancing thermoelectric materials into practical applications

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A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Thermoelectrics is an emerging technology for effective recovery of waste heat and its conversion into useful electricity without moving parts, noise or the release of harmful chemicals. Therefore, such converters exhibit a high potential to contribute to the global efforts to reduce CO₂ emissions from fossil fuels and towards a cleaner and sustainable environment. Currently available converters can only work in a limited temperature range, resulting in limited efficiencies of only up to several percent, and exhibit insufficient mechanical properties.

In this talk the potential of both n- and p- type novel and highly efficient materials including the TiNiSn-based half-Heusler, HH, compounds, as well as Mg₂Si- and GeTe- based alloys will be described via understanding the role and controlling of meso-scale defects, such as grain-boundaries, separated phases, dislocations/twinning and chemical impurities on the thermoelectric properties. Such materials, containing available constituents, can be optimized for better mechanical endurance and are capable at different temperature ranges of operation up to 700°C, and therefore expected to enhance the Carnot efficiency with all of the other associated advantages. The efforts of maximizing the potential of such materials by both electronic and phonon effects will be described in detail in the talk and the routes approaching practical energy conversion devices will be addressed.

Investigation of Structure and Electrical Properties Modifications in Layered Oxyhalide Nanoplates Induced by Anion Exchange and UV Irradiation

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A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Layered oxyhalides from the Sillén family form a diverse group of materials with potential applications as photocatalysts, photocathodes, and photodetectors, as well as alternatives to lead-halide perovskites [1-4]. This wide range of applications stems from their unique structure, where positively charged $[\text{Bi}_2\text{O}_2]^2$ layers and halide ions are stacked along the [001] direction through van der Waals forces. As a result, these anions are mobile, and their selective replacement can significantly influence the electrical properties of nanoplates. Additionally, surface modifications in layered nanoplates can impact their characteristics, such as catalytic activity. Notably, these surface changes can be induced directly through UV light irradiation, leading to the formation of oxygen vacancies and alterations in the oxidation state of bismuth ions [3].

In this study, two approaches were used to modify the properties of bismuth oxychloride (BiOCl) nanoplates: anion exchange and oxygen vacancy formation. The effects of these modifications were analyzed using dielectric spectroscopy, which enabled real-time monitoring of changes in the electrical properties of nanoplates under UV irradiation. Structural changes were further examined through X-ray diffractometry, transmission electron microscopy, UV-Vis spectroscopy, and X-ray photoelectron spectroscopy.

The findings demonstrate how layered oxyhalides' dielectric and optical properties can be tuned for specific applications. The anion exchange approach provided insight into how different ions affect the dielectric properties of these materials while minimizing morphological effects. Meanwhile, UV-induced modifications on the nanoplates' surface revealed how charge carrier type and concentration variations influence their high-frequency properties.

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Magnetite nanoparticles coated by hydrochar-like structure: the influence of synthesis methods on drug delivery and magnetic hyperthermia effect

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Polysaccharide-modified magnetite nanoparticles are a growing research focus due to their potential in targeted and controlled drug delivery. Surface functionalization is crucial, with organic modifiers like polysaccharides (e.g., dextran, starch) enhancing biocompatibility, stability, and targeted drug conjugation. These biopolymers create a biocompatible environment, minimizing toxicity and immune responses while enabling prolonged circulation and selective tissue targeting. The choice of polysaccharide significantly impacts drug release kinetics, allowing for sustained or triggered release, which improves therapeutic efficacy and reduces side effects. Starch, a widely available, low-cost, and biodegradable polysaccharide, is particularly promising for drug carriers and nanoparticle coatings. Functionalized starch-coated iron oxide nanoparticles enhance stability by balancing magnetic and van der Waals forces, while polymer surface complexing agents help control particle size during magnetite formation.

In our research, we created magnetite-based materials modified with wheat starch using a high-temperature decomposition process. This study explores how synthesis methods influence physicochemical properties. Structural analysis was conducted using X-ray diffraction to determine phase composition and crystallite size, while scanning and transmission electron microscopy provided detailed insights into morphology. UV-VIS spectroscopy assessed drug adsorption on ferrite nanoparticles, and drug release studies revealed significant differences in adsorption capacity based on the applied modifiers. The polysaccharide layer proportion was determined using thermogravimetric analysis. Additionally, we evaluated the magnetic hyperthermia effect of polysaccharide-modified magnetite nanoparticles and compared it with unmodified magnetite.

Interface Modification in Fe/Pt Spintronic Bilayers for Superior THz Emission

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Layered ferromagnetic/non-magnetic (FM/NM) nanostructures have attracted significant interest for spintronic applications due to efficient spin transport across epitaxial interfaces in Fe/Pt bilayers [1]. These bilayers are promising for THz spintronic devices [2], with interface quality playing a crucial role in spin current transmission. Optimizing interfacial structure and defect density can enhance spintronic THz emitter performance [3]. This study investigates structural modifications of the Fe/Pt interface by varying growth and annealing temperatures, correlating interfacial features with THz emission properties.

Fe/Pt bilayers with Fe (12 nm) and Pt (6 nm) were deposited on MgO(100) substrates via electron beam evaporation. To maintain total thickness, Pt layer growth temperature was varied to modify the Fe/Pt interface. A 12 nm Fe film was deposited at 300°C and annealed for 30 minutes, followed by a 6 nm Pt layer deposited at 300°C, 450°C, or 600°C, with subsequent annealing at corresponding temperatures. THz emission was characterized by using terahertz time-domain spectroscopy (THz-TDS). Structural investigations included X-ray diffraction (XRD), transmission and scanning transmission electron microscopy (TEM/STEM), energy-dispersive X-ray spectroscopy (EDXS), and Z-contrast high-resolution STEM (HRSTEM) imaging along with HRSTEM image simulations.

The Fe/Pt(450°C) sample exhibited the highest THz emission, nearly twice that of Fe/Pt(300°C), while Fe/Pt(600°C) showed negligible signal [4]. XRD revealed an almost strain-free Fe/Pt structure for Fe/Pt(300°C), while the 450°C sample showed an additional $L1_0$ -FePt peak, suggesting interface modification. The 600°C sample exhibited new peaks corresponding to the fct lattice of $L1_0$ -FePt, indicating complete transformation into an ordered alloy. TEM analysis confirmed distinct Fe and Pt layers for Fe/Pt(300°C). HRTEM imaging of Fe/Pt(450°C) revealed a 2 nm interlayer (IL) at the Fe/Pt interface with a periodic intensity modulation, signifying a chemically ordered $L1_0$ -FePt structure. Z-contrast HRSTEM imaging and simulations confirmed chemical ordering. STEM-EDXS showed localized Fe and Pt interdiffusion. In contrast, TEM analysis of Fe/Pt(600°C) showed full interdiffusion into a chemically ordered $\text{Fe}_x\text{Pt}_{1-x}$ alloy with fct symmetry.

The Fe/(2 nm) $L1_0$ -FePt/Pt interface in Fe/Pt(450°C) significantly enhanced THz emission. In contrast, complete intermixing and the absence of a non-magnetic Pt layer in Fe/Pt(600°C) suppressed emission. These findings highlight the potential of engineered interlayers for optimizing spintronic THz emitter performance and advancing spintronic device design.

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High-temperature stability of Al-based structured electrodes

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A2_10, Machuca Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Sensors working at high temperatures are required in industry to monitor and optimize high-temperature processes. Wireless devices, such as surface acoustic wave (SAW) sensors, allow measurements at locations which are difficult to access by wired systems. To realize a high-temperature stable SAW sensor, a high-temperature stable piezoelectric substrate as well as a high-temperature stable metallization are required.

The two Al-based metallizations TiAl and RuAl are investigated as an alternative to the expensive high-temperature stable Pt-based solutions reported in literature. The high-temperature long-term stability of extended thin films as well as of structured electrode systems were analyzed for both alloys.

Ti-Al multilayer films were deposited by e-beam evaporation from pure material with a total thickness of 200 nm. The RuAl films were deposited by co-sputtering from elemental targets with additional thin Al layers on top, in the center and at the bottom with a total film thickness of 130 nm. The films were deposited on $\text{Ca}_3\text{TaGa}_3\text{Si}_2\text{O}_{14}$ (CTGS), which is a high-temperature stable piezoelectric substrate, as well as on thermally oxidized Si as a reference. The samples were annealed in high vacuum or in air for a duration up to 192 h and at temperatures up to 800 °C. Scanning electron microscopy (SEM) and especially transmission and scanning transmission electron microscopy (TEM and STEM) in combination with energy dispersive X-ray spectroscopy (EDX) were performed to analyze the morphology and possible degradation of the thin films.

First experiments revealed a chemical reaction between the CTGS and the Al-based alloys, proving the necessity of the addition of suited barrier layers between the metallization and the substrate. In addition, an oxidation protection layer on top of the samples was required. For these additional layers, SiO_2 , AlNO or a combination of both was used.

In case of the TiAl samples, the experiments demonstrated a long-term high-temperature stability in air up to at least 500 °C and for 192 h and a short-term stability at 600 °C. In contrast to this, due to the noble character of Ru, the RuAl samples showed hardly any degradation at 600 °C. A long-term stability was achieved at 700 °C and the samples were almost completely oxidized after annealing at 800 °C for 192 h. For both material systems, a strongly improved high-temperature stability will be achieved in high vacuum or by a suited encapsulation of the sensors.

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Synthesis and Characterization of Titanium Niobium Oxides for Advanced Photocatalytic Applications

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A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Titanium niobium oxides (TNOs) have gained significant attention as electrode materials in lithium-ion batteries due to their stability, high energy storage capabilities, and tunable electronic properties [1,2]. However, these same characteristics—unique electronic structures, adjustable band gaps, and excellent stability—also make TNOs promising candidates for photocatalysis [3,4]. Photocatalysts are widely used in environmental applications, including hydrogen production via water splitting, CO₂ reduction, and the degradation of organic pollutants. Despite their potential, the photocatalytic properties of TNOs remain relatively unexplored, with only a few studies investigating their capabilities.

One of the key advantages of TNOs is their ability to modify their electronic band structure when titanium is incorporated into niobium oxide Wadsley-Roth lattices. This modification extends light absorption into the visible spectrum, improves charge carrier mobility, and reduces recombination losses, enhancing overall photocatalytic efficiency. Given their established role in the energy storage industry, TNOs present an exciting opportunity as scalable, multifunctional materials that can bridge the gap between energy storage and photocatalysis.

In this study, we synthesized TNOs with the most common stoichiometries—TiNb₂O₇ and Ti₂Nb₁₀O₂₉—using three different synthesis methods: solid-state, hydrothermal, and solvothermal routes. Among these synthesis methods, the hydrothermal and solvothermal routes are the most efficient for photocatalytic applications. This is related to the smaller particle size obtained through these routes, along with optimized morphology, and crystallinity, leading to improved light absorption and charge separation properties.

Through extensive characterization, we gain deeper insights into the photocatalytic performance of TNOs and their potential to drive sustainable chemical transformations. By further exploring these materials, we hope to contribute to the development of next-generation photocatalysts with enhanced efficiency and stability for environmental and energy-related applications.

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Acoustically-driven Hybrid Nanocrystals for In Vivo Pancreatic Cancer Treatment

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A2_7, Machuca Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Background

Pancreatic ductal adenocarcinoma (PDAC) is one of the deadliest tumors, projected to become the second leading cause of cancer-related death in the United States by 2030. PDAC is marked by hypoxia, intrinsic chemoresistance, a “cold” tumor microenvironment and dense desmoplastic stroma, which hinders drugs penetration. In the continuous effort to develop alternative treatments, this study proposes a multimodal therapy leveraging a nanomedicine-based approach.

Methods

A nanoconstruct based on iron-doped zinc oxide nanoparticles (NPs) was developed, and a tailored lipidic formulation - inspired by those employed in COVID-19 vaccines - was implemented to shield the NPs while enhancing their stability in biological media. It was hypothesized that NP administration, followed by local ultrasound stimulation, could elicit a tumor response through the generation of reactive oxygen species (ROS) via a process called inertial cavitation. This effect was enhanced by incorporating a lipophilic molecular sonosensitizer (IR780) into the lipidic shell. After in vitro validation on KPC cells, the approach was translated in vivo using mouse models bearing subcutaneous KPC pancreatic tumors.

Results

The resulting nanoconstructs were thoroughly characterized from a physico-chemical perspective. The in vitro results showed that the combined therapy triggered significant ROS production and the death of KPC cells. In vivo, the antitumor efficacy was particularly pronounced when both the sonosensitizer and the ultrasound stimulation were employed. In fact, the experimental group receiving lipid-coated NPs incorporating the sonosensitizer (lipid-coated-IR780 NPs) and subjected to ultrasound stimulation showed a clear reduction in tumor size. Moreover, increased immune cell infiltration, enhanced cancer cell apoptosis and prolonged survival of treated animals were achieved.

Conclusions

These results underscore the potential of a combined therapeutic strategy that integrates lipid-coated, sonosensitizer-loaded nanoparticles with ultrasound stimulation, offering a potent treatment option for PDAC and in situ monitoring. Most importantly, these results were achieved by combining two safe-by-design treatments and employing an FDA/EMD-approved ultrasound transducer, paving the way for future clinically translatable therapies suitable for deep-seated tumors such as PDAC.

Clinoptilolite functionalization with antimicrobial nanoparticles using a green in situ reduction process

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A2_6, Machuca Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Natural zeolites are extensively investigated due to their impressive ability to adsorb toxic substances, reduce airborne pathogens, and promote cleaner air. Among them, clinoptilolite has attracted significant attention in air purification and wastewater treatment. Furthermore, the introduction of antimicrobial nanoparticles on their surface can enhance their pathogen removal efficiency.

In this study, clinoptilolite powders were functionalized with silver and copper nanoparticles (NPs) to provide antimicrobial properties, using an environmentally friendly approach. The process concerned the in situ reduction of antimicrobial NPs on the surface of zeolites with tannic acid (TA) as a green reducing agent. The multi-step functionalization process was investigated from a morphological-compositional and structural point of view using Fourier-transform infrared (FTIR) spectroscopy, field emission scanning-transmission electron microscopy (FESEM, STEM, TEM) equipped with energy dispersive X-ray spectroscopy (EDS), and X-ray diffraction (XRD). The absorption properties were evaluated through BET analysis, while the antibacterial effect was assessed via the zone of inhibition and bioaerosol contamination tests.

FTIR analysis confirmed the successful functionalization of clinoptilolite powders with tannic acid. Morphological and compositional analyses showed the presence of antimicrobial NPs on the zeolite surface, and XRD confirmed the presence of metallic silver and copper or copper oxide NPs. The functionalized clinoptilolite exhibited antibacterial activity against both Gram-positive and Gram-negative bacterial strains. In conclusion, the environmentally friendly process of functionalization of clinoptilolite with NPs with antimicrobial effect proved to be a promising strategy to develop natural materials capable of adsorbing toxic compounds and effectively inhibiting the growth of pathogens.

Unveiling Surface Dynamics: In Situ Oxidation of Defective WS₂

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A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Defects on transition metal dichalcogenides (TMDs) surfaces influence their surface reactivity, stability, and performance in electronic and catalytic applications. In this work, we investigated the oxidation dynamics of defective WS₂ using in situ X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) simulations. Sulfur vacancies are introduced via grazing incidence Ar⁺ sputtering, leading to the emergence of a shoulder in W 4f core-level spectra at low binding energy, indicative of reduced tungsten states. Upon controlled O₂ exposure, oxidation proceeds in a pressure-dependent manner: at low pressures (<10⁻⁴ mbar), oxidation is minimal, while at higher pressures (>10⁻² mbar), rapid conversion to W⁶⁺ occurs, signifying WO₃ formation. XPS analysis shows the disappearance of defect-related features as vacancies become passivated. DFT calculations reveal that vacancy clusters reduce the effective charge on tungsten atoms, lowering the activation barrier for O₂ dissociation (<0.3 eV). Electron transfer from the surface to the O₂ molecule facilitates oxygen incorporation into the lattice, driving oxidation. Understanding these oxidation pathways is crucial for tuning WS₂ stability in applications such as catalysis and gas sensing, where surface reactivity plays a key role. By controlling defect densities and oxidation conditions, WS₂ can be engineered for sustainable energy applications, including hydrogen evolution reaction (HER) catalysts and chemical sensors for environmental monitoring. These insights provide a pathway for optimizing TMD-based materials for long-term stability and functionality in green technology and device applications.

Atomic-scale metastable structure formation in nickel-aluminum alloys synthesized far from equilibrium

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A2_10, Machuca Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

The present study reports on the structure formation in epitaxial nickel-aluminum (Ni-Al) films (Al content up to ~25 at.%) grown on MgO(001) substrates by magnetron sputtering. Nanoscale structure and chemistry probes, along with and theoretical calculations consistently demonstrate that the alloy films consist of face-centered cubic (FCC) solid solution (denoted as γ phase) and/or ordered $L1_2$ Ni_3Al phase (denoted as γ' phase) domains. The Al contents in the range ~10-25 at.% the γ and γ' -phase domains are homogeneously intermixed at the atomic-scale, forming a coherent matched lattice with one overall lattice parameter. The lattice parameter expands as the Al content increases, with γ -phase domains being progressively replaced by their γ' -phase counterparts. Isothermal annealing of films containing ~14 at.% Al, coupled with structural and nano-mechanical characterization, reveal that the nanostructure retains its integrity for temperatures up to 673 K , while the film hardness increases from ~5 (as deposited films) to ~6 GPa . Further increase of the annealing temperature to 873 K and 1073 K cause the coherent to dissolve leading to discrete γ and γ' phases and reduction of hardness to values of ~4 GPa. These observations confirm the metastable nature of the as-deposited nanoscale structure of the thin-film Ni-Al alloy system providing new insights for meta-stable intermetallic thin film synthesis.

Dynamical studies (liquid/gas/corrosion strain & crystalline- amorphous-phase maps) using in situ 4D-SPED in advanced materials

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A2_8, Machuca Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Automatic crystal orientation & phase mapping (ASTAR technique) can be applied in a variety of materials [1,2] using 4D-SPED (scanning Precession Electron Diffraction), where beam precession (to improve ED patterns quality [3,4]) in TEM is used in synchronization with beam scanning. ASTAR technique has significant spatial resolution down to 1-3 nm (in case of FEG-TEM).

In situ methods have been extensively applied towards dynamical studies. The combination of 4D-SPED ASTAR with the new generation of pixelated detectors allows the use of extremely low electron dose with significantly fast acquisition times (500-1000fps). For example, we have obtained orientation /texture maps on Au colloidal nanoparticles in water by monitoring local orientation changes over time.

Another in-situ study, regards Zirconium- (Zr-) based alloys, that utilized as cladding material for nuclear reactor fuel, are susceptible to oxidation under harsh reactor operation conditions. Using a MEMS-based environment holder, we have studied Zr metal oxidation mechanism by monitoring local orientation/phase changes using ASTAR and strain mapping by integrating four-dimensional scanning transmission electron microscopy (4D-STEM), ambient pressure gas-cell holder, precession electron microscopy (PED), and direct electron detector (DED). This type of setup can be used to conduct in situ/ in operando corrosion studies across a broad range of materials.

Again, the recent development of e-PDF mapping analysis (pair distribution function by electron diffraction) in TEM enables the study of amorphous materials at nm scale resolution and distinguish between various complex amorphous phases (e.g. phase separated glasses for industrial use, semiconductor thin amorphous layers, etc.)

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Electronic and optical properties of GaN/AlN heterostructures in relation to their strain state

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Heterostructures composed of successive thin mGaN/nAlN bicrystals with a wurtzite-type structure are crucial for the development of optoelectronic devices. Here, (m and (n) denote the periodicity of the thickness along the c-axis [1,2,3]. This study aims to optimize their electronic and optical properties by selecting appropriate m/n ratios with relatively low thicknesses, avoiding the condition of plastic relaxation.

Two structural models are considered in this contribution:

1. Free-Standing Model: This model assumes complete relaxation with zero stress.

2. Pseudomorphic Model: This model includes thin pseudomorphic GaN wells on a thicker AlN layer.

The energetics of both models are investigated through computer simulations using DFT calculations with the Quantum ESPRESSO ab initio package [4]. A series of structural configurations are analyzed with $m, n = 1 \div 10$ for the free-standing model and $m = 1 \div 10$ with $n = 8$ for the pseudomorphic GaN case. Special attention is given to the detailed analysis of the $m=4, n=8$ pseudomorphic configuration, which corresponds to the experimental case reported in [1].

Elastic models are developed to minimize the elastic energies of the bicrystals. These combined DFT and elastic calculations also provide data to extract the interfacial energies. The electronic and optical properties are approximated by including the Hubbard correction for strongly correlated systems using DFT+U and Hubbard parameter calculations [5,6]. The results demonstrate a correlation between the elastic models and electronic structures.

Computation work in this report has been produced using the High-Performance Computing (HPC) Infrastructure and Resources of the Aristotle University of Thessaloniki (AUTH).

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Elastic limit and plastic relaxation of GaAs/In(Al,Ga)As core shell nanowires for bandgap engineering

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Core-shell nanowires (CSNWs) exhibit pseudo-uniaxial strain along their long axis. Specifically, narrow and flexible GaAs cores can sustain large elastic strain energy without plastic relaxation, leading to a bandgap reduction of up to 40% [1] and a 50% increase in electron mobility [2] when overgrown with sufficiently thick In_x(Al,Ga)_{1-x}As shells. Using high resolution transmission and scanning-transmission electron microscopy (HR(S)TEM) combined with atomistic and continuum calculations, we determined experimentally the critical indium composition for the onset of plastic relaxation and characterized the 3D strain fields and plastic relaxation mechanisms [3].

GaAs/In_x(Al,Ga)_{1-x}As CSNWs (0.2 < x < 1) were grown via the self-catalyzed VLS mode using MBE, with a fixed 20 nm core diameter and 80 nm shell thickness. HR(S)TEM observations were conducted using a 300 kV ThermoFisher Titan Themis 60/300 and a 200 kV JEOL JEM F200 CFEG microscope. The 3D strain fields were measured using geometrical phase analysis and were compared to theoretical finite element analysis and atomistic empirical potential calculations. Density functional theory (DFT) calculations were employed to analyze the electronic properties of the strained heterostructures.

It was found that, while axial strains remain uniform, elastic relaxation induces radial and tangential strain gradients in the core and shell due to strain concentration at their interface, even after plastic relaxation of the CSNW. GaAs/In_{0.5}Al_{0.5}As CSNWs sustained the highest elastic strain in their cores while exhibiting a coherent interface [4]. In contrast, CSNWs with higher indium contents in the shell underwent plastic relaxation through specific mechanisms introducing extended defects in the shells. These included Frank partials delineating horizontal intrinsic stacking faults (SFs), misfit dislocations gliding along inclined {111} planes, and stair-rod dislocations forming at SF junctions. The preferential accumulation of specific defects on either side of the core suggested that transient bending, caused by asymmetric shell deposition at the early growth stages, can affect defect formation. Despite the presence of significant strain gradients at the core-shell interface, DFT calculations confirmed that the heterojunction maintained a type-I alignment without significant band bending in the core.

We thank the High-Performance Computing (HPC) Infrastructure and Resources Center of the Aristotle University of Thessaloniki (AUTH) for providing computing resources.

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Inkjet printing of hard magnetic iron-platinum layers

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A2_6, Machuca Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

In recent years, hard magnetic thin films have attracted considerable attention due to their wide applicability in the field of advanced electronics. Their capability to retain some degree of permanent magnetization proved essential for magnetic recording systems, telecommunication devices, magnetic sensors or spintronic applications [1]. The equimolar alloy formed by iron and platinum, in particular, is of major interest due to its exceptional coercivity and remanence, coupled with superior corrosion and wear resistance.

FePt thin films can be deposited using physical evaporation techniques like sputtering [2] or wet deposition techniques like electrodeposition [3]. In both cases, coercivities of many kOe can be easily obtained. Beside these well-established techniques, one of the most promising approaches to deposit the thin FePt layers required for advanced magnetic applications is inkjet printing (IJP). This process, still largely unexplored for the deposition of hard magnetic thin layers, relies on the controlled jetting of an ink, containing the material in the form of solubilized compounds or suspended nanoparticles (NPs), through a nozzle and towards a suitable substrate. The jetting of small amounts of ink, corresponding to single droplets, allows for optimal material usage. This aspect, together with the dimensional precision and the scalability typical of this technique, make IJP highly promising for the controlled patterning of FePt layers.

In this context, the aim of the present work is to deposit, for the first time, thin layers of FePt using IJP. The alloy is synthesized, in the form of NPs, operating the reduction of simple inorganic precursors. The resulting NPs are dispersed, without the aid of surfactants, in an environmentally friendly solvent and subsequently inkjet printed. The FePt thin layers obtained are annealed in a H₂/Ar atmosphere to sinter the NPs and promote the formation of the highly ordered, hard magnetic, L10 phase. Finally, they are characterized from the morphological, microstructural and magnetic point of view. In particular, the coatings obtained evidence good hard magnetic properties, with a remanence in the order of 34 emu/g and a coercivity in excess of 7 kOe.

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Solution growth of one-dimensional wide bandgap semiconductor nanostructures

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A2_8, Machuca Room (Level -2), septiembře 17, 2025, 10:30 - 13:10

One-dimensional wide-bandgap semiconductor nanostructures have garnered increasing attention in recent years, due to their promising potential for future electronic and optoelectronic devices. While the growth of these nanostructures from the vapor phase has been extensively investigated both experimentally and theoretically, the growth from solutions is predominantly addressed through empirical methods, without a fundamental understanding of the growth phenomena. In its basic form, growth is conducted in batch reactors, where reactants are introduced to induce supersaturation by controlling the thermodynamic properties of the system. However, these simple reactors exhibit poor control of supersaturation and its temporal dependence.

We introduce the concept of continuous-flow reactors and demonstrate that supersaturation can be precisely controlled in these reactors. In conjunction with lithographic techniques, growth in continuous flow reactors enables the elucidation of fundamental growth phenomena by combining experimental results with theoretical modeling. The significance of understanding the fundamentals of growth is demonstrated on (a) the growth of ZnO nanowires (NWs) by chemical bath deposition (CBD) with controlled morphology on p-type GaN epitaxial layers and on GaN NW arrays grown by plasma-assisted molecular beam epitaxy (PAMBE) for UV light sources and (b) on NW networks for gas sensors. The electrical properties of the individual NW heterojunctions and the fundamental building blocks of their networks were investigated within the chamber of a scanning electron microscope equipped with nanomanipulators.

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Identification and evaluation of interphase properties of polymer nanocomposites based on a multiscale approach

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A2_2, Machuca Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

It is known from experiments that adding nano-sized filler particles to polymers shows a pronounced strengthening of the material compared to larger filler sizes. To understand the mechanisms behind this observation, simulations can supplement experimental studies and provide insights into the processes taking place at time and length scales hardly accessible by experiments. In addition, numerical techniques may help to develop targeted strategies to improve the material performance and reduce the effort and cost for material development. In this regard, numerical models of high precision are required that can appropriately capture the processes of relevance.

This contribution presents a numerical methodology based on the Capriccio method, which integrates molecular dynamics and finite element simulations in a multiscale framework. In this approach, the elementary interactions between atoms form the foundation to eventually obtain matrix-filler interphase profiles, which can be used for higher level investigations based on continuum techniques. In our approach, we first characterise the material behaviour separately for the neat polymer and the filler particles using pure molecular dynamics. To this end, we perform numerical “pseudo” experiments to obtain the material properties and to set up appropriate constitutive relations. In the next step, we numerically manufacture nanocomposite samples at purely molecular resolution together with their finite element counterparts exhibiting the same nanoparticle arrangement. From an inverse parameter identification, we extract spatial profiles of the material properties changing throughout the interphase.

Eventually, we use these interphase profiles to set up simulations at the level of representative volume elements and compare the overall material behaviour to that obtained in experiments. Together with subsequent parameter studies, we demonstrate that our methodology is able to reproduce trends observable in reality based only on the elementary interactions between atoms. Hence, it provides a suitable mean to link the material behaviour at the nanoscale to the resulting macroscopic properties. As such, it paves the way to targeted material development which integrates experiments and simulations across a wide range of scales.

White light emission in tailored nanostructured thin films produced by pulsed laser deposition

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A2_9, Machuca Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Energy consumed for lighting accounts for 15-20% of world electricity consumption and is responsible of a 5% of total CO₂ emissions. This is why conventional incandescent and fluorescent light sources are being replaced by the more efficient and sustainable solid-state white-light emitting diodes (W-LEDs). Current commercial W-LED technology for lighting is based on InGaN blue LEDs combined with crystalline YAG:Ce³⁺ phosphors embedded in an epoxy resin coating. However, they show a deficient red emission and thermal constraints that limits their performance. Thus, exploring non-traditional doping elements is essential for the development of more efficient and reliable phosphors with improved color rendering. Specifically, in the current trend of reducing device dimensions it is very important to design thin film nanostructures with new concepts to increase efficiency and improve sustainability.

Pulsed laser deposition (PLD) has demonstrated to be an optimum technique to synthesize artificial nanostructures with a predesigned configuration thanks its ability to sequentially deposit layers of materials in a single step.[1] In this work, we exploit this characteristic of PLD to obtain near-white light emission nanostructured materials by precisely controlling the dopant distribution and nanostructure configuration along the growth direction. In particular, we will show two successful examples of this approach: i) The inclusion of Ag nanoparticles in europium oxide (EuOx) thin films, which leads to a broad PL white emission band that is related to the simultaneous presence of Eu²⁺ and Eu³⁺ ions in the nanostructure, and the coupling of Eu ions with Ag NPs; and ii) The synthesis of Bi and V-codoped MgAl₂O₄ nanostructured thin films consisting of undoped, Bi-doped or V-doped MgAl₂O₄ spinel layers, in which the optimum Bi/V concentration ratio and the adequate distribution of the different types of layers lead to near white light emission by the combination of the characteristic PL response of Bi³⁺ ions and that of V⁵⁺ ions present in [VO₄]³⁻ groups.

[1] X. Wang, R. Morea, J. Gonzalo, B. Palpant, Nano Lett. 15 (2015), 2633–2639

Wind turbine blade erosion monitoring and predictive maintenance: combining microstructural and machine learning approaches

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A2_6, Machuca Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Achieving 2000 gigawatts of offshore wind power by 2050, on a global scale, has significantly boosted the development of wind energy sector. Wind turbine blades are crucial components, and their structural integrity is essential for uninterrupted operation and downtime minimization. Blade erosion forms one of the main failure modes that lead to high production losses and maintenance expenses. Several studies have used time-domain and frequency-domain features alongside machine learning techniques to predict faults in wind turbine blades, such as erosion and cracks. However, a key gap remains in integrating these methods into a unified framework for fault prediction, which could offer a more comprehensive solution for diagnosing faults.

In this study, a combination of fault classification in wind turbine blades by leveraging well-known signals and analysis with machine learning techniques, along with microstructural investigations of faulty/eroded blade sections is presented. The methodology involves a detailed feature engineering process that extracts and analyzes features from the time and frequency domains. The time- and frequency-domain features were extracted and analyzed using various machine learning algorithms. It was found that erosion and crack faults have unique time- and frequency-domain features. The crack fault introduces an amplitude modulation in the vibration time wave, which produces sidebands around the fundamental frequency in the frequency domain. However, erosion fault introduces asymmetry and flatness to the vibration time wave, which produces harmonics in the frequency-domain plot. The results also highlighted that utilizing both time- and frequency-fault features enhances the performance of the machine learning algorithms. As a complementarity approach, microstructural analysis, predominately using optical and electron microscopy techniques in various scales has been performed in order to assess the effect of fault and erosion in the blades and for a direct comparison with the machine learning data. These findings provide valuable insights into optimizing predictive maintenance strategies and advancing renewable energy reliability.

Precise control over nanocomposite mechanics via polymer branching and grafting

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A2_2, Machuca Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Novel developments in polymer synthesis have allowed in recent years precise control over polymer branching and grafting, techniques that can be used to control the nanoscale structure and dynamics of new polymer-based nanomaterials. This includes a wide variety of materials such as grafted nanoparticles, thin films, composites for applications such as protective coatings, adhesives, membranes, and many more.

Theoretical and computational investigations in this field allow for a great level of control and insight into the nanoscale structures formed from different building blocks often inaccessible to experiments, guiding predictions of structure-property relationships and rational material design.

I will broadly discuss recent advancements in this area and the key principles behind them, and I will then focus on our contribution, particularly in manipulating the glass transition behavior and mechanical response of bulks and thin films using star polymers, polymer-grafted nanoparticles, or polymer-grafted graphene sheets. I will show that polymer grafting offers a unique avenue to control the dispersion, local dynamics and gradients in mechanical properties around nanofillers.

ALIAS: an Atomistic Local Identification of Stiffness method

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A2_8, Machuca Room (Level -2), septembre 17, 2025, 10:30 - 13:10

This study tackles the problem of identification of elastic continuum model by atomistic simulations for graphene polymer nanocomposite. The Atomistic Local Identification of Stiffness method, so-called ALIAS method, is developed to estimate the local stiffness tensor at all points of polymer graphene laminate nanocomposite. Results suggest that the graphene can be modeled at continuum scale by a general imperfect interface with zero thickness. Moreover, the identification procedure reveals the existence of interphase on either side of the graphene with a thickness of 1 nm, which is one and a half times stiffer than the polymer bulk matrix. The identified continuum model is used to study the effective elastic properties of nanocomposites with sandwich microstructure. This study at continuum scale reveals a softening effect due the very low stiffness of slip along graphene plane. The softening due to the interfaces is preponderant in relation to the interphase stiffening. Finally, the continuum model also suggests that the wrinkling of graphene increases the stiffness of nanocomposites.

Nanoscale Strengthening and Toughening of Polymers

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A2_2, Machuca Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Strong and tough polymers are always highly desirable for engineering structural applications. However, many well-established approaches for polymer toughening and strengthening are usually accompanied by unwanted compromises in other properties, such as drops in T_g and modulus, poorer processability, and inadequate low temperature performance. The emergence of nanotechnology has led to attempt to develop novel strong and tough polymers through incorporation of nanoparticle tougheners. In many cases, incorporation of nanoparticles does not show benefit over the micro-sized. Fundamental knowledge on nanoscale phenomena of polymer toughening and strengthening is still lacking. In this talk, a few intriguing examples of nanoscale phenomena that show great benefits in toughening and strengthening of polymers are presented. Issues regarding the preparation of strong and tough polymers will be discussed.

Advances in supported 1D organic nanowires growth as soft-templates for conformal multifunctional coatings by vacuum and plasma deposition techniques

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A2_8, Machuca Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Surface nanoarchitectures exhibit optical, electronic, and chemical properties that can be exploited in a myriad of applications. Among these, supported one-dimensional (1D) nanostructures are of relevance in notable areas such as energy (nanogenerators, batteries, solar cells and hydrogen), microelectronics, catalysis, photonics, biomaterials and biomedicine, and nanosensors.

Our approach to produce these 1D nanostructures is to grow single crystalline organic nanowires (ONW) by organic physical vapor deposition of planar molecules. These molecules adhere to the substrate in preferential spots that elongate when more molecules arrive and attach to themselves by π - π stacking. The control of the deposition parameters and surface structure and chemistry provides the ability to regulate density, thickness and length to the one suitable for the required application. By using vacuum deposition, this method avoids organic solvents and hazardous reagents, therefore being clean, reproducible and industrially scalable. During the last years, we have demonstrated the compatibility of the protocol with relevant substrates ranging from polymers (PDMS, PET, EcoFlex) to metal meshes, cellulose, graphene and carbon paper, including on-device formation on silicon wafers and TCOs.

Furthermore, these ONWs can be used as soft templates for coatings to be deposited conformally by a range of vacuum and plasma deposition techniques. Being organic, the ONWs can be easily removed after the coating by sublimation or plasma treatment, leaving a nanotube of the coating material behind. In addition, the space between the nanotubes can be filled with a soluble material by solution processing. This allows for a wide collection of materials, both organic and inorganic, and thus of possible applications to profit from the 1D nanoarchitecture.

This communication reports our recent advances in the growth of several supported 1D ONWs for energy, optic, electronic and sensing applications. We will specifically cover the use of non-planar molecules, the benefits of growing ONWs with a low sublimation point, the control of ONW density and length, the variety of suitable substrates, and the possibility of producing complex 3D nanoarchitectures. We will also examine a diversity of materials that can conformally coat these ONWs. Finally, we will present a few examples of applications of these surface nanoarchitectures.

ACKNOWLEDGEMENTS

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US: VI and VII PPITUS

Design and Engineering of Carbon Defects in TiO₂ Nanoparticle Architectures

Mr. Guillem Vives Ollé¹, Dr. Thomas Berger¹, Dr. Gilles Bourret¹, Dr. Oliver Diwald¹

¹Paris Lodron Salzburg University, Salzburg, Austria

A2_5, Machuca Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

The photoconversion of CO₂ into valuable molecules using solar radiation offers a promising approach to recycle the vast amounts of CO₂ emitted by modern society. Titanium dioxide (TiO₂) particle-based systems are useful for this purpose, as they are efficient photocatalysts with high performance under UV irradiation. However, their practical applications remain constrained due to the low lifetime of electron-hole pairs and unidentified trapping sites.¹ In this context, defect engineering constitutes a powerful strategy to enhance charge generation and separation in photocatalysts.² Despite its potential, systematic investigations on how the design of nanoparticle architectures (NPAs) and carbon dopants influence defect states and charge carrier dynamics are limited. In this work, we present strategies to engineer carbon impurity-based trapping sites, termed Carbonecks, in different NPAs. These Carboneck defects function as electron traps, promoting charge redistribution under UV irradiation.

We investigate four different TiO₂ architectures: (NPA1) unsupported TiO₂ nanoparticles synthesized via Chemical Vapour Synthesis (CVS), (NPA2) unsupported cast TiO₂ nanoparticles, (NPA3) silicon-supported cast TiO₂ nanoparticles, and (NPA4) silicon-supported TiO₂ heterostructured films, prepared by combining a cast TiO₂ nanoparticle film on a sputtered TiO₂ film. Excess electrons are generated upon oxygen removal from the TiO₂ lattice at 973 K under high vacuum conditions. Electron Paramagnetic Resonance (EPR) spectroscopy is used to characterize (EPR-active) electron traps. In addition to superoxide radicals (O₂⁻), all slurry-derived NPAs (i.e. NPA2-4) exhibit an isotropic signal at $g = 2.0042$, which is attributed to carbon impurities inside the contact area between aggregated nanoparticles.³ For silicon-supported cast TiO₂ nanoparticles (NPA3), an additional isotropic signal at $g = 2.0020$ is observed, which we assign to paramagnetic carbon impurities at the silicon/TiO₂ interface. The organic constituents of the nanoparticle slurry are identified as the main source of these carbon trapping sites. However, when a TiO₂ sputtered film is deposited on the silicon substrate before the casting process (NPA4), it acts as a protective layer, preventing the Carboneck formation. UV excitation of the NPAs leads to charge redistribution involving the Carboneck signals.

This contribution will discuss the implications of these findings for converting particle powders into functional materials like photocatalytic layers and electrodes.

(1) Schneider, J. et. al. Understanding TiO₂ photocatalysis: mechanisms and materials. 2014

(2) Dozzi, M. V. et. al. Doping TiO₂ with p-block elements: Effects on photocatalytic activity. 2013

(3) Elser, M. J. et. al. On the Importance of Nanoparticle Necks and Carbon Impurities for Charge Trapping in TiO₂. 2023

Chiral Nanomaterials

Prof. Iouri Gounko¹

¹Trinity College Dublin: The University Of Dublin Trinity College, Dublin, Ireland

A2_8, Machuca Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Symmetry and chirality are properties commonly found throughout the natural world. Chirality is one of the most important factors in molecular recognition, with chiral compounds having a major role in chemistry, biology and medicine. Chirality has also been envisaged to play an important role in nanotechnology. Over the last years the area of chiral nanoparticles has received a great deal of attention due to the range of potential applications offered by these materials. The main aim of our work is to develop new types of technologically important inorganic nanoparticulate materials possessing optical activity and chirality, study their properties, investigate their nature and explore their applications. We have developed a range of new chiral nanomaterials including chiral ternary silver indium sulfide and selenide based semiconducting nanoparticles (quantum dots). In addition, we started to explore the properties of new anisotropic chiral 2D nanostructures. The new nanomaterials have shown a very interesting optical activity and unusual chiral morphologies which were confirmed by various instrumental techniques. Several critical aspects on the nanocrystals growth, characterization, and the optimisation of the surface passivation by the chiral ligand in order to optimize the nanoparticle chirality are thoroughly investigated. Optical spectroscopy as circular dichroism and luminescence are exploited to analyze the coordination processes leading to the formation of the ligand-nanocrystal chiral interface. The study highlights the dynamic nature of the interaction between the nanocrystals surface and the chiral ligand and clarify some fundamental aspects for the transfer and optimization of the chiroptical activity. We have also explored potential applications of chiral quantum dots for chiral recognition and luminescent chemo- and bio- sensing. Finally, we overview chiral nanomaterials within the framework of synthesis-structure-property-application relationships and provide insights on how to leverage machine learning for the study of these complex relationships.

Tailoring the plasmonic response of Ag/NiO heterostructures by solid state dewetting for spintronic applications

Mrs. Carmen del Pino-Batlles¹, Cayetano Hernández-Gómez¹, Pilar Prieto², Jesús López-Sánchez¹, Juan Rubio-Zuazo^{3,4}, Dóra Zalka⁵, Alba Berja¹, Latiff Ullah Khan⁶, Messaoud Harfouche⁶, Alexey Maximenko⁵, Noemí Carmona⁷, José Francisco Fernández¹, Adrián Quesada¹, Aída Serrano¹

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A2_10, Machuca Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Antiferromagnetic materials (AFM) have recently attracted attention for their potential use as active elements in spintronic applications. A key challenge is the manipulation of AFM domains in the absence of external magnetic fields, with light irradiation being one possible way. In this line, the activation and manipulation of spin waves in AFM by plasmonic nanomaterials through light is a challenge. This approach in the field of spinplasmonics has been scarcely investigated and its potential is impressive.

In this work, a hybrid system based on Ag nanoparticles (NPs) on an AFM NiO film is fabricated from bilayer deposition by dual ion beam sputtering plus subsequent solid-state dewetting of Ag by post-annealing processes. The epitaxial growth of the system has been controlled by different types of substrates (MgO, SrTiO₃ and Al₂O₃), obtaining commensurate and incommensurate growth of layers in different crystallographic directions depending on the substrate and its crystallographic orientation. In addition, the morphological characteristics of Ag NPs are controlled as a function of the different substrates and thermal post-treatments. A study of the chemical state of the Ag NPs and the stability of the system as a function of thermal post-treatments and over time is also carried out. All these features allow the control of the plasmonic characteristics of heterostructures for future application.

The use of artificial intelligence to rapidly optimize nanomaterials production

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A2_6, Machuca Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Hydrothermal synthesis is a key route to the sustainable manufacture of nanomaterials and is used in laboratories around the world. Some researchers prefer to use batch systems, whilst others use exclusively use continuous flow reactors, with a few laboratories using both approaches. Whilst continuous flow systems are inherently more scalable, they also have drawbacks, particularly around understanding the relationship between operating variables with product characteristics. There are more than 10 variables (e.g. temperature, precursor type, concentration, flow rate, flow ratio), that can operate across a wide range of conditions. Essentially this creates an infinite number of experiments that could be attempted when seeking to make a nanomaterial for the first time.

Design of Experiments is one approach which seeks to correlate variables with outcomes, whilst minimizing the amount of test work. This is still time consuming and generally still separates production from characterization from correlation.

Artificial Intelligence methods are perfectly suited to continuous hydrothermal flow systems because they can monitor products (in real time) and use self-optimizing algorithms to directly control process variables in order to quickly find out how to make materials that match target characteristics (size, shape, crystal structure etc).

This approach can reduce the development cycle for a new material and can also contribute to a more sustainable route to manufacture with more favourable sustainability metrics.

Examples of different types of AI algorithm and self optimization experiments will be given during the developments of functional nanomaterials such as MOFs (metal organic frameworks) and metal oxides (Fe₂O₃, ZrO₂, ZnO).

Fabrication and Nanosecond Laser Processing of TiN Nanoislands for Robust Plasmonic Applications

Mrs. Stavros Panos¹, Mrs. Nikolaos Pliatsikas¹, Ms. Tamara Odutola¹, Mrs. Spyridon Kassavetis¹, Mrs. John Arvanitidis¹, Mrs. Dimitrios Christofilos², Ms. Eleni Pavlidou¹, Ms. Maria Gioti¹, Mrs. Panos Patsalas¹

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A2_9, Machuca Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

The rapid development of clean energy technologies requires innovative research methodologies that enable scalable, high-throughput fabrication of functional nanostructures. Nanosphere lithography (NSL) has emerged as a promising, cost-effective technique for nanostructures fabrication, offering a rapid and scalable approach compatible with wafer-scale manufacturing. This study improves NSL-based fabrication by adding nanosecond laser annealing as a fast post-processing step to improve the structural and functional integrity of titanium nitride (TiN) nanoislands, a type of refractory conductive nitride, along with ZrN, HfN, NbN, and TaN that have a lot of potential for uses in plasmonics and energy harvesting.

To accelerate the production of defect-free, highly conductive TiN nanoislands, process parameters were systematically optimized, including UV ozone treatment to refine the interstitial voids in the nanosphere mask and reactive magnetron sputtering conditions tailored to enhance deposition precision. The introduction of nanosecond laser heating as a rapid, non-contact annealing technique ensures superior structural stability while preserving the optical and electronic properties of the fabricated nanoislands. The resulting nanostructures demonstrate exceptional resilience to thermal and optical stress, positioning them as ideal candidates for applications in plasmonic-enhanced solar energy harvesting, high-efficiency photodetectors, and advanced catalysis.

Study of the evolution of AgxAuy plasmonic nanoparticles on NiO antiferromagnetic layers for spintronics applications

Mr. Cayetano Hernández-Gómez¹, Mrs. Carmen del Pino-Batlles¹, Dr. Adrián Quesada¹, Dr. Aida Serrano¹, Dr. Pilar Prieto²

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A2_10, Machuca Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Spintronics is presented as a novel route for a whole new era of data processing devices which will exploit the great properties of spin-waves or magnons, such as non-linear dynamics, low energy consumption and ultra-fast responses. In this line, hybrid systems based on plasmonic nanoparticles (NPs) on antiferromagnetic (AF) layers show high potential to stimulate spin-waves by light through plasmon-magnon interactions. However, developing these hybrid systems requires a detailed comprehension of physical-chemical interactions between AF and plasmonic NPs.

In this work, we study the evolution of AgxAuy NPs on NiO AF layers after the solid-state dewetting (SSD) of plasmonic nanostructures. AgxAuy and NiO bilayers were grown by dual ion-beam sputtering at high-vacuum environment and subsequently a post-annealing at 500 °C was carried out to generate the nanostructuration of metallic layer. The evolution of plasmonic NPs and their interaction with the AF layer was evaluated varying annealing time and the atmosphere during the SSD process. The nanostructuration of the AgxAuy film has been studied in terms of Scanning electron microscopy (SEM), UV-visible absorbance and Raman spectroscopies, as well as by X-ray photoelectron spectroscopy (XPS). When the annealing process is performed in a 10⁻² Pa oxygen partial pressure, AgxAuy nanoparticles are formed, while a semi-dewetted AgxAuy nanostructure film is observed when the annealing is performed in high vacuum conditions (10⁻⁵ Pa). The AgxAuy composition, around 60% Au and 40% Ag atomic concentration, have been determined by EDX and XPS. The chemical state of the different elements present in the hybrid AM-plasmonic system during the nanostructuration process was followed by XPS in situ when the annealing is performed in high vacuum and ex situ when it is performed in oxygen atmosphere, finding changes in the XPS spectra depending on the dewetting state of plasmonic NPs.

FeCoNi nanowires as candidates for 3D magnetic memory units

Dr. Malgorzata Kac¹, Dr. Anna Nykiel¹

¹Institute of Nuclear Physics, Polish Academy of Sciences, Krakow, Poland

A2_8, Machuca Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Nanomaterials have been among the most studied objects in the last few decades. Their unique electrical, optical and magnetic properties make them attractive for various applications from biomedicine to environmental protection and consumer electronics. A particularly interesting aspect is connected with spintronic applications, where one-dimensional magnetic objects such as nanowires may be promising materials for a new type of three-dimensional magnetic memory units called racetrack memory.

In this study, FeCoNi nanowires (NWs) will be presented as a candidate for magnetic memory in a 3D approach. To meet the required criteria, they should demonstrate well-defined morphology, chemical composition, structure, and magnetic properties. Thus, nanowires with a diameter of 40 and 100 nm and a length of 6 μm were electrodeposited in polycarbonate membranes using a template-assisted method. Their chemical composition was modified by an appropriately selected cathodic potential and resulted in an increase in Ni content while decreasing Fe and Co concentrations when the applied voltage was shifted towards more cathodic values. These nanowires crystallized in the fcc structure with significant changes in the lattice parameters and crystallite size associated with various elemental content and different current density. The geometry, chemical composition, and structure of nanowires influenced their magnetic properties. All samples showed an easy magnetic axis along the NW axis due to the dominant role of shape anisotropy. The coercivity and squareness values decreased for 40 nm diameter nanowires with increasing cathodic potential, but showed an opposite relationship for nanowires with a diameter of 100 nm because of dominant contribution of dipolar interactions. Studies of angular coercivity dependence exhibited the vortex domain wall propagation at the angles close to the easy direction and switching of the magnetization reversal mechanism to coherent rotation or transverse domain wall movement at the angles close to the hard directions. First-order reversal curve analysis together with Lorentz TEM observations revealed the single-domain structure of both nanowire diameters and confirmed non-interacting system in the case of 40 nm diameter nanowires. Segmented nanowires composed of FeCoNi alloys with different concentrations showed domain walls located at the segment boundaries. Therefore, the obtained nanowires meet the criteria required for 3D racetrack memory applications.

Physics-based simulations and machine learning for nano-materials and nano-devices

Prof. Alejandro Strachan¹

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A2_7, Machuca Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

This presentation will highlight recent work in our group on combining machine learning (ML) and physics-based simulations to explore nano-materials. The first example uses density functional theory (DFT) to explore 2D materials as building blocks for layered ceramics for high-temperature applications. High-throughput DFT calculations predict the stability of the structures and their elastic constants; this is followed by ML models that use these properties to predict melting temperature, a property that is very computationally intensive to calculate directly. We discovered 67 new hexagonal, layered materials with thermal stability comparable to or better than previously observed zeta phases. A second example focuses on phase change materials, leading candidates for future non-volatile memory storage devices. We use ML interatomic potentials to perform molecular dynamics simulations of the operation of these devices. Simulations of amorphization and recrystallization of carbon-doped Ge₂Sb₂Te₅ with temporal and spatial scales matching those of current devices reveal the role of C atoms in the nucleation and growth processes.

Pr³⁺-ACTIVATED NaY₉Si₆O₂₆ LUMINESCENT NANOPOWDERS: PREPARATION, STRUCTURE, MORPHOLOGY, AND PHOTOLUMINESCENCE

Ms. Madalina Ivanovici², Dr. Zeljka Antic^{1,2}, Prof. Miroslav Dramicanin^{1,2}

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Pr³⁺ luminescence centers in solids provide diverse emissions across the ultraviolet, visible, and infrared spectral ranges, originating from both interconfigurational [Xe]4f15d1 → [Xe]4f2 and intraconfigurational [Xe]4f2 → [Xe]4f2 electronic transitions. These emissions can be of any type, including scintillation, downshifting, downconversion, and upconversion. They can exhibit fast decay times in the nanosecond range, making them ideal for scintillating applications, or slower decay times in the microsecond range, suitable for lighting phosphors and sensing applications. Additionally, Pr³⁺ optical centers may provide long-lasting luminescence. For these reasons, Pr³⁺-doped materials have found widespread use in a variety of practical applications, particularly in lighting, displays, healthcare, sensing, and security fields.

Here, we report a thorough examination into the structural, morphological, and photoluminescence features of Pr³⁺-activated NaY₉Si₆O₂₆ (x = 0; 0.5; 1; 3; 5; and 7 mol% Pr³⁺) oxyapatite phosphors, prepared using hydrothermal synthesis. Differential thermal analysis was used to determine the optimal calcination temperature, and an exothermic peak was found at 995°C. This peak is attributed to the transformation of the NaY₉Si₆O₂₆ from an amorphous to a crystalline form. The X-ray diffraction patterns of six NaY₉Si₆O₂₆ samples doped with different Pr³⁺ concentrations revealed a single-phase hexagonal structure with the P6₃/m (176) space group. Transmission electron microscopy images of samples showed agglomerates of round-shaped nanoparticles with an approximate size of ~55 nm. The room temperature photoluminescent emission spectra, excited at 450 nm, revealed distinct emission bands in the visible spectral region. These emission bands correspond to the Pr³⁺ electronic transitions, specifically the [Xe]4f2 → [Xe]4f2 transition. The optimal Pr³⁺ doping concentration, based on observed emission intensities, is 0.5 mol%.

Funding: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7017, TECHNOLOGY FOR REMOTE TEMPERATURE MEASUREMENTS IN MICROFLUIDIC DEVICES – REMTES. This study was also supported by Romania's National Recovery and Resilience Plan, NRRP, [project grant number C9-I8-28/ FC 760107/2023]. Authors from Vinča Institute would like to acknowledge funding of the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia under contract 451-03-136/2025-03/200017.

Electrophoretic deposition of Pr³⁺-doped Lu₂SiO₅ thin films for antimicrobial applications

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),

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In this study, we utilized electrophoretic deposition to create antibacterial thin films from Pr³⁺-activated powders. The motivation for this research stems from the unique luminescent properties of Pr³⁺-doped materials. In cases where the Pr³⁺ lowest-energy 4f5d state is located below the 4f2 1S0 state, Pr³⁺ ions facilitate two-photon blue light upconversion to the ultraviolet C (UVC) spectral range. UVC light has widely known germicidal properties, which means it may effectively kill microorganisms such as bacteria, viruses, and fungi. As a result, UVC is employed in a variety of disinfection processes, including water and air purification and surface sterilization in healthcare settings. This study intends to develop functional coatings with biocidal capabilities under visible light using the upconversion properties of Pr³⁺-doped materials.

At first, single-phase Lu₂SiO₅ doped with 0.5 mol% Pr³⁺ was produced by a Pechini-type polymerized complex technique. This method involves a polyesterification reaction between citric acid and ethylene glycol, yielding a precursor material subsequently utilized for electrophoretic deposition. Subsequently, we fabricate thin films on conductive aluminum substrates using the electrophoretic deposition of the precursor powder. Both films and precursor powders undergo full characterization employing several analytical techniques. The methods employed comprised X-ray diffraction for analyzing the crystal structure, scanning electron microscopy for examining morphology and surface characteristics, and photoluminescence spectroscopy for evaluating upconversion emission. To assess the efficacy of thin films for germicidal applications, experiments were conducted on gram-positive bacteria (*Staphylococcus aureus*), gram-negative bacteria (*Escherichia coli*), and fungus (*Candida albicans*), chosen due to their relevance in clinical and environmental settings.

Acknowledgement: This research was supported by the Science Fund of the Republic of Serbia, #GRANT No 7017, TECHNOLOGY FOR REMOTE TEMPERATURE MEASUREMENTS IN MICROFLUIDIC DEVICES – REMTES. Authors from Vinča would like to acknowledge funding of the Ministry of Science, Technological Development, and Innovation of the Republic of Serbia under contract 451-03-136/2025-03/200017.

A bottom-up approach for multifunctionality optimization in nanoreinforced polymers

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A2_7, Machuca Room (Level -2), septembre 16, 2025, 17:00 - 19:00

A novel fabrication methodology for nanocomposites with precise size control and optimal dispersion of spherical nanoparticles will be presented. In contrast to conventional methods of mixing nanoparticles

with polymeric materials, we propose to circumvent the traditional approach by synthesizing the nanoparticles in situ within the polymer matrix. Nanoparticles are synthesized in a mixture of solvent and polymer. In addition to the established parameters (standard synthesis) that govern the morphology

and size of the nanoparticles, the polymer composition and macromolecular architecture are hypothesized to play a significant role in determining the resultant nanoparticle size and dispersion within the surrounding matrix. This latter approach considered the polymer macromolecular chains as a

critical parameter to control both the size and three-dimensional organization of nanoparticles within a

polymeric matrix. By exerting control over both crucial parameters (size and distribution), the obtained properties (NP size distribution and dispersion in the polymeric matrix, induced magnetic and strengthening effects of the composite material) that exceeded expectations.

These results constitute a precious data base to validate modeling approach, from the atomistics to finite

element crossing by micromechanics. During this seminar, an overview on previous challenges and the opportunities given by our new results will be presented in details.

Numerical simulations of the elastic energy associated with a buried hexagonal network of dislocations and its application to semiconductor heterostructures

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

With its nanoscale and discrete energy spectrum, the technology of self-assembled quantum dots (SAQDs) is becoming very alluring to provide a variety of advancements for electronics, including greater efficiency, lower power requirements, faster operating speeds, and many novel electronic proprieties [1,2].

Some prospective uses of semiconductor nanocrystals, including nanoscale memory devices and intersubband photo-detectors, have significant challenges in terms of how to arrange themselves in a very accurate way and how to manage their size distributions during the fabrication process [3].

One way to control the location of quantum dot nucleation and their size is the use of a functional substrate inducing a lateral self-organization by a buried dislocation network [4-6]. Let us note that more researches are still needed to determine the fundamental relationship between the dislocation network and SAQD nucleation.

In this work, the anisotropic elasticity theory based on the analyze of the elasticity of dislocations in subsurface layers [7-10], is used to determine the elastic field (displacements and stresses) and the stored elastic energy E_s , generated by an hexagonal network of buried dislocations located between a thin layer bonded onto a semi-infinite substrate. The effect of the thickness of the layer and the misfit mismatch are also shown. Finally numerical applications are presented for different heterosystems: CoSi₂/Si, GaAs/Si and CdTe/GaAs.

Thermohydraulic Performance and Optimization of a Double-Pipe Heat Exchanger with Perforated Annular Fins and clove functionalized GNP nanofluids

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study proposes a compound heat transfer enhancement method that integrates clove-functionalized graphene nanoplatelet (CGNP) nanofluids with perforated annular fins. The thermohydraulic performance and flow structure of a double-pipe heat exchanger fitted with fins of 0.2-0.7 porosity are investigated numerically in the Reynolds number (Re) ranging from 561 to 7,945. The CGNP nanofluid 0.025 wt% and distilled water (DW) were employed as the working fluid. This study filled the gap in research on the porosity of perforated fins. The numerical result showed that all fin designs could induce secondary flows and vortices, which intensified fluid mixing and thinner thermal boundary layers, resulting in heat transfer enhancement. Compared to the full annular fin, although the perforated structure resulted in a slight decrease in the Nusselt number (Nu), it was accompanied by a significant decrease in the pressure drop. A porosity of 0.4 was considered to better balance the heat transfer enhancement and pressure drop. Compared to the smooth circular pipe, the perforated fin with 0.4 porosity increased the Nu by 78% and the pressure drop by 87% at Re = 2270, at which time the highest PEC value of 1.46 was obtained. Furthermore, the CGNP nanofluid improved the heat transfer coefficient by 15.7 % and 19.5 % for a pipe with annular fins of porosity 0.4 and a smooth pipe, respectively, with a negligible change in pressure drop. The compound method strengthened the velocity-temperature field synergy, resulting in optimized convective heat transfer.

TEM investigation of hybrid MXene coatings of Ti₃C₂T_x and Nb₂CT_x for lubrication

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Tribology plays an important role in improving the lifetime of mechanical systems with moving components. The aim is the reduction of friction-related losses [1], so the simplest and most efficient solution is the application of a lubricant to separate the interacting surfaces. Two-dimensional (2D) materials with layered structures have emerged as a highly researched class of solid lubricants. 2D materials are thin, sheet-like structures that consist of one or a few atomic layers in thickness. MXenes are 2D-materials consisting of layered transition metal carbides, nitrides, and carbonitrides. The MXenes properties are strongly influenced by factors such as the number of nanosheets, the orientation of the individual monolayers, the lateral flake size, or the film thickness.

Two different MXenes, namely Nb₂CT_x- and Ti₃C₂T_x-MXene as pure flakes, as well as a hybrid solid lubricant coating, were examined in more detail. For comparison, uncoated AISI 304 steel substrates were used as reference materials, and the tribological performance of individual Ti₃C₂T_x and Nb₂CT_x coatings was also investigated against an Al₂O₃ counterbody. The excellent lubricating performance of the hybrid coating is attributed to the tribo-induced formation of a compact, patchy tribofilm, which effectively reduces the coefficient of friction and protects the substrate from wear.

Transmission electron microscopy (TEM) was used to study the pure MXene flakes, as well as the tribofilm after wear tests. The detailed microstructural characterization included imaging by transmission electron microscopy, high resolution TEM, phase analysis by selected area electron diffraction patterns (SAD) as well as measurements of the lattice space distances of the HRTEM images. A chemical analysis (elemental mappings) was done by energy dispersive x-ray analysis (EDX).

As a result, one important realization was, that the two-dimensional structure of the MXenes was retained within the tribofilm after sliding, and it kept its crystallinity. This could be proven by high resolution TEM imaging after preparing a TEM lamella cut by Focused Ion Beam (FIB). The crystal structure could be verified with Ti₃C₂ and Nb₂C, respectively.

So in the end it can be concluded, that a hybrid tribo layer consisting of Nb₂CT_x- and Ti₃C₂T_x-MXene flakes, provides a promising basis for future tribological films to reduce friction-related losses.

[1] K. Holmberg und A. Erdemir, „Influence of tribology on global energy consumption, costs and emissions“, Friction, Bd. 5, Nr. 3, S. 263–284, Sep. 2017, doi: 10.1007/s40544-017-0183-5.

Compressive strength as a screening tool for quality control of tubular honeycomb ceramic filters

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Honeycomb tubular ceramic filters are the most common ceramic filter design, whose standard quality control in the industry is based on assessing whether or not a relevant filtration parameter, typically permeability, of one or more randomly selected filters meets the desired specification. Ceramic filters are however particularly prone to fracture, yet it is not common to measure their strength as an integral part of quality control, or to do so inadequately. Because a lower-than-expected strength is an indication of processing problems, strength-based screening can be an ideal complementary tool for the quality control of ceramic filters. The aim of this work is to assess the mechanical integrity and reliability of commercial honeycomb tubular ceramic filters at their typical processing stages using simple compression testing and Weibull analysis, and to show the usefulness of this methodology as a complementary screening tool for quality control.

Assessing the mechanical strength of multi-channelled flat-sheet ceramic filters

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A methodology is presented for assessing the mechanical strength of multi-channelled flat-sheet ceramic filters, and applied to a flat-sheet SiC filter designed for submerged outside-inside vacuum-driven filtration. To this end, four-point bending, tensile, and compressive tests were performed, and the experimentally measured failure loads were converted to failure stresses and analysed by Weibull diagrams. This ceramic filter was found to be ~1.4 times stronger and ~2.9 times less reliable under compression than in bending, and in turn ~3.3 times stronger and ~5.4 times more reliable in bending than in uniaxial tension. These differences in mechanical performance are explained in terms of the corresponding fracture modes and the critical flaw populations responsible for failure. Finally, relevant implications for ceramic “membranologists” interested in mechanical characterization are discussed.

Investigation of phase transformation in zeolitic imidazolate frameworks (ZIFs) under operating conditions using in-situ TEM

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A3_2, U2 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

Zeolitic imidazolate frameworks (ZIFs), an intriguing class of metal-organic frameworks (MOFs) with zeolite-like topologies and composed of metal ions connected by imidazolate linkers, have attracted great attention due to their promising applications in gas separation and catalysis. To gain important insights into their behavior and performance when ‘in use,’ in-situ transmission electron microscopy (TEM) has shown great potential to study the structural evolution of ZIFs under such operating conditions. However, investigating such delicate soft materials by TEM is challenging due to potential radiation damage by the TEM’s electron probe.

In our study, we systematically investigated the stability and phase transformation of ZIFs under different temperature and gas environments using advanced in-situ environmental TEM techniques. First, we evaluated the stability of ZIF crystals under electron beam exposure using electron diffraction, i.e. by measuring the attenuation of relative intensities in Bragg planes over time as a function of the applied total electron dose. We established a critical electron dose threshold of $30 \text{ e-}\text{\AA}^{-2}\text{s}^{-1}$ at room temperature for ZIF-8 and ZIF-L. If a larger electron dose than this critical total dose is applied during any TEM experiment, electron-beam-induced structural degradation will occur. Further, we investigated the effect of elevated temperature and found that at temperatures above 550°C , ZIF-L undergoes a structural collapse and amorphization. Using EDX and EELS mapping in STEM, changes in composition and chemical state have been tracked.

Now controlling the electron beam effects, we then investigated the pyrolysis of ZIF-L at temperatures between 700°C and 1100°C to establish a structure-property correlations for its performance in oxygen reduction reaction (ORR). We found that nitrogen-doped graphitic carbon, formed during pyrolysis, is a key factor in improving the properties of pyrolyzed ZIF-L.

Furthermore, we investigated the stability of ZIF-8 in an oxygen atmosphere. Under 2.7 mbar O_2 pressure and temperatures ranging from 350°C to 550°C , we studied the transformation of ZIF-8 into ZnO nanoparticles, identified by contrast changes in TEM bright-field images and confirmed by selected area diffraction (SAED) patterns.

Our comprehensive study demonstrates the power of in-situ TEM techniques in elucidating structure-property relationships when overcoming the challenges associated with electron-beam experiments on beam-sensitive MOFs. Our findings provide valuable insights into the behavior of ZIFs under realistic operating conditions and contribute to developing more efficient and stable MOF-based materials for various applications.

Metal-organic frameworks for Li-S batteries

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembere 17, 2025, 13:10 - 14:30

Energy is currently one of the most important human needs and is also necessary for the development of technology and human civilization. Currently, rechargeable lithium-ion batteries (Li-ion) with energy densities of 200-400 Wh/kg, 500-1300 Wh/L, which have dominated the market since the 1990s, are the most commercially used. Although continuous Li-ion battery research is progressing, and batteries are achieving energy densities approaching their theoretical values, they are no longer sufficient for current energy consumption demands.

The electrochemical reduction of sulfur in lithium-sulfur (Li-S) batteries is not based on an intercalation/deintercalation process like Li-ion batteries but on a conversion reaction mechanism where intermediates are formed during the charging/discharging. The operating potential of the Li-S battery is 2.1 V versus Li/Li⁺, representing a theoretical energy density of 2500 Wh/kg and 2800 Wh/L. Li-S batteries are the most widely investigated due to their high storage capacity and are considered as the next-generation energy-storage technology.

However, challenges such as low sulfur conductivity ($\sim 5 \times 10^{-30}$ S/cm), significant volume expansion ($\sim 80\%$) during cycling, and the polysulfide "shuttle effect" lead to electrode degradation and rapid capacity fading. Metal-organic frameworks (MOFs) have been investigated as sulfur hosts in Li-S battery cathodes to address these limitations. Porous materials with high surface area and stability have been shown to effectively confine polysulfides and limit their unwanted migration, improving battery performance.

MOF-based materials, including MIL-101(Fe)-NH₂, MOF-76(Gd), and STAM-1, have demonstrated the ability to enhance cathode conductivity and facilitate electrolyte and sulfur infiltration. MIL-101(Fe)-NH₂, with a surface area of ~ 3500 m²/g, achieved an initial discharge capacity of 705 mAh/g at 0.5C and retained 476 mAh/g after 200 cycles, with a low capacity fading rate of 0.162% per cycle. Similarly, carbonized MOF-76(Gd) exhibited an initial capacity of 658 mAh/g and maintained 93% of its capacity after 200 cycles. STAM-1, a Cu(II)-based MOF, provided a discharge capacity of 452 mAh/g at 0.5C, retaining 430 mAh/g after 100 cycles with a Coulombic efficiency of 97%.

In addition to stabilizing the cathode structure and mitigating volume fluctuations, these MOFs accelerated the conversion of sulfur species, enhancing overall battery efficiency. The results confirm that well-engineered metal-organic frameworks can significantly improve the performance, cycle life, and energy storage capabilities of Li-S batteries, paving the way for more efficient and durable next-generation energy storage systems.

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Sustainable water purification using UiO-66 MOF gels for PFAS remediation

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A3_1, U2 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

Perfluoroalkyl substances (PFAS) or "forever chemicals" pose significant concern regarding their impact on the environment and overall health due to their toxicity and long-term durability. Among them, perfluorooctanoic acid (PFOA) is responsible for various complications in malignant diseases and developmental disorders, and its long-term persistence with respect to degradation processes in nature makes its removal from water particularly challenging.

This study investigates the use of zirconium terephthalate metal-organic framework (MOF) gel UiO-66 to extract PFOA from contaminated water using powder X-ray diffraction (PXRD), scanning / transmission electron microscopy (STEM & TEM) imaging and energy dispersive X-ray spectroscopy (EDS), as well as nuclear magnetic resonance (NMR) spectroscopy.

The gel form of UiO-66 exhibits a similar structure to the powder form of UiO-66, but has improved processing and usability capabilities. PXRD and TEM analysis confirmed the nanocrystalline character (with an average size of about 20 nm) and the hierarchical porous structure of the gel. Quantitative evaluation using ¹⁹F-NMR showed an extraction efficiency of 96% for PFOA, while solid-state NMR confirmed the interactions between the fluorine groups in PFOA and the carbonyl groups in the gel network. In addition, STEM-EDS analysis showed a homogeneously dispersed distribution of PFOA in the gel and thus confirmed its efficient absorption mechanism. In addition, satisfactory performance in its membrane form, with a harvesting efficiency of over 95%, was displayed through successive membrane filtering processes. Notably, the filtering process did not require any external pressure, and it relied purely on gravity, providing a cost-effective and efficient alternative to traditional water purification processes.

Given these findings, the use of UiO-66 MOF gels for water ultrafiltration is very promising as a feasible and scalable process for PFAS remediation and, more generally, for environmental pollution control with an effective and environmentally-friendly approach.

Bulk nano-structured porous martensitic alloys: a sustainable synthesis attempt via reactive vapor phase dealloying-alloying

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A3_5, U2 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

For millennia, alloying has been the greatest gift from metallurgy to humankind: a process of mixing elements, propelling our society from the Bronze Age to the Space Age. Dealloying, by contrast, acts like a penalty: a corrosive counteracting process of selectively removing elements from alloys or compounds, degrading their structural integrity over time. In this presentation we will show that when these two opposite metallurgical processes meet in a reactive vapor environment, profound sustainable alloy design opportunities become accessible, enabling bulk nano-structured porous alloys directly from oxides, with zero carbon footprint. We will discuss thermodynamically well-grounded treasure maps that turn the intuitive opposition between alloying and dealloying into harmony, facilitating a quantitative approach to navigate synthesis in such an immense design space. We demonstrate this alloy design paradigm by synthesizing nano-structured Fe-Ni-N porous martensitic alloys fully from oxides in a single solid-state process step, and substantiating the critical kinetic processes responsible for the desired microstructure.

Mixed-matrix membranes modified with nano-SiO₂ for technical applications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The aim of the research was to obtain mix matrix membranes (MMM) which properties are modified by the addition of nanoparticles such as: TiO₂, SnO₂ or SiO₂. The MMM is a mesoporous composite material in which dispersed particles are embedded in a polymer matrix. The function of the matrix is to keep the particles dispersed, providing selective permeability due to interactions at the particle-polymer interface. The type of the filler influences the membrane properties such as; mechanical strength, selectivity towards particles/ions, increased permeability compared to polymeric membranes and higher thermal stability. The choice of the filler allows new properties to be imparted to the membrane resulting in an increase in service time, e.g. by reducing the deposition of inorganic as well as organic compounds (organic macromolecules produced by bacteria). The antifouling and immobilising properties of particles on the membrane surface represent a new research trend in MMMs, and allow to extend the range of membrane applications, which can be used both for gas separation and in wastewater treatment or water desalination processes. Our proposed approach is based on the use of nano-fillers in the form of SiO₂ or its forms modified with organic salts, altering the surface charge of the membrane and thus hindering adsorption of macromolecules as well as bacteria, or to bind the contaminant to the surface. Modifying the particles surface improve their compatibility with the matrix and facilitate their dispersion. A high degree of dispersion is a prerequisite for improving the mechanical properties of the membranes.

In this study, SiO₂ nanoparticles chemically modified with organic salts such as polypyrrole were used. The characterisation of the powders consisted in determining particle size by DLS or TEM observation and assessing their wettability. The effectiveness of the particle modification was verified using the FTIR. The prepared particles were introduced into the PSU matrix. The effect of the particles on the polymer structure was investigated using FTIR and thermal analysis methods (DSC). Microstructural studies of the membranes consisted of SEM observations and determination of pore size distribution by the capillary flow porometry. An important step was the determination of the surface properties of the membranes, surface energy and electrical charge i.e. the surface zeta potential. The information on the surface state was contrasted with the adsorption of bacteria on the membrane surface. Results of the studies may help selection of membranes with properties suitable for medical, environmental and industrial applications.

Silica derived from Industrial Waste as Catalyst Support: Characterization of Morphological and Surface Properties.

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A3_4, U2 Room (Level 0), settembre 18, 2025, 10:30 - 13:10

The sustainable recovery of Silica from industrial waste presents a promising opportunity to develop high-performance materials with tailored properties, which can be applied and functionalized as catalytic support for Carbon Dioxide Capture and Re-Use Process (CCSU). This contribution is focused on the investigation and development of the synthesis, characterization, and application of silica derived from hexafluorosilicic acid (H_2SiF_6), a hazardous by-product of the phosphate and aluminum fluoride industries. Through controlled precipitation using ammonia and the incorporation of organic templates, silica nanoparticles, mesoporous, and macroporous silica supports were produced with diverse morphological and surface characteristics.

Silica nanoparticles exhibited spherical morphology with diameters of 20–40 nm and surface areas of 115–130 m^2/g , and fluoride impurity levels reduced below 0.5 wt.% through optimized washing and drying procedures. Porous silica synthesized with organic templates achieved specific surface areas in the range 1100–400 m^2/g , pore volumes of 0.94–1.15 cm^3/g , and ordered pore sizes ranging from 3 to 30 nm. Also, macroporous silica have been prepared using different organic templates, obtaining materials with a pore diameter between 150–350 nm and a surface area of 110 m^2/g . FTIR-spectroscopy confirmed the presence of diverse silanol groups across all samples, with surface characteristics modulated by porosity and residual fluoride species. The FT IR analysis of hydroxyl (OH) groups revealed a combination of free, geminal, and hydrogen-bonded silanol groups, with weak protonic acidity evaluated using pivalonitrile adsorption-desorption studies. These waste-derived and recovered silica-samples demonstrated physicochemical properties comparable to commercial silica benchmarks.

The tunable porosity, high surface areas, and weak acidity indicate these material as promising candidates for advanced applications such as a sustainable catalytic support. These materials, once functionalized with suitable promoters (metals, basic oxides), will be tested for environmental remediation processes through CCSU.

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Hierarchical pore formation in iron nitride foils investigated at nano-scale by phase-contrast tomography

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A3_4, U2 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

Metallic materials displaying a high porosity in form of sponges or foams have gained increasing interest since the turn of the century. It is widely understood that the presence of pores within a material can alter the range of applications significantly. In more detail, pore size, morphology and volume fraction govern the function of the respective material. Catalytic materials, for example, benefit significantly from an increased surface area based on open-pore systems. Recent studies suggest the suitability of iron nitride as a catalyst due to its high activity¹ and long-term stability². Experimentally, a quantitative analysis of pore connectivity, size and distribution remains challenging for pores in the submicron range. Therefore, this study investigates systematically the pore formation during nitriding and denitriding of 38 μm thin, free-standing iron foils. For this, the samples were treated in an NH_3/N_2 atmosphere with different temperature sequences^{3 4}. Subsequently, the samples were analyzed by employing phase-contrast tomography at the ID16B beamline at the ESRF allowing for a voxel size down to 25 nm. Individual scans of the full foil thickness were recorded for areas of up to $125 \times 125 \mu\text{m}^2$. This combination of high resolution and large scan volume are significant advantages compared to standard scanning electron microscopy and focused-ion beam tomography.

The overall results indicate an open-pore system with hierarchical pore formation dependent on the process temperature. The foils exhibit μm - and nm-sized pores towards the edge and middle of the foil, respectively. Additionally, elongated pores oriented parallel to the surface are visible in the center, in contrast to perpendicular pores allocated towards the surface. The study demonstrates the potential of the ID16B beamline to facilitate quantitative data for materials exhibiting hierarchical pore systems in an easy manner. Furthermore, it sheds light on the overall pore formation in iron nitride foils dependent on the process temperature. The results can be a valid stepping stone to further finetune the porosity properties for specific applications such as catalysis.

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Porous and luminescent coordination networks from new tailored ligands

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A3_4, U2 Room (Level 0), settembre 18, 2025, 10:30 - 13:10

Coordination Polymers (CPs) and Metal-Organic Frameworks (MOFs) continue to attract great scientific interest due to their application in many different fields. Alongside well-known and studied MOFs the search for new materials through the development of tailored organic ligands is still an active topic in the field.

In our long standing interest in the synthesis, structural and topological characterization of new CPs and MOFs we are exploiting the coordination ability of new organic ligands to obtain homo and heterometallic porous networks. In particular, MOFs assembled with β -diketone and derived ligands which show large crystallographic void and structural flexibility will be presented. Their synthesis, crystal structures and porous properties will be discussed.

In addition, will be also presented the use of the triimidazo[1,2-a:1',2'-c:1'',2''-e][1,3,5]triazine (TT) molecule as a platform to develop new organic ligands of trigonal symmetry for the assembly of new CPs. The interesting luminescent properties of TT together with the great versatility in chemical functionalization is very promising for obtaining new luminescent and porous CPs.

Unraveling Ion-Exchange behavior in ZnAl LDH: The Impact of Functional Substituents and Isomeric Variations

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A3_4, U2 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

This study provides a comprehensive investigation into how both functional substituents and isomeric arrangements influence the intercalation and ion-exchange behavior of ZnAl layered double hydroxides (LDHs). Two distinct systems were examined. In the first, isophthalic acid (IPA), 5-aminoisophthalic acid (AIPA), and 5-nitroisophthalic acid (NIPA) were intercalated into ZnAl LDHs via a co-precipitation method to understand the impact of $-\text{NH}_2$ and $-\text{NO}_2$ substituents. UV-Vis quantification revealed that loading capacity followed the sequence $\text{NIPA} \geq \text{AIPA} > \text{IPA}$, whereas release kinetics in NaCl solution proceeded in the order $\text{AIPA} > \text{IPA} > \text{NIPA}$. Density functional theory (DFT) simulations attributed these differences to varied binding affinities driven by deprotonated carboxylates on the aromatic ring, showing a higher affinity for NIPA2-

than AIPA2- or IPA2-. Moreover, $-\text{NO}_2$ group stabilized the intercalated species by additional interactions with hydroxide layers, while the $-\text{NH}_2$ group led to weaker interlayer stability due to the positively charged hydrogen atoms.

In the second system, three isomers of pyridinedicarboxylic acid (PDA)—2,3PDA, 2,5PDA, and 3,4PDA—were intercalated into ZnAl LDHs via ion exchange to examine the role of molecular geometry. Structural characterizations showed distinct interlayer orientations leading to varying stabilities, release profiles, and chloride ion uptake capacities. ZnAl-2,3PDA exhibited the highest stability and minimal release due to nearly vertical orientation and strong electrostatic interactions, whereas ZnAl-2,5PDA showed moderate stability with the highest chloride ion uptake. Conversely, ZnAl-3,4PDA demonstrated rapid release and instability owing to a disordered interlayer arrangement. DFT analysis supported these findings, highlighting the correlation between binding strength, charge distribution, and isomeric configuration.

Overall, these results underscore the pivotal influence of both functional substituents and isomeric arrangements on the ion-exchange and intercalation properties of LDHs. Such insights pave the way for the development of predictive models and the rational design of LDH-based materials for targeted applications in controlled release, environmental remediation, and catalysis.

Metal-Organic Frameworks for the Production of Radionuclides of Medical Interest

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A3_2, U2 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

Metal-Organic Frameworks (MOFs) have emerged as promising materials for various applications, including the production of radionuclides for medical imaging and therapy. In this study, we demonstrate the potential of MOFs as:

i) Adsorbents in the $^{99}\text{Mo}/^{99}\text{mTc}$ generator, a device used in over 80% of diagnostic nuclear imaging procedures, accounting for the diagnosis of 30-40 million patients every year. Our results show that MOFs can achieve high adsorption capacities, exceeding 500 mg/g, and exhibit excellent radiation stability, making them suitable candidates for replacing traditional adsorbents in the $^{99}\text{Mo}/^{99}\text{mTc}$ generator. The molybdenum adsorption performance of MOFs, including adsorption kinetics and isotherms, was determined, and the adsorption mechanism was studied using various analytical techniques, such as X-ray photoelectron spectroscopy, Raman spectroscopy, zeta potential, and density functional theory calculation.

ii) Radiation targets for the production of ^{51}Cr , a radionuclide with applications in labelling red blood cells, diagnosing gastrointestinal bleeding, and assessing the life span of red cells. The radiation stability of these MOFs is assessed using two different facilities, and the results show that MIL-100 (Cr) and MIL-101 (Cr) exhibit excellent radiation stability after exposure to gamma radiation doses up to 5 MGy, without showing a dose rate dependency. The Cr-MOFs were irradiated in a nuclear reactor, and the ^{51}Cr yield and specific activity were determined at different irradiation times, extracting agents, and extraction times. The most optimal results show that high enrichment factors (>500) and yields (>50%) can be achieved, appearing to be a promising ^{51}Cr production route for nuclear medicine.

iii) Precursors to produce materials containing mono-atomically dispersed molybdenum which can be utilized for producing molybdenum-99 with high specific activity. This approach enables the selective isolation of molybdenum-99, enhancing its specific activity and ultimately yielding a product with a purity and quality comparable to that obtained through traditional fission-based methods, thereby providing a viable alternative for the production of this crucial medical isotope.

Our research highlights the potential of MOFs in the production of radionuclides for medical applications, and we believe that these emerging porous materials will play a crucial role in the development of innovative technologies for the healthcare sector.

Optimizing MOF morphology for enzyme immobilization: Insights from Nanoscale Characterization

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Imagine enzymes, nature's catalysts, can operate efficiently under the extreme conditions (i.e., high pressure, temperature, salt concentration) and revolutionize biocatalysis applications. Enzymes are highly efficient catalysts, playing a vital role in biocatalysis, biosensors, and biomedical applications. However, their use is often limited by lack of stability, loss of activity under harsh conditions, and limited reusability. These limitations demand the development of advanced support materials that can improve enzyme stability, preserve long-term catalytic efficiency, and enable easy recovery and reuse. In this regard, metal-organic frameworks (MOFs) have emerged as highly tuneable hierarchical materials known for their chemical and thermal stability. Their synthesis process allows precise control over structural properties, including composition, size, morphology, and crystallinity, making them well-suited for enzyme immobilization and encapsulation. With their high porosity and structural adaptability, MOFs provide a protective yet accessible environment for enzymes, enhancing their stability and catalytic performance for various applications.

The aim of this study is to improve enzyme stability and catalytic efficiency by precisely controlling MOF properties and immobilization strategies. By systematically investigating enzyme immobilization via adsorption and covalent bonding strategies as well as varying enzyme concentrations, we aim to understand how these parameters affect the structural integrity and catalytic properties of enzyme-MOF nanocomposites. Advanced (electron) microscopic and spectroscopic techniques were employed to confirm the successful attachment of enzymes onto the MOF surfaces and to elucidate the interactions at the enzyme-MOF on the nano scale. Immobilization efficiency and enzymatic properties were measured.

Our results demonstrate that controlling the MOF chemistry as well as morphology and choosing the right immobilization strategy significantly improves enzyme stability and minimizing leaching, while optimal enzyme concentration ensures a balance between catalytic efficiency and structural integrity. High-resolution scanning/transmission electron microscopy reveals uniform distribution of enzymes inside the MOF at the nanoscale level.

By addressing the critical challenges in enzyme immobilization on MOFs, this study lays the foundation for the rational development of MOF-based biocatalytic systems and paves the way for more sustainable and efficient biocatalysis applications.

Smart food packaging based on Metal-Organic Frameworks: one platform with multiple possibilities

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A3_1, U2 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

Reducing food loss is a major global challenge, approximately 30% of the food is wasted throughout the supply chain. In this context, packaging plays a fundamental role by helping to minimize waste, protecting food during production, transport and storage and ultimately extending its shelf life. Smart packaging technologies are being explored for their ability to prevent contamination (mainly water sources), regulate the internal conditions of packaged products, and preserve food quality through the incorporation of active components.¹

Here, we propose two strategies for integrating metal-organic frameworks (MOFs) into smart packaging to avoid contamination and increase the food shelf-life: use of intrinsically active MOFs, or encapsulation of active ingredients in porous frameworks. For the first strategy, a new MOF, IEF-32 ($[\text{CaC}_{24}\text{H}_{22}\text{N}_3\text{O}_9\text{P}_3]$) based on the micronutrient Ca and a triazine derivative ligand with potential antimicrobial properties, has been synthesized and fully characterized. IEF-32 demonstrated high preservation capacity in grapes for one month. A second strategy is the encapsulation of eugenol, a natural essential oil with remarkable antifungal and antimicrobial activities,² in the microporous Zn bispirazolate MOF ZnBDP ($[\text{ZnC}_{12}\text{H}_8\text{N}_4]$; SBET $\approx 2000 \text{ m}^2/\text{g}$; square channels of 1.1 nm).³ The successful encapsulation of eugenol was performed using two different approaches (vapour and liquid phase), achieving significant cargoes of 22 and 60 wt.%, respectively. Further, eugenol was slowly and progressively released in water (60% in 2 weeks), demonstrating its efficient preservation against fungal infections in strawberry and grape fruits. These results highlight the potential of MOFs in preservation of foodstuffs.

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Synthesis of novel porphyrin-based MOFs for environmental remediation

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A3_1, U2 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

The increase in atmospheric CO₂ concentration due to the combustion of fossil fuels is one of the major environmental challenges of the 21st century. In pursuit of a total decarbonization, a key research focus is the development of advanced technologies for CO₂ utilization. Metal Organic Frameworks (MOFs) have emerged as promising candidates for CO₂ capture, owing to their high specific areas, remarkable sorption capacities and tuneable physicochemical features [1]. However, their industrial implementation remains limited due to relevant drawbacks, i.e., the lack of stability and catalytic efficiency. In this context, the development of new MOFs based on highly conjugated linkers and high-valence metals is particularly encouraging. The combination of abundant and non-toxic cations, such as Ti(IV), Zr(IV) or Fe(III), which exhibit hard Pearson acidic behaviour, with polydentate linkers (e.g. porphyrins), presenting hard Pearson basic coordinating moieties (e.g. carboxylates) is expected to yield highly conjugated and stable coordination polymers [2]. Furthermore, the use of these macrocyclic linkers also allows the generation of dual-site catalysts by introducing additional, non-structural metal ions into the coordination network through ligand metalation. This enhanced stability, combined with the optoelectronic properties ascribed to the selected linkers [3] and the synergetic effects of simultaneous metal sites, is expected to improve the catalytic performance of these materials towards a more efficient CO₂ conversion.

Herein, we report the synthesis of two novel MOF families based on the combination of two carboxy-substituted trans A2-B2 porphyrins (i.e., 5,15-(di-4-carboxyphenyl)-10,20-(diphenyl)porphyrin (DCPP) and 5,15-(di-4-carboxyphenyl)porphyrin) (BDP), both barely described in the literature, and three M(III) lanthanides (Dy, Nd, Y). These materials were prepared through both solvothermal and MW-assisted methods leading to different porous isostructural series (BET surface areas up to 700 m²/g). Materials were physicochemically characterized with a broad palette of techniques, including X-ray diffraction, infrared and UV-Vis spectroscopies, elemental analysis, gas sorption studies (affinity towards CO₂), electron microscopy, and thermogravimetric analysis, among others, and their chemical/structural stability evaluated under different conditions (aqueous media at different pH, different organic solvents). These novel MOFs are currently being tested as potential CO₂ catalysts and luminescent sensors.

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Lanthanide and bi-lanthanide loaded zeolites for wastewater treatment

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The pharmaceutically active substances, widely used in human medicine, veterinary medicine, and aquaculture, represent an important group of emerging pollutants. They often enter the aquatic ecosystems through various sources such as municipal wastewater, inappropriate disposition of expired medicines, human and animal excretions, livestock farming. Numerous pharmaceutically active substances can be found in various water sources at concentrations ranging from ng/L to µg/L, because traditional methods for water treatment are insufficiently effective for their removal. During the past decade fluoroquinolone (FQ) antibiotics, norfloxacin (NOR) and ciprofloxacin (CIP), have been often detected in the environment. Long-term exposure to these compounds can cause harmful effects on aquatic organisms and human beings. Therefore, development of materials efficient for their removal, using simple and inexpensive methods, is an important research area.

Zeolites are microporous hydrated crystalline aluminosilicates of alkali or alkali earth elements (e.g. sodium, calcium). Because of well-defined structures made of pores and channels, large surface area, and high thermal stability, these materials are frequently used in adsorption, separation, and catalysis. Zeolites exhibit three-dimensional open framework structure composed of TO₄ (T = Si, Al) tetrahedra which are connected via corner oxygen atoms. The negatively charged framework is neutralized by charge-balancing cations, that are located in pores and channels and can be easily replaced by other cations via simple ion exchange procedure. Additionally, the amount of cation dopants is controlled by the aluminum content and zeolite structure.

In this work, two structurally different zeolites (FAU, BEA) have been loaded with lanthanide cations Eu, Ce and Tb, using cost effective and simple ion-exchanged procedure from diluted aqueous solution of lanthanide nitrate salts. The physicochemical characterization of prepared materials Eu-Y and Eu-β, as well as CeTb-Y and CeTb-β zeolites was done by X-ray powder diffraction analysis, FTIR spectroscopy, scanning electron microscopy with energy dispersive spectroscopy, ultraviolet–visible diffuse reflectance spectroscopy, X-ray photoelectron spectroscopy, fluorescence spectroscopy, and low temperature N₂ adsorption-desorption. Photoluminescence, adsorption and photodegradation with exposure to simulated solar light of NOR and CIP served as a tool to estimate potential application of prepared multifunctional materials. The photocatalytic degradation of NOR and CIP after 180 minutes of irradiation was ~30 % for both Eu-Y and CeTb-Y zeolites. The results showed the highest removal efficiency after 180 minutes of irradiation for Eu-β (~75 %) and CeTb-β (~65 %) zeolites, that resulted from two processes: adsorption and photocatalytic degradation.

Electrospun Lignin/ZIF-8 Hybrid Nanofibers for Sustainable Catalysis and Environmental Applications

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A3_3, U2 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Metal-organic frameworks (MOFs) are highly attractive due to their structural and chemical tunability, electrical insulation properties, adjustable pore size, and chemistry, which allow specific interactions with ions. Recent advancements in processing have enabled the synthesis of self-supporting membranes [1]. Additionally, MOFs exhibit stability in aqueous environments, making them suitable for water capture in aggressive or toxic conditions. Their production can also be cost-effective using low-cost metal precursors and organic building blocks. Among MOF materials, zeolitic imidazolate framework (ZIF) structures stand out for their exceptional properties, such as high thermal and chemical stability. ZIF-8, with the molecular formula $\text{Zn}(\text{2-methylimidazolate})$, is one of the most studied.

Nevertheless, the inherent fragility of MOF crystals hinders the fabrication of membranes composed solely of MOFs, requiring their integration with polymeric substrates to enhance their flexibility and handling. Recently, the electrospinning route has revealed as an efficient process for incorporating MOFs into polymeric nanofibers, combining porosity and high surface area with additional functionality. This advancement expands their applicability in fields such as energy and environmental science [2].

The increasing demand for sustainable materials in energy and environmental applications has intensified the search for non-fossil alternatives to conventional polymers. In this context, lignin, an abundant biomass-derived biopolymer, has emerged as a promising candidate for hybrid nanofiber fabrication. In this work, electrospun lignin/ZIF-8 hybrid nanofibers were developed. Lignin was blended with polyethylene oxide (PEO) to optimize electrospinnability and nanoscale ZIF-8 particles were integrated, which improves catalytic activity due to its high surface area and tunable porosity. This combination enhances catalytic performance, enabling applications in energy storage (dye-sensitized solar cells, batteries, capacitors, and supercapacitors) and environmental remediation. Moreover, the nanofibers serve as efficient catalyst support for various catalytic processes, including photocatalysts, and as adsorbents for water purification and volatile organic compound (VOC) removal, providing a sustainable approach to advanced catalysis and environmental protection. [3]. The hybrid nanofibers of ZIF-8/lignin, after thermal treatment, were analyzed in terms of morphology (SEM and TEM), enabling a detailed assessment of nanoparticle incorporation and distribution within the fibers. Their structural integrity was verified through XRD and FTIR analysis, while textural properties were also assessed using N_2 adsorption isotherms (BET), pore size distribution, and CO_2 sorption and co-sorption capacities (DVS and BTA).

Porosity evolution along simultaneous synthesis and sintering of zinc ortostannate

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Zinc ortostannate (Zn_2SnO_4) has received broad attention due to its excellent optical and electrical properties, as well as its stability. However, some research has shown the anomalous expansion that presents when synthesis and sintering are performed simultaneously. This research demonstrates that it could be used to obtain porous ceramics without the addition of any pore generator.

The starting point was a stoichiometric mixture of ZnO and SnO_2 . Its analysis in a hot stage microscope at $25\text{ }^\circ\text{C}\cdot\text{min}^{-1}$ showed that contraction begins around $1000\text{ }^\circ\text{C}$, but an expansion occurs between 1080 and $1200\text{ }^\circ\text{C}$, that presumably generates an increase in porosity. This fact was confirmed by firing dry-pressed specimens of the mixture (samples of $2\times 8\text{ cm}^2$ compacted at $250\text{ kg}\cdot\text{cm}^{-2}$) during 1 hour at different temperatures between $950\text{ }^\circ\text{C}$ and $1350\text{ }^\circ\text{C}$. The bulk density of fired specimens at $1050\text{ }^\circ\text{C}$ and $1150\text{ }^\circ\text{C}$ ($2,77$ and $3,14\text{ g}\cdot\text{cm}^{-3}$ respectively) was lower than the value corresponding to $950\text{ }^\circ\text{C}$ ($3,33\text{ g}\cdot\text{cm}^{-3}$). However, bulk density increased for specimens fired at higher temperatures ($3,92$ and $4,37\text{ g}\cdot\text{cm}^{-3}$ for the samples fired at $1250\text{ }^\circ\text{C}$ and $1350\text{ }^\circ\text{C}$ respectively).

Mercury intrusion porosimetry showed that total pore volume shows an inverse trend with respect to bulk density, peaking for the samples treated at $1050\text{ }^\circ\text{C}$. Concretely, samples fired at $1050\text{ }^\circ\text{C}$ had a pore volume of $0,20\text{ cm}^3\cdot\text{g}^{-1}$, a 42% higher than $0,14\text{ cm}^3\cdot\text{g}^{-1}$ obtained at $950\text{ }^\circ\text{C}$. However, the mean diameter increases with a nearly exponential trend with the sintering temperature, from $0,15\text{ }\mu\text{m}$ at $950\text{ }^\circ\text{C}$ to $1,22\text{ }\mu\text{m}$ at $1350\text{ }^\circ\text{C}$. These characteristics are compatible with a microfiltration membrane, with the advantage that no pore generator, as starch, was introduced in the composition. Consequently, the thermal cycle did not require a slow step for oxidise/decompose the additive, shortening the firing step and reducing the energy cost.

The abnormal behaviour under firing around $1050\text{ }^\circ\text{C}$ of the stoichiometric mixture of ZnO and SnO_2 around $1050\text{ }^\circ\text{C}$ generates a ceramic with high porosity and sub-micronic mean pore size that allows their use as microfiltration membranes with the advantage that no pore generator was needed.

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Design and optimization of zeolite-CZA tandem catalysts for CO₂-to-ethylene conversion: towards green polymer production

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A3_3, U2 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

As the demand for sustainable carbon sources grows, carbon dioxide (CO₂) has emerged as a promising feedstock. Its catalytic conversion can yield valuable chemicals, offering both environmental and industrial benefits. One exciting possibility is the production of light hydrocarbons (C₂–C₄), which are essential for the energy, chemical, and manufacturing sectors, through a carbon-negative approach. Ethylene (C₂H₄), a major contributor to the olefin market, is traditionally derived from high-energy processes involving naphtha and ethane, which emit harmful pollutants. Developing sustainable, economically viable production routes has therefore become a key focus. The direct catalytic hydrogenation of CO₂ to ethylene faces challenges due to C–C coupling barriers. A promising alternative is using tandem heterogeneous catalysts for sequential reactions, with methanol as an intermediate. In the first step, CO₂ is hydrogenated to methanol using Cu- and Zn-based catalysts. In the second step, methanol is converted into ethylene via a methanol-to-olefins (MTO) process, typically using zeolite catalysts with acidic sites to facilitate C–C bond formation. Herein, we explored a tandem catalytic approach with porous materials, combining Cu/ZnO/Al₂O₃ (CZA) catalyst for CO₂ hydrogenation to methanol and a zeolite-based catalyst for methanol-to-olefins (MTO) conversion. The zeolite-CZA composite catalyst was synthesized via coprecipitation in an automated synthesis system (Atlas Potassium, Syrris) to facilitate the scale-up process. Zeolites were either used as received or surface-functionalized. Structural, textural, and compositional characterization studies are being performed to understand how synthesis processes and material selection influence its catalytic properties. Powder X-ray diffraction (PXRD) confirmed the retention of crystalline CuO and ZnO phases in both the CZA and zeolite-CZA samples, indicating preservation of the crystallinity of both catalysts. Scanning electron microscopy (SEM) analysis revealed that CZA had an irregular morphology, while the zeolites displayed well-defined crystalline structures. Additional textural studies, including N₂-physisorption, are being conducted to assess the surface area and pore size distribution, crucial factors influencing catalytic performance. Furthermore, inductively coupled plasma (ICP) spectroscopy is being utilized to determine the elemental composition of the catalysts. Future work will focus on fine-tuning synthesis parameters and evaluating the material's efficiency as a tandem catalyst for ethylene production from CO₂. This study highlights the significance of porous materials in CO₂ valorisation. We aim to demonstrate the potential of zeolite-CZA as an efficient tandem catalyst for real-world industrial applications, particularly for ethylene production, supporting global carbon-neutral efforts through the production of green polymers.

Aerogels and Xerogels from Biogenic Phenols and Furfural

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Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Both climate change and the depletion of fossil feedstocks drive the demand for high performance materials based on renewable natural resources. Due to their remarkable thermally insulating and light-weight properties that can be traced back to their unique microstructure, aerogels and xerogels based on phenolics, such as resorcinol-formaldehyde (RF), have received increasing attention.[1] Furthermore, high char yields resulting from carbonization of RF gels render them attractive precursors for porous carbons, which- in turn- are interesting for electrochemical applications. However, RF is made from fossil precursors, and thus biogenic alternatives to these phenolic aerogels are highly sought-after.

In that context, we report on three phenolic aerogels and xerogels made from bio-based monomers, namely cardanol-furfural, thymol-furfural, and eugenol-furfural.[2] We have investigated the conditions of gelation, solvent exchange, and drying, and characterized properties such as chemical structure, density, surface area, pore size and -volume, microstructure, thermal stability and wetting behavior. Furthermore, we report on the carbonization of these bio-based aerogels and xerogels. Especially carbon xerogels based on eugenol-furfural show promising pore characteristics and significantly higher char yield when compared to carbons based on cellulose aerogels. These gels can, thus, be considered attractive candidates for larger scale production and further studies in electrochemical applications.

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Hydrogen storage in nanoporous carbons: A path towards sustainable and scalable solutions

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A3_5, U2 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

Hydrogen is a crucial clean energy carrier with a high gravimetric energy density. However, its low volumetric energy density presents significant storage challenges. Beyond energy-intensive methods such as compressed hydrogen (700 bar) or liquid hydrogen (20 K), physisorption-based storage in nanoporous materials offers a promising alternative at moderate pressures and cryogenic temperatures. Nanoporous carbons have shown great potential for hydrogen storage due to their high specific surface area and tunable pore structures. However, research has largely focused on lab-synthesized materials with limited scalability. This study systematically investigates 16 commercially available nanoporous carbons, derived from various precursors and in macroscopic forms (granules, pellets, powders, spheres), to assess their viability for large-scale hydrogen storage applications. Structural characterization via Raman spectroscopy and X-ray diffraction confirmed the turbostratic nature of the studied materials, while N₂ (77 K) and CO₂ (273 K) adsorption provided insights into their pore structure characteristics. Hydrogen storage capacity was initially evaluated at 77 K under low pressures (<1 bar), followed by high-pressure measurements (up to 100 bar) at 77, 87, and 111 K for a subset of five promising materials with varying microporous and mesoporous structures. The storage performance was analyzed in both gravimetric and volumetric terms, considering bulk densities to assess the practical storage potential. The obtained results are compared with pore structure characteristics. In addition, a techno-economic analysis determined material costs per unit of stored H₂, correlating the findings with the U.S. Department of Energy targets. Several commercially available nanoporous carbons demonstrated hydrogen storage capacities competitive with these targets, underscoring their potential for scalable hydrogen storage applications.

Fixed-bed column adsorption of activated biochar towards purification of landfill leachate

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A3_5, U2 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

The purpose of this study was the purification of landfill leachate collected at the output of Sequencing Batch Reactor (SBR). The adsorption of total polyphenols (TPh) and color was studied using palm leaves biochar after pyrolysis and activation with the addition of KOH. The activated biochar was used in batch adsorption experiments (kinetic studies), and in fixed-bed column adsorption studying the effect of dilution rate of the initial leachate and the regeneration of the adsorbent material. Two-times activated biochar was also produced to perform adsorption at different flow rates. Furthermore, activated biochar with titanium loading was investigated in batch and fixed-bed column experiments. The materials were characterized for specific surface area, morphology and surface structure by BET, SEM-EDS and FTIR analyses. For the fixed-bed column adsorption experiments, performance modeling was studied using the Thomas, Bohart-Adams and Yoon-Nelson models. For the batch experiments, the higher TPh adsorption yield appeared 73-93% at pH 5, while for the activated biochar with titanium loading the TPh adsorption yield reached 98%. For the column experiments, the breakthrough time was 300 min for the 1/20 dilution rate, 240 min for the 1/10 and 130 min for the 1/5. During regeneration experiments (1/20 dilution rate), the 2nd round regeneration lasted 1310 min, the 3rd regeneration 1110 min and the 4th regeneration 1030 min. For the two-times activated biochar (1/20 dilution rate, 1 ml/min flow rate), it yielded a breakthrough time of 680 min. For the activated biochar loaded with titanium (1/20 dilution rate), the 1st round had a breakthrough time of 740 min, the 2nd round regeneration 1130 min and the third 860 min. The models Thomas and Yoon-Nelson described adequately the TPh adsorption in the fix-bed column experiments.

Electromagnetic Interference Shielding: Carbon-Based Materials and aluminosilicate Ceramic Fiber Composites

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

With the rapid advancement of technology, electromagnetic (EM) pollution has become a significant concern, as modern electronic devices and systems emit microwave radiation. This radiation can interfere with electronic circuits, leading to malfunctions and operational failures. To address this issue, the development of effective electromagnetic interference (EMI) shielding materials has become a critical area of research. Ideal shielding materials must meet several requirements, including chemical and corrosion resistance, lightweight properties, flexibility, tunable morphology, ease of processing, and cost-effectiveness. Carbon-based materials, such as graphene, carbon nanotubes, and reduced graphene oxide (rGO), have emerged as promising candidates for EMI shielding due to their exceptional electrical conductivity, lightweight nature, and ability to interact with electromagnetic waves. These materials can be incorporated into polymer matrices or used in hybrid composites to create efficient and versatile shielding solutions.¹

In this study, we propose a novel approach to developing EMI shielding materials by utilizing an aluminosilicate-based ceramic fiber as a template. This fiber was selected due to its inherent porosity, thermal stability, and compatibility with high-temperature processes. The fiber was incubated in an aqueous dispersion of graphene oxide (GO), allowing the GO to infiltrate its porous structure. The composite was then subjected to hydrothermal synthesis and thermal treatments to reduce the GO into reduced graphene oxide (rGO) within the fiber. This process imparted conductive properties to the composite material, making it suitable for EMI shielding applications. The resulting carbon-based material was characterized using electrochemical impedance spectroscopy to evaluate its conductive properties, and its morphology was analysed using scanning electron microscopy.

The proposed method offers several advantages. The aluminosilicate-based ceramic fiber is highly resistant to high temperatures, making it compatible with thermal synthesis processes. Additionally, the reduction of GO to rGO within the fiber is an eco-friendly procedure that uses only water as the reaction medium, eliminating the need for hazardous chemical reducing agents. This approach is scalable and aligns with sustainable manufacturing practices. The findings of this work demonstrate the potential of silicate-based ceramic fibers combined with rGO as a promising material for EMI shielding, offering a balance of performance, sustainability, and scalability for future applications in electronic protection.

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MOF-Polymer Composites for Enhanced Atmospheric Water Harvesting

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A3_3, U2 Room (Level 0), settembre 17, 2025, 17:00 - 19:00

The development of highly efficient sorbent materials is crucial for advancing atmospheric water harvesting (AWH) technologies, particularly in arid and semi-arid climates. In this work, we report the synthesis, characterization, and performance evaluation of novel MOF-polymer composites designed for efficient water capture.

A series of zirconium-, iron-, and chromium-based MOFs were synthesized and functionalized with hydrophilic linkers to optimize water uptake under low relative humidity conditions. The resulting MOFs demonstrated water adsorption capacities exceeding 45 wt.% at 70 % RH, with rapid adsorption kinetics and excellent structural stability over multiple cycles. Novel more sustainable solvothermal synthesis routes were optimized to minimizing energy-intensive processing and reduce the environmental impact, while maintaining high yield and good crystallinity.

To enhance scalability and mechanical stability, these MOFs were incorporated into polymeric matrices, including alginate and polyvinylpyrrolidone, forming robust and versatile composite structures. The polymer integration preserved MOF adsorption efficiency while increasing the mechanical integrity and processability of the materials. The MOF-alginate composites were prepared as beads. Beads provide better mechanical stability than powders, maintaining structural integrity over multiple cycles. Their uniform packing ensures consistent moisture distribution, preventing aggregation and improving sorption kinetics. Additionally, beads are also easier to handle, transport, and reuse, making them ideal for scalable and sustainable AWH applications. On the other side, MOF-PVP composites have been used as coatings to enhance the performance of sorption-based thermal energy storage (TES) and AWH systems. These composites exhibited an improvement in long-term cycling stability. The coating plays a vital role in improving heat and mass transfer efficiency between the sorbent material and the heat-exchanger, ensuring material stability, and enabling scalability.

Further performance enhancement was achieved through the incorporation of carbon-based photothermal harvesters, enabling solar-driven water desorption. Spectroscopic and thermal imaging analyses confirmed an increase in surface temperature upon solar irradiation, facilitating efficient moisture release at low energy inputs.

This study highlights the potential of engineered MOF-polymer composites as next-generation materials for sustainable AWH. Ongoing work focuses on refining composite formulations, optimizing photothermal efficiency, and scaling production methodologies to further enhance their viability for real-world applications. and solar-driven desorption.

Influence of Microstructure on Dealloying Kinetics and Nanoporosity in AgAu Thin Films for Electrocatalytic Applications

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A3_4, U2 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

Dealloying corrosion is a well-established technique for fabricating high-surface-area nanoporous metals, which hold great potential for catalytic applications, particularly in alkaline water electrolysis [1]. This process selectively dissolves the less noble metal from a solid-solution alloy, resulting in a chemically enriched, three-dimensional open-pore nanostructure primarily composed of the more noble metal [2]. These nanoporous metals offer a highly tunable platform for optimizing composition, morphology, and surface-to-volume ratio—key factors influencing catalytic and electrochemical performance.

Utilizing thin film precursors presents several advantages over bulk solid-solution alloys, including reduced production costs by minimizing noble metal consumption, the introduction of a high density of microstructural defects that act as preferential sites for dealloying initiation, and enhanced integration into energy storage and catalytic devices due to their inherent substrate-support characteristics [3]. Moreover, thin films deposited via magnetron sputtering enable precise control over thickness and composition, making them highly adaptable for targeted application [4]. Therefore, a fundamental understanding of the microstructure of precursor samples is essential for optimizing dealloying mechanisms and tailoring critical nanoporous features, such as ligament size and composition.

In this study, we investigate the influence of microstructure on the dealloying behavior of AgAu thin films deposited at 400°C with either a (111)-textured or a non-textured grain orientation. Electron backscatter diffraction (EBSD) confirms the distinct crystallographic textures. At the same time, atom probe tomography (APT) reveals that the textured film retains a higher Ag content in the nanoligaments after chemical dealloying. In contrast, the non-textured film undergoes more pronounced coarsening and exhibits lower residual Ag concentration. These findings underscore the critical role of microstructure in controlling dealloying kinetics, and final ligament composition. Understanding such structure-property relationships is essential for optimizing nanoporous metals in catalysis, where stability and active surface area are crucial for long-term performance.

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Accelerating MOF Synthesis Through AI: Building the Lab-of-the-Future

Dr. Manuel Tsotsalas¹

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A3_2, U2 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

Metal–organic frameworks (MOFs) present a vast chemical landscape, offering diverse structures and exceptional tunability for applications ranging from catalysis to sensing. While computational tools have long guided MOF discovery and design, recent advancements in Artificial Intelligence (AI) are transforming their experimental realization—potentially accelerating R&D by up to tenfold. However, technology alone will not suffice; to unlock AI’s full impact, we must integrate data-driven methodologies into everyday lab practices.

In this presentation, I will provide an experimentalist’s perspective on merging AI with established laboratory routines. Drawing on examples from our work at the Karlsruhe Institute of Technology (KIT), we have successfully leveraged closed-loop AI systems to optimize growth conditions for Surface-anchored MOFs (SURMOFs), achieving improved crystallinity, uniform orientation, and minimal surface roughness. I will further illustrate how automated data extraction and machine learning predict initial synthesis conditions for new MOF structures, which can be refined through iterative, AI-guided cycles.

The second part of the presentation focuses on our journey toward the “Lab-of-the-Future,” facilitated by Aixelo Inc.—a KIT spin-off dedicated to AI software, strategy consulting, and professional services. Our EDISON-4.0™ platform empowers chemists to adopt AI without specialized coding or data science expertise, much like using apps on a smartphone. Key capabilities include:

1. Automated Data Extraction & Machine Learning – Rapid predictions for optimal synthesis conditions and reduced trial-and-error.
2. Adaptive Experimental Planning – Autonomous optimization that continually refines parameters based on real-time feedback.
3. Integration of Large Language Models – Streamlined data management and accelerated knowledge extraction across experiments.

By bridging AI innovation with practical application, our platform lowers barriers to AI adoption and fosters significant productivity gains. Ultimately, this presentation underscores how AI-driven strategies can fast-track MOF research, transform traditional workflows, and pave the way for a more efficient, data-centric era in materials science.

Exploiting the potential of Metal-Organic Frameworks to improve the therapeutic efficiency of Glycodrugs

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A3_1, U2 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

Glycomimetics have attracted much interest as therapeutic agents for a wide variety of diseases; however, their optimal delivery in cells is still a major concern. The therapeutic potential of many bioactive glycomimetics is often limited by poor biodistribution due to issues such as quick degradation or clearance, or low solubility or aggregation in biological media. The latter is the case of sp²-iminoglycolipids, a family of glycolipids endowed with immunomodulatory capabilities but requiring high doses (in the micromolar range) to exhibit an effective cellular response.

In this context, the use of nanosized metal-organic frameworks (MOFs) has been recognized as a promising strategy to achieve more efficient delivery of small bioactive compounds; however, the efficient encapsulation of large biomolecules such as carbohydrates is not trivial, and probably for that reason has been little investigated until now. Our group has recently optimized a synthetic procedure for the encapsulation of a variety of glycolipids within a zeolitic-imidazolate framework-8 (ZIF-8) nanostructure, giving rise to several GlycoZIFs with distinctive therapeutic potential depending on the specific glycolipid encapsulated. We have performed computational studies to disclose the favorable glyco-ZIF interactions and propose a plausible mechanism of formation of these GlycoZIFs.

From the application point of view, the therapeutic activity of two different GlycoZIFs have been evaluated in in vitro and ex vivo experiments. These works demonstrate the potential of GlycoZIFs to: (1) modulate the oxidative stress in endothelial cells, by exploiting the antioxidant properties of a GlycoZIF that encapsulates Se-glycolipids, and (2) treat diabetic retinopathy, thanks to the anti-inflammatory effect exerted by a GlycoZIF that contains SO₂-glycolipids. In conclusion, these examples serve to illustrate the promising future of carbohydrate/MOF-hybrid materials in the biomedical field.

Nanosized Porphyrinic Metal-Organic Frameworks for the Construction of Transparent Membranes as a Multiresponsive Optical Gas Sensor

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A3_1, U2 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

The well-known and excellent colorimetric sensing capacity of porphyrins, along with the exceptional structural properties of metal-organic frameworks (MOFs), make porphyrin-based MOFs, such as PCN-222, ideal candidates for the generation/construction of a chemical sensor based on absorbance. However, there are two key requirements for this end which remain challenging: (i) the synthesis of nanoscale PCN-222 in order to minimize/avoid scattering in the absorbance measurement, and (ii) the deposition/integration of the PCN-222 into thin transparent membranes/films in an homogeneous manner without compromising the performance of the PCN-222 (i.e., accessible porosity to interact with analytes and distinctive optical response as a function of the analyte). Fortunately, using an optimized microwave-based synthetic method, we were able to prepare high-quality PCN-222 nanoparticles with a rod-shape and lateral size of ca. 100 nm, and almost negligible scattering in the absorbance spectrum when dispersed in water solution, thanks not only to the small size of the particles but also to their high colloidal stability. Moreover, using poly(dimethylsiloxane) (PDMS) for the formation of flexible and transparent membranes, we have proposed a simple method for the integration of the PCN into the membrane resulting in a multi-responsive optical gas sensor with excellent sensitivity, capable of discriminating between different VOCs through pattern recognition identification.

Exploiting Cross-Responsiveness of Fluorescent Interpenetrated Zirconium–Organic Frameworks Integrated in Polymeric Membranes as a Multi-Analyte Gas Sensor Array

Ph.D. Juan Jesús Romero Guerrero¹, Dr Francisco G. Moscoso¹, Dr David Rodríguez-Lucena³, Dr Said Hamad¹, Dr Carolina Carrillo-Carrión², Prof José María Pedrosa Poyato¹

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In this work, a series of Zr metal-organic frameworks, whose hexanuclear clusters of Zr are connected with luminescent rodlike dicarboxylic acids, are used for the construction of a sensor array to selectively detect various analyte vapors. The chemical functionalization of the ligand (HOOC[PE-arylEP]COOH) (which alternates phenylene(P) and ethynylene(E) units) through the aryl core, is focused on obtaining six Porous Interpenetrated ZirconiumOrganic Frameworks (PIZOFs) with distinctive luminescent properties.

Particularly, the synthesis of two new ligands (aryl = nitrobenzene; aryl = pyrazine) enabled the preparation of new PIZOFs (UPO-1 and UPO-2) with submicron sizes, thanks to the use of a microwaveassisted synthetic method. The fluorescence properties of these two new PIZOFs, along with four others already reported, are thoroughly evaluated and noticeable changes are observed in their optical properties based on variations in the aryl core of the ligands. Furthermore, the presence of various volatile analyte vapors particularly modified their characteristic emission, resulting in multiple optical responses that are combined to achieve selectivity in detecting these analytes. Specifically, the construction of a fluorescent sensor array is proposed, incorporating the six PIZOFs into polyvinylidene-fluoride (PVDF) films, capable of producing unique identification patterns for each analyte by leveraging the cross-responsiveness of these sensing materials.

Immobilization of Lipase on Hafnium based MOF for heterogenous biocatalysis

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A3_2, U2 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

Most transport fuels and chemicals are currently derived from fossil resources but concerns about depletion and pollution have driven interest in renewable alternatives. Biomass offers a sustainable carbon source for biofuels and valuable chemicals, and specifically 5-Hydroxymethylfurfural (HMF), a versatile platform molecule derived from hexoses can be reduced to 2,5-bis(hydroxymethyl)furan (BHMF) followed by the esterification of BHMF for its potential use as alternative to petroleum-derived phthalates [1,2]. To date, metal catalysts effectively facilitate this transformation, however, often require severe conditions and suffer of metal leaching and deactivation. Here, we propose a heterogeneous biocatalyst based on the enzyme lipase immobilized on a hafnium-based Metal-Organic Frameworks (MOF), capable of performing a cascade reaction to obtain BHMF-DE.

Pure microporous UiO-66(Hf) and hierarchical HPUs-(X), where X indicates the volume of water added on the synthesis, were prepared following a procedure reported in the literature [3]. Since the pore size of the materials plays a critical role in enzyme immobilization efficiency, according to lipase from *Candida Rugosa* diameter (5 nm [4]), the MOFs' cavities have been rationalized to have different size and thus different degree of lipase immobilization. Moreover, to increase the possibility of immobilization, MOF's surface has been functionalized with proline. Lipase was loaded according to the adsorption method [3]. All the materials were characterized by means XRD, N₂ physisorption, and FE-SEM while the amount of immobilized lipase was determined using the hydrolysis reaction of 4-nitrophenyl palmitate catalyzed by the enzyme.

In all the tested materials, lipase retained the catalytic activity after immobilization, with a slower kinetics compared to the free enzyme. The cascade catalytic reaction from HMF to BHMF-diester as well as the reusability of the bifunctional material were finally studied. The MOF catalyzes the Meerwein-Ponndorf-Verley reduction of HMF to BHMF, while lipase is involved in the transesterification step to produce BHMF-diester. A full cascade reaction test achieved a 57% yield for BHMF-diester with the most promising material, confirming the catalyst's efficiency. Recycling tests showed that the lipase remained stable over three cycles, and enzyme immobilization improved its stability at higher temperatures, supporting the enzyme's potential for extended use in catalytic processes.

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The structure-mechanical properties relations of nanoporous Ag as obtained from molecular dynamics simulations

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A3_5, U2 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

The mechanical behavior of nanoporous gold (NPG) is governed by a complex interplay of ligament-scale deformation mechanisms, topology-dependent elasticity, and size-dependent plasticity. In this study, we employ molecular dynamics (MD) simulations to investigate the compression and creep response of NPG nanopillars and nanowires, focusing on their size-dependent mechanical properties, plasticity evolution, and deformation mechanisms. Compression simulations of NPG nanopillars reveal that their elastic modulus depends not only on solid fraction but also on ligament topology and nanopillar dimensions. The elastic response is primarily governed by ligament compression, with the effective number of load-bearing ligaments influencing the modulus. In the plastic regime, compression stress-strain curves exhibit an initial nonlinear response, followed by a plateau and a strong hardening stage. Our analysis of dislocation activity shows that the elastic-plastic transition occurs at lower strains than previously assumed. By skeletonizing the ligament structure, we track the evolution of load-bearing ligaments and find that at the onset of the plateau, 40% of ligaments have already yielded, suggesting the plateau stress corresponds to the topology of the unyielded ligaments. Furthermore, tensile creep simulations of NPG nanowires highlight the interplay between dislocation slip and atomic diffusion, revealing a transition from diffusion-dominated deformation at low creep stresses to a mixed displacive-diffusive mechanism at higher stresses. The contribution of dislocation activity decreases as ligament size increases, which manifests as changes in creep exponents. Remarkably, the calculated activation volumes and creep stress exponents align with those measured in indentation creep experiments, despite differences in length and time scales. Our findings provide a comprehensive understanding of how ligament-scale plasticity, structural topology, and diffusion-mediated mechanisms contribute to the mechanical response of NPG structures. This study advances the predictive modeling of porous materials and offers insights for the design of NPG-based functional and structural applications.

Synthesis and characterization of hybrid composites for marine biotoxins by surface-enhanced Raman scattering (SERS)

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A3_3, U2 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

The efficient, rapid, and cost-effective detection of marine biotoxins remains a critical scientific and technological challenge, exacerbated by the increasing prevalence of harmful algal blooms (HABs). These blooms, driven by excessive algal accumulation in aquatic ecosystems, can produce toxins that pose serious risks to human health. The rising frequency and intensity of HABs, further amplified by ocean warming and climate change, highlight the urgent need for innovative detection strategies. Beyond health concerns, HABs also have substantial economic consequences, particularly for marine-related industries such as aquaculture. Hence, developing advanced, rapid, and selective detection methods is essential to mitigate these risks, ensuring both public safety and the resilience of marine economies [1].

To address this challenge, we have developed a microfluidic system for surface-enhanced Raman scattering (SERS)-based detection of marine biotoxins. This innovative platform integrates an organic-plasmonic hybrid composite designed for high-affinity, selective toxin adsorption. The composite consists of covalent organic polymers (COPs) or covalent organic frameworks (COFs) as chemoreceptor with high-affinity, preferential toxin adsorption [2,3] and gold nanoparticles (GNPs) as optical enhancer, which allow the SERS detection, enabling selective trace-level detection. In this communication, the exploration of different COPs and COFs, their different structures (e.g., bulk, core-shell, and surface-functionalized forms) alongside various GNPs morphologies (spherical particles, aggregates and anisotropic gold nanostars) will be discussed. Preliminary assessments of these hybrid composites demonstrate promising sensitivity for trace toxin detection, laying the groundwork for an integrated detection system optimized for aquaculture farms in open-sea environments.

Additionally, the designed system leverages on density functional theory (DFT) calculations, to validate the resulting SERS signals, ensuring precise toxin identification and quantification, and will incorporate automated detection powered by chemometrics and machine learning algorithms, enhancing efficiency, accuracy, and real-time monitoring capabilities.

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Covalent Organic Frameworks for the Efficient Adsorption and Detection of Contaminants of Emerging Concern in Runoff Waters

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A3_1, U2 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

Urban runoff is widely recognised as an important pathway for pollutants released in the urban environment.¹ Common contaminants include sediments, heavy metals, pesticides, fertilizers, oil, and bacteria from urban, industrial, and agricultural areas. Although the toxicological profile of some of these pollutants remains poorly characterized, they can exhibit biological activity even at very low concentrations, potentially harming non-target organisms. Additionally, they can persist in the environment, leading to long-term ecological damage.²

Many pesticides classified as Highly Hazardous Pesticides (HHPs), along with tire wear particles, and other emerging contaminants, are frequently detected in runoff waters.³⁻⁴ Under the European Water Framework Directive (WFD), the EU Commission regulates surface water quality to preserve, protect and improve the aquatic ecosystem and human health by setting environmental quality standards (EQS) for surface waters.⁵

Within this framework, the Horizon Europe project D4RUNOFF focuses on contributing to the development of innovative detection methods and sensors for characterizing runoff pollutants and enabling rapid in-situ monitoring. It aims to support the implementation of cost-effective hybrid mitigation solutions that integrate nature-based strategies with water infrastructures.

Innovative nanomaterials, such as covalent organic frameworks (COFs), have been explored as adsorbents for the efficient removal of micropollutants from water and wastewater.⁶ COFs are a class of crystalline porous organic polymers composed entirely of organic building blocks. Thanks to their tuneable functionality and pore aperture sizes, as well as structural stability under various conditions, they are widely favoured for adsorbing various molecules. This study assessed COFs as alternative adsorbents to solid-phase extraction (SPE). Several COFs (i.e., TpBD-(CF₃)₂, TpBD-(CH₃)₂, TpBD-DMTP) were tested for the extraction of different triazines and 6-PPD-quinone. Results demonstrated that TpBD-(CF₃)₂ and TpBD-(CH₃)₂ show strong potential as alternative SPE adsorbents for these substances. Subsequently, contaminant detection was achieved using the Surface-Enhanced Raman Scattering (SERS) technique. Furthermore, the combination of COFs for contaminant adsorption and concentration with a microfluidic device for detection enables real-time runoff water monitoring, ensuring a rapid and in-situ response.

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Covalent Organic Framework in combination with Surface-enhanced Raman scattering for Ultrasensitive Antibiotic Detection

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A3_2, U2 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

In modern days, antibiotics are indispensable in human and animal therapy. However, their rapid and accurate detection is crucial in environmental and biological samples for contamination monitoring and antimicrobial resistance control [1]. Surface-enhanced Raman Scattering (SERS) is a powerful tool that benefits from signal enhancement caused by plasmonic metallic nanostructures, enabling fast and highly sensitive detection of different molecules, including antibiotics.

A pre-concentration step is needed due to the very low concentration of the target compound found in the environment and food matrices. A covalent organic framework (COF), a crystalline porous material, was selected as pre-concentrator since these materials have been demonstrated to adsorb pharmaceuticals efficiently. [2]

In this study, sulfonamides were chosen as the target antibiotic family to test the COF's pre-concentration efficiency and the SERS strategy's performance due to the special interest and urgency of their monitoring. In particular, sulfamethoxazole, a widely used antibiotic to treat gram-positive and gram-negative bacteria, is an emerging contaminant of concern in groundwater worldwide. The EU has established a detection limit of 10 ng/L for sulfamethoxazole in surface water [4] and a maximum residue limit of 100 µg/Kg for total sulfonamides in milk [5].

Our results demonstrate that our COF-SERS combinative strategy enables the detection and differentiation of at least sulfamethoxazole, sulfathiazole and sulfapyridine (also in mixture) at 0.1 µg/L. This is achieved through spectral pre-processing, followed by artificial intelligence (AI)-driven analysis. Combining material-enhanced SERS performance and AI, this platform represents a promising tool for on-site antibiotic detection with high sensitivity and selectivity.

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ACKNOWLEDGEMENTS

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Integrated SERS-based microdroplet platform for antibiotics detection in water

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The detection of antibiotics in marine environments is a growing concern, as their presence can lead to environmental imbalances and contribute to antibiotic resistance [1]. In our study, we explore the use of surface-enhanced Raman scattering (SERS) as a promising analytical tool for detecting these contaminants owing to its high selectivity, being one of the most sensitive techniques currently available. Additionally, SERS has other advantages that hold particular significance in sensor development, including reduced time requirements and the potential for in-situ measurements, which are important for real-time water monitoring [2].

The analytical applicability of SERS is intricately linked to the fabrication of highly efficient SERS substrates. In this work, a series of hybrid composites were developed by integrating covalent organic frameworks (COFs) with gold nanoparticles (GNPs). COFs are crystalline, high-surface-area materials that can act as chemoreceptors for the antibiotics. When attached to a plasmonic surface such as GNPs, these highly porous hybrid composites facilitate the concentration of molecules near the plasmonic surface, generating a unique SERS fingerprint spectrum that enables the antibiotic detection [3].

We integrate the highly sensitive SERS detection enabled by the composites in a microdroplet-sensing platform, which facilitates an automated, reproducible and ultra-fast multiplexed detection in nanoliter volumes [4]. First, we evaluated the encapsulation and stability of the hybrid composite inside the microdroplets, which were fabricated using a T-junction microfluidic device paired with a mixer to enhance the interaction between the composite and the antibiotics using an in-house developed detection microfluidic device. The antibiotic detection was carried out using a portable Raman system with a 785 nm laser line. The initial results indicate that this approach shows great potential for developing an autonomous, in-situ sensor with high sensitivity for monitoring antibiotics in water systems.

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Improving the electrocatalytic behaviour of ZIF-67 nanomaterials via fast eco-friendly cold plasma treatments

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A3_2, U2 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

Coordination polymers, known as metal-organic frameworks (MOFs), exhibit remarkable properties such as high crystallinity, well-defined porosity, large surface areas, and great structural and compositional versatility. Moreover, the metal nodes forming the 3D frameworks —together with the organic linkers— are homogeneously distributed at the nanometric scale, providing numerous active sites for (electro)catalysis in various energy-related processes. However, these promising nanomaterials face several challenges, including limited accessibility to active sites, low electrical conductivity, and moderate stability under working conditions. In this context, advanced cold plasma treatments (highly reactive, non-equilibrium systems formed by the partial ionization of a gas or gas mixture) emerge as a powerful and environmentally friendly tool to enhance the electrocatalytic performance of MOFs. These treatments enable precise modifications of their nanostructures—through functionalization, nanoparticle formation, defect engineering, etc.—with a high degree of control over the extent of these alterations. Recently, our research group has begun exploring the compositional and structural modification of ZIF-67-based materials (a MOF composed of Co^{2+} ions and 2-methylimidazole ligands) using plasmas derived from different precursors. We have observed that short treatments —on the order of minutes— can significantly improve the electrocatalytic activity of these nanomaterials toward the oxygen evolution reaction (OER), a key process for green hydrogen production in electrolyzer devices.

Exploring CO₂ capture dynamics in CALF-20 using positron annihilation lifetime spectroscopy

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A3_3, U2 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Reducing atmospheric CO₂ levels is crucial to mitigate climate change. This study investigates the effectiveness of the zinc-based metal-organic framework CALF-20 (Zn) for CO₂ capture across varying temperatures. The unique structure of CALF-20 allows it to maintain high CO₂ selectivity and efficiency in a broad range of temperatures.

Positron annihilation lifetime spectroscopy (PALS) played a crucial role in this research, providing detailed insights into the CO₂ adsorption dynamics within CALF-20.

The variable temperature PALS experiments demonstrate that CO₂ molecules are spatially localized within the CALF-20 cages, leaving temperature- and pressure-dependent gaps between them. PALS results indicate that CO₂ initially spreads across cage centers, 1D chains, and ultimately adheres to pore walls. Interestingly, positronium intensity, which increases with CO₂ adsorption pressure, closely aligns with the Langmuir-Freundlich isotherm and reflects gas uptake behaviour.

These findings highlight CALF-20's potential for effective CO₂ capture and storage, demonstrating its capability to perform well across a range of temperatures. The study underscores the vital role of PALS in investigating and understanding the structural and functional characteristics of CALF-20 for CO₂ capture applications

Optimizing Electrospun Ceramic Fibers: A Direct Aqueous Approach for Cost-Effective Production

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Optimizing the production of electrospun ceramic fibers is a relevant challenge in materials science, driven by the synergy between the intrinsic properties of ceramics and the unique advantages offered by electrospun fiber morphology. That is, high thermal stability, mechanical robustness, chemical resistance, high surface area, porosity and high potential for selective functionalization make electrospun ceramic fibers highly versatile and valuable at industrial level, for cutting-edge applications such as energy conversion, aerospace, heterogeneous catalysis, filtration and more.

Traditionally, a sol-gel approach has been employed for electrospinning ceramic fibers, offering precise control over chemical composition and structural homogeneity while allowing for the incorporation of dopants or additives to tailor material properties. However, it has several disadvantages that directly impacts its practicality and efficiency, that being expensive precursors and large volumes of organic solvents required, which can further escalate costs and raise environmental concerns.

Direct electrospinning of commercial ceramic powder aqueous suspensions represents a straightforward route, with fewer steps and less chemical handling compared with sol-gel electrospinning-based approach. This route is especially promising for industrial applications where simplicity, cost-effectiveness and scalability are priorities. For this, an example system of commercially available Al₂O₃ powder is presented, providing an in-depth discussion on the colloidal suspension details and resulting fiber characteristics and the intended applications.

Development of Sustainable and Functional Materials from Textile Waste for the Circular Economy

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The textile industry is one of the main culprits of environmental pollution, generating around one million tons of textile waste per year in Spain, of which more than 90% corresponds to used clothing. This problem, aggravated by the rise of fast fashion and the fact that only between 10% and 12% of this waste is recycled, poses a critical challenge: reusing textile waste to mitigate its ecological impact. In view of these data, a new European directive on textile recycling will be issued by 2025.

In parallel, there is a growing need to develop sustainable and functional materials that contribute to a circular economy model, where waste is transformed into valuable resources.

This work focuses on the design of a composite material with a biodegradable polymeric matrix reinforced with recycled textile fibers. The objective is to develop an optimal material with conditions that allow its application in an industrial design product, with the aim of reintroducing it into the market. Thus, the aim is to promote the circular economy.

Over the course of a year and a half of research, multiple tests have been carried out to optimize the mechanical, structural and functional properties of this new material. In the initial stages, the focus was on the search for organic materials that would improve its characteristics. Subsequently, tests were carried out to test their strength, durability and impermeability. Thus, it was possible to select a small group of samples, since they obtained the best results in the different tests.

Currently, the study has been focusing on the incorporation of conductivity in the material. For this purpose, different options have been proposed and are being tested and analyzed. In addition, by incorporating graphene nanoplatelets in varying concentrations (0%-3%), it was possible to provide the material with conductive properties. Experimental tests showed that an optimum content of 2% in nanoplatelets allows electrical resistivity values of 1.2 k Ω -mm to be achieved, which is suitable for industrial applications. This opens up a whole range of new possibilities for using the material in a real application: a product to be introduced into the current market.

4D Printing of a Transformable Exoskeleton Protector using Shape Memory Polymer

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A4_1, Z2 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

In this study, a 4D printing technology was developed to fabricate a transformable exoskeleton protector using a shape memory polymer. The proposed approach aimed to meet specific requirements: high elongation, thermo-responsive deformation capability, and shape-recovery characteristics. To achieve thermo-responsive deformation, a polyurethane (TPU)-based shape memory polymer with a glass transition temperature of 55°C was employed. The exoskeleton protector was designed using a re-entrant honeycomb structure with dimensions of 70 × 40 × 2 mm, capable of elongating up to 70%. The exoskeleton protector was additively manufactured using an extrusion-type 3D printer. Tensile elongation and shape-recovery behaviours were evaluated under varying temperature conditions, with the protector heated in a 60°C water bath prior to elongation. Comparative tensile tests with other porous structures, including square and circular hole arrays, revealed that the re-entrant structure achieved the highest elongation (up to 70%) compared to other structures (approximately 20%), confirming its suitability as a transformable exoskeleton protector. This high elongation provides sufficient length to wrap around half of an adult's wrist, making it an effective protective structure. Furthermore, the deformed protector exhibited excellent shape recovery, with a recovery ratio of 98%. Once recovered, the protector returned to its original compact dimensions of 70 × 40 × 2 mm. This slim profile, combined with its shape transformation capability, makes it highly portable and convenient for use as a practical exoskeleton protector.

Next generation of stimuli responsive materials for 4D macro- and microprinting

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A4_1, Z2 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Emerging in the 1980s 3D printing has undergone a prosperous development, enriching multiple fields in academia and industry, increasing its societal impact as high-tech 3D fabrication method continuously. Beside extension of the available technological toolset, one key breakthrough was the conceptualization of 4D printing in 2013. 4D printing describes the implementation of time as fourth dimension to standard 3D printing allowing the generation of smart 4D structures. Such 4D objects can change their shape or material properties in controlled fashion upon exposure to a suitable stimulus such as light, temperature or pH, etc, contrasting traditional 3D printing that produces static structures. Due to its inherently dynamic and functional characteristics 4D printing has established as ideal fabrication approach for smart and dynamic applications in advanced fields such as soft robotics, smart optics and life science among others.[1] Basis for the success of 4D printing in the last decade was the large progress made in smart ink design enriching the 4D material library. However, the current set of materials for 4D printing is still limited in several aspects: The versatility and extent of response respectively actuation, the adjustability of material properties postprinting, as well as aspects such as biocompatibility highly relevant for application in life sciences.

Our main focus is to tackle these challenges by designing and developing new smart materials for light-based 4D printing at the macro- and microscale. For this purpose, we employ our knowledge as organic and polymer chemists to introduce new functionalities and smart characteristics by chemical engineering of materials at the molecular level. Exemplary we investigated new polymeric architectures equipped with functional units such as bottlebrush polymers, or linear prepolymers according to their printability and extended their range and quality of actuation. By implementation of dynamic covalent chemistry into our printed structure at the macro- and microscale we were able to show highly dynamic features by reversible mechanical property adjustment via simple postprinting protocols.[2],[3] Furthermore, we succeeded in the design of bioinks based on proteins such as collagen achieving new printable 4D biomaterials for the next generation of smart devices in life sciences.[4]

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Comparative Analysis of NiTi SMAs Powder Produced via Ultrasonic Atomization: Virgin Powder vs. Re-Powder from 3D Printed Parts

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The selection and management of feedstock have become increasingly critical to the economic efficacy of the entire process as additive manufacturing (AM) technologies have advanced at a rapid rate. The repurposing of discarded powders and scrap printed parts is of considerable industrial interest because of the recycle, particularly as the adoption of 3D printing continues to grow. In this study, the feasibility of recycling scrap NiTi shape memory alloy (SMA) parts that were produced through laser powder bed fusion (LPBF) has been examined in order to optimize material utilization and decrease expenses. The scrap parts were remelted using the ultrasonic atomization Re-Powder Amazemet machine, and fine, homogeneous powders with particle sizes below 75 μm were produced using an ultrasonic sonotrode operating at 20 kHz, which is appropriate for LPBF applications. Carbon and oxygen contamination were monitored and controlled at all stages of the process, from the initial feedstock to the melted ingot and final powder, to guarantee process integrity, in accordance with ASTM F3049 standard. The final powder exhibited properties that were analogous to the initial feed material, as evidenced by detailed analyses of the powder, including microstructural characterization, martensite-to-austenite transformation hysteresis, and chemical composition. These findings underscore the potential of ultrasonic atomization to facilitate the efficient recycling of waste, providing a promising solution to improve the economic and sustainable viability of AM processes.

Pioneering NiTi-Cu Shape Memory Alloys via Binder Jetting Additive Manufacturing: Process Optimization and Microstructural Refinement

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A4_3, Z2 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

This study introduces a novel application of Binder Jetting Additive Manufacturing (BJAM) to produce NiTi-Cu shape memory alloys (SMAs), marking the first exploration of this method for such alloys. Fine pre-alloyed NiTi and pure Cu powders (<20 µm) were utilized to fabricate components, with the process parameters: temperature, Cu percentage, and sintering time carefully optimized to achieve high-performance SMAs. The parts were sintered in a controlled furnace under an inert atmosphere to minimize contamination and enhance microstructural integrity. The investigation revealed that process optimization significantly influenced the resulting microstructure, minimizing defects and ensuring homogeneity. The study also examined the impact of Cu content and sintering conditions on phase transformations, transformation temperatures, and temperature hysteresis. This pioneering work demonstrates the potential of BJAM as an effective and scalable method for producing NiTi-Cu SMAs with tailored properties, offering a new avenue for additive manufacturing of functional shape memory alloys with minimal defects and superior performance characteristics.

Development of Bio-Based Photocurable Resins for High-Resolution 3D Printing with the Incorporation of Quantum Dots for Advanced Photonic Applications

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A4_3, Z2 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Vat photopolymerization-based 3D printing, such as stereolithography (SLA), has become an essential technique for manufacturing complex structures with high resolution. However, the reliance on photocurable resins derived from petrochemical-based (meth)acrylates poses significant challenges in terms of sustainability and toxicity. In this context, research has focused on developing sustainable alternatives using bio-based monomers.

This study presents the synthesis and characterization of novel photocurable resins developed from natural derivatives, with a significantly higher bio-based content than previously reported values for vat photopolymerization. Structural (FTIR, NMR), thermal (DSC, TGA), and mechanical (tensile, flexural) analyses were performed to characterize the properties of the obtained resins. The 3D printing capability of the resins was evaluated by fabricating test objects using a stereolithography (SLA) apparatus. The mechanical properties of the printed objects were analyzed and compared with those of the commercial resins. The synthesized bio-based photocurable resins demonstrated mechanical and thermal properties comparable to those of commercial resins used in stereolithography 3D printing.

Additionally, within the framework of the National QD-PAVANE project, the incorporation of quantum dots (QDs) into these bio-based resins was explored for photonic and optoelectronic applications in the visible and infrared spectrum. QDs, known for their unique tunable emission and absorption properties, offer the possibility of developing functionalized materials with adaptable optical responses. The combination of bio-based resins with QDs expands the range of applications in detection, lighting, and energy devices, promoting sustainable solutions in cutting-edge technologies. The incorporation of quantum dots (QDs) into bio-based resins allowed for the modulation of their optical properties, opening up new possibilities for applications in photonic and optoelectronic devices. A significant effect of the QDs on the light emission and absorption of the resins was observed, suggesting their potential for the development of sustainable sensors, lighting devices, and solar cells. This study demonstrates the potential of bio-based photocurable resins as a sustainable alternative to conventional resins in high-resolution 3D printing. The incorporation of quantum dots (QDs) into these resins expands their functionalities and opens new perspectives in the fields of photonics and optoelectronics. This approach promotes the development of advanced materials and more sustainable manufacturing technologies.

Exploring the Influence of Stimuli on 4D Printed Components: A taxonomy of Stimulus, Smart Materials and Transformation Effects

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Exploring the Influence of Stimuli on 4D Printed Components: A taxonomy of Stimulus, Smart Materials and Transformation Effects

Jiayue Qin

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Abstract

4D printing is a significant advancement in additive manufacturing, enabling dynamic, self-actuating structures through stimuli-responsive materials. While widely explored in engineering and biomedical fields, its application in fashion and footwear remains underdeveloped due to the challenges of integrating material science with design aesthetics and functionality. The key gaps include the absence of accessible design frameworks for non-technical designers and a comprehensive taxonomy linking stimuli, smart materials, and transformation effects. These limitations hinder informed decision-making in material selection, transformation predictability, and adaptive functionality in design. This study addresses these challenges by investigating the influence of thermal, humidity, light, pH, electric, magnetic, and mechanical stress on 4D-printed components, developing a structured design application guide to facilitate creative industry adoption.

This study follows a qualitative research approach within the Design Research Methodology, progressing from literature review to experimental studies and expert interviews. The literature review establishes an initial classification of stimuli, revealing that thermal and humidity stimuli induce gradual, reversible transformations, light and pH stimuli allow localized or selective changes, and mechanical, magnetic, and electric stimuli enable rapid, on-demand actuation. Furthermore, this research introduces a new classification framework integrating stimuli, smart materials, and their transformation effects. This taxonomy forms the basis of the proposed design application guide, structured using the Technology Acceptance Model, which categorizes stimuli and materials based on perceived ease of implementation and usefulness in creative design, ensuring accessibility for non-technical designers. To refine and validate the guide, experimental studies will investigate how different sources and combinations of stimuli, along with printing techniques, influence material responses. Additionally, semi-structured interviews with experts in 4D printing and fashion design will assess the guide's practicality, feasibility, and clarity. Experts will apply the guideline in design and provide feedback to enhance its usability.

This study contributes to the broader adoption of 4D printing in the fashion industry by offering (1) a categorized taxonomy of stimuli-responsive materials, (2) practical design methodologies tailored for creative applications, and (3) a conceptual framework promoting interdisciplinary collaboration. The proposed guide provides structured insights into material selection, deformation simulation, and printing workflows, enabling designers to create garments and footwear that dynamically adapt to environmental conditions.

Transforming Jewelry Design: Shape Memory Polymers and the Advances of three- and four-dimensional Printing

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A4_2, Z2 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Shape memory polymers (SMPs) belong to the class of smart materials¹. Thermoresponsive SMPs can retain a temporary shape after thermomechanical treatment, also known as programming, until they are heated above their switching temperature, whereupon they largely recover the original shape. Among the various SMPs, thermoplastic polyurethanes (TPUs) have proven to be promising material candidates for the development of new applications due to their modifiable mechanical and thermal properties. Researchers have used additive manufacturing (AM) to process TPUs because it fulfills the criteria of design freedom and cost efficiency for prototyping in equal measure, so that the hurdles for small series production are low. This makes the technology attractive in new application contexts, e.g. in the jewelry industry.

In the field of jewelry design with smart materials, first steps were taken by the development of shape memory alloy-based rings that open to reveal embedded gemstones² and SMP flower rings that can move dynamically and are produced by digital light processing³. Basically, AM of objects with good structural resolution is essential to manufacture jewelry from SMP. In this context, fused filament fabrication (FFF) is a promising platform to print filigree structures, e.g. from polyester urethane⁴.

For this contribution, a polyester urethane characterized by shape memory properties was synthesized and compounded with dye particles to improve its optical appearance. The obtained filament was used to produce demonstrators for jewelry in the form of earrings and bracelets using the FFF process. The pieces of jewelry were modified by programming so that they were temporarily stabilized in a new shape and could later be switched back to their original shape. In a further approach, a polyether urethane was developed and employed to carry out four-dimensional printing via FFF, a method which allows manufacturing thermoresponsive objects without the need of programming⁵. This time, the investigation of shrinkage effects was the primary focus against the background of the transformation of the jewelry into another shape. In any case, the additively manufactured jewelry was evaluated from a functionality point of view and against the background of sustainability aspects.

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In-depth Mechanism of Corrosion and Mechanical behavior of Ni-rich NiTi Alloys through Optimized Heat Treatment and Phase Transformation

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A4_3, Z2 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

NiTi-based SMAs are widely employed in biomedical applications owing to their distinct properties, such as shape memory effect (SME) and pseudoelastic effect (PE), resulting in extraordinary shape recoverability. Along with high corrosion resistance, impressive biocompatibility plays a significant role. The present study investigates the in-depth mechanism of corrosion and mechanical behavior of a Ni-rich NiTi alloy (50.80 at% Ni) under different heat treatment conditions. The as-received alloy is initially solution treated at 850 °C for 2 h (ST) and subsequently aged at either (i) 350 °C for 2 h, named as HT_1, or (ii) 550 °C for 2 h, named HT_2. Primarily, equiaxed grains of size of $\sim 35 \pm 4.37 \mu\text{m}$ are noted to form in both the aged alloy specimens. Transmission electron microscopy analysis confirms the presence of the B2 phase, R-phase, and Ni-rich (Ni₄Ti₃) precipitates in them. However, the volume fraction of these phases and size of precipitates are different in the aged alloys. These microstructural modifications attained through thermal treatment are noted to influence the corresponding corrosion and mechanical properties of the NiTi alloys. Among the aged conditions, HT_2 alloy is effective in altering the microstructure and improving the corrosion resistance of NiTi alloy in physiological solutions like Hank's solution at 37 °C. Notably, after 30 days of long-term immersion, HT_2 alloy develops another Ca-P layer along with a uniform TiO₂ oxide layer, which is beneficial for the cell growth during immersion period. In contrast HT_1 alloy forms a thin and inhomogeneous oxide layer, which leads to pitting corrosion over time. Furthermore, mechanical characterization reveals that HT_2 alloy exhibits optimized tensile properties with respect to the solutionized alloy. Most importantly, HT_2 alloy exhibits larger transformation strain plateau of 2.5 % and lower critical transformation stress ($377 \pm 9 \text{ MPa}$) for stress-induced martensite transformation (SIMT) as compared to that for ST and HT_1 alloys. Careful scrutiny of the tensile deformation behaviour, analysed via digital image correlation. Interestingly, it reveals that SIMT initiates and extends in an inhomogeneous and localized manner through Lüders-like band. Overall, such improved mechanical, functional, and corrosion characteristics of NiTi alloy in the HT_2 condition are of particular significance for its biomedical application.

key words: SMA, Ni-rich precipitates, corrosion resistance, Lüders band formation

A new generation of bio-renewable vitrimer based on vanillin

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A4_2, Z2 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

The development of sustainable polymers has become a key focus in materials science, with a strong emphasis on creating recyclable, self-healing, and high-performance alternatives to conventional plastics. Vanillin, a bio-derived aromatic compound, has emerged as a promising building block for polymeric materials due to its renewable nature, structural rigidity, and functional versatility. Among the various dynamic covalent networks, the category of vitrimer stands out. In fact, vitrimers possess the unique ability to undergo network rearrangement through associative bond exchange reactions while maintaining overall crosslink density. This characteristic allows vitrimers to combine the durability of thermosets with the re-processability of thermoplastics, distinguishing them from traditional polymer classes. With its aldehyde functionality, vanillin serves as an excellent precursor for imine formation, reacting with amine compounds to create a stable yet adaptable polymer network. This imine reversible bond allows the material to exhibit self-healing capabilities and recyclability without compromising mechanical strength. Therefore, vanillin-based vitrimers utilizing imine chemistry present a compelling alternative for a wide range of applications.

This work carefully investigated a vanillin-based imine vitrimer with various techniques. After successfully confirming the vanillin-based building block formation with Fourier Transform Infrared Spectroscopy (FTIR) and Nuclear Magnetic Resonance (NMR) ; the kinetic of the reaction was investigated by real-time rheology test. Subsequently, Differential Scanning Calorimetry (DSC), Dynamic mechanical thermal analysis (DMTA) and thermogravimetric analysis (TGA) were performed to determine the glass transition temperature (T_g) and thermal stability of the new crosslinked network, providing insights into the material's thermal behaviour. Rheological analyses were conducted to evaluate the viscoelastic properties and the dynamic exchangeability of imine bonds, confirming the vitrimer nature of the material. Furthermore, the mechanical strength, flexibility, and toughness of the polymer were investigated by tensile test.

Finally, self-healing and chemical recyclability tests, such as scratch recovery and different reprocessing cycles, demonstrate the material's durability and sustainable potential.

In conclusion, vanillin-based vitrimers utilizing imine chemistry represent an innovative and eco-friendly approach to developing a new class of sustainable polymer materials. Further optimization of these materials can unlock new possibilities for next-generation sustainable applications in various industries.

Improving the thermal hysteresis of NiTi Melt-spun ribbons for faster actuation with the Cu addition and optimized annealing time.

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A4_3, Z2 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

NiTi shape memory alloys (SMA) have unique properties that make them very suitable for various electrical actuator and sensor applications. These attributes include the shape memory effect and superelasticity. It is essential to enhance their response to attain faster actuation. Investigating the phase transformation properties of NiTi shape memory alloy (SMA) is crucial for this objective. This study compares the transformation temperatures and thermal hysteresis of Ni50Ti50 shape memory alloy with Ni45Ti50Cu5 shape memory alloy in ribbon form. The ribbons are manufactured using the melt spinning technique at two distinct velocities: 20 m/s and 45 m/s. They undergo annealing at 470 °C for one hour. Analytical methods, including XRD, DSC, SEM, and EDX, have verified the existence of Ni₄Ti₃-Cu precipitates in all specimens. The DSC results indicate that the incorporation of 5 at. % Cu alloying partially alleviates multistep phase change in the R45 sample. A slight reduction in *M_s* temperature and *H_t* values is noted with the incorporation of Cu and subsequent annealing treatment in both R20 and R45. This research offers significant insights into the impact of Cu addition and an appropriate annealing treatment on the transformation temperatures of NiTi shape memory alloys.

Phase and microstructure formation of α'' Ti-Nb: Laser powder bed fusion (LPBF) vs. single track laser melting

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A4_3, Z2 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Titanium alloys containing moderate amounts of β stabilizers (e.g. Nb, Ta) exhibit remarkable functional properties including shape memory effect and tailorable thermal expansion, which are rooted on the orthorhombic martensite α'' . Conventional fabrication of those alloys involves classical ingot metallurgy, thermomechanical processing, and shaping by forming and subtractive methods, limiting geometric freedom and restricting application specific design. In contrast, additive manufacturing techniques like laser powder bed fusion (LPBF) combine the benefits of (near-) net-shape production of complex parts from Ti alloys with the intrinsic potential to locally tailor microstructures to the requirements dictated by the end application. In addition, due to its characteristic rapid cooling rates, LPBF favours the formation of metastable phases as-built, such as hexagonal martensite α' in β stabilizer-lean parts, and metastable β phase in β stabilizer-rich parts. LPBF may also allow controlled formation of orthorhombic martensite α'' – which is an open question that needs systematic validation and exploration.

However, the limited availability and relatively high cost of commercially pre-alloyed, atomized powders is a significant challenge for the widespread production of LPBF α'' parts. Taking Ti-Nb as example, this work thus explores the fabrication of α'' Ti-Nb via LPBF from pre-alloyed Ti-29Nb powders, prepared by mechanical alloying of elemental Ti and Nb powders. The powders were characterized for homogeneity, particle size, and phase constitution, and subsequently consolidated into cuboids via LPBF. Various combinations of laser power and scan speed were tested to study their effects on as-built microstructures and porosity. To isolate the influence of the layerwise build process on the resulting phases and microstructures, experiments will be discussed, for which α'' martensitic substrates were remelted along single laser tracks. Single track remelting revealed different microstructures depending on the melt pool location, including planar growth at the roots and cellular-dendritic growth near the surface.

The results of this study suggest that proper selection of alloy content and LPBF parameters can lead to α'' martensitic Ti-Nb parts for functional 3D-printed components.

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A sustainable approach to design electrode in structural battery composite applications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

A simple, cost-effective, scalable and increasingly efficient structural battery composite (SBC) is under development in our group now. To follow through this innovation aspects, a sustainable anode material for SBC is developed and demonstrated. A low-cost, abundant and most importantly the raw material sourced from a spent brewery waste (draff) that is used to synthesise activated carbon at relatively low temperature (≤ 500 °C) under pyrolytic environment and without using any harsh and toxic chemicals. These draff derived engineered activated carbons (DEACs) are characterised by different physical characterisation techniques such as XRD and Raman spectra which revealed the mixed amorphous and graphitic crystalline nature of the DEACs whereas FE-SEM and BET analysis results highlighted the high porous nature of DEACs. The DEACs anode further showed a promising rate capability and an excellent reversible specific capacity of 43-236 mAh g⁻¹ at 0.2 A g⁻¹ current density after 100 cycles. The sample synthesised at 500 °C using 1:4 pyrolysed C: KOH showed the highest quality and demonstrates superior electrochemical performance as anode material in a sodium ion battery coin cell with 87% capacity retention over 100 cycles and >99% coulombic efficiency. Hence, this work will promote the development of sustainable SBC utilising the low cost, green and high-performance electrode produced from the waste stream.

Multi-functional Rotating triangular metamaterial for vibration isolation and energy harvesting applications

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A4_4, Z2 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

This work presents novel multi-functional rotating triangular metamaterials designed for simultaneous vibration isolation and electricity generation. The core innovation lies in the incorporation of rotating triangular joints, which introduce bending deformations in the cell walls under compressive loads. This rotational mechanism reduces the structural stiffness from a positive value to a quasi-zero stiffness (QZS) regime, effectively lowering the system's natural frequency and enhancing its ability to isolate external vibrations. The deformation mechanisms within the metamaterial involve bending, compression, and tension of cell walls, each playing a crucial role in energy harvesting. The integration of piezoelectric materials (PZTs) on the tensioned walls enables efficient electricity generation due to applied tensile loads, while the attachment of piezo benders (PBs) on bending-dominant regions further enhances energy conversion efficiency. By leveraging these synergistic mechanical and electromechanical properties, the proposed structure provides a lightweight, efficient, and scalable solution for vibration mitigation and energy harvesting applications at the same time. Potential applications include automotive systems, where the metamaterial can be embedded in vehicle suspension components, car seats, or chassis structures to dampen external excitations encountered during driving. The harvested energy can be used to power small electronic systems, enhancing their overall energy efficiency and sustainability. Beyond automotive applications, these multi-functional metamaterials hold promise for use in aerospace structures, civil infrastructure, and wearable technologies, where vibration isolation and self-powered sensing are critical.

Effect of printed material stiffness on the curvature of 4D textiles: experimental and computational analysis

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A4_1, Z2 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

4D textiles are a unique class of 4D printed materials, i.e. 3D printed materials capable of shapeshifting after printing. They are created by printing 2D structures onto elastically pre-tensioned fabrics, enabling them to transform from flat systems into 3D objects. This transition occurs either through a rapid self-shaping process when the tension on the fabric is released, or through a delayed, remote actuation triggered by a thermal stimulus. The resulting objects typically assume curved shapes, whose curvature is dictated by the mechanical equilibrium between the textile's recovery stress and the stiffness of the printed structure.

This study investigates how the final curvature is influenced by the stiffness of printed elements and the pre-stretch of the textile. An FDM printer was used to prepare the specimens by printing on Lycra fabric both simple and complex geometries (a longitudinal bar on a monoaxially stretched textile, and single or multiple star-shaped patterns on biaxially stretched textiles). A systematic variation of the realization parameters allowed to produce various states of curvature, from a flat state where curvature is hindered, through more regular curvatures, to multi-stable buckling conditions. While Lycra was selected for its compliance (Young's modulus, $E \sim 1$ MPa) and high stretchability, the flexural stiffness of printed elements was modulated by varying their thickness and using materials with different Young's moduli: i) PLA ($E \sim 10^3$ MPa); ii) TPE ($E \sim 10$ MPa); iii) PLA later heated above its T_g to reduce the modulus to a value similar to that of the textile, while also investigating shapeshifting via thermal actuation.

The curvature and local strain evolution during shape transformation was analyzed using a stereoscopic digital image correlation (DIC) system, to explore the relationship between strain fields and the 4D textiles' structural and kinematic behavior. This helped provide key data for developing and validating analytical models to predict the final shape of both simple and complex structures.

A finite element model was created, calibrating it on the specific properties of the various constituents, and attempting to describe the whole 4D textile history, from textile stretching, through the printing phase, to the shape transformation upon stress release. The model was shown to be capable of accurately reproducing the behavior of 4D textiles, especially regarding the shape and the displacement of the curved elements and the occurrence of multi-stability, although some discrepancies also emerged, which could be addressed by implementing the model with better defined parameters.

Carbon-Nanotubes Embedded Strain Sensors for Monitoring of Structural Carbon Fibre Composites

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A4_4, Z2 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Carbon nanotubes (CNTs) offer a promising piezoresistive sensing approach and have been extensively investigated as strain sensors in wearables, healthcare applications, and human-machine interaction devices. This study presents the development of piezoresistive strain sensors based on CNT yarns for structural applications.

Typically, CNT-based sensors consist of discrete CNT fillers embedded in elastomeric polymers, designed to accommodate a broad range of deformations—often exceeding the strain levels relevant to aerospace structural materials, which are typically below 2000 microstrain. While these sensors have demonstrated the capability to detect low strains, they incorporate epoxy or elastomeric polymers, such as thermoplastic polyurethane, which exhibit lower thermal stability than the high-performance polyetherketoneketone (PEKK) family.

In contrast, continuous ensembles of highly aligned CNTs joined together into macroscopic fibres or yarns could help eliminate the associated problems by taking advantage of their hierarchical structure and properties not attainable to discrete CNTs. CNT yarns exhibit piezoresistive behaviour and have already been employed in various flexible materials, including self-recoverable artificial muscles, soft bioelectronic sensors, and smart textiles. The piezoresistivity mechanism in CNT fibres differs from that of percolated nanocarbon networks formed by discrete nanoparticles.

The sensors developed in this study consist of PEKK-coated thermoplastic filaments reinforced with continuous CNT yarns, fully integrated into structural thermoplastic-matrix carbon fibre-reinforced laminates. The PEKK coating enhances the piezoresistive behaviour of the CNT yarns by improving internal stress transfer. When embedded in a laminate, the CNT sensors exhibited a gauge factor of up to 10 for strains of 2000 microstrain under both tensile and compressive loading.

The CNT sensors were calibrated and compared with commercial strain gauges at the coupon level through three- and four-point bending tests conducted at room temperature. The analysis was subsequently extended across a range of temperatures to evaluate the feasibility of the proposed sensors under operational conditions. Additionally, high-cycle fatigue tests demonstrated no degradation in sensing performance, confirming the sensors' suitability for long-term structural applications.

Finally, the sensor's ability to detect damage was assessed by subjecting the test specimens to low-speed impact. A change in signal behaviour was observed, enabling clear damage identification while maintaining a proportional relationship between the sensor signal and the experienced deformation.

Bioinspired approach to autonomous deployment of 4D-printed structures for space applications

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A4_1, Z2 Room (Level -3), septembre 17, 2025, 10:30 - 13:10

The pursuit of advanced space exploration requires innovative solutions that reconcile minimal stowage volume with rapid and reliable deployment. Traditional deployable structures often rely on intricate mechanical systems involving multiple moving parts, which are not only prone to mechanical failure but also often present high energy expenditure, making them ill-suited for missions where energy conservation is paramount. In this work, we propose potential solutions that harness adaptive materials produced via 4D printing—a process integrating time-dependent functionality into 3D-printed structures—to achieve autonomous and rapid deployment upon external stimuli, such as temperature variations.

Our design leverages shape-memory polymers (SMPs), known to be able to store and release elastic energy in response to thermal stimuli [van Manen, 2017]. Advances in additive manufacturing have enabled precise control over material composition and internal architecture, allowing the anisotropic properties of the resulting structure to be tailored in order to achieve the desired deployment kinetics [Jourdan, 2023]. Upon exposure to a temperature change, the structure transitions from a compact, stowed configuration to a fully deployed state. This mechanism eliminates the need for additional actuators or energy-consuming systems, thereby reducing the complexity and potential weak points inherent in conventional designs. This work aims to present concepts leading to structures that can reliably and rapidly deploy, with potential for applications where both speed and energy efficiency are critical.

The inspiration for our study is drawn from natural organisms that have achieved efficient passive deployment strategies with millions of years of evolution. For instance, the rapid opening of seed pods [Hofuis, 2016] and the unfolding of insect wings [Phan, 2024] serve as models for energy-efficient, self-actuating systems. These biological mechanisms typically exploit stored elastic energy and material anisotropy to achieve swift morphological changes without active control, and provide solutions that can be abstracted and implemented in passive deployable architectures for space applications that benefit from nature's optimization.

This work builds upon progress in both adaptive materials [Le Duigou, 2025] and bioinspired design [Poppinga, 2010], demonstrating that 4D printing can produce structures that are not only compact during launch but also capable of rapid, autonomous deployment. By combining insights from materials science and biological systems, this study is intended as a step towards the development of deployable structures that meet the stringent requirements of modern space exploration.

Oxidation resistance of self healing carbon ceramic nanocomposites

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Carbon materials are highly attractive for aerospace applications due to their exceptional properties, such as high thermal stability, low thermal expansion coefficient, excellent electrical conductivity, and low density. However, their use in this field is limited by their susceptibility to combustion reactions at temperatures above 500°C. Therefore, improving their oxidation resistance is crucial to ensure their viability in extreme aerospace environments.

To address this challenge, carbon materials reinforced with ceramic nanoparticles, such as silicon carbide (SiC), zirconium carbide (ZrC), and titanium carbide (TiC), as well as submicrometric particles of boron carbide (B₄C), Tantalum carbide (TaC) and hafnium carbide (HfC), have been developed. These composites enable the creation of self-sintering carbon materials with self-healing properties during oxidation.

During oxidation, the carbides oxidize to form a protective glassy layer that acts as a barrier against further oxidation of the carbon. This layer primarily consists of boron oxide (B₂O₃) and silicon oxide (SiO₂), forming a borosilicate glass. The introduction of metal carbides not only reduces the evaporation of boron oxide but also enhances the stability of the protective layer, leading to improved oxidation resistance. Additionally, these additives improve the wettability and dispersion of carbon, optimizing the properties of the composite material.

To study the behaviour of these materials, thermogravimetric analysis (TGA) was conducted in air up to 1600°C to observe the weight loss of the samples. Isothermal oxidation tests were also performed at different time intervals, exposing the samples to temperatures as high as 1500°C. These tests allowed for the evaluation of thermal stability and the effectiveness of the protective layer formed.

Samples have been characterised by X-Ray Diffraction (XRD) to identify the crystalline phases present in original, Stereomicroscopy and Scanning Electron Microscopy (SEM), to obtain a detailed view of the surface and the integrity dispersion of nanoparticles and sintering of the material. The protective layer generated during oxidation was characterized using techniques, including Scanning Electron Microscopy (SEM), to analyse the morphology and structure of the layer and XRD.

The incorporation of ceramic nanoparticles into carbon materials represents a promising strategy for enhancing their oxidation resistance in aerospace applications. The formation of a protective glassy layer, combined with the stabilization provided by metal carbides, not only increases the material's durability but also optimizes its performance under extreme conditions. These advancements open new possibilities for the use of carbon materials in the aerospace industry, where thermal resistance and stability are critical.

Elastocaloric effect on laser-sintered thermoplastic polyurethanes

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A4_4, Z2 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Refrigeration has traditionally played a crucial role in several industrial sectors. Almost all current refrigeration systems are based on vapor-compression refrigeration, where a fluid refrigerant evaporates and condenses. Although vapour-compression has been the dominant technology, there is an increasing concern about the primary global warming and environmental impact from air-conditioning and refrigeration systems. It is thus paramount to investigate new plausible alternatives with similar or higher efficiencies than the current refrigeration cycles. In the last few years, some solid-state refrigeration techniques have been analyzed as potential candidates to replace the traditional refrigeration systems. Solid-state refrigeration through elastocaloric cooling leverages the elastocaloric effect (eCE), where certain materials exhibit temperature changes under mechanical stress due to reversible phase transformations.

Although there is a notorious scientific effort in the field of caloric materials, not all materials are great potential candidates from the technical, economical or ecological perspective. Additionally, designing efficient driver mechanisms that can apply and recover mechanical loads effectively remains complex, so the use of new manufacturing techniques like 3D-printing could accelerate the introduction of new cooling systems.

The present work investigates the elastocaloric effect (eCE) of a thermoplastic polyurethane (TPU) produced using Selective Laser Sintering (SLS) to explore the potential of 3D-printed TPUs for solid-state refrigeration applications. Mechanical testing, including uniaxial tensile tests, is conducted to characterize the stress-strain response, including the non-linear elastic response and stress softening behavior. Differential Scanning Calorimetry (DSC) measurements are performed to analyze the thermal transitions of the TPU, such as melting and crystallization temperatures, in order to provide insights into the material's microstructural properties, including its phase behavior. Cyclic loading and infrared thermal measurements are conducted at room temperature to evaluate the eCE by measuring the temperature changes during loading/unloading phases. Finally, Small-Angle and Wide-Angle X-ray Scattering (SAXS/WAXS) experiments are conducted during mechanical cycling to investigate the microphase-separated structural changes and possible Strain Induced Crystallization (SIC) phenomena in the TPU. The focus is on understanding how strain-induced crystallization and other microstructural transformations contribute to the eCE. The experimental results obtained through infrared camera measurements show an increase in temperature above ambient temperature during the loading phase of the cycles and a decrease below it during the unloading phase. These results seem to indicate the formation of crystals during strain increase, which melt upon load removal. The SAXS/WAXS tests show a clear correlation between temperature variations and the appearance of new phases in the loading direction.

Superelastic Behavior Improvements of Ti–Nb–Mo Alloys via Heat Treatment

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

There is a rising demand for nickel-free vascular stents due to concerns over the release of nickel ions from conventional NiTi stents, which may cause allergic reactions and potential long-term health risks. Ti-Nb-Mo alloys have emerged as a promising alternative, offering excellent biocompatibility along with superelasticity and shape memory properties. However, optimizing their mechanical performance, particularly their superelasticity, remains challenging.

Hence, this study aims to investigate the effect of heat treatment on the microstructure and mechanical properties of Ti-Nb-Mo alloys, focusing on enhancing their superelastic behavior. The alloys were fabricated using a vacuum arc melting furnace and subjected to various heat treatment conditions to regulate their phase composition and grain structure. Scanning electron microscopy (SEM) and X-ray diffraction (XRD) were employed to analyze the microstructural evolution, while tensile tests were conducted to evaluate the mechanical response.

This research provides insights into the correlation between heat treatment parameters, microstructural evolution, and the resulting superelastic properties of Ti-Nb-Mo alloys. The findings are expected to contribute to the development of nickel-free vascular stents with improved mechanical performance and biocompatibility..

Melt-electrowritten smart light-responsive lamellar structure with carbon nanoparticles incorporated into polymer matrix

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A4_2, Z2 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Nowadays, the interest in smart materials is increasing. These materials can change their properties under different external stimuli such as temperature, light and others. These materials can be used in wetting applications such as microfluidic devices, oil/water separation and others. Wettability can be changed in two common ways: changing their topography or chemical modification of the surface. The topography of smart materials can be controlled by external stimuli. For example, melt-electrowritten lamellar structure of polyether-urethane with poly(1,10-decylene adipate) (PEU-PDA) wrinkles at 70°C [1]. Although the heating is not localized and cannot heat a local part of the sample. On the other hand, light has the advantage due to localization and can be converted into heat energy, which is better absorbed by dark surfaces. A solution to this problem was presented for a lamellar structure with coated blank ink that was locally heated by laser exposure [2].

Here, we present a novel approach to fabricate lamellar structure with a dark surface by using PEU-PDA with incorporated 0.2 wt.% graphene nanoplates (GN) or multi-walled carbon nanotubes (MWCNT). The incorporated particles increase the melting point of the soft segments up to 10°C. When exposed to an infrared (IR, 808 nm) laser, the coated lamellae wrinkle due to thermal expansion, confirming the local heating of the irradiated area. The temperatures of covered lamellae reach 50°C and 70°C for GN and MWCNT composites respectively. The main drawback of wrinkling is the lack of a certain direction, in this case capillary forces can determine the bending direction of the lamellae. Water droplets placed between two lamellae cannot bend the lamellae at room temperature due to the high elastic modulus of the lamellae. When exposed to the laser, the coated area of the lamellae bends in the presence of droplets due to the decreased elastic modulus of the lamellae. In addition, the direction of the bending can be changed by adding an additional droplet in a neighboring position. This approach allowed us to obtain a lamellar structure with programmed topography due to capillary forces and local heating. These adjustments may help us to create a new type of microfluidic devices or soft robotics.

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Micro-structural and Mechanical Characterization of Wire and arc additive manufactured Fe-Mn-Si shape memory alloy

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A4_3, Z2 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Iron-based shape memory alloys (Fe-SMAs) have attracted considerable interest due to their economical production, pseudo-elastic properties, shape memory effect (SME), and exceptional mechanical characteristics, making them ideal for civil engineering applications. This study proposes that integrating a Fe-SMA lattice structure with advanced micro-structural engineering could enhance the material's recover-ability through SME, potentially resulting in negative stiffness and improved energy dissipation. Thin walls of Fe-SMA were fabricated using Wire Arc Additive Manufacturing (WAAM). To assess the energy absorption capabilities of Fe-SMA lattice structures, it is essential to gain a thorough understanding of the interplay between manufacturing variables, micro-structure, and functional performance. The primary aim of this research is to conduct a micro-structural and mechanical characterization of WAAM-fabricated Fe-SMA samples in both their as-built and heat-treated states. The findings indicate that post-processing heat treatment, specifically aging at 760 °C for 8 hours, significantly enhances the pseudo-elasticity and recovery strain of the samples.

Shape memory behavior of wetting-programmable lamellar surface

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A4_2, Z2 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Developing wetting-programable shape-changing topographical surfaces is essential for creating new materials and technologies that enable droplet manipulation and the creation of actuators. Smart materials, such as shape memory polymers, are used to fabricate surfaces capable of switching their mechanical properties to modify their wetting behavior. In this research, high-aspect-ratio lamellar surfaces composed of shape memory polymers exhibited significant deformation under water droplet dynamics. The lamellar surface topography was fabricated using melt-electrowriting (MEW) of polyurethane microfibers. Two different types of stimuli – temperature and light exposure – were applied to modify the mechanical properties, thereby influencing the deformation and recovery of the original surface. Wetting studies demonstrated that the deformation of the high-aspect-ratio lamellar surface can be tuned not only manually but also by the presence of a liquid droplet. This behavior is controlled by temperature variations induced through direct heating/cooling or light exposure when the lamellae were stained with black ink. The forces exerted on the system were analyzed for the deformation of both fixed and non-fixed (cantilever-like) lamellae. The interaction between the liquid and the thermo-responsive topography introduces a novel wetting behavior. This feature opens new possibilities for applying such topographies in the design of smart elements for microfluidic devices, such as smart valves.

Programmable meta-material composites for regulating force, energy dissipation & recovery

Prof. Mahdi Bodaghi¹

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A4_1, Z2 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

The development of programmable meta-material composites offers new frontiers in smart manufacturing, where materials can be engineered to regulate force and stiffness, dissipate energy, and recover mechanical properties after deformation. This talk presents our latest advancements in meta-material composites, leveraging principles of non-linear instability, visco-pseudo-elasticity, shape recovery, sustainability, and additive manufacturing.

By developing programmable lattice architectures and reinforcing them with bio-based additives, these meta-composites exhibit programmable stiffness profiles (positive, negative, or zero), shape recovery, and hysteretic energy dissipation. They can regulate force and stiffness, while efficiently absorbing and releasing mechanical energy on demand. This makes them highly applicable components for automotive/rail/aerial vehicle, protective sports gear, and medical devices, where impact mitigation, energy dissipation and recovery play a crucial role.

This presentation will discuss novel computational and experimental approaches for developing these structures, including finite element modelling, composite development, and thermo-mechanical testing. The research explores how the interplay between material properties and geometric design can significantly enhance response tuneability, impact resilience, lightweighting, comfort, and durability, promoting sustainability by reducing material waste before and after fabrication. By integrating nonlinear mechanics with sustainable material innovations, this study lays the foundation for next-generation high-performance, responsive, and energy-dissipating structures.

Novel triboelectric graphene polymer sensor for risk mitigation in different environments

Ph.D. José Sánchez del Río Sáez^{1,2,3}, Ph.D. Carolina Hermida-Merino¹, Ph.D. Elena Cerro¹, Prof. Yolanda Ballesteros³, Ph.D. Antonio Vázquez-López⁴, Ph.D. Xiang Ao², Prof. Deyi Wang²

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A4_4, Z2 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

The increasing demand of free energy in modern society, coupled with the urgent need to find clean and sustainable energy sources, the same as monitoring physical magnitudes in order to either improve the life quality of citizens in smart cities or to mitigate risks against catastrophes, have propelled research and development in innovative areas of energy generation and sensing. One of these innovative approaches is harnessing the triboelectric effect as a viable source of electricity generation. The triboelectric effect, based on generating electrical charge from mechanical energy in the form of friction or contact between materials, offers significant potential for energy harvesting in everyday environments and situations where conventional electrical infrastructure is limited or inaccessible. In addition, the use of specific materials that enhances sensitivity and gives novel properties to the sensors such as electromagnetic shielding or fire retardancy is a key challenge for scientists specialized in novel smart materials. In this work novel triboelectric sensor made of different charged polymer layers and with graphene and fire retardancy elements in its polymer matrix is presented. Its use as a risk mitigation warning alarm system in areas with fire or with high radioactive doses in the air makes this novel sensor a very good candidate to operate in smart buildings. An electrical and mechanical characterization was performed and a high efficient mechanical-electrical energy conversion is shown, reaching power values of mW for applied forces of dozens of newtons. Furthermore, its radiation shielding capacity and its applications as a smart sensor resistant to fire conditions was tested with a novel communication system based on LoRA and Wi-Fi protocol.

MATERIAL AND DESIGN SOLUTIONS RELATED TO BODY PROTECTION AND MEANS OF DIRECT COERCION WITH HIGH COMMERCIALIZATION POTENTIAL

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The presentation discusses the experience of the Institute of Security Technologies "MORATEX" in the development of ballistic personal shields, in particular ballistic helmets, ballistic vests and shields used in the area of demining, incl. humanitarian demining based on the composite technologies. Material solutions protecting humans against a number of ballistic phenomena and scenarios related to situations with the use of melee weapons will be presented.

The aim of the research was to develop a number of material system solutions and utility forms conducive to increasing the comfort of use and aesthetics of the product using the principles of design thinking.

Solutions with high commercialization potential will be presented in the field of: hybrid ballistic helmets, composite ballistic inserts based on atmospheric plasma or low-temperature plasma modification technologies, body shields used in demining processes or during operational activities of sapper services.

Ballistic and other functional requirements specified in the research will also be presented, conducive to increasing the level of user protection while at least maintaining the ergonomics of the developed personal protections.

Other technological solutions related to coercive technologies selected as part of the implemented processes of mapping technologies with the greatest commercialization potential, including the use of multi-criteria analysis, will also be presented.

The presented design and material solutions were indicated as part of the analysis of the commercialization potential and technology mapping as part of task No. 1 "Development Incubator", as part of the project entitled "Science4Business - Science for Business".

3D Printed Methyl cellulose/Gelatin-based Scaffolds for Cartilage regeneration

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Articular cartilage is an avascular tissue with limited regenerative capacity. Older population often has degenerative diseases of articular cartilage which causes pain and difficulty with daily activity. Therefore, there is extensive biomaterials research for treatment of regenerative disease of the articular cartilage. Current treatment method is replacement surgery which has disadvantages, such as prolonged recovery times, need of revision surgery and relatively high cost. In this study, the mechanical properties of the natural cartilage is mimicked with 3D printing methylcellulose(MC)-gelatin-

based scaffolds by varying gelatin concentration of MC/gelatin bioink. The scaffolds were printed with 20% infill density with a speed of 8 mm/sec at 42 degrees with dimensions of 10x10x2 mm. The printing pressure was varied between 8 to 30 psi depending on the viscosity of the prepared ink. The produced scaffolds were characterized by Fourier Transform Infrared (FTIR) spectroscopy, contact angle measurements, degradation studies and mechanical tests. FTIR results confirmed successful blending of MC and gelatin homogeneously within the 3D printed scaffolds which is essential for successful 3D printing. Printing accuracy of the scaffolds were determined by Image-J analysis which showed that the scaffolds had upto 92% accuracy with the input images. Contact angle values were found to be within the suitable range for human tissue which was ranging in between 40-70 degrees. Mechanical tests revealed that the produced scaffolds had a stiffness of about 10 kPa and compressive strength of approximately 90 kPa. The % strain values were about 45% which showed remarkable degree of ductility of the scaffolds. Swelling and degradation tests revealed that pH range of the scaffolds were within the physiological range (pH: 7.1-7.6) of human tissue. % weight loss of the scaffolds were found as 50% within 14 days period. Overall, the mechanical properties of the scaffolds require to be further developed by incorporation of an effective filler such as calcium phosphates or bioactive glasses. Due to their remarkable degree of ductility and shape fidelity, the produced scaffolds were found to be promising for future applications for articular cartilage regeneration. Furthermore, the results revealed that the potential application of the scaffolds may be extended for soft tissue engineering and drug delivery applications.

Mechanical in-situ investigation of Ni/PU hybrid foams for energy absorption and protection applications using X-ray computed tomography

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Metallic foams are porous materials that exhibit unique properties, making them valuable for a wide range of applications. Their high strength-to-weight ratio and excellent thermal conductivity make them ideal for use in lightweight construction and as heat exchangers. Additionally, their exceptional energy absorption capabilities make them well suited for crash protection in automotive and aerospace industries, enhancing safety during impacts. Metallic foams are also incorporated into protective equipment to absorb shocks and mitigate damage.

In this study, Ni/PU hybrid foams produced via electrodeposition and optimized for energy absorption are investigated. These foams are designed for use as mobile protective barriers in explosive ordnance disposal services and as façade elements for critical infrastructure, such as embassies. To enable the attachment of large foam elements to a façade, inserts must be embedded into the foam. Consequently, inserts are incorporated into the PU foam and subsequently coated via electrodeposition to ensure a secure bond with the foam. This critical interface, along with the foam's compression behavior, is analyzed using X-ray computed tomography (CT).

X-ray CT is a powerful, non-destructive technique for three-dimensional (3D) imaging of materials. It enables in-situ analysis of microstructures and their evolution during mechanical testing, providing detailed insights in 3D. The study presents mechanical in-situ investigations using a load cell to perform compression tests. Additionally, the load cell is adapted to conduct pull-out tests to evaluate the connection strength between the inserts and the foam. These experiments are performed on foams with varying pore sizes, allowing for a comprehensive understanding of the influence of pore size on mechanical behavior and insert bonding.

Aging of High-Density Polyethylene - Characterisation and identification methods

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Polyolefins represent one of the most used polymer types in packaging applications. The application in packaging sets specific requirements on the needed material properties. For rigid packaging, a central material is high density polyethylene (HDPE), which is used in bottles, canisters and large packaging such as IBCs. These products are usually produced in the blow moulding process. The used polymer needs to have fitting mechanical properties in the finished product to withstand the repeated mechanical stresses and be chemically stable to the packaged goods. With a more sustainable perspective on the use of plastic packaging one needs to investigate the longevity of HDPE products and HDPE. Answers to the question of how long a product can be used, need to be found, if a longer lifetime is a goal for more sustainability. An easy access to data and small experimental effort is desirable, ruling out long experiments on a product.

Over the lifetime of a product, material properties change and can lead to a premature failure of a product. Polymers are affected by many environmental stressors. These vary by application and can include:

- temperature,
- UV exposure,
- medium in which they are used, or
- repeated mechanical stresses.

This is known as aging of polymers.

Real products can be used to analyse the effects of aging in a polymer with the drawback that the history of use is often not clear. To better differentiate between environmental aspects, simulated accelerated aging can be utilised, zeroing in on individual aging parameters and defining the impact of e.g. raised temperature during use. When comparing to real aged products or found polymer debris, an understanding of the effects of environmental impacts can help to assess the age and condition in which an unknown product has been used.

In this work methods to characterise types of aging in HDPE were assessed and ranked for usability, preciseness and finding fitting testing conditions. The samples are artificially aged with parameters such as raised temperature. The analysed methods will be split in to mechanical (e.g. tensile testing), optical (e.g. microscopy) and chemical characterisation (e.g. FTIR-identification) to detail the effects of environmental stresses on the material properties. A comparison is drawn between real products and lab-aged polymer samples. Material properties and aging mechanisms need to be assessed to be used as a base for material models to easy experimental effort and allow prediction of a products lifetime.

Rheoelectrical properties of Multi-Walled Carbon Nanotubes-based electrofluids for soft electronics applications

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A5_2, Andalucía III Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Electrofluids can be understood as conductive liquid composites, where conductive filler particles are suspended in a non-conductive liquid matrix. In order to achieve electrical conductivity, the filler concentration should be enough to create a 3D network that spans through the entire volume, where the particles are in contact with each other. This concentration is defined as the percolation threshold. The addition of filler particles has an impact on the mechanical network of the electrofluids. At increasing concentrations, the particles form a colloidal gel. We adapted the electrical percolation theory with mechanical parameters to determine the transition from liquid to solid-like behaviour of the electrofluids, i.e., the formation of a mechanical network. Here, we will present how the interplay of these two networks dominates the properties of electrofluids and exploit them as soft sensors and conductive interconnections.

Electrofluids composed of Multi-Walled Carbon Nanotubes (MWCNTs) as the conductive filler and glycerol as the liquid matrix at different concentrations were investigated. The electrical resistance was obtained from I-V curves using a 4-point probe setup for each concentration. The mechanical values (storage modulus, G') were obtained from frequency sweeps in the linear viscoelastic (LVE) region at low frequencies. We found that the electrical percolation was reached at a lower filler concentration than the mechanical: 0.04 wt% and 0.16 wt% MWCNTs, respectively. We propose three regimes to describe the electrofluids depending on which networks are present that allows us to predict their mechanoelectrical responses. Electrofluids were encapsulated in EcoFlex tubes and underwent uniaxial tensile tests coupled to electrical resistance measurements. Electrofluids with concentrations between the electrical and the mechanical percolation exhibited a strong electrical relaxation under strain, due to the MWCNT rearrangement, whereas electrofluids with mechanical network retain the electrical response. This behaviour correlates what observed in rheoelectrical tests (amplitude sweeps). Flow curves showed that the electrical resistance remains constant until a shear rate value of 50 s⁻¹, demonstrating that the electrical and the mechanical networks are independent. We employed electrofluids as conductive interconnections for metal joint components and successfully reduce the change in electrical resistance by 80% compared to an empty ball joint during rotation.

Tailoring Mechanical Properties of Polymer Foams at Constant Density: The Impact of Pore Shape, Pore Size, and Fabrication Processes.

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A5_2, Andalucía III Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Polymer foams are especially sought after in energy absorbing applications like safety gear or packaging, due to their lightness and mechanical properties. However, adjusting the properties of a polymer foam often involves trade-offs. For example, increasing the density increases the mechanical properties but also the weight [1]. This leads to the question whether the structure of a polymer foam can tailor its mechanical properties while the density is kept constant. In this work, we investigate polymer foams with defined pore shapes, pore sizes and a pore size gradient. The unit cells range from 10 to 2.5 mm in edge lengths and have either spherical pores (7.5 to 1.8 mm in diameter) or cubic pores (7.6 to 1.9 mm in edge length). The unit cells were assembled by a computer aided design (CAD) software into uniform and graded materials with constant density but varying pore sizes, and subsequently fabricated by stereolithography 3D printing.

We found that materials with cubic pores have a higher E-modulus but a lower yield strength compared to materials with spherical pores. In contrast, the graded materials have lower mechanical properties as their uniform counterparts, no matter the pore shape. Moreover, the pore size influences the material's mechanical response, which is linked to the fabrication process. FEM simulations combined with μ -CT scans were used to analyze the stress distribution during compression, and the effects of fabrication-induced geometric deviations. Consequently, our study emphasizes the critical role of identifying and considering fabrication process related defects and deviations for material property characterization. Apart from this, it demonstrates that mechanical properties of polymer foams can be tailored not only via the density but also by the morphology: shape matters.

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Fabrication, characterization and applications of electrospun polymer-inorganic nanocomposites

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A5_2, Andalucía III Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The design and development of functional, polymer-based nanocomposites attracts significant attention nowadays owned to their unique properties, deriving from the combination of polymers with nanostructured materials of either organic or inorganic origin. Electrospinning – which has already reached the industrial sector – is one of the most powerful and versatile fabrication methods used in the production of nanocomposite materials in the form of micro- and nanofibers [1]. Such fibrous nanocomposites are highly attractive in various research fields, owned to their unique properties including high surface to volume ratios, high porosity and multifunctionality. This presentation provides an overview of our recent research activities on the fabrication, characterization and applications of polymer-based electrospun nanocomposites in the form of nano- and microfibers and corresponding microrods. More precisely, the fabrication strategies followed in the preparation of the afore-mentioned systems, along with the materials' characterization and investigation of their potential applicability in various fields including biomedicine [2, 3], catalysis [4], environmental remediation [5], optoelectronics [6, 7] and sensing [8] are presented and discussed.

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INJECTABLE SODIUM ALGINATE BASED HYDROGEL WITH METRONIDAZOLE FOR PHARMACOLOGICAL APPLICATIONS

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

A drug delivery system (DDS) is a pharmaceutical dosage form that releases one or more active ingredients in a modified manner in terms of site, rate, and time and ensures that certain systemic or local therapeutic concentrations of the molecules are achieved or maintained. In this work a complex reservoir-like vaginal ring was considered as DDS. Fused deposition modeling (FDM) 3D printing was exploited to manufacture the reservoir wall with controlled dimensions, and macroscopic porosity. The drug, Metronidazole (MTZ) was chosen as antibiotic for the treatment of bacterial vaginosis. It had to be transferred into the reservoir by an easily injectable carrier. Further, once in the reservoir, the carrier should not leak through its pores, to obtain a sustained drug release. An alginate-based hydrogel was developed for this task. Alginate was selected for the gel due to its low cytotoxicity; CaCO₃ and glucono-delta-lactone as crosslinking agents allowed for a controlled gelation process, with the aim to fill the reservoir with a flowable precursor solution that reached the solid-like consistency of the hydrogel in the cavity. Given the therapeutic need of a MTZ load higher than the amount soluble in the aqueous alginate solution, a MTZ dispersion had to be considered. The effects of the composition of the drug-loaded precursor dispersion and the resultant filled hydrogel were investigated from a rheological standpoint. In steady state rotational tests, the precursor dispersions exhibited a flow threshold, followed by a pseudoplastic behavior. By combining this information with a purposely developed capillary rheometry approach their injectability was predicted and assessed. The ability of the suspension to crosslink despite the very high MTZ solid content was confirmed performing dynamical mechanical tests. The solid fraction showed a predominant effect on mechanical properties if compared with alginate. Loss factor increased with increasing dispersed drug content probably due to energy dissipation caused by friction between solid particles. The alginate-content controlled hydrogel stability. Further considering the hydrogel as an independent DDS, alginate content controlled the MTZ release rate. However, once into the reservoir, the release rate controlling factor was demonstrated to be the reservoir porosity, with very little effect from the hydrogel composition.

PREPARATION AND CHARACTERIZATION OF ROTOMOLDED FOAMED POLYETHYLENE BLENDS WITH IGNIMBRITE DUST

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

ABSTRACT

Ignimbrite powder (Ig), a byproduct of stone extraction, was used as reinforcement with an azodicarbonamide-based chemical foaming agent (CBA) to produce polyethylene (PE) parts via rotational molding. The outer layer of the sample was a polyethylene composite with 0-10 wt% mineral, while the inner layer was foamed polyethylene (using 3 wt% CBA) blended with 0-30 wt% ignimbrite. Mechanical characterization showed an increase in maximum stress and elastic modulus in both bending and tensile tests with mineral addition. The composite with 10 wt% ignimbrite in the outer layer and 30 wt% in the foamed inner layer exhibited the greatest difference. Impact tests showed no major differences from neat polyethylene, though impact resistance slightly increased with 10 wt% ignimbrite in the outer and 20 wt% in the layer. Thermogravimetric tests indicated no differences between the blends used, thus keeping the thermal stability of PE even when adding mineral powder and foaming agent. Based on this work, a balance between mechanical, thermal and aesthetics properties of the rotomolded parts can be achieved by selecting the composite with neat PE in one layer.

ACKNOWLEDGEMENTS

Rock'n'Rot Project (PID2023-149534NA-I00, MCIU/AEI/10.13039/501100011033/FEDER, UE) funded by the Ministry of Science, Innovation and Universities of Spain. Francisco Romero acknowledges ULPGC for the funding of his PhD,(reference ULPGC-2023-2-3-4).

Hydrophobic Eutectics-based Supramolecular Gels and Cellulose-based Nanosponges: Breakthrough Solutions for Water Remediation

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Clean water is a fundamental goal of the 2030 Agenda for Sustainable Development [1] and the European Green Deal's Zero Pollution Action Plan [2], making water remediation a critical focus in research. Conventional extraction techniques like dispersive liquid-liquid and solid-liquid microextraction (DLLME and DSLME) face challenges, including the use of volatile organic solvents and non-sustainable sorbents with limited capacity.

This study addresses these challenges by introducing new classes of sustainable materials based on hydrophobic non-ionic eutectic solvents (HES) [3]. HES offer several advantages, including being chloride-free, easy to prepare from natural precursors, 100% atom economy, and high sustainability [4]. To expand their use beyond liquid-liquid extraction, two innovative HES-based materials are developed: hydrophobic eutectogels (HEG) and HES-loaded cellulose nanosponges (HECS).

HEG are supramolecular gels formed by the rapid thermoreversible self-assembly of low molecular weight gelators (LMWG) [3]. HECS are hybrid materials obtained by combination of HES with cellulose nanosponges (CNS), eco-safe nanostructured cellulose-based materials made from TEMPO-oxidized cellulose [5], branched polyethyleneimine and citric acid [6,7], a particularly attractive option for sustainable water remediation.

Preliminary studies with HES and HEG composed of terpenes, long chain carboxylic acids and phosphine oxides have demonstrated promising extraction abilities in water remediation from phthalates and bisphenol A.

The materials' structure and extraction mechanisms are thoroughly investigated using NMR and UV-Vis spectroscopy, and HPLC-UV. This comprehensive analysis allows for precise control over their properties, making these materials highly adaptable for various water remediation applications.

The development of these materials marks a breakthrough in sustainable water treatment. By overcoming the limitations of current extraction methods, this research offers a safer, more efficient, and eco-friendly solution for removing harmful contaminants. These materials have the potential to play a crucial role in achieving global clean water goals and advancing the field of green chemistry.

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Development and Weather Aging Evaluation of Thermoplastic Eco-Friendly Composites Reinforced with Pyrolyzed Biochar

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A5_2, Andalucía III Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The increasing demand for sustainable materials has spurred interest in eco-friendly composites utilizing renewable resources. This study investigates the impact of aging on the performance of thermoplastic matrices reinforced with biochar inclusions. A carbon-rich material was produced via the pyrolysis of agricultural waste. The biochar was incorporated into the thermoplastic via the twin roll method, to enhance its mechanical and thermal properties, including tensile modulus, tensile strength, bending modulus, and melting point. A key focus of the study was assessing the long-term durability of the composites through a comprehensive aging analysis.

Samples were subjected to accelerated weather aging, simulating prolonged exposure to environmental conditions, and compared with physically aged samples under real-time conditions. This comparison enabled the estimation of an aging factor specific to the material, providing deeper insights into its long-term performance and reliability.

The mechanical and thermal properties of pristine, accelerated-aged, and physically aged materials were thoroughly evaluated.

This study highlights the potential of pyrolyzed biochar-reinforced thermoplastics, offering a viable route for repurposing agricultural waste into high-value, eco-friendly materials.[1-3]

Graphene-based electrospun nanofibers in the removal of U(VI) from aqueous media

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Water is one of the most valuable natural resources on earth. Nowadays, rapid growth of industrialization and human activities lead to water contamination by toxic metals such as radioactive metal ions, which pose significant environmental and public health challenges. Adsorption is a widely used treatment method that can be used in removing such hazardous elements [1]. Electrospinning is a versatile technique employed in the fabrication of nano- and microfibers, exhibiting high surface area to volume ratio and tunable properties, particularly well-suited for water treatment applications [2]. In this study, methacrylic random copolymers containing tertiary amino groups were synthesized by conventional free radical polymerization and characterized in respect to their chemical composition and molar mass. These polymers were combined with polyethylene oxide (PEO) to produce blended fibers by means of electrospinning. PEO is well-known for its highly electrospinnability, biocompatibility and good mechanical properties [3]. By altering the electrospinning conditions including the applied voltage, the needle-to-collector distance, the polymer solution concentration, etc., the optimum electrospinning conditions were determined. Moreover, these materials were further functionalized with carbon-based nanomaterials such as graphene oxide (GO) to enhance their adsorption capabilities [4]. The resulting fibers were characterized in respect to their morphology and they were evaluated for their efficiency in the removal of radioactive elements such as uranium ions (U(VI)).

Acknowledgements:

This work was supported by the University of Cyprus.

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Enhancing silicone rubber functionality with thermally conductive fillers

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A5_3, Andalucía III Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Soft materials, especially silicone rubber, have gained attention in recent years, with efforts to develop multifunctional materials. Silicone materials now face stricter requirements, particularly in long-term temperature resistance. To manage high temperatures and reduce thermal load, thermally conductive particles are added for heat dissipation. These materials are particularly useful in e-mobility, where faster charging generates more heat that needs to be managed. Despite their advantages, elastomers exhibit low thermal conductivity compared to metals and ceramics, typically ranging from 0.1 W/m*K to 0.5 W/m*K.

This study investigates the influence of ceramic fillers – aluminum oxide (Al_2O_3), boron nitride (BN), and a combination of aluminum oxide and zinc oxide (ZnO) – with different particle sizes, on the thermal conductivity of solid silicone rubber. Additionally, the impact of potential synergistic interactions from the simultaneous addition of selected fillers is explored to identify pathways for enhancing thermal conductivity. In addition to the interactions, the mechanical properties of the thermally conductive silicone rubber are also determined.

Our study demonstrates that by using a combination of different ceramic fillers with optimal particle sizes and distribution, we can enhance the thermal conductivity from 0.2 W/mK to over 2.0 W/mK.

Furthermore, the thermal conductivity of the silicone compounds is examined under various pressure and temperature conditions to better understand its behavior under realistic application conditions. The results reveal that the influence of pressure and temperature on thermal conductivity is linear within pressure ranges from 10 bar to 200 bar and temperatures from 30 °C to 200 °C.

Comparison of mechanical and rheological characterization for multifunctional magnetic hydrogels for 3D printing applications

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Developing new material characterization strategies that combine mechanical and rheological methodologies is essential for optimizing biomaterials [1] used in medical applications such as pharmaceuticals, implants, 3D bioprinting, and tissue engineering. The rapid development of 3D printing techniques has been a driving force in personalized material manufacturing, offering the creation of complex structures and versatility in material selection. Such control in material architecture and mechanical properties is crucial in the tissue engineering sector as when engineered biomaterials come into contact with biological materials, it is crucial for them to closely mimic the dynamic natural environment for optimal integration. However, the required mechanical and rheological properties of biomaterials for 3D bioprinting applications have not been systematically correlated to material printability.

This study aimed to compare various mechanical and rheological characterization techniques of soft magnetic biomaterials and explore how combining these methods, can provide a broader understanding of biomaterial properties, ultimately guiding the selection of appropriate biomaterials for tissue engineering, with a focus on 3D bioprinting applications. The mechanical and rheological properties of various magnetic hydrogels, based on polysaccharides and proteins with varying concentrations [2,3], were measured using a universal testing machine, a rheometer, and a Dynamic Mechanical Analyzer to enable a comparative analysis of the collected data. Furthermore, the effects of material anisotropy were studied through magnetic particle structuring within the hydrogel using triaxial magnetic fields [4].

The universal testing machine applied controlled tensile and compressive forces to the biomaterial sample and measured the resulting deformation, accommodating larger deviations in force and displacement. Using oscillatory shear stresses through rheology, the storage and loss moduli were evaluated. DMA provided a more versatile measurement setup that combined the principles of the universal testing machine and rheology to simulate real-world conditions under extension and torsion. Although the maximum achievable force in DMA was lower than that of the universal testing machine, it offered improved resolution. This setup proved essential for a comprehensive analysis of soft biomaterials' static and dynamic mechanical and rheological properties.

This work was supported by the ArchiFun European Union's Horizon 2022 research program co-financed by Marie Skłodowska-Curie Action COFUND 01.

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FATIGUE CRACK GROWTH BEHAVIOUR OF POLYACRYLAMIDE ALGINATE DOUBLE NETWORK HYDROGELS

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A5_3, Andalucía III Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

A hydrogel is an aggregate of water and polymers, and usually contains more water than polymers. This structure makes them very soft and flexible and biocompatible. These materials, traditionally employed in the biomedical field, are emerging as candidates for potential applications in tissue engineering, flexible electronic devices, etc, where they are required to sustain prolonged static and cyclic loads. The main drawback is that the fatigue response of these materials is still limited, and many uncertainties are still unsolved concerning the fatigue analysis. Thus, this work investigates the fatigue crack propagation in polyacrylamide-alginate double-network hydrogels, materials known for their outstanding mechanical properties. Unlike previous studies in the literature, which have been performed under dry or partially hydrated conditions, this study focuses on tests performed under full immersion conditions, an aspect so far unexplored in the scientific literature. Therefore, the objective is to analyze the effect of alginate concentration on the fatigue crack propagation response of polyacrylamide-alginate double-network hydrogels when the specimens are fully immersed in an aqueous medium. The effect of delayed fracture is also analyzed, a phenomenon in which a specimen cracked under the action of a static load, below which fracture would occur, experiences crack growth.

Structural integrity of sustainable thermoplastic elastomers

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A5_3, Andalucía III Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

To be more sustainable and move towards green technology, more and more efforts are being made to use more environmentally friendly materials. In this context this research is proposed, where sustainable thermoplastic elastomers (TPE) are analysed to replace the non-sustainable polymeric materials currently employed for protective mask frames for cleanroom applications. Considering the mask's reuse requirement, the durability is an important concern, especially the fracture resistance of TPEs, to ensure safe and long-term usability of protective masks. Therefore, the main objective of this work is to evaluate the fracture resistance of TPEs with a reduced environmental impact. Due to the marked viscoelastic nature of these materials, it will be necessary to apply the Viscoelastic Fracture Mechanics approach to determine the fracture resistance curves and the specific energy associated with the onset of crack propagation. Load relaxation tests in tensile mode will be performed and the Single Edge Notch Tension (SENT) configuration will be chosen for the fracture characterization. Evaluating fracture parameters, together with other indicators also determined in previous works, will help to discriminate among potential candidates the best TPE to replace the unsustainable material used in the protective mask frames.

Effect of steam and gamma-irradiation sterilization treatments on sustainable thermoplastic elastomers

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This work is part of a research activity aimed at redesigning from a sustainability perspective a reusable protective mask for cleanroom applications, currently produced with conventional non-sustainable polymeric materials. This study examines the mask frame, produced by injection moulding in a thermoplastic elastomer (TPE), and the possibility of using sustainable TPEs to replace the one currently used is investigated. To this aim, considering the requirement of reusability of the mask, and that the mask must be subjected to adequate sterilization treatments after each use in the cleanroom, the attention was directed to the study of the effects of industrial sterilization processes on the properties of the candidate TPEs. Six industrially relevant TPEs with a reduced environmental impact, differing for the chemical nature, were examined in the form of specimens cut out from injection moulded 2 mm thick plates specially prepared. The ordinary TPE currently employed to produce the frame was also analysed. Both steam and gamma irradiation sterilization treatments were considered as these are the two types of sterilization methods to which the mask is exposed when in service. The TPE samples underwent steam sterilization in the laboratory, by means of an autoclave, following a standard sterilization cycle (121°C-30 minutes) repeated for up to 55 times. Gamma-irradiation treatments were carried out externally, by a company that provides gamma sterilization services for industrial goods, and different increasing radiation doses (up to 125 kGy) were used. The effects of the various sterilization treatments were assessed by structural (Wide Angle X-ray Scattering, WAXS) and calorimetric (Differential Scanning Calorimetry, DSC) analyses, as well as by mechanical tests. Concerning these latter experiments, both uniaxial tensile tests in quasi-static conditions and instrumented impact tests were carried out. The impact tests were performed with a pendulum in tensile-impact configuration on double-edge notched specimens. For the various TPEs examined, the effects promoted by the sterilization processes on the mechanical performances are discussed based on the outcomes from the structural and thermal characterization, in the attempt to identify the best sustainable TPE candidate for the obtainment of the protective mask frame.

Biopolymer-modified double-network PVA hydrogels: A comparative analysis of additive effects on material properties

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Abstract:

Polyvinyl alcohol (PVA)-based double-network hydrogels, incorporating agarose, chitosan, or silk fibroin as biopolymer additives, were systematically evaluated for their structural, mechanical, tribological and biocompatibility properties. Although these polymers are commonly used in cartilage tissue engineering, their precise effects on hydrogel properties have not been systematically compared under uniform synthesis conditions, making this study critical for understanding their role in tailoring mechanical and biological performance. Designed using a consistent freeze-thaw process, these hydrogels address limitations of pure PVA, such as insufficient mechanical strength and bioactivity, providing a deeper understanding of structure-property relationships in soft materials.

Mechanical testing revealed additive-specific effects: PVA-agar hydrogels exhibited the highest compressive modulus, PVA-chitosan hydrogels demonstrated improved elasticity and durability, and PVA-silk fibroin hydrogels displayed superior energy dissipation. These findings suggest their suitability for diverse functional applications. All hydrogels exhibited a high water content (>80%), advantageous swelling characteristics, and interconnected porous structures, essential for supporting hydrated, tissue-like environments. Preliminary cytotoxicity studies confirmed minimal adverse effects, supporting their potential for bioengineering applications.

This study lays the groundwork for developing hydrogels with improved mechanical and biological properties, which are crucial for applications such as cartilage tissue engineering. The fabrication techniques and characterization methods used provide insights into how specific biopolymer additives influence the material's structural and functional performance.

Analysis of piezoionic phenomenon in ionic conductive hydrogel materials for the fabrication of innovative self-powered tactile sensors

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A5_2, Andalucía III Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Nowadays the lack of tactile devices able to replicate skin functions has prompted researchers to look for and create novel technology that takes advantage of the physical properties of specific materials to develop diverse types of sensors. The piezoionic phenomenon is an effect that occurs in ionic conductive hydrogels. When pressure is applied to the material, ions migrate away from the deformed region, inducing a strain-driven ion flux. If anions and cations mobility differs, their diffusion within the hydrogel will also differ under load, causing a charge imbalance measurable as an electrical voltage in the device, leading to a current in the external circuit, both of which are proportional to the applied pressure. This physical mechanism behaves in an analogous way as the mechanoreceptors in the skin, therefore, can be useful to describe the perception of touch, so its study can lead to the creation of new self-powered sensors and a variety of smart healthcare devices. This study analyses the piezoionic effect in a photocurable semi-interpenetrated polymeric network hydrogel composed of Poly (vinyl alcohol) (PVA), acrylic acid (AAc) and Poly (ethylene glycol) diacrylate (PEGDA). The impact of ionic mobility on the electrical response of the material was validated using different chloride salts, keeping the same anion and altering the cations with various alkali metals. To assess the electrical behavior of the various mobile ions, flat samples with parallel and sandwich copper electrodes underwent a variety of electromechanical and electrochemical characterizations. Furthermore, 3D printed samples were subjected to the same studies to evaluate the impact of complex geometry on the piezoionic response. The results demonstrate that complex 3D geometries enhance the electrical response because of mechanical strain concentration induced by the structure with respect to bulk samples. After the functional characterization of the material, the hydrogel was implemented as a biometric self-powered sensor and as a potential mechanical harvester to recover energy from human motion. The findings pave the way to employ piezoionic phenomenon in the development of new tactile sensors as well as innovative devices useful in soft robotics, flexible and wearable electronics and health monitoring.

Thermal treatment on a silica-filled NBR preliminarily softened by stretching: effect on fracture toughness and fracture propagation process

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A5_3, Andalucía III Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

When filled rubber compounds are deformed, they exhibit a softening depending on the applied stretch level: in subsequent loading cycles, lower stresses are observed for strains below the maximum strain applied in the first loading cycle. Several studies have shown that the pristine uniaxial tensile behaviour of the material can be recovered through the application of appropriate thermal treatments. However, limited research has been conducted on the thermally induced recovery of fracture behaviour after stretch-induced softening.

This work investigates the effect of stretch-induced softening and its thermally induced recovery on the fracture behaviour of a silica-filled NBR. A thermal treatment has been defined that preserves the tensile behaviour of the pristine material but allows an almost complete recovery of the tensile behaviour of the material preliminarily softened through load-unload cycles under uniaxial tensile conditions. The fracture behaviour was assessed by performing quasi-static tensile tests on notched specimens in pure shear deformation conditions. Tests were video recorded to identify the crack onset and measure the crack advancement. Initially, stable crack propagation occurs, which stops if the specimen elongation is kept constant and no further strain energy is supplied to the specimen. Subsequently, crack propagation becomes unstable, causing the crack to propagate even without a further increase in overall deformation. The energy-based J-integral parameter was evaluated until the initiation of unstable crack propagation and plotted versus the crack advancement, obtaining a resistance curve. The stable crack propagation rate was also evaluated and represented as a function of the J-integral, similarly to the Paris-Erdogan representation. The J-integral values at the onset of both stable and unstable crack propagation were considered as a measure of material's fracture toughness.

The softening induced by stretching the material up to 350% deformation caused a decrease in the fracture toughness due to the less dissipative behaviour of the softened material. After thermal treatment, the softened material showed a partial recovery of the overall force-displacement response. However, the J-integral values at crack onset and unstable fracture initiation remained comparable to those of the softened material, with the resistance curve even lower than that of the softened material. From the analysis of the crack propagation rate, it was observed that the thermal treatment accelerates the fracture propagation. As a result, the response of the thermally treated softened material derives from the superposition of a beneficial effect (recovery of stretch-induced softening) and a deleterious one (acceleration of crack growth).

Fracture toughness evaluation for filled rubbers towards the most appropriate energy parameter and test conditions

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A5_3, Andalucía III Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Filled elastomers are widely used in industrial products such as tyres, hoses and sealings, whose integrity is essential to maintain their function. A proper characterization of materials fracture behaviour is therefore fundamental for the appropriate material selection. Currently, there is not a standard for the evaluation of fracture toughness of rubber materials in quasi-static loading conditions and different fracture tests are proposed in literature. Their consistency has been verified for unfilled elastomers, for which the critical value of the tearing energy (T) at fracture initiation in mode I fracture tests has been found to be independent of the loading conditions and thus proposed as a measure of materials' fracture toughness. Further, the critical value of the tearing energy of unfilled rubbers at fracture onset resulted to be consistent to that of an alternative energy-based parameter, J -integral. For filled rubbers, literature reports both differences between the results obtained from different loading conditions and between the values of T and J critical for fracture onset (T_c , J_c).

In this work, a study on the fracture behaviour of three filled elastomers differing in the type of rubber matrix (NBR, SBR) and/or filler type (CB, silica) was performed. Single-edge notch tensile tests, biaxial tension on centre-notched squared specimens and fracture tests in pure shear deformation on single-edge notched specimens were performed at 23°C and 1 min⁻¹. The values T_c and J_c were evaluated from the different tests and compared. Analytical formulations and, in some cases, finite element analysis-based solutions were adopted to assess the parameters' critical value for the occurrence of fracture. A quite good correspondence between T_c and J_c has been obtained for a highly CB-filled NBR, irrespectively of the loading conditions. For the more deformable silica-filled NBR, higher T_c and J_c values were obtained from SENT tests. Regarding the effect of specimen geometry on the SENT tests results, it was investigated if the notch length, a_0 , affects fracture phenomenology and the T_c value and whether the observed effects depend on the material (the above-mentioned CB-filled NBR and a silica-filled SBR). A a_0/W ratio value in the range between 0.07 and 0.33 was adopted ($W = 30$ mm is the width of the 120 mm long specimens of SENT tests). For both materials T_c seems to be not significantly affected by a_0/W . However, the two materials seem to differ in the fracture phenomenology, with the SBR showing a crack deviation during fracture propagation.

Gelatin-Based Hydrogels with Carrageenan and Chitosan for Soft Tissue Engineering

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Bioresorbable hydrogels are leading materials in soft tissue engineering for the realization of scaffolds that can promote the reconstruction of damaged or diseased tissue by hosting cells capable of building new functional tissue. Their superior regenerative performance is favored by the close similarity between their hydrophilic macromolecular network and the structure of the extracellular matrix (ECM).

Inspired by the variegated combination of proteins and carbohydrates in native ECM, novel hydrogels were developed with a composition based on gelatin and enriched with polysaccharides of natural origin: one containing carrageenan (G-PEG-CARR), one with chitosan (G-PEG-CH), and one containing both (G-PEG-CARR-CH). These three materials were synthesized by crosslinking with poly(ethylene glycol) diglycidyl ether and freeze-dried, in order to obtain an interconnected porous structure suitable for cell colonization through a green procedure, without using any toxic solvent or foaming agent.

The swelling, degradation, and mechanical behavior of the scaffolds were evaluated along time upon immersion in water at body temperature. G-PEG-CARR, G-PEG-CH and G-PEG-CARR-CH exhibited high water uptake (about 550%, 730% and 830% after 24 h, respectively) and rather fast hydrolysis (~40%-50% mass loss at 6 weeks), nevertheless maintaining their structural integrity up to 6 weeks. During compression tests, the three materials showed a nonlinear elastic response with high compliance (stiffness of 30 kPa, 40–250 kPa and 60 kPa, respectively) and good deformation reversibility for repeated compressive cycles at 50% strain. They also exhibited natural tissue-like viscoelasticity with fast stress-relaxation (half stress relaxation time ~1-3 s), and their mechanical behavior became more and more compliant after prolonged immersion in water, as degradation gradually occurred.

In order to investigate the hydrogels as potential carriers for cell delivery in tissue engineering, they were seeded with human Mesenchymal Stromal Cells (hMSCs), featuring the potential for self-renewal and capacity to differentiate into several cell lineages. hMSCs spread homogeneously throughout the scaffolds and maintained their growth and viability for at least 21 days, with an increasing proliferation trend.

Altogether, these findings revealed that encapsulating hMSCs in gelatin-based hydrogels containing carrageenan and/or chitosan could be a promising strategy for cell delivery in regenerative medicine, deserving further studies targeting specific tissue engineering applications. In particular, at the light of their soft viscoelastic behavior, compatibility with cyclic loading, and efficient hydrolysis, these scaffolds showed great potential for the reconstruction of soft tissues such as skin, muscles, cartilage, or adipose tissue.

SUBBIMATT - Sustainable, Biobased and Bio-inspired Materials for Smart Technical Textiles

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The SUBBIMATT project aims to develop a new generation of sustainable, biobased, and bioinspired smart technical textiles to address energy efficiency challenges in key applications such as adaptive building envelopes, automotive interiors, and advanced garments.

Objectives

SUBBIMATT follows a Safe and Sustainable by Design approach and focuses on:

- Developing circular textile intermediates from biobased materials.
- Engineering smart textile materials for motion actuators, energy harvesters, and tunable openness fabrics.
- Demonstrating real-world applications in construction, automotive, and wearable technologies.
- Creating innovative business models and integrating external developments to ensure market adoption.

Methodology

The project is structured into three key phases:

1. Preparation Phase: Development of novel debondable adhesives, bio-polyurethane, and negative thermo-responsive materials to produce high-end coated fabrics, nanomembranes, and shape-memory filaments.
2. Enabling Phase: Integration of smart textile functionalities for mechanical actuation, energy harvesting, and tunable fabric openness.
3. Demonstration Phase: Implementation and validation of these materials in real-world use cases across the built environment, automotive, and fashion industries.

Expected Impact

SUBBIMATT is expected to generate significant industrial, environmental, and societal benefits:

- Boosting Industry Competitiveness: Strengthening the European textile sector through circular economy principles and innovative materials.

- Enhancing Sustainability Awareness: Promoting eco-friendly alternatives in buildings, mobility, and apparel.
- Improving Energy Efficiency: Showcasing smart materials that contribute to energy management in daily applications.
- Supporting EU Policies: Aligning with the EU Bioeconomy Strategy, Industrial Strategy, Textile Strategy, and Fit for 55 objectives.

By leveraging biobased and bioinspired materials, SUBBIMATT contributes to the transition toward a more sustainable and resilient textile industry.

A study of the mechanical behaviour of a 3D printed thermoplastic polyurethane: from material-controlled Mullins effect to process-dominated fracture behaviour

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A5_3, Andalucía III Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

This work is the result of a collaboration between Politecnico di Milano and Instituto Superior Técnico, Lisboa. The aim is to study the mechanical behaviour of 3D printed components based on a thermoplastic polyurethane and produced through the filament fused fabrication (FFF) technique. The TPU92A from Fillamentum characterised by T_g of $-40\text{ }^{\circ}\text{C}$ and T_m of $200\text{ }^{\circ}\text{C}$ was used.

A preliminary mechanical characterization was performed using 3.2 mm thick dumbbell shaped specimens, printed with YXZ (flatwise) printing orientation (ASTM F2921 terminology): in the 7.4 mm wide and 33 mm long gauge area, each layer consists of 19 deposited material beads, aligned along the direction of the specimen's gauge-length. Uniaxial tensile tests have been carried out at 23°C , at different strain rates (0.6 and 6 min^{-1}) to highlight any viscoelastic response of the material. Loading-unloading cyclic tests were also carried out up to different strains, to evaluate the dissipative response of the material and its dependence on the applied strain.

Rectangular-shaped specimen 1.6 mm thick, with a gauge area 100 mm wide and 20 mm long, were 3D printed with the YZX (Edgewise) printing orientation (ASTM-F2921). Each layer consists of 4 beads aligned along the X axis. A 15 mm long notch was introduced on one edge of the specimen, at its mid-plane, using a razor blade. Fracture tests were performed at 23°C and nominal strain rate of 0.6 min^{-1} , stretching the notched specimen in the direction perpendicular to the layer planes. The energy-related parameter, J-integral, was evaluated to characterize the inter-layer adhesion strength.

Different nozzle temperature (235 or 240°C), layer thickness ($t_L=0.2$ or 0.3 mm), deposition paths (aligned-rectilinear or concentric), and the use or absence of a cooling fan were considered in the printing process.

The uniaxial tensile tests show: (i) a change in the structure of the material, induced by the preliminary stretching, (ii) a residual strain present at the end of the unloading step, partially recovering with time, (iii) no significant effect of the printing parameters on the 3D printed specimen tensile response within the explored ranges.

From the fracture tests, a higher fracture resistance value was obtained for pure shear specimens printed at 240°C , with $t_L=0.2\text{ mm}$ and non-use of the cooling fan. Microscopic observations of the fracture surfaces are in progress to try to correlate the measured fracture toughness with the actual contact area and morphology of the fracture surfaces.

A soft hydrogel for processing and 3D molecular imaging of the human brain

Prof. Juhyuk Park¹

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Understanding the intricate architecture and function of the human brain is crucial for advancing treatments for neurological disorders. However, conventional imaging and histological techniques are constrained by the fragility and complexity of brain tissue, often requiring small biopsy samples that limit organ-scale investigations. To overcome these challenges, we introduce a functional soft material that chemically transforms intact human brain tissue into a stretchable, transparent biohybrid, termed mELAST (magnifiable entangled link-augmented stretchable tissue-hydrogel).

At the core of mELAST is an in situ polymer synthesis strategy that forms highly entangled, superhydrophilic polymer chains within the brain's native nanoporous network. By integrating with endogenous biomolecules, this soft material stabilizes delicate neural structures while preserving molecular integrity, enabling repeated mechanical thinning and controlled physical expansion of large tissue samples for multiscale imaging.

This functional soft material seamlessly integrates with existing histological and imaging pipelines, facilitating advanced tissue phenotyping at unprecedented speed and resolution. By maintaining native protein configurations and molecular markers, mELAST enables rapid multiplexed immunostaining and structural interrogation of neural circuits. The expanded tissues provide a high-fidelity platform to study cellular architecture, morphology, and connectivity in both healthy and diseased brain states.

Applications of mELAST in neurodegenerative disease research demonstrate its potential to uncover micro/nanoscale pathological features, such as amyloid plaques and neurofibrillary tangles in Alzheimer's disease, within large intact brain samples. The ability to spatially map neuronal and glial populations at an organ scale offers transformative insights into disease progression and neural network dysfunction.

By harnessing the principles of functional soft materials, mELAST transcends traditional limitations in brain tissue analysis. Its tunable thickness/size and molecular preservation capabilities redefine how we visualize and understand the human brain, providing an innovative platform for fundamental neuroscience, neuropathology, and precision medicine. This breakthrough paves the way for next-generation approaches in 3D human brain mapping, advancing our ability to decipher complex neural systems and develop targeted interventions for neurological diseases.

Aging and properties of sodium silicate hydrogels in subsurface environments

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A5_1, Andalucía III Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Hydrogels made from sodium silicate have been used as grout to reduce soil permeability and reinforce soil in civil engineering projects. However, their application as a grouting material is becoming more challenging due to urbanization and climate change adaptation, which require deeper injections in increasingly complex soil and groundwater conditions. At the same time, recent legislation mandates more comprehensive environmental impact assessments of hydrogels upon application.

Despite these challenges, little is known about the behavior of hydrogels in the subsurface. A thorough investigation is needed to understand how soil and groundwater composition influence their in-situ performance.

This presentation explores the impact of environmental factors on sodium silicate hydrogels, including soil organic matter, iron-bearing minerals, calcite, soil pH, groundwater composition, and hydrogel properties. Our experimental work characterizes gel properties based on rheology, porosity, microstructure, mechanical strength, chemical composition, and deformation rate. Using this characterization, we assess how soil and groundwater composition affect gel performance.

Overall, this study provides a database to support the selection of optimal grout formulations for soft gel applications aimed at reducing permeability, considering both environmental and engineering conditions.

3D-hydrogel matrix for *Synechocystis* sp. cultivation: mutual influence between microenvironment and microbial growth

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Physical confinement in natural highly hydrated 3D microenvironments influences the dynamics of bacterial growth [1]. Microbial loaded hydrogels have potential application in biocatalysis, bioremediation, and production of synthetic communities. However, the understanding of how engineered microenvironments influence microbial growth and metabolic activities is still limited.

One of the main features affecting microbial growth is the mechanical properties of the soft matter [2]. Here we study how an engineered 3D microenvironment affects microbial growth by providing structural cues that influence proliferation and metabolism. Besides, we want to evaluate how microbial activity can alter material stability. To this, *Synechocystis* sp. PCC 6803 was encapsulated in calcium alginate hydrogels, and the system was analyzed from both biological and material science perspectives.

The hydrogel composition was based on internal gelation of alginate with Ca²⁺, and its viscoelastic final properties were evaluated by frequency sweep in oscillatory dynamic mechanical measurement in linear viscoelastic regime. The crosslinking kinetic was followed by a time sweep test. We produced samples with a cell concentration of 107 cells per mL of hydrogel (Syn-Hy) and control hydrogels (C-Hy) without the addition of cells. The stability of the hydrogels, and bacterial growth and physiology (cytofluorimetry, microscopy, microelectrodes) were evaluated up to 27 days of culture at r.t. under controlled light conditions.

BG-11 was used as solvent for the hydrogel precursor solutions. However, the resulting hydrogels were not stable upon bacterial cells inclusion. Therefore, BG-11 composition was adjusted increasing Ca²⁺ concentration. The crosslinking times were minimally changed by the medium compositional change. The initial values of G' and G'' increased during the first day of immersion. For longer immersion times, Syn-Hy samples were macroscopically degraded, while C-Hy ones remained stable. Rheological properties steeply decreased for Syn-Hy, while C-Hy were slightly affected. From flow cytometry, *Synechocystis* growth rate in the hydrogel was comparable to that of the bacterial suspension in BG-11. Microscopy investigations showed the presence of heterogeneous microhabitats and the synthesis of extracellular polymeric substances within the hydrogel. Oxygen production confirms the photosynthetic activity of *Synechocystis*.

The obtained results indicate a reciprocal interaction between *Synechocystis* and the produced hydrogel, thus guiding the design of 3D matrices for microbial growth.

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Performance-optimized diatom-SiO_x anodes for Li-ion batteries by preserving the nanostructured SiO₂ shells of diatom microalgae and tailoring oxygen content

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Nanostructured silicon oxides (SiO_x) are promising anode materials for lithium-ion batteries (LIBs) due to their high capacity and excellent cycling stability. Nanostructured SiO₂ sourced from diatom microalgae holds great potential as a sustainable template for SiO_x synthesis via scalable magnesiothermic reduction (MgTR), which requires SiO₂ and Mg as reactants. However, the successful application of diatom-SiO_x in LIB technology relies on the ability to achieve precise control over SiO_x oxygen content while preserving the intricate nanoporous structure of diatom-SiO₂. This work explores, for the first time, the use of diatom-SiO₂ from industrially cultured microalgae as a precursor for SiO_x anodes through MgTR. Our findings reveal that partial reduction of diatom-SiO₂ to diatom-SiO_x occurs through the formation of Si nanocrystals embedded on the SiO₂ matrix. Particle nanostructure was found to be highly sensitive to the heat generated during MgTR, and it could only be preserved by adding controlled amounts of NaCl heat scavenger. Distinctive electrochemical performance of SiO_x anodes was achieved by modifying the amount of Mg on the reactants mixture. Anodes prepared with 1:1:2.5 SiO₂-to-Mg-to-NaCl molar ratio delivered optimal electrochemical performance, with superior capacity stability after 200 cycles. These findings provide key enablers for developing performance-optimized sustainable diatom-SiO_x anodes.

Multiscale porous carbon supports for PEMFC electrocatalysts

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A6_1 - Hydrogen generation - I, Machado Room (Level -2), septembre 15, 2025, 14:30 - 16:30

Proton Exchange Membrane Fuel Cells (PEMFC) are devices that produce electricity and heat from hydrogen and oxygen. They are foreseen to replace combustion engines in the future. However, they currently lack strong performances and durability. The cathode, one of the most critical component, is made of a nanostructured porous carbon layer decorated with electrocatalysts. Such mesoporous materials provide high specific surface area and encapsulates the electrocatalysts nanoparticles (Pt NPs), slowing down the degradation coming from NP coalescence, detachment or Ostwald ripening. However, upon electrochemical cycling, their small pores hamper the diffusion of species to the electroactive sites, thus limiting the performances of the PEMFC.

In our laboratory, we aim at developing graphene-based aerogels (GBA) which are carbons that are expected to show high durability since they display larger graphitic domains than regular porous activated carbon and could provide more stable anchoring sites for NPs. They are characterized by a hierarchical porosity, which should enable the fast diffusion of species through the larger macropores (up to 100 μm) to the interconnected micro and mesopores (1-100 nm) where the electrocatalysts NPs are located. We functionalize these carbons with Pt nanoparticles controlled in size and dispersion for the electrocatalysis of the oxygen reduction reaction. We then investigate the impact of the materials porosity on the electrochemical performances and durability of the PEMFC.

In this presentation, we will describe the different synthesis process specifically developed to design these materials with controlled surface chemistry and structure. The correlation between these materials porosity and electrochemical performances will then be discussed.

Hydrophobic materials and treatments for outdoor electrical insulation

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A6_8 - Energy harvesting from heat - II, Machado Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Outdoor electrical insulation materials are of fundamental importance for electrical distribution systems and related devices, such as instrument transformers, sensors, and embedded poles. On top of good electrical insulation, to withstand the outdoor environmental conditions, hydrophobic properties and UV protection contribute substantially to achieve good, long-time performance. Essentially, hydrophobicity is crucial for outdoor electrical insulation for several reasons:

Prevents water tracks: Hydrophobic surfaces resist the formation of water tracks, which can conduct electricity and increase leakage currents. Therefore, hydrophobicity helps in reducing the probability of flashovers and other deterioration effects.

Self-cleaning property: Outdoor insulators are often exposed to pollutants. Hydrophobic surfaces prevent contaminants from adhering, maintaining the insulator's electrical performance and reducing maintenance needs.

Improves longevity: Some self-healing hydrophobic materials can recover their hydrophobicity even after exposure to harsh conditions. This self-healing property extends the lifespan of the insulators by retaining self-cleaning properties and preventing water tracks.

These properties make hydrophobicity a key factor in ensuring the reliability and durability of outdoor electrical insulation devices. On top of their surface performance requirements, the material composition of outdoor insulation systems needs to comply with current and future regulations. Therefore, we are looking at sustainable material solutions with good hydrophobic properties, while at the same time, we investigate the possibilities of having a circular approach for the end-of-life products. Given the fact that these insulating materials are typically thermosetting polymers in their nature to survive the long-term exposure to outdoor conditions, their recyclability is an additional challenge.

In this work we are exploring 3 pathways to find alternative, more eco-friendly materials for serving the needs of outdoor electrical insulation. Specifically, we look at 1) bulk composition modification, 2) coatings, and 3) physical surface roughening towards the enhancement of hydrophobic performance. We discuss the advantages and disadvantages of these approaches, and we show a few examples. We also discuss methods for characterizing their performance which includes the evaluation of static and dynamic wetting properties, as well as more specific to the application tests, such as the measurement of leakage currents, tracking and erosion, etc. Based on such measurements we define what experimental outcomes are desired for a material to be considered as a good performing outdoor electrical insulator.

Finally, we also analyze potential recycling strategies of decommissioned products, that so far are typically sent for landfilling or being incinerated. We discuss how this could contribute towards a circular economy and responsible waste management.

All-day Passive Radiative Cooling Performance of Porous Materials

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A6_5 - Improving Energy in Buildings - II, Machado Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Nowadays, a third of the total energy demand is destined for cooling due to the consequence of the global warming, which results in higher temperatures and heatwaves. All-day passive daytime radiative coolers (PRC) offer a promising solution for energy-free cooling of buildings and devices. At the same time, it is important to develop low-cost, easy-scalable to industry materials. In this talk, I will present 1D and 3D- anodic aluminium oxide (AAO) nanostructures on Al as a passive daytime radiative cooler. I will analyse how all the morphological properties and chemical structure of porous alumina nanostructures on Al influence on their optical properties and their radiative cooler properties. A maximum cooling temperature of 10.2 °C was reached under direct sunlight in a summer day in Spain for 3D-AAO. This cooling performance results of AAO nanostructures are higher than over previous studies, demonstrating the potential of AAO nanostructures to be used in thermal management applications. Moreover, I will present the use of various cellulose-derivative networks (porous materials) to achieve optimal and stable cooling performance. Our results showed that nitrocellulose network showed the highest cooling temperature, with a significant reduction of 14 °C from the ambient temperature and a power of 124 W/m² during the daytime and at night of 7.7 °C and 72.8 W/m². This study also analysed the dampness's effect on the cooling performance of cellulose-derivative networks. We observed that the cooling performance of nitrocellulose network drops ~3 °C (from 14 to 11.3 °C) when the humidity exceeds ~30%. Our findings indicate that the capacity of a material to absorb water from the surrounding air significantly influences its performance as a passive cooler, primarily due to changes in its optical properties. This is an important insight, as it highlights the need to consider environmental factors like humidity and sample hydrophobicity for PRC systems.

Flexible OPC-Polymer Composites for thermal management

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A6_4 - Improving Energy in Buildings - I, Machado Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Thermal management has become a key factor for a wide range of industrial areas, from buildings and renewable energy to automotive and electronics. Moreover, the increasing miniaturization and higher power density of the new generations of electronic devices require more efficient solutions for thermal management in ever smaller spaces. In addition, the emergence of flexible devices, such as wearables and foldable displays, introduces new challenges requiring materials that combine thermal efficiency, flexibility and shape adaptability.

In this context, phase change materials (PCMs) are considered outstanding tools for thermal management due to their ability to absorb or release large amounts of energy during their phase transitions. However, solid-liquid PCMs present safety-related limitations, such as the risk of leakage, which complicate their integration into advanced devices.

A promising alternative is the use of solid-solid PCMs, which eliminate these problems due to their shape stability during phase changes. Within this category, organic plastic crystals (OPCs) are promising materials with highly energetic phase transitions and the possibility to tune their working temperature over a wide temperature range, spanning 40 to 180 °C. These characteristics make them ideal candidates for specific thermal applications. However, the lack of flexibility and limited shape adaptability of OPCs restrict their use in flexible thermal management systems, posing a significant challenge for their implementation in practical applications.

In this sense, the aim of this work is to fabricate new flexible solid-solid PCMs based on OPCs in a simple way. For this purpose, Neopentyl glycol (NPG) powder is mixed and processed with PTFE particles in a mortar. During the processing step, these particles undergo spontaneous fibrillation, which leads to the formation of a nanofiber network that traps the NPG powder, resulting in a shape-stable material. The materials obtained by this method show good flexibility and shape adaptability, being able to be kneaded, folded and implemented on a variety of surfaces, as well as being shaped into films or pellets. DSC and TGA analysis show that the melting temperature, enthalpy and degradation temperature of NPG are not affected by the addition of PTFE. Furthermore, it is observed that the subcooling of NPG is reduced by 30% when combined with 5% PTFE. Finally, the hydrophobic properties of NPG are also improved, drastically increasing the contact angle with water. Overall, the results show that this strategy gives rise to materials with potential for being implemented in complex device thermal management systems.

Direct evidence of the presence of hybrid charge transfer state in a perovskite nanocrystal -polythiophene blend solid state film

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A6_9 - Supercapacitors, Machado Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

In recent years, metal halide perovskite semiconductors (MHPs) have demonstrated their exceptional capabilities in the optoelectronic field. This can be ascribed to their outstanding intrinsic photoelectric properties, such as high light harvesting abilities, long and balanced carrier diffusion lengths, high defect tolerance, high photoluminescence quantum yields and readily tunable bandgaps. Despite these interesting features, the lack of long-term operational stability still prevents the use of lead halide perovskites in general, and of their nanocrystals [NCs] in particular, in commercially available devices. To overcome this problem interesting is the possibility of blending perovskite NCs with semiconducting polymers, able to stabilize perovskites by improving film morphology and environmental stability. Additionally, their electronic properties enable the creation of hybrid materials that combine the electrical and optical characteristics of both components. In this work we investigate by ultrafast spectroscopy and morphological characterisation the photophysical properties of a hybrid material composed by a conjugated polymer and perovskite nanocrystals. The relaxation dynamics of a drop-casted film from the semiconducting polythiophene (P3HT) and a green-emitting CsPbBr₃ (zwitterionic sulfobetaine -capped) perovskite nanocrystals (NCs) solution is studied. The transient spectroscopy presents a very long photobleaching signal peaked at 516 nm not present in the single components of the blend. The scanning electron and confocal fluorescence microscopy images show that the P3HT and the CsPbBr₃ NCs are finely mixed in the film. We propose the presence of a very efficient charge transfer from the nanocrystal to the polymeric chain which induces the formation of a long-lived charge-transfer state as we see in the pump-probe measurements. The theoretical model reveals the important role of the zwitterionic sulfobetaine capper in this process. The perovskite strongly adsorbs the surfactant, while the polythiophene chain is not directly bound to the perovskite. Instead, it interacts with the surfactant itself, contributing to the electronic properties of the overall system.

Internal Structure and Cycling Performance of Atomized Silicon Composite Anodes for Lithium-Ion Batteries

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Silicon is a promising anode material for high-energy-density lithium-ion batteries due to its high theoretical capacity. However, its practical application is hindered by significant volume expansion during charge-discharge cycles, leading to mechanical degradation and capacity fading. To address this challenge, we synthesized multicomponent silicon composite powders using gas atomization. These powders were primarily composed of silicon, aluminum, copper, nickel, and boron, with tailored composition ratios designed to optimize their internal structure and electrochemical cycling stability. This study discusses how the internal structure of each powder, influenced by differing compositions and manufacturing process conditions, affects their initial specific capacity and capacity retention over 35 cycles. It further explores the relationship between the internal structure and electrochemical cycling stability, tested in coin cells using lithium metal as the counter electrode and an electrolyte containing LiPF₆, with formation and cycling conducted in a voltage range of 0.005–1.5 V vs. Li/Li⁺.

Focused Ion Beam (FIB) milling at 300 nm intervals, combined with Energy-Dispersive Spectroscopy (EDS), was employed to characterize the internal structure and composition of the powders with a diameter of 2 μm . The cross-sectional structure of the multicomponent silicon powder consists of discrete silicon-rich regions of approximately a few hundred nanometers embedded within a continuous silicide matrix. The volume fraction of silicon within this matrix was quantitatively assessed. Additionally, cross-sectional nanoindentation tests were conducted to evaluate the mechanical properties of each powder and their relationship to structural features.

Results indicated that powders with higher silicon volume fractions exhibited greater initial specific capacity. However, powders with higher nano-hardness exhibited lower capacity retention after 35 cycles. This phenomenon is attributed to the lack of deformation capability of the silicide matrix in high-hardness powders, which hinders its ability to buffer the volume changes of silicon during cycling. The silicide matrix likely acts as a mechanical buffer, mitigating the volume changes of silicon during charge-discharge cycles and enhancing the structural integrity of the composite. This study provides insights for further optimizing atomized multicomponent silicon composite anodes in next-generation LIBs, contributing to the development of durable and high-capacity silicon anodes for more efficient and reliable energy storage systems.

The discovery of Ta₂Ni₃S₈: a new fiber-like crystal structure with promising thermoelectric properties

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A6_7 - Energy harvesting from heat - I, Machado Room (Level -2), septembre 17, 2025, 14:30 - 16:30

Our quest for new materials for thermoelectric applications has led to the discovery of a completely new material, previously undescribed in any material database. The novel compound, Ta₂Ni₃S₈, was synthesized in a quartz ampoule in the form of low-dimensional fibrous grains, making the determination of its crystal structure highly complex. Conventional X-ray diffraction tools were insufficient for resolving its structure. Consequently, the precession electron diffraction tomography method [1-3], combined with dynamical calculations [4-5], was employed to solve and refine the structure on an individual fiber isolated on a carbon grid. The material is characterized by the space group I4/m (No. 87), with unit cell parameters $a = 23.853(4)$ Å and $c = 3.2962(4)$ Å.

The evaluation of the transport properties was carried out on pellets fabricated by spark plasma sintering. However, due to its fibrous nature, the material exhibits strong anisotropy (up to 6x between along and across fibers) in transport properties. Intrinsically, Ta₂Ni₃S₈ shows n-type conductivity, with a Seebeck coefficient ranging from -100 to -150 µV/K. To assess the thermoelectric potential of this material, several doping trials were performed using W, Cu, Cl, Ni, and Sb. Notably, Ta₂Ni₃S₈ doped with Cu demonstrated a power factor along the fibers of 700 - 1200 µW·K⁻²·m⁻¹ from RT to 460°C making this material an interesting candidate for further optimization.

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EFFECT OF THE SINTERING TEMPERATURE ON THE WEATHER RESISTANCE OF ANTI-SOILING COATINGS FOR SOLAR APPLICATIONS

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A6_4 - Improving Energy in Buildings - I, Machado Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Anti-soiling (AS) coatings are critical for improving the performance of concentrated solar thermal (CST) systems by reducing surface soiling and maintaining high transmittance in glass covers. These coatings are particularly valuable as they help reduce the frequency and amount of water needed for cleaning, contributing to the sustainability and cost-effectiveness of CST operations. The coatings were prepared by dip-coating from sol-gel precursor solutions. Two fluorinated compounds with different chain lengths (F1 and F2) were used to provide hydrophobic character to the coatings. In addition, two sol-gel processes: one involving reflux and another without reflux (NR) were studied. In this work, the effect of sintering temperature on the properties of hydrophobic AS coatings was evaluated.

Three sintering temperatures were studied: 200 °C, 400 °C, and 500 °C. At higher sintering temperatures, an increase in transmittance was observed, which is attributed to the removal of organic components, resulting in more transparent coatings. However, the static water contact angle (WCA) decreased as the sintering temperature increased. Abrasion resistance was assessed over 500 cycles, and the results showed differences based on the fluorinated compound and the sol-gel process used. The coatings abrasion resistance was studied by using a Taber linear abraser. The coatings prepared with the longer fluorinated chain (F2) exhibited better resistance to abrasion, as demonstrated by the lower increase in surface roughness (Ra) over 500 cycles and the higher retention of normalized transmittance compared to those prepared with F1. This behavior indicates that the longer fluorinated chain enhances the mechanical durability and optical stability of the coatings under abrasive conditions. Notably, the difference between F1 and F2 was more pronounced at higher sintering temperatures, where F2 coatings consistently maintained lower roughness and higher transmittance. Similarly, coatings obtained through the reflux method displayed superior abrasion resistance compared to the NR variants. This advantage is evident in the slower degradation of normalized transmittance and the more stable roughness values for the reflux coatings, regardless of the fluorinated compound used.

The results indicate that sintering temperature, fluorinated compound, and sol-gel process all influence the mechanical behavior of AS coatings. In addition to the abrasion tests, results from accelerated aging and further environmental durability studies will also be presented, providing a comprehensive evaluation of the performance of these coatings under real conditions.

Intrinsic Plasmonic Heating in Bismuth Telluride Nanostructures: Enhancing Thermoelectric Performance through Geometric and Nanostructure Modifications

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A6_7 - Energy harvesting from heat - I, Machado Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

This study explores the potential of plasmonic heating in bismuth telluride (Bi_2Te_3) nanostructures as a pathway to enhance their thermoelectric performance without the need for external metallic plasmonic nanoparticles. By harnessing surface plasmon resonances inherent to nanostructured Bi_2Te_3 , we demonstrate localized temperature increases that improve thermoelectric efficiency. Utilizing template-assisted electrochemical deposition, we fabricated 1D nanowire arrays and 3D nanowire networks, systematically evaluating their plasmonic heating performance through Raman spectroscopy under various excitation wavelengths.

Our results reveal that 3D nanowire networks exhibit significantly higher plasmonic resonance intensities compared to 1D arrays, leading to more pronounced localized heating. This enhanced thermal gradient, driven by plasmonic heating, can improve energy conversion efficiency in thermoelectric applications. Unlike traditional approaches that rely on metallic nanoparticles to induce plasmonic effects, our findings underscore the capability of Bi_2Te_3 nanostructures to independently generate and optimize plasmonic heating through geometric and structural modifications. The unique plasmonic properties of Bi_2Te_3 , a topological insulator, stem from its topological surface states, which enable visible-range surface plasmon resonances. These resonances can be tailored by engineering the size, shape, and arrangement of nanostructures, offering a versatile platform for enhancing both plasmonic and thermoelectric functionalities. The 3D nanowire networks, in particular, demonstrate superior plasmonic heating capabilities due to their increased surface area and enhanced light-matter interactions, highlighting their potential for next-generation thermoelectric devices.

This work not only advances the understanding of plasmonic interactions in topological insulators but also opens new avenues for the design of sustainable energy technologies. By strategically optimizing Bi_2Te_3 nanostructures to exploit plasmonic heating mechanisms, we provide a pathway for developing high-efficiency thermoelectric devices. These findings emphasize the importance of integrating plasmonic and thermoelectric properties at the nanoscale, offering a transformative approach to energy conversion and thermal management in advanced material systems.

In summary, our study establishes the foundation for leveraging intrinsic plasmonic heating in Bi_2Te_3 nanostructures, paving the way for innovative applications in thermoelectric energy conversion. Future research can build upon these insights to further enhance device performance through precise nanoscale engineering of plasmonic and thermoelectric interactions.

Enhancing Lithium-Ion Batteries: Advanced Architectures for High-Performance LiFePO₄ Cathodes

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A6_6 - Batteries - II, Machado Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

The increasing demand for sustainable energy solutions and the rapid expansion of the electric vehicle (EV) market have placed significant focus on lithium-ion batteries as a critical enabler of these technologies. Among the various cathode materials, lithium iron phosphate (LiFePO₄, or LFP) has emerged as a compelling option due to its superior thermal stability, inherent safety, and cost-effectiveness. LFP's long cycle life and resistance to thermal runaway make it an ideal candidate for large-scale applications, including EVs and renewable energy storage systems. Moreover, its reliance on abundant, non-toxic raw materials positions it as a sustainable alternative to nickel- and cobalt-based chemistries. However, despite these advantages, LFP suffers from kinetic limitations that hinder its performance under high-power and fast-charging conditions, restricting its broader adoption in energy-intensive scenarios such as electromobility.

The primary objective of this study is to overcome the kinetic limitations of LFP by designing and optimizing a novel cathode architecture. This approach aims to enhance the transport of lithium ions and electrons, thereby improving the electrochemical performance of LFP-based batteries at high current rates.

To achieve this, the research focused on combining the morphology of LFP particles with conductive additives to act synergistically, enhancing ion and electron transport. Through the optimized manufacturing and drying process of the cathode film, the alignment of internal structures was achieved, resulting in highly interconnected networks. The microstructural characterization of the cathodes and their components was conducted using advanced techniques, revealing improved structural connectivity and alignment. Electrochemical characterization, including rate capability tests and cycling stability, demonstrated the superior performance of the proposed architecture compared to alternative designs.

The results showed that the aligned cathode architecture significantly improves energy transfer efficiency, enabling enhanced performance under high current rates. Additionally, this design mitigates traditional kinetic challenges while improving durability and energy efficiency. These findings highlight the scalability and practicality of the proposed approach, offering a promising pathway for industrial-scale production of fast-charging LFP-based batteries.

This study presents a significant advancement in LFP cathode engineering by integrating material design with alternative and low cost manufacturing techniques. Unlike prior studies, which often focus on improving either the material properties or the electrode structure in isolation, this work demonstrates the transformative impact of aligning both aspects. The resulting architecture not only bridges the gap between material performance and industrial application but also sets a new benchmark for high power, fast charging lithium ion batteries.

Towards printed zinc-lignin batteries

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Printed electronics involves using printing technologies as a mass production tool to integrate electronic circuits, sensors, and wireless communication on a flexible label, making any kind of object interactively connected to the internet. This is the "Internet of Everything," which is expected to connect billions of electronic labels to the internet. Powering these devices with conventional batteries presents a sustainability challenge in terms of material recycling and expensive maintenance. Today, bulky batteries are increasingly being replaced by low-power energy harvesters (e.g., thermoelectrics, solar cells, piezoelectrics) that charge thin batteries without the need for maintenance. The technical specifications for these types of thin batteries include high cyclability, high power, green materials, low cost, and compatibility with printed technologies, rather than the high energy density required in other sectors such as mobile phones.

The greenest materials come from biomass. Lignin is of particular interest because it is an aromatic biopolymer that carries catechol groups capable of storing charges through electrochemical reactions. First, we explore the design of lignin electrodes by compositing with carbon or conducting polymers [1-3]. Second, a new class of electrolyte operating in the "water-in-polymer salt electrolyte" regime is considered to enable aqueous organic batteries with low self-discharge behavior [4-6]. Finally, we integrate these materials into a robust and promising zinc-lignin battery [7-8].

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Phase Changing Materials for efficiency improvement of Luminescent Solar Concentrators smart windows

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A6_4 - Improving Energy in Buildings - I, Machado Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Commercial and residential buildings are the source of almost 40% of global CO₂ emissions and energy consumption. Building Integrated Photovoltaics (BIPV) and Phase Change Materials (PCMs) are promising technologies for reducing the carbon footprint of buildings.

PCMs can store large amounts of energy through their phase transition while maintaining constant temperature, releasing that stored energy with a significant time delay. Luminescent Solar Concentrators (LSCs) are photovoltaic devices perfect for BIPV applications thanks to their transparency. They are made of a waveguiding material encapsulating a film functionalized with a fluorophore that partially absorbs solar radiation and emits fluorescence light that is waveguided to PV cells optically coupled to the edges. However, the Power Conversion Efficiency (PCE) of LSCs is limited by three main factors: amount of light absorbed, emitted and waveguided to the cell, efficiency of PV cells and efficiency derating of cells caused by high operational temperature. The first two factors are hard to modify in BIPV applications because of implementation costs and light management for indoor visual comfort. Thermal management of the Nominal Operating Cell Temperature (NOCT) via PCMs is an effective and low-cost solution to achieve higher PCEs without changing the other conditions. Above 25°C NOCT, a silicon PV cell can experience a PCE derating of 0.4-0.65%/°C.

This work consists of thermal simulations performed via "COMSOL Multiphysics" of LSCs solar windows combined with PCMs to evaluate the impact of PCMs on the NOCT of PV cells coupled to the LSCs. The simulations employ the Finite Element Method (FEM) and were performed based on weather data from different geographic locations. The 1m*1.4m simulated windows in both single- and double-glazed structures are framed in a PVC structure modeled to be full of air in one case and full of PCMs in the other.

Preliminary results show that the integration of a PCM with a melting point of 36°C and latent heat capacity of 240 kJ/kg can significantly reduce the NOCT of PV cells, up to 6°C in the considered locations. The temperature decrease leads to a +2.95% PCE per each cell, meaning +11.80% for the entire LSC. Performances can be further optimized by considering the coupling of several PCMs with different melting points. The effects of the PCMs are not only seen around the melting point but also at lower temperatures as their lower thermal diffusivity compared to air strongly attenuates the temperature increase inside the frame.

Exceptional stability of solid-state radical-anions in perylenediimide-polyethyleneimine polymers for energy applications

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A6_9 - Supercapacitors, Machado Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The search for organic materials with tunable redox properties and high stability is crucial for advancing electro-optical devices for energy conversion and storage. Perylenediimide (PDI)-based radical anion has emerged as promising candidates for solar energy harvesting due to their broad absorption in the visible and near-infrared (NIR) regions and their ability to participate in Consecutive Photoinduced Electron Transfer (ConPET) processes, offering significant potential for applications such as photocatalysis, photobatteries, and dye-sensitized solar cells. However, the limited stability of these radicals under ambient conditions, particularly in the solid state, remains a major obstacle.

In this communication, we present the synthesis and characterization of a series of novel materials based on polymers composed of perylenediimide and hyperbranched polyethyleneimine (PDI-PEI). By varying the PEI/PDI ratios, we achieved the isolation of the radical anion exhibiting exceptional solid-state stability for several months. The presence of the radical anion was assessed in all synthesized materials. Their unprecedented stability was confirmed by various spectroscopic techniques, including electron paramagnetic resonance (EPR) and Raman spectroscopy. We hypothesized that the anion radical is generated through internal electron transfer between the amine groups of PEI and the carbonyl groups of PDI promoted by light absorption. Furthermore, we propose that PEI enhances the stability of the PDI radical anion by providing steric protection. The photoactive behavior of the materials was assessed by solid-state UV-Vis-NIR absorption spectroscopy, revealing strong absorption across the visible and NIR regions, making them suitable for broadband solar light harvesting. Furthermore, the redox properties of the radical anion are also investigated. Structural information about the molecular arrangement and chemical composition of the materials is evaluated by solid ¹³C-RMN and X-Ray diffraction (XRD) and thermal stability is evaluated by Thermogravimetric analysis. Finally, the compatibility of the material with indium tin oxide (ITO) substrates is demonstrated by depositing thin and homogeneous films using spray coating and spin coating techniques, maintaining the anion radical stability at the PDI-PEI/ITO interface. Future studies are planned to investigate device performance, including its evaluation as an interlayer in solar cell prototypes, and modulating the material's properties through chemical modifications to optimize its performance in energy applications.

Ion beam engineered earth-abundant electrocatalysts for Hydrogen generation

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A6_1 - Hydrogen generation - I, Machado Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Electrocatalysts are at the heart of green hydrogen and ammonia production. Cost-competitive hydrogen requires GW-scale electrolyser production coupled with a significant drop in current manufacturing costs. Earth-abundant alternatives to platinum compatible with large-scale manufacturing is therefore highly desirable. On the other hand, realising electrochemical ammonia production demands highly selective catalysts for dinitrogen activation. In this work, we present a novel electrocatalyst fabrication approach based on ion implantation that can be optimised for both hydrogen evolution reaction (HER) and nitrogen reduction reaction (NRR).

Transition metal carbides (TMC) and nitrides (TMN) have attracted significant interest as cathode electrocatalysts for HER and NRR, respectively. The inability to manufacture TMCs as ultra-fine nanoparticles (to achieve high surface area) has hindered their catalytic potential for HER. Conventional routes require high synthesis temperatures leading to uncontrollable agglomeration, drastically reducing their active surface area. Using ion implantation, we demonstrate synthesis of tungsten and molybdenum carbides with high activity towards HER (TOF > 10 H₂ s⁻¹) [1-3]. With high-resolution TEM and X-ray photoelectron spectroscopy, we demonstrate synthesis of rare metastable phases of TMCs (e.g., γ' -MoC known for HER activity comparable to Pt) at dimensions as low as 2-3 nm. We show that by careful selection of synthesis parameters, the phase and size of the TMC particles can be controlled consequently affecting their HER activity.

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Evolution of defects for high thermoelectric power factor in copper iodide films

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A6_8 - Energy harvesting from heat - II, Machado Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Copper iodide (CuI) is a wide-bandgap semiconductor and a sustainable thermoelectric material suitable for transparent thermoelectric and smart window applications[1]. However, it suffers from poor electrical transport properties due to its low electrical conductivity (σ), which leads to a low power factor ($\alpha^2\sigma$), where α is the Seebeck coefficient, thereby reducing its thermoelectric energy conversion efficiency. Defect engineering is an effective method for tuning its electronic band structure and modifying defect complexes to improve the power factor[2]. Ion implantation is a versatile microfabrication doping technique that allows for controlled introduction of suitable dopants and modulation of point defects[3].

In this paper, we report on the defect engineering by implanting noble gas ions (Ne, Ar, and Xe)[4] or chalcogen ions (S, Se, and Te)[5,6] into cubic zinc blende γ -CuI films[7] using a GNS low-energy ion implanter. Density functional theory and Monte Carlo calculations revealed that the substitution of chalcogen elements (Ch) at the iodine site (ChI) and the copper vacancy (VCu) defect complex exhibited a shallower acceptor transition than isolated ChI and VCu defects. Noble gas ions led to the abundant production of Frenkel pairs, which suppressed compensating donors in CuI and increased hole density. The implantation generated point defects favored formation of defect complexes with the dopants, simultaneously increasing α and σ , resulting in a high power factor. Our results demonstrate that defect engineering via implantation is an effective strategy for enhancing the power factor and achieving high thermoelectric efficiency.

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Modification of the stoichiometric and the reduced SnO₂ (110) surface by transition metal doping: density functional study

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembere 15, 2025, 13:15 - 14:30

SnO₂ is a wide gap semiconductor, which has excellent properties for selective detection of various gases, catalysis and optoelectronic devices. Many experimental studies showed that the transition metal (TM) doping is a way to enhance its performances. Using the modified density functional calculations we study the relative stability of the stoichiometric and the reduced SnO₂ (110) surfaces, as well as the influence of transition metals doping on their stability and electronic structure. In our study we consider models of the surface with different positions and concentrations of oxygen vacancies. We find that the substitutional doping of TM for Sn induces the structural relaxation and the charge modification around the involved atoms. In some of the investigated cases it also introduces surface states within the band gap. The obtained results for the structural relaxations and energetics are compared with available previous theoretical and experimental data.

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Functionalized PVDF-based terpolymers for pyroelectric energy harvesting

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A6_10 - Polymers for energy, Machado Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Polyvinylidene fluoride (PVDF) and its copolymers is recognized as the most performing ferroelectric polymer, with applications in energy harvesting, sensing, haptics, high-k dielectrics, and others. Recently, the relaxor ferroelectric terpolymer P(VDF-TrFE-CFE) that comprises trifluoroethylene (TrFE) and chlorofluoroethylene (CFE) monomers has been functionalized with addition of fluorinated alkyls (FA). The obtained tetrapolymer P(VDF-TrFE-CFE-FA) was found to display an unprecedented electromechanical coupling and a gigantic piezoelectric coefficient of 1000 pm/V [Science 375, 1418 (2022)], similar to the best inorganic materials. It would be interesting to explore the perspective of employing the tetrapolymer in pyroelectric harvesting applications. However, reports on its pyroelectric performance are currently lacking. In this work we functionalized P(VDF-TrFE-CFE) and P(VDF-TrFE-CTFE) terpolymers (where CTFE stands for chlorotrifluoroethylene monomers) with fluorinated alkynes of various fractions. After verification of the successful chemical modification by means of NMR, the phase transitions of the resulting tetrapolymers have been studied by DSC. The polymer structure (crystalline phases, crystallite domain size, crystallinity) has been studied by means of x-ray scattering in bulk and film form. Simple capacitors have been fabricated and the generated pyroelectric current has been recorded. The structure-function relationships are derived and rationalized.

Effect of Deposition Temperature on the Thermoelectric Properties of MnFe_2O_4 Thin Films

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A6_8 - Energy harvesting from heat - II, Machado Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

This study investigates the influence of deposition temperature in the pulsed laser deposition (PLD) process on the structural and thermoelectric properties of manganese ferrite (MnFe_2O_4) thin films. Deposition temperature plays a crucial role in determining crystallinity and preferential growth orientation, with higher temperatures enhancing crystallinity and promoting growth along the [311] crystallographic direction. These trends were confirmed through X-ray diffraction (XRD) analysis and morphological examination via scanning electron microscopy (SEM) and transmission electron microscopy (TEM), which revealed well-defined crystalline structures at elevated deposition temperatures.

To further optimize the thermoelectric performance, post-deposition annealing was carried out under different atmospheric conditions, including air, oxygen, argon, and a reducing environment ($\text{Ar} + 1\% \text{H}_2$). The thermoelectric properties were characterized in terms of the Seebeck coefficient (S) and sheet resistance (R_s) at room temperature, revealing significant anisotropy effects influencing charge transport. Among the investigated samples, the highest Seebeck coefficient was observed for the film deposited at 700 °C, with a value of $-665 \mu\text{V/K}$ at room temperature, indicating n-type semiconductor behavior.

However, thermoelectric measurements conducted over a temperature range from room temperature to 350°C exhibited variations, suggesting a complex interplay between crystallinity, grain orientation, and charge transport mechanisms. Notably, the highest power factor of $6.5 \mu\text{W}/(\text{m}\cdot\text{K}^2)$ was achieved at 350°C for the film deposited at 200 °C, despite its lower crystallinity at room temperature. This finding suggests that thermally activated charge transport mechanisms significantly contribute to the overall thermoelectric performance.

Post-deposition annealing played a crucial role in modifying the film structure and transport properties. Annealing in oxidizing atmospheres (air or O_2) led to phase transformations into hematite, drastically reducing electrical conductivity. In contrast, reducing conditions ($\text{Ar} + 1\% \text{H}_2$) altered the preferential crystal orientation from [311] to [111], introducing an additional unidentified phase. Annealing in pure argon at 300°C successfully preserved the [311] orientation while maintaining favorable electrical conductivity, highlighting the importance of controlled thermal treatments for optimizing thermoelectric performance.

This work demonstrates that both deposition temperature and post-deposition annealing significantly affect the crystallographic orientation and thermoelectric behavior of MnFe_2O_4 thin films. The findings provide valuable insights into tailoring the structural and electronic properties of spinel ferrites for thermoelectric applications.

ALL-PRINTED, ORGANIC THERMOELECTRIC GENERATORS ON FLEXIBLE SUBSTRATES

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A6_7 - Energy harvesting from heat - I, Machado Room (Level -2), septembre 17, 2025, 14:30 - 16:30

To meet current environmental challenges, researchers are looking to develop new methods of energy production that would provide an alternative to fossil fuels, while also reducing the greenhouse gas emission. Within this context, thermoelectric materials, i.e. materials capable of converting heat into electricity, have been arousing growing interest over the last twenty years, as they could help to meet the quest for energy.¹ The many advances on organic semiconductors (OSCs) are showing ever better conductive properties, in addition to their improvable high electrical conductivity, and an intrinsic low thermal conductivity, which is in line with the optimisation of the figure of merit quantifying thermoelectric efficiency, namely zT . This makes OSCs ideal candidates for thermoelectric devices. Compared with inorganic semiconductors, OSCs offer several advantages, such as their better processability in the liquid phase (enabling the use of printing techniques), their flexibility, their mechanical robustness and their competitive cost². In this work, we will present the fabrication and characterisation of fully printed thermoelectric generators on flexible polyimide substrates. These generators are composed of two legs, electrically connected in series. The first leg is made using a p-type OSC, namely poly(3,4-ethylenedioxythiophene) polystyrene sulphonate (PEDOT: PSS), in the form of a commercial ink deposited by ink-jet printing. The second leg is made using an n-type OSC, namely poly(3,7-dihydrobenzo[1,2-b:4,5-b']difuran-2,6-dione) (PBDF) synthesised from protocols described in the literature³ and deposited here by ink dispensing. We will present the formulation of the inks, the characterisation of their rheological properties and the electrical properties of the printed layers. Then, we will describe the fabrication of the full generators and their complete thermoelectric characterisation (I/V and V/T curves, output power measurements). While exposed to a temperature gradient of 13K/cm, our generators exhibit a Seebeck coefficient as high as 35 $\mu V/K$ and an output power of 2 nW for a p-n pair measuring 6 cm² and approximately 1 μm thick. Finally, we will present the outcome of the mechanical tests of these flexible thermoelectric generators, in order to investigate the impact of flexibility on their thermoelectric performances.

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Ambient deposition of single atoms for enhancement of nanostructured metal oxide electrodes

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A6_2 - Hydrogen generation - II, Machado Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Cutting-edge technology utilizes single-atom decoration to enhance heterogeneous catalysis at the atomic level. However, single atoms often aggregate into nanoparticles due to high surface energy. To counter this, we modify surfaces with nanostructured support layers like TiO₂ nanotubes, nanosheets, and NiO nanosponge. Anodization facilitates precise fabrication of well-ordered oxide nanostructures and nanotubes. Gentle defect-engineering methods like room-temperature sonochemical treatment, UV-light irradiation or pH-control are employed to trap Pt, Ir and V single atoms effectively. UV-light radiation induces Ti³⁺ and oxygen vacancies onto TiO₂ nanosheets, enabling efficient Pt single-atom decoration. Sonochemically treated TiO₂ nanotubes exhibit promising performance in H₂ evolution catalysis. Thermal annealing in a reductive atmosphere facilitates the anchoring of single Ir atoms onto NiO nanostructures, further stabilized by ultrasound-driven methods. Characterization involves microscopy (FESEM, TEM, HAADF-STEM) and spectroscopy (XPS, ToF-SIMS). Especially time-of-flight secondary ion mass spectrometry (ToF-SIMS) shows a unique capability of identifying co-catalysts in a single-atomic state on the support. Gas chromatography evaluates H₂ photocatalytic performance, while linear sweep voltammetry assesses H₂ and O₂ electrochemical activity. The demonstrated deposition techniques significantly enhance the efficiency of nanostructured oxide electrodes modified with stable single-atom co-catalysts through gentle treatments.

High Thermoelectric Performance of Copper Selenide and Silver Selenide electrodeposited films

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A6_7 - Energy harvesting from heat - I, Machado Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

The growing interest in thermoelectric applications has driven a shift towards affordable, sustainable and easily scalable materials that continue to offer high performance, such as copper selenide (Cu₂Se)[1-2] and silver selenide (Ag₂Se)[3]. In this work, copper selenide and silver selenide films with different compositions were grown by electroposition using new optimized solutions. The structural, morphological and compositional characteristics of the films were analyzed by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and X-ray fluorescence (XRF). The thermoelectric properties, such as electrical conductivity (σ), Seebeck coefficient (S) and thermal conductivity (k) of the films were also measured. Maximum power factors ($PF=\sigma \cdot S^2$) of $912 \pm 188 \mu\text{W}/\text{m}\cdot\text{K}^2$ and $3464 \pm 714 \mu\text{W}/\text{m}\cdot\text{K}^2$ were obtained for the copper selenide and the silver selenide films, respectively, surpassing all previous records reported in the literature for films[4-5]. These results set a new benchmark for electrodeposited Cu₂Se and Ag₂Se films, advancing high-performance thermoelectric materials.

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Passive Radiative Cooling Performance of Nanostructured Poly(vinylidene fluoride) (PVDF) inside Aluminium Anodic Oxide (AAO)/Al

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A6_5 - Improving Energy in Buildings - II, Machado Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

The last few decades have seen a significant increase in energy consumption associated with conventional refrigeration, which aggravates environmental problems related to pollution and global warming. In this context, new technologies that do not rely on external energy supply, like Passive Daytime Radiative Coolers, are being developed. For a material to have potential as a 24-hour radiative cooler, it must have a high reflectance in the solar spectrum and a high emittance in the infrared, in particular, in the atmospheric transmission window between 8-13 μm .

Among the materials used for this application are polymers, like Poly(vinylidene fluoride) (PVDF). This material has a high infrared emissivity associated with the vibrational modes of the functional groups that compose them. Furthermore, studies have shown that their nanostructuration enhances their solar reflectance. One way to achieve this is through their infiltration inside one- and three-dimensional Aluminium Anodic Oxide (AAO) templates. Their morphological properties such as inter-channel distance or pore diameter can be tuned to obtain the highest reflectance values possible.

In this work, 1D- and 3D- PVDF metamaterials have been obtained by their infiltration inside AAO templates, with the optimization conditions carried out from the beginning. As well as that, three different cooling rates have been applied to study the polymer's different phases: natural cooling, fast cooling with a cold heat dissipator and ultrafast cooling with liquid nitrogen.

Moreover, the morphological, chemical characterization, and the crystallographic structure of the nanostructures were analysed conducted under different infiltration conditions. Additionally, the optical characterization of the polymeric (PVDF) metamaterials was performed by measuring the reflectance in the solar spectra, in the wavelength range from 300 nm to 1200 nm, and the emittance in the IR, from 2.5 μm to 17 μm . From these values the theoretical cooling power and cooling temperature of the material under direct sunlight and at night was calculated. The maximum cooling power and temperature were found to be $\sim 135 \text{ W/m}^2$ and 10°C , respectively, for the case of 3D-PVDF without AAO / Al and fast cooling.

Carbon fiber Cu/CuO coatings and the effect of composite fabrication methods on the mechanical performance in energy storage multifunctional devices

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A6_9 - Supercapacitors, Machado Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

Smart mobility has emerged as a solution to reduce carbon dioxide emissions by utilizing cleaner and more efficient energy sources. A key focus is vehicle electrification, where multifunctional supercapacitors and composite-based batteries serve both energy storage and structural functions. Woven carbon fibers (WCF) used as electrodes require modification to enhance electrochemical performance by increasing their specific surface area (SSA). Various modifications using carbon nanostructures or nanoparticles of metals, metal oxides, metal sulfides, and selenides have been explored. Among these, metal oxides stand out as promising materials for pseudocapacitive energy storage mechanisms due to their lower toxicity compared to sulfides and selenides. Copper oxide has been widely studied for enhancing carbonaceous electrodes. It is typically hydrothermally synthesized on carbon fibers using a copper salt (e.g., nitrate) and a reducing agent (e.g., hydrazine or HMTA). While effective for CuO nanowire growth, the toxicity of reducing agents necessitates more sustainable alternatives. Yokohama et al. synthesized copper nanowires from copper chloride using PVP, NaCl, and ascorbic acid as a reducing agent. We recently applied this method to modify high-modulus carbon fibers and demonstrated their use in flexible supercapacitors [1]. For structural composites, mechanical characterization is essential. Traditionally, tensile testing is used, but interlaminar shear strength (ILSS) tests have gained importance due to the role of interfaces in stress distribution. Only a few examples can be found in the literature when the ILSS is study for structural supercapacitors [2]. This study focuses on optimizing hydrothermal growth conditions for Cu, CuO, and Cu/CuO nanoparticles on WCF and evaluating their electrochemical performance as electrodes. Structural supercapacitors were fabricated using two different methods, and their mechanical properties were analyzed. The hydrothermal process was found to be critical, as complete surface coverage is essential for effective performance. These findings open new possibilities for Cu-based nanostructures on WCF in energy storage and multifunctional applications.

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High Power Factor Silver Selenide thin films deposited at low temperature by pulsed hybrid reactive magnetron sputtering (PHRMS)

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A6_8 - Energy harvesting from heat - II, Machado Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Thermoelectric materials convert a thermal gradient into a voltage difference. This quality makes them candidates for increasing the efficiency of energy generation, through the harvest of waste heat. Thermoelectric generators (TEGs) can be applied for waste heat recovery, like is the case of human heat harvesting, which can be useful for powering wearables and Internet of Things (IoT) devices (1). Thermoelectric efficiency is evaluated with the figure of merit zT , defined as $zT = S^2 \cdot \sigma \cdot T / \kappa$, being S the Seebeck coefficient, σ the electrical conductivity, κ the thermal conductivity and T the temperature. Therefore, materials with high power factor ($PF = S^2 \cdot \sigma$) and low thermal conductivity are highly interesting.

Silver selenide (Ag_2Se) is a high-performance thermoelectric material near the room temperature range (2,3). Although this material has been widely studied in bulk form, thin film works remain scarce in comparison, due to its fabrication complexity. To fabricate these films our group developed pulsed hybrid reactive magnetron sputtering (PHRMS) (4,5). In this technique, Ag is deposited by DC magnetron sputtering and Se is added using a pulsed flux effusion cell. This technique avoids Se overpressure or high substrate/cell temperatures to obtain Ag_2Se films with good thermoelectric properties, therefore, it is totally compatible with the use of polymer substrates, also flexible ones, for producing wearable devices. The PHRMS process is implemented in EUROPHAS, a newly developed semi-industrial multi-chamber deposition system, designed for the fabrication of 2" size samples.

In this work, we present our first experimental results of Ag_2Se thin films grown on amorphous borosilicate glass substrates at room temperature by PHRMS in the EUROPHAS system where we obtain thin films showing β -phase crystallization and a PF around $4000 \mu W / (m \cdot K^2)$, surpassing actual values from the literature (4,6). The structural and thermoelectric characterization are shown and discussed as well as the effect of stoichiometry variation on the properties of the films.

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Improving thermoelectric properties of calcium manganites using co-doping strategy

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Due to the relatively low thermoelectric properties of oxide ceramics, fixed A-, and variable B-site doped CaMnO_3 materials were prepared and studied for raising their thermoelectric performances. $\text{Ca}_{0.97}\text{Y}_{0.01}\text{La}_{0.01}\text{Yb}_{0.01}\text{Mn}_{1-2x}\text{Nb}_x\text{Mo}_x\text{O}_3$ ($0 \leq x \leq 0.03$) samples were prepared using planetary milled precursors, to reduce the initial particle size and increase their reactivity. The mixture was calcined at 1050°C for 1h, milled again, cold uniaxially pressed in form of pellets (about $3 \times 3 \times 15 \text{ mm}^3$), and sintered at 1310°C for 12h. Powder XRD patterns showed that sintered samples are nearly single phase, with only small amounts of CaMn_2O_4 . SEM analysis performed on the samples surfaces revealed that grain size decreases with Nb, and Mo dopant content, while porosity variation with dopant content is negligible. This was confirmed through density measurements using Archimedes' method, which indicates that all samples are around 91-94% of the theoretical density of CaMnO_3 . Electrical resistivity (ρ) of samples decreases with the dopant content, reaching the minimum at 800°C ($6.1 \text{ m}\Omega \text{ cm}$) in $x=0.03$ samples, 60% lower than that of the pristine ones. On the other hand, Seebeck coefficient (S) decreases with doping, and the highest values at 800°C among the doped samples have been determined for $x=0.005$ ($210 \mu\text{V/K}$). The highest power factor ($\text{PF}=S^2/\rho$) at 800°C has been obtained for $x=0.01$ samples ($0.46 \text{ mW/K}^2\text{m}$) due to their best compromise between electrical resistivity and Seebeck coefficient. Thermal conductivity (κ) measured in the same direction as ρ , and S , did not significantly vary with composition, but the combination of PF and κ , leads to the highest figure of merit ($\text{ZT}=S^2/\rho\kappa$) values at 800°C for the $x=0.005$ samples (0.27), which is among the best reported in the literature. These results clearly show that co-doping approaches are very useful to raise the thermoelectric performances of CaMnO_3 materials, and open new paths for integrating high-performance calcium manganite-based materials in TE modules for power generation at high temperatures.

Use of fast preparation method to produce n- and p- thermoelectric legs and their integration into a thermoelectric module for power generation

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A6_7 - Energy harvesting from heat - I, Machado Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

It is well known that the massive use of thermoelectric generators (TEG) requires not only high-performance p- and n-type thermoelectric materials, but also good compatibility among the different elements used to build the TEG. Moreover, the highest output power, low cost per watt, and long life span are other features that should be achieved in these TEG. Based on previous works, $\text{Ca}_{0.91}\text{Yb}_{0.03}\text{La}_{0.03}\text{Yb}_{0.03}\text{MnO}_3$, and $\text{Ca}_{2.93}\text{Sr}_{0.07}\text{Co}_4\text{O}_9$ materials were prepared as n- and p-type legs. The stoichiometric amounts of precursors were attrition milled for 2h, dried and manually milled. The mixtures were calcined at 1100, and 850°C for 1h, for the n-, and p-type, respectively, and cold uniaxially pressed. The pellets were sintered at 1310°C for 6h, and 900°C for 12h for the n-, and p-type materials, respectively. Powder XRD patterns showed that the thermoelectric phase is the major one in both cases, accompanied of small amounts of secondary phases. Microstructural studies confirmed the XRD data, and showed much lower porosity content in the n-type material than in the p-type one. Electrical resistivity showed semiconducting-like behaviour for both types of samples, and the values at 800°C are 5.7, and 17mΩ cm for the n- and p-type legs, respectively. Seebeck coefficient is negative for the n-type, and positive for the p-type. Furthermore, the absolute value is increased with temperature in both cases, reaching 190, and 290μV/K for the n-, and p-type legs, respectively. Thermal conductivity decreases with temperature for the p-type material reaching 1.60W/K m at 800°C, while it is approximately constant for the n-type (1.20W/K m). These results lead to ZT values of 0.56, and 0.53, for the n-, and p-type materials, respectively. Once the materials have been fully characterized, a large number of p-, and n-type legs were prepared, and their resistance at room temperature has been determined, followed by Ag paint of their ends and sintered at 900°C for 2h to assure good adhesion. At the same time, Ag has been used to design the electrical circuit on the top and bottom alumina layers, and sintered at 900°C for 2h. Finally, the thermoelectric legs were integrated in the TEG using Ag paint and the whole system has been sintered at 900°C for 2h, and the final prototype has been characterized with a cold side temperature fixed at 16°C, while the hot side has been heated at temperatures between 100 and 900°C.

Development of Silicide Thermoelectric Devices for Energy Harvesting based on Recyclable Silicon from PV industry

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A6_7 - Energy harvesting from heat - I, Machado Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Taking into account that ca. 66% of global energy consumption is emitted to the environment as waste heat, thermoelectric (TE) devices can offer a promising approach for waste heat recovery and energy savings when applied in combustion engines and industrial processes. Solid-state TE Generators (TEGs) are able to provide great advantages since they directly convert heat into clean electrical power through the Seebeck effect, and operate without any CO₂ or toxic emissions, vibration, or noise. Silicide thermoelectrics have attracted considerable attention because these compounds consist of earth-abundant and eco-friendly elements, combining good TE properties and suitable stability for mid-temperature TE applications. From the point of view of materials, the TE efficiency is determined by the dimensionless figure of merit, ZT, depending on the Seebeck coefficient, the electrical conductivity, the absolute temperature, and the thermal conductivity.

In an effort to establish a circular economy approach and provide a cost-effective solution for the manufacturing of high-performance TEGs, the European program ICARUS attempts to utilize effectively recycled Si from PV manufacturing industry for the development of silicide thermoelectrics. Two types of recycled Si kerf are used for the synthesis of n-type Mg₂Si_xSn_{1-x}, (0.6 ≤ x ≤ 1.0) solid solutions and p-type Higher Manganese Silicide (HMS) MnSi_x phases. The investigated materials are developed by Mechanical Alloying (MA) which is an energy-efficient, straightforward and scalable method. Material characterization is carried out by using X-ray diffraction and the crystal structure of final products is confirmed through the Rietveld method, while SEM analysis is also performed to study the microstructure of developed phases. Promising TE efficiencies are achieved for the kerf-based materials which are used for the fabrication of TE modules (TEM). The developed devices are characterized using a TEM testing apparatus. High power density is achieved for the Si-kerf-based TEM devices, and a good agreement between experimental and simulated performance is observed. The aforementioned results validate that this research work is a successful paradigm of circular economy approach, providing sustainability and a strong silicon recycling solution in the field of green energy technologies.

This work is part of ICARUS project funded by Horizon 2020 research and innovation programme under grant agreement No 958365. ICARUS project aims to process and refine secondary raw materials from silicon PV manufacturing.

Nitrogen-based polymeric solid electrolytes for next-generation multivalent batteries: An environmental impact analysis.

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A6_10 - Polymers for energy, Machado Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

In the last decade, the growing global energy demand has provoked a need for the use of intermittent renewable energy sources, as alternative and sustainable energy strategies. However, these strategies require the development of innovative efficient and sustainable energy storage methods in order to reduce the carbon emissions in various sectors, as well as to ensure electricity supply in remote and disadvantaged regions, contributing to improved quality of life and significant health benefits.

In this context, current manufactured lithium batteries have significant challenges, from an environmental point of view, because of their manufacturing require scarce materials, with a high environmental impact associated with their extraction and processing methodologies, particularly transition metals. As an alternative, in the last years rechargeable organic batteries have emerged as a promising economical and environmentally friendly alternative; however, they are currently in the early stages of development, and it is necessary to thoroughly investigate new materials for optimizing their efficiency from an energy storage perspective, as well as their environmental impact to medium-long-term application.

In this context, this research focuses on the development of a new concept of organic solid electrolytes, based on nitrogen-based structures, which could solve the current limitations of rechargeable organic batteries. In particular, we investigated an innovative polymer solid-state electrolyte, with good mechanical stability, low heat transfer, high ion conductivity and high stability, based on aminotriazole-type repeating units (monomers), which has rendered promising properties as electrolyte for rechargeable multivalent ion batteries, such as calcium or zinc.

Six different polymers based on triazole-type structures have been obtained using an easily scalable methodology through soft reaction conditions and avoiding polluting solvents. The polymers were characterized by using different techniques such as Nuclear Magnetic Resonance (NMR), elemental analysis and Differential Scanning Calorimetry (DSC). Then, the polymer electrolytes were mixed with different calcium and zinc salts (concentrations ranging from 80% to 50% polymer), resulting in solid membranes, which were assessed as electrolytes for calcium secondary batteries through electrochemical measurements as Electrochemical Impedance Spectroscopy (EIS).

In addition, an evaluation of the environmental impact of the developed solid electrolyte manufacturing process was performed using Life Cycle Assessment (LCA) methodology, with sigmaPro software and the Ecoinvent database. The LCA showed promising results in terms of carbon footprint with values equal or lower than other polymer electrolytes previously reported in literature.

Direct Ink Writting of NiFe electrodes for the Oxygen Evolution Reaction

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A6_1 - Hydrogen generation - I, Machado Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Water splitting is a critical process for generating the so-called green hydrogen. Specifically this green hydrogen can be produced by water electrolysis as far as sustainable energy is used in the process. In order to accomplish the viability of this technology, affordable electrodes with improved performance are required for both the hydrogen and oxygen evolution reactions (HER and OER, respectively). Focusing in the OER in alkaline conditions, Ni and NiFe electrocatalysts have demonstrated competitive results. On the other hand, additive manufacturing (AM, aka 3D printing) is revolutionising the design and fabrication of electrocatalysts by enabling tailored architectures that improve efficiency and durability while reducing costs. In this work, we explore the possibility of enhancing the performance of Ni and NiFe electrodes in alkaline conditions for the OER by customising their geometries. Specifically, electrodes with different lattice patterns were designed and printed using a custom-made direct ink writing (DIW) 3D printer. The first challenge was thus to obtain Ni pastes that could be printed by DIW. This was successfully overcome using adequate F127 Pluronic®/water formulations that allowed high Ni powder loads (over 75 wt% solids content). The rheological properties of the resulting aqueous Ni pastes were optimal for DIW, showing shear-thinning and self-supportive behaviour. The equilibrium storage moduli (G'_{LVR}) were high enough to assure a good printing resolution. The printed electrodes were thermally treated under inert atmosphere up to 900 °C to completely remove the paste carrier and sinter the Ni micro-particles. After post-processing, the different geometries of 3D printed Ni electrodes exhibited good mechanical properties and further NiFe electrocatalysts were electrodeposited by a chronopotentiometry (-3mAcm⁻² 10 min 60°C) using chlorides as metallic precursors. Finally, they were tested by linear sweep voltammetry (LSV) for the OER reaction and compared to a benchmark NiFe catalyst electrodeposited onto a commercial Ni-foam. The 3D printed electrodes showed a 10% reduction of the OER overpotential with respect to the benchmark.

Improvement in the production of green hydrogen from a freeze-cast porous Fe₂O₃ material by the use of small amounts of Al₂O₃ and TiO₂

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A6_2 - Hydrogen generation - II, Machado Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Hydrogen has become the new energy vector because its combustion produces neither pollutants nor greenhouse gases.

Current production is still based on fossil fuels, with a small but growing proportion coming from renewable resources. However, storage and transport remain a challenge.

Iron oxide is a low-cost raw material that can be used to produce high-purity hydrogen through the Chemical Looping Water Splitting (CLWS) process. First, a carbonaceous fuel from organic waste such as biogas, bioethanol or biomass reduces the hematite to wustite (FeO), which is later re-oxidised with steam to produce pure hydrogen.

However, the efficiency of this reaction is dominated by the available surface area, the formation of coke due to the use of bioethanol as a reductant source, and the deactivation phenomenon caused by the high working temperature after numerous redox cycles.

Here we show an Fe₂O₃ freeze-casting porous material doped with Al₂O₃ and TiO₂ capable of yielding 8 mmolH₂/g sample on each redox cycle with negligible traces of CO. We found that TiO₂ has the potential to enhance the reduction reaction of the iron oxide, while Al₂O₃ helps to withstand the prolonged heat treatment. These properties, which double the hydrogen production reported for similar systems are relevant to the proper operating of PEM fuel cells. Our porous materials were fabricated using a camphene-based suspension of synthesised nanoparticles with different compositions. Fe₂O₃ nanoparticles doped with Al₂O₃ and TiO₂ oxide (95 wt% Fe₂O₃ - X wt% Al₂O₃ - (5-X) wt% TiO₂; X= 2, 2.5 and 3) were prepared by the co-precipitation method. This procedure produces a single solid solution matrix with an interconnected porosity of approximately 70%. After redox test, the formation of coke deposit over the surface is neglected at 675°C for samples with 3 wt% TiO₂, leading to a high-purity hydrogen produced during steam oxidation. This study is important to further improve the chemical design of oxygen carriers and also to improve the mechanical strength of porous catalyst materials. As the surface reactions produce a significant stress due to volumetric changes.

Intercalation-Conversion Hybrid Cathode Enabled by MXene-Driven TiO₂/TiS₂ Heterostructure for High-Energy-Density Li–S Battery

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A6_6 - Batteries - II, Machado Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

A dense electrode with high sulfur loading is a straightforward approach to increasing the energy density of lithium–sulfur battery (LSB), but the development of dense electrodes suffers from both fabrication challenges and electron/ion transport limitations. In addition, the shuttle effect of soluble lithium polysulfides and sluggish reaction kinetics cause declined utilization efficiency of the active material and poor cycling stability. Herein, a dense intercalation-conversion hybrid cathode is prepared using MXene-driven TiS₂ nano-needles decorated with TiO₂ nanoparticles. The TiO₂/TiS₂ heterostructure simultaneously possessing a high adsorption capability (TiO₂) and bidirectional electrocatalytic effect (TiS₂) is observed to effectively suppress lithium polysulfide shuttling and facilitate the sulfur conversion reactions. Furthermore, it is believed that TiS₂ provides additional capacity from the intercalation reaction and functions as a multichannel network to feed both Li⁺/e[−] to the active sulfur material due to its high electronic and ionic conductivities. Thanks to these synergistic effects, the LSB assembled using the TiO₂/TiS₂ heterostructure exhibits high gravimetric and volumetric energy densities of 331 Wh kg^{−1} and 730 Wh L^{−1}, respectively, as well as superior cyclability at a high sulfur mass loading of 7.5 mg cm^{−2} and lean electrolyte of 2.5 μL mg^{−1}.

PHASE CHANGE MATERIALS IN INSULATING ELEMENTS TO INCREASE BUILDING ENERGY EFFICIENCY AND THERMAL CONFORT

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A6_5 - Improving Energy in Buildings - II, Machado Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

The increasing demand for energy-efficient solutions in buildings has brought significant attention to advanced materials with synergistic thermal properties. The integration of phase change materials (PCMs) into polyurethane or geopolymer foams presents a promising way to improve the thermal comfort in buildings. PCMs are particularly appealing due to their high latent heat storage capacity that could confer higher apparent thermal capacity to insulating materials in defined temperature ranges, with effect of shaving and shifting temperature peaks. This approach combines the thermal insulation ability of porous lightweight materials with high thermal mass, thus increasing energy efficiency and thermal comfort.

In this work, composite materials with polyisocyanurate or geopolymeric foams incorporating organic PCMs at concentrations of up to 20 wt% were developed, while preserving the inherent thermal insulation properties of the pristine foams. In case of polyisocyanurate foams the process involved emulsifying a PCM formulation into the polyol component, while in case of geopolymers an emulsion of micro-encapsulated PCMs was used in the formulation. The selected PCMs were commercial materials with nominal melting point of 28 or 31 °C. The use of a nucleating agent to mitigate subcooling effect was also investigated.

The thermal performances of developed materials in static and dynamic conditions were analysed through Differential Scanning Calorimetry (DSC), Hot Disk Thermal Diffusivity measurements, Hot plate device and Infrared Thermography. These analyses provided insights into the thermal conductivity and demonstrated the impact of PCM latent heat on thermal peak shaving and shifting. The results indicate that increasing PCM concentrations lead to progressively larger time shifts in thermal oscillations as they propagate through the material.

Acknowledgement: The authors would like to thank the project “PRESTO – Phase change materials for Energy Saving and building thermal cOMfort” financed by European Union, Next Generation EU, Mission 4, Component 1, CUP B53D23008790006”.

Towards Efficient Energy Harvesting: Flexible Piezoelectric Fibrous Mat with PDA@Modified Nanofillers

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This study aims to create a nonwoven fibrous mat composed of biopolymer fibers for energy harvesting, integrating polydopamine (PDA)-modified carbon nanofibers (CNFs) and gallium nitride (GaN) nanostructures. GaN exhibits robust piezoelectric characteristics, whereas CNFs enhance electrical conductivity depending on their degree of graphitization. The incorporation of these functionalized fillers seeks to enhance the piezoelectric response and mechanical flexibility of the composite fibrous mat.

This study investigates the possible synergy of piezoelectric and conductive fillers to increase energy harvesting efficiency, motivated by recent developments [1,2] in using PDA for improved dispersion and interfacial bonding of functional nanomaterials. As shown in comparable systems for piezoelectric and strain-sensing applications, PDA modification is expected to resolve issues with agglomeration and interfacial compatibility. Additionally, PDA functionalisation improves filler distribution and interfacial bonding, further mitigating common agglomeration challenges in nanocomposites.

This study presents preliminary findings on PDA-modified nanostructures in nonwoven biopolymer-based fibrous mats for energy harvesting applications. The findings may contribute to the development of next-generation sustainable smart materials for wearable electronics and human-machine interaction systems.

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Experimental assessment of computationally designed Complex Concentrated Alloys (CCAs) for Molten Salt Reactors (MSR)

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A6_2 - Hydrogen generation - II, Machado Room (Level -2), septembre 15, 2025, 17:00 - 19:00

Compositionally Complex Alloys (CCAs) have recently emerged as attractive structural materials in the nuclear sector, primarily due to their suggested superior irradiation tolerance when compared to conventional alloys [1]. Their expansive compositional space allows for fine-tuning of diverse properties, including electrochemical behaviour, making them interesting for demanding reactor environments [2].

This study focuses on the evaluation of newly designed corrosion- and irradiation-resistant CCAs for Generation IV Molten Salt Reactors (MSRs), where materials must endure chloride-based molten salts at temperatures ranging from 550 to 750°C. Building upon the work of Herschberg et al. [3], both novel CCAs and literature-based "reference alloys" were fabricated through cold crucible induction casting. The obtained Ni-rich alloys incorporate Al or Mo as principal alloying elements along with Cr. Comprehensive microstructural characterisation of both as-cast and homogenised samples employed X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), Electron Backscatter Diffraction (EBSD), and Transmission Electron Microscopy (TEM). In addition, the predictions made by ThermoCalc software were compared with the experimental findings in order to assess phase stability and guide alloy development.

Mechanical properties were examined via Vickers hardness measurements, room-temperature tensile tests, and hot compression tests. So as to investigate corrosion resistance, prolonged static immersion tests were performed in eutectic LiCl-KCl salt at 450°C for 24 and 168 hours. Heavy-ion irradiation experiments utilised 6 MeV Ni ions at 450°C, and subsequent TEM analyses evaluated resulting microstructural changes. Furthermore, the interplay between irradiation and corrosion was explored through sequential heavy-ion irradiation and corrosion testing.

Preliminary results highlight that these "MORA" alloys not only display robust high-temperature phase stability and favourable mechanical performance but also exhibit commendable resistance to corrosive chloride salts.

Acknowledgements

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Investigation of Co-doped Iron Oxide Electrocatalysts for AEM Electrolysis

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Recent advancements in catalyst development for anion exchange membrane (AEM) water electrolysis have highlighted iron oxides doped with cobalt as efficient and cost-effective alternatives to noble metal-based catalysts. Studies demonstrate that Co doping enhances the oxygen evolution reaction (OER) activity and durability of Fe-based oxides, optimizing their electronic and structural properties for improved performance. These findings [1-2] emphasize the potential of Co-doped Fe oxides to boost AEM electrolysis efficiency, offering a promising pathway toward scalable and sustainable hydrogen production.

In this study, we present a systematic investigation into transition metal oxides, specifically Fe₂O₃ thin films doped with cobalt, as highly active and robust catalysts for OER. The thin films were fabricated using reactive magnetron sputtering, a precise deposition technique enabling control over film composition, microstructure, and thickness.

Comprehensive characterization of the Co-doped Fe₂O₃ thin films revealed improvements in catalytic activity and stability compared to undoped Fe₂O₃. Structural analysis using X-ray diffraction (XRD) indicated that cobalt incorporation enhances the crystallinity and modifies the lattice structure, promoting favorable electronic and surface properties. Scanning electron microscopy (SEM) and atomic force microscopy (AFM) provided insights into the surface morphology and uniformity of the films, which directly impact their electrochemical performance.

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Novel $\text{Na}_{0.75}(\text{Ni}_{0.2}\text{Co}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Ti}_{0.2})\text{O}_2$ high entropy cathodes for sodium-ion batteries with superior capacity and stability

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A6_6 - Batteries - II, Machado Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

The great abundance of sodium, its low cost and the similar chemistry to lithium, makes sodium-ion batteries (SIBs) a promising alternative to traditional lithium-ion batteries. However, the development of sustainable, low-cost, high-capacity, and stable cathode materials is still an open challenge for the SIBs technology. Layered oxides ($\text{Na}_x(\text{TM})\text{O}_2$, with TM being a transition metal ion) are among the most promising candidates. They can exhibit a set of flexible crystallographic structures, differing on the layer stacking and the metal connectivity, which proved to be efficient with respect to Na reversible insertion and extraction. A critical aspect of layered oxides is that high specific capacity can be achieved at the expense of cycling stability. The latter can be improved by exploiting the high entropy concept, i.e. by designing materials with a large configurational entropy, characterized by more cations sharing the same crystallographic site. Indeed, the combination of different transition metals helps to increase the reversibility of the phase transitions occurring during the charging/discharging cycles.

Here we report on a novel composite cathode active material (CAM) with composition $\text{Na}_{0.75}(\text{Ni}_{0.2}\text{Co}_{0.2}\text{Mn}_{0.2}\text{Fe}_{0.2}\text{Ti}_{0.2})\text{O}_2$ produced with a homemade spray pyrolysis setup, which led to well separated grains with submicrometric size. The CAM is composed for three parts of a mixture of two layered oxides, and for one part of some residual rock salt and spinel phases. The electrochemical performance combine high capacity and stability: the cathode reaches initial discharge capacities of approximately 180 mAh g⁻¹ (0.08C, 15 mA g⁻¹) and exhibits capacity retention of 69% after 300 cycles at a current density as high as 200 mA g⁻¹ (1C). The post mortem analysis revealed no major changes in microstructure and phase composition.

To assess the impact of the microstructure, we prepared a CAM with the same chemical composition using a more conventional synthesis method, specifically sol-gel. This approach yielded a nearly phase-pure material with smaller and more irregular grains. In comparison to the CAM produced via spray pyrolysis, it exhibited electrochemical performance consistent with existing literature, with reduced capacity and stability.

Enhanced triboelectric performance in 3D-nanonetworks biodegradable PLA metamaterials

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A6_10 - Polymers for energy, Machado Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Modern electronics, which are essential for human health, safety, and communication, provide a wide array of opportunities to evolve our society into an intelligent world. However, with the rapid growth of the Internet of Things (IoT), the energy supply for electronics and sensors has become a critical challenge. Triboelectric nanogenerators (TENGs) have been developed as a key technology for mechanical energy harvesting, but further improvements in their triboelectric properties are still necessary to meet the demands of practical and functional devices.

Three-dimensional anodized aluminum oxide (3D-AAO) features hexagonal column-shaped cells with cylindrical central holes of varying diameters and transversal channels. Due to this structure, it can be used as a template for nanostructuring processes. This nanostructuring method offers several advantages over lithography-based techniques, such as cost-effectiveness, broad accessibility, and the ability to fabricate with nanoscale precision from the top down.

Poly(lactic acid) (PLA), one of the most promising biopolymers due to its non-toxicity, and excellent mechanical properties, has found industrial and medical applications thanks to its wide range of properties, from amorphous to crystalline states.

This study investigates the potential of TENGs for efficient mechanical energy harvesting through contact-separation triboelectrification and electrostatic induction. Nanoengineered PLA films with controlled nanostructuring, enabled by the use of 3D-AAO, are utilized in a simple, fast, controllable, and cost-effective process. The influence of 3D nanocavities within PLA films on triboelectric power generation is examined, revealing a correlation with the triboelectric charge density and the polymer's relative permittivity.

Acknowledgements

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Toward High-rate Carbon-based Supercapacitors: New Insights into the Structural Characterization and Electrochemical Performance of Hierarchical Porous Carbons

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A6_9 - Supercapacitors, Machado Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

Conventional porous carbon materials, such as activated carbons and carbon blacks, are attractive supercapacitor electrode materials due to their low cost of production and ultrahigh specific surface areas. However, their small electrolyte-accessible surface areas and slow ion transport in their micropores at high charging/discharging rates result in low specific capacitances, thereby limiting their energy densities. Recent research has shown that hierarchical porous carbons (HPCs) offer the ultimate solution by combining the high surface area of micropores with the improved mass transport of ions in mesopores and macropores, thus rendering HPCs as promising high-rate supercapacitors.

Herein, we report the facile synthesis of pristine and N-doped HPCs utilizing the ice-templating method coupled with hard-templating using LUDOX[®] colloidal silica particles. In a typical synthesis, an aqueous mixture of glucose (or glucose-and-urea) and colloidal silica particles is flash-frozen in liquid nitrogen. The ice fronts formed in the flash freezing process act as a soft template for macropores that can be removed by lyophilization, thereby yielding the dry glucose-silica (or glucose-urea-silica) matrix. The latter is then pyrolyzed, and the resulting carbon-silica (or N-doped carbon-silica) matrix is stirred in an alkaline medium under reflux to etch out the hard colloidal silica template and create the mesopores. Microporosity can then be introduced into the carbon matrix via either physical or chemical activation, using CO₂ or KOH as activating agents, respectively. Nitrogen porosimetry and small-angle X-ray scattering were utilized to analyze the porous structures of the HPCs. Elemental analysis and X-ray photoelectron spectroscopy were employed to determine the nitrogen content and bonding configurations, respectively, in the N-doped HPCs. The electrochemical performance of the HPCs was assessed using the cyclic voltammetry and cyclic galvanostatic charge-discharge techniques.

High-performance lithium-ion battery electrodes based on ion-implanted germanium thin films

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Germanium (Ge) has emerged as a promising anode material for lithium-ion batteries (LIBs) due to its high theoretical capacity and superior lithium-ion diffusivity compared to conventional graphite. However, its significant volume expansion during cycling remains a major challenge, leading to mechanical degradation and capacity fading. Nanostructurization appears an interesting solution to enhance structural stability and electrochemical performance. In this study, we explored ion-implanted Ge thin films as negative electrodes. The Ge films were fabricated using plasma-enhanced chemical vapour deposition (PECVD) followed by ion implantation to modify their microstructure morphology. The implantation process introduced controlled defects and altered the the Ge films, aiming to improve their mechanical resilience and lithium storage capability. The morphological and structural characteristics of the implanted films were analysed using scanning electron microscopy (SEM). This technique provided insights into surface morphology, film uniformity, and the evolution of the electrode structure after cycling. Additionally, X-ray diffraction (XRD) and Raman spectroscopy were employed to assess changes in crystallinity and phase transformations induced by ion implantation. Focused ion beam (FIB) cross-section analysis was also conducted to evaluate film integrity after the nano structuring process.

Electrochemical characterisation was carried out through galvanostatic charge-discharge cycling and cyclic voltammetry, measurements which allow the evaluation of capacity retention, rate performance, and reaction mechanisms of the ion-implanted Ge electrodes. The results demonstrated that the ion-implanted Ge films exhibited improved cycle life and higher stability compared to pristine Ge electrodes. Specifically, the modified Ge electrodes retained a higher capacity over prolonged cycling, with reduced initial capacity loss and enhanced coulombic efficiency. At a current density of 1C, the ion-implanted Ge films maintained a reversible capacity significantly higher than conventional graphite electrodes. These findings indicate that ion implantation is a viable strategy for tuning the structural and electrochemical properties of Ge-based anodes, mitigating volume expansion, and enhancing battery performance.

Thermoelectric efficiency enhancement of sputtered L21 Fe₂VAI, Fe₂V_{0.8}Al_{W0.2} and Ti-doped Fe₂VAI (100) and (110) epitaxial thin films

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Thermoelectric materials are capable of transforming thermal gradients into an electrical voltage difference. This quality makes these materials a possible solution to the global energy crisis through the harvest of diffusive heat waste.

Thermoelectric efficiency is measured with the figure of merit zT , which is defined as $zT = S^2 \cdot \sigma \cdot T / \kappa$, being S the Seebeck coefficient, σ the electrical conductivity, T the temperature and κ the thermal conductivity (1). For that reason, materials that exhibit high S , high σ and low κ are very interesting. Thermoelectric thin films are of great interest because they reduce considerably the κ through nano-structuration.

Among all thermoelectric materials, Fe₂VAI is a full Heusler alloy that has attracted considerable interest due to its non-toxic and earth abundant constituents and its great thermoelectric properties. The thermoelectric properties in this alloy can be tuned via doping with elements like Ti, Si or W (2,3), making the alloy p or n type, and in some cases, resulting in a significant increase in thermoelectric performance (4).

Besides doping, chemical order of Fe₂VAI has an impact on the alloy's band structure. So, a systematic study of the thermoelectric properties according to its chemical order is of high interest. Also, other parameters like crystal orientation may influence the thermoelectric properties, for example, via changes in the grain morphology and size.

In this work, we present experimental thermoelectric and structural results of Fe₂VAI and Fe₂V_{0.8}Al_{W0.2} thin films grown by magnetron sputtering from nominal composition targets at deposition temperatures ranging from RT to 950°C, on Al₂O₃ (1 1 -2 0), and on MgO (1 0 0) substrates, exhibiting (1 1 0) and (1 0 0) orientations, respectively, and varying degrees of chemical order. Moreover, a doping optimization of L21 Fe₂VAI with Ti, in a co-deposition configuration was performed, obtaining higher values of Seebeck and power factor ($PF = S^2 \cdot \sigma$) reaching the range of 100 μV/K and 2000 μW/(m·K²) respectively.

Acknowledgements

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Novel Polyperyleneimide-Based Organic Cathodes with Graphene-Like Structures for Calcium Multivalent Secondary Batteries.

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A6_6 - Batteries - II, Machado Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

The green and digital transition, as well as the associated transformation of our economy, industry and society to achieve climate neutrality in Europe by 2050 is a challenge, which cannot be faced without considering the development of new energy storage technologies, as crucial components in promoting alternative and sustainable energy strategies, including wind or solar energy harvesting. Traditionally, the energy storage systems are based on lithium materials and transition metals, whose extraction and use are associated with a high environmental, social and economic impact. For this reason, it is vitally important to find new energy alternatives that are ecologically, socially and environmentally sustainable. Among these new energy alternatives are calcium batteries, which are part of the group called transition-metal-free energy storage systems, and although they are expected to be safe, efficient and economically viable, its application is limited due to the difficulty of finding efficient cathodes for calcium-type batteries.

Numerous studies have evaluated the electrochemical properties of Organic Electrode Materials (OEMs), including conductive polymers, organosulfur compounds, and carbonyl compounds. While strategies such as structural engineering, polymerization, hybridization, and amorphization have been employed to enhance cathode performance, the use of OEMs in multivalent batteries remains limited. Challenges such as low cell voltage, reduced specific power/energy, poor electrical conductivity, and dissolution in electrolytes continue to hinder their practical application.

In this study, we present our latest advancements in developing organic cathodes based on polyperyleneimide redox-active materials integrated with graphene-like structures. Utilizing directed methodologies, we achieved highly conductive hybrid cathodes with a redox-active molecule content of 90%-95% and capacities reaching 2-3 mAh/cm². These innovative cathode materials were synthesized using a novel, cost-effective, reproducible, and sustainable approach, eliminating the need for expensive and environmentally harmful solvents such as DMF and DMSO. Thus, the developed polymer synthetic strategy is straightforward, scalable to gram quantities, and without complex purification or isolation processes.

The developed hybrid materials were structurally characterized using a combination of techniques, including nuclear magnetic resonance (NMR), differential scanning calorimetry–thermogravimetric analysis (DSC-TG), and infrared spectroscopy (IR), among others. Upon confirming their structures, their electrochemical properties were analyzed using electrochemical techniques such as cyclic voltammetry and impedance spectroscopy, and others related methods, which provided promising properties as efficient and stable organic cathodes for calcium batteries.

Finally, they were studied in symmetric calcium cells, yielding promising results.

Fabrication and characterization of 3D printed ceria structures for solar thermochemical water splitting reactors

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A6_2 - Hydrogen generation - II, Machado Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Solar thermochemical cycles are considered for the production of renewable fuels at large scale. The direct conversion of heat, generated by concentrated solar radiation, into chemically stored energy and the usage of the full solar spectrum enable in theory high process efficiencies and respectively low fuel production costs. One of the most investigated redox cycle in this area is the two-step ceria cycle with temperature-swing, pressure-swing operation. In this process ceria is partially reduced at moderate vacuum conditions and temperatures of around 1500°C and oxidized at around 1000°C. In recent years substantial improvements of related receiver-reactors have been experimentally demonstrated [1]. Further improvement potential is claimed for advanced receiver-reactor concepts like R2Mx [2].

The redox material is often applied as an open porous monolithic structure to allow deep penetration of solar radiation and a high surface area for fast kinetics during reduction and oxidation. While the most efficient systems so far have been using reticulated porous ceramics, 3D printing is seen as an option to further improve and tailor the design of the redox structures [3]. First tests have been reported for structures used in directly irradiated receiver-reactors.

R2Mx creates a different set of requirements for the redox structures and adapted designs have been developed. For the fabrication 3 different printing methods are investigated: Binder Jetting, Material Extrusion, and Vat Photopolymerization. Ceria pellets and rods have been printed and characterized in order to iteratively elaborate and improve the fabrication methods. More advanced designs which are closer to the application as well as a proof-of-concept test rig for the testing of the 3D printed ceria structures including first experimental results will be presented.

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Utilization of Waste Triglycerides and Sulfur for the Production of Triboelectric Nanogenerators

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In recent years, there has been a significant increase in the interest in sustainable materials aimed at reducing environmental impact and promoting efficient resource utilization. A promising approach involves the reuse and recycling of industrial byproducts to create functional materials, minimizing waste and transforming residues into valuable resources. This study focuses on the production of high-sulfur-content materials with sustainable properties, utilizing elemental sulfur and waste triglycerides from plant oils representing traditional low-value residues. These materials are synthesized through inverse vulcanization, where sulfur copolymerizes with unsaturated compounds such as waste vegetable oils, acting as a solvent, initiator, and monomer in the process.

The resulting sulfur-based polymers exhibit outstanding properties such as thermal stability, chemical resistance, and thermoplastic behavior. To comprehensively analyze the produced material, various characterization techniques were employed, including scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, 3D profilometry, differential scanning calorimetry (DSC), dielectric analysis (DEA), and mechanical property evaluation.

A key aspect of this study is the assessment of the triboelectric properties of the synthesized sulfur-based copolymers. The copolymer was paired with two different waste-derived materials to form triboelectric pairs: discarded goat leather and a blend of recycled refuse waste polymers (RRWP), primarily composed of polyolefins. The triboelectric response was found to be highly dependent on the pairing material. When combined with goat leather, the composite exhibited a tribonegative character, whereas when paired with RRWP, it demonstrated a tribopositive nature. Notably, this trend intensified with cycling during the triboelectric experiment, stabilizing after approximately 150 cycles under conditions of 14 kPa applied pressure and a sliding velocity of 0.6 m/s.

The findings provide valuable insights into the relationship between copolymer composition and triboelectric behavior, demonstrating the potential of sulfur-based thermoplastics for sustainable energy harvesting applications.

Development of high porosity bifunctional materials for Sorption Enhanced Steam Reforming (SESR) of ethanol using colloidal process and freezes-casting technique.

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Sorption enhanced steam reforming of ethanol is an intensified process, in which it is possible to produce high purity hydrogen with low content of carbon oxides. Ideal for the production of hydrogen for fuel cells applications, minimizing the purification stages downstream the reforming reactor. Considering the production of hydrogen for fuel cells applications, the main advantage of this process is that it allows H₂ production and purification in one stage, minimizing the purification stages downstream the reforming reactor.

Among the most active catalysts for the ethanol reforming reaction are the ones based on Ni as active phase supported on alumina, since they are highly active and low cost. Regarding the CO₂ capture process, the CaO has shown high CO₂ capture capacity under the reforming temperature range, rapid CO₂ capture kinetics, as well as high availability and also low cost. However, both materials have some disadvantage, as Ni is susceptible to deactivation by both carbon formation and sintering, and CaO is prone to sintering at high temperatures (around 850 °C).

Then, the development and synthesis of bifunctional materials with high active surface minimizing the distance between CO₂ generation sites and CO₂ sorption sites has gained relevance. Nevertheless, many researchers are developing bifunctional materials using low-tech techniques such as impregnation method, co-precipitation method, wet-mixing method or, high-tech techniques such as atomic layer deposition method and template-assisted method.

Here we show a simpler method of manufacturing high porosity Ni(Al₂O₃-MgO)-CaO bifunctional material combining co-precipitation and colloidal process, with freezes-casting technique. The resulting structure showed an open porosity of 70% with a significant number of Ni/CaO interfaces. It reached a complete reforming of ethanol without coke formation. The CO₂ capture rate was kept constant throughout the entire test. Also, no microstructure degradation was noticed.

These findings are significant to confirm the improvement in the efficiency of the SESR process, by an adequate design of the manufacturing technique of the active material

Optical properties of Sb-Ge and Ge-Se thin films for applications in photovoltaic devices

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The current global context, marked by growing concern over environmental issues stemming from the overexploitation of conventional energy resources, is driving a research effort focused on developing more sustainable, adaptable, and efficient photonic and photovoltaic devices [1-2]. In this context, advances in the development of semimetal-based and chalcogenide -based materials for sustainable solar photovoltaic cells as a potential energy alternative [3], are particularly relevant. In recent years, efforts have been made to find new solutions to eliminate the toxicity of Cd and the scarcity of elements such as In, Ga, and Te, which are present in traditionally used CIGSe and CdTe-based thin-film solar cells. Among the compounds that have attracted interest for both photonic and photovoltaic applications are those based on SbGe and Sb₂(S,Se)₃ and related materials [4]. They show unique properties as absorbers for thin-film solar energy harvesting.

This work focuses on the optical characterisation of the of Ge-Sb and Ge-Se thin films. These films were deposited by thermal evaporation o co-evaporation followed by a selenization process in the case of the chalcogenides. By using spectroscopic ellipsometry we have determined their dielectric optical function that give access to the determination of the band gap energy and absorption coefficient. We correlate the optical properties to the composition and morphology of the films. This study was carried out at the Optical Characterization of Materials Service (SCOM) of the Institute of Optics (IO-CSIC) [5], using advanced techniques such as spectroscopic ellipsometry [6], reflectance, and transmittance [7] measurements.

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Scalable Hybrid Organic-Inorganic Solid-Solid Phase Change Materials for Thermal Management in Lithium-Ion Batteries

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A6_4 - Improving Energy in Buildings - I, Machado Room (Level -2), septembre 16, 2025, 14:30 - 16:30

As the demand for safer and more efficient lithium-ion (Li-ion) batteries intensifies across diverse sectors, innovative solutions for thermal management are critical to addressing challenges in performance, safety, and lifespan. This study presents groundbreaking advancements in hybrid organic-inorganic solid-solid phase change materials (SS-PCMs), focusing on their synthesis, scalability, and application in passive thermal management for Li-ion batteries.

Hybrid SS-PCMs, including both perovskite and non-perovskite types with the general formula $(\text{CnH}_{2n+1}\text{NH}_3)_2\text{MIIX}_4$ ($\text{M} = \text{Cu}, \text{Zn}; \text{X} = \text{Cl}$), were synthesized at a 20-liter scale, demonstrating industrial viability. These materials feature tunable phase change temperatures (54°C – 95°C) tailored through organic structural modifications, validated via advanced characterization techniques such as synchrotron X-ray diffraction, ensuring compatibility with energy storage systems. Notably, these SS-PCMs remain solid during phase transitions, eliminating risks associated with liquid-phase leakage. Remarkably, despite their solid-state behavior, we successfully shaped these materials using compression and injection molding, enabling their integration into various battery configurations. Thermal characterization revealed enthalpy changes of 72–85 J/g and thermal stability up to 180°C , ensuring effective heat management and reduced degradation risks. Mechanical testing demonstrated a rigidity of 1 GPa, further highlighting their robustness. These features make them ideal for addressing the thermal challenges of energy storage systems. Herein, we present for the first time, copper-based SS-PCMs integrated into a 7-cell Li-ion battery module, achieving superior passive thermal management, optimized temperature regulation, and enhanced performance under high thermal loads.

This work highlights the very promising role of SS-PCMs in advancing the thermal management of energy materials, demonstrating their scalability, versatility, and impact on next-generation energy storage technologies.

Fluorine-Free Materials for Sustainable-By-Design Electrolysis Cells

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A6_1 - Hydrogen generation - I, Machado Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

FASTCH2ANGE aims to pioneer a sustainable-by-design method for developing TRL4-compliant 100% PFAS-free proton exchange membrane-based electrolysis (PEMEL) cells. It will focus on developing four fluorine-free components: proton exchange membranes, catalyst-supporting layers, transport and gas diffusion layers, and new sealing components like gaskets and insulation plates.

FASTCH2ANGE will achieve this by designing, developing, and testing new PFAS-free PEMs at TRL4. These PEMs will be made using TEOS-based hybrid organic-inorganic ionomers, targeting an operating current density of 3.0 A/cm² at 1.8 V cell voltage, with a degradation rate under 5 μ V/hr by 2030. Innovations in catalyst coating technologies will be explored, including an optimized ink deposition technique.

Additionally, fluoroelastomers-free liquid-gas diffusion layers will be prepared using a sol-gel process with silicon alkoxides to improve hydrophobicity and thermal stability. FASTCH2ANGE also plans to develop PFAS-free sealing components using silicon-based sol-gel formulations and advanced materials like stainless steel, polyetheretherketone, and polyphenylene sulfide, employing high-performance coatings such as diamond-like carbon and ceramic.

Hence, an advanced testing platform utilizing multisingle cells proprietary technology will test the newly developed catalyst-coated membranes (CCMs), achieving a first-of-its-kind PFAS-free 5-cells stack with optimal components.

Harmonized European testing protocols will be used, and the cross-integrability with fuel cell technologies will be assessed in close synergy with SUSTAINCELL and EVERYWH2ERE projects.

FASTCH2ANGE new components will allow the replacement of 10-11% by weight of a new generation of electrolysis systems with harmless materials, that for the envisioned European 140 GW capacity would mean saving up to 10500 tons of PFAS crafted into PEMEL components by 2030.

The authors are presenting this work on behalf of the FASTCH2ANGE Consortium”.

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The catalytic effect of cobalt and influence of mechanical milling on hydrogen storage system MgH_2 – Co using small milling time

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The addition of cobalt to MgH_2 powder and forming MgH_2 - Co composites was investigated for small milling times. The composite powders were synthesized for 15, 30, and 45 min and characterized by XRD, SEM-EDS, PSD, DSC, and TPD methods. During TPD analysis, a kinetic model for the hydrogen desorption process was also determined. The hydrogen desorption reaction in catalyzed samples is described by the Avrami-Erofeev model with the value of parameter $n=4$. The E_a (apparent activation energy) for the hydrogen desorption reaction was decreased with the increase in milling time and the addition of transition metal. The uniform distribution of transition metal decreases hydrogen desorption temperature by more than 100 °C compared to the pure MgH_2 and purely milled MgH_2 . The quantity ratio of released hydrogen reached the highest value ($LT/HT=3.38$) for a sample with the highest amount (20 wt.%) of additive and the longest milling time (45 min). LT maxima appear at 310 °C, significantly reducing desorption temperature compared to commercial MgH_2 (480 °C). The short milling times improve desorption properties by lowering the hydrogen desorption temperature enhancing the effect of catalyst. In this approach, mechanosynthesis can be analyzed as two independent processes—grinding and catalytic effects. For the studied milling times, the catalytic influence of Co is dominant in the hydrogen desorption process.

Electrospun PEO-based membrane enriched with recovered lignin: towards sustainable solid-state electrolytes for Li-ion batteries

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Nowadays the demand for rechargeable energy storage devices has increased, driven by the proliferation of electrical applications across various sectors, including household appliances, electric vehicles, computers, smartphones, and stationary energy storage systems coupled with renewable sources. Notably, lithium-ion batteries are broadly diffused due to their high energy density, high specific capacity, operating voltage, relatively slow self-discharge rate, good cycle stability, and fast charging capabilities. However, the use of liquid electrolytes is associated with several potential safety risks including poor heat dissipation, leakage and the uncontrolled growth of lithium dendrites. These issues can provoke short-circuits, fires, and explosions, raising some concerns about safety and environmental impact. Solid state electrolytes (SSEs) have emerged as a viable alternative to address these limitations, owing to their exceptional flexibility, good chemical stability, and high energy density, thereby enhancing battery safety. Additionally, SSEs permit a simplification of the internal structure, which makes the assembly process easier and saving cost. With this perspective, the present contribution aims at demonstrating the potential of a novel and sustainable solid polymeric electrolyte (SPE), based on electrospun PEO-Lignin-LiTFSI membranes. Electrospinning was chosen as manufacturing technology due to its versatility, cost-effectiveness, and potential scalability and since it allows to produce highly porous and flexible nanofibrous membranes with a high surface-to-volume ratio and a controlled entanglement of polymer chains thanks to the rapid evaporation of the solvent. PEO is typically used for the production of SPEs because of its cost-effectiveness, ease of processability, and the capacity to dissolve lithium salts, thus allowing for ion conductivity. The incorporation of lignin proved to be essential to enhance the mechanical strength of the resulting membranes and ensure their stability during electrochemical cycles, due to the excellent thermal stability and favourable rigidity. Moreover, lignin is a by-product of the paper industry, thus offering a sustainable solution for the reuse of a waste polymer in a valuable application, thereby promoting the production of SPE within a circular economy model. As a proof of concept, the PEO-Lignin-LiTFSI membrane was tested in a symmetric Li|Li electrochemical cell at 55 °C, demonstrating compatibility with Li plating and stripping; the addition of lignin turned out to be effective in counteracting the growth of Li dendrites and thus preventing the resulting battery breakdown for a longer time with a reference membrane prepared with only PEO-LiTFSI.

Cu-Mo-O mixed oxides as anodes in high performance lithium-ion batteries

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The mixed oxides of the Cu-Mo-O (CMO) system have attracted significant interest in recent years due to their remarkable redox properties, which enable applications in various fields such as catalysis, photochemistry, sensing, and energy storage systems [1]. Specifically, the 3:2 stoichiometry phase ($\text{Cu}_3\text{Mo}_2\text{O}_9$) exhibits a high theoretical capacity (916 mAh g^{-1}), high electronic conductivity, and a non-toxic nature compared to other metal oxides containing cobalt, which are commonly used in lithium-ion batteries (LIBs). Various synthesis methods and additional strategies have been employed to modify the microstructure and enhance the electrochemical performance of phases with different stoichiometries [2].

In this work, materials with nominal composition $\text{Cu}_3\text{Mo}_2\text{O}_9$, are synthesized using (i) ball milling of metals followed by oxidative heating, (ii) ball milling of metals oxides followed by calcination, (iii) solvothermal synthesis and (iv) coprecipitation method. Structural and compositional characterizations are performed using various techniques: XRD, Raman, SEDX, SEM and TEM. The electrochemical performance as anodes for Lithium-ion Batteries (LIB) is evaluated through cyclic voltammetry, charge-discharge curves at different rates, and impedance spectroscopy. The materials show high rate cyclability and long-term stability. Thus, capacity values of around $910 \text{ mA h} \cdot \text{g}^{-1}$ after 10 cycles at $0.1 \text{ A} \cdot \text{g}^{-1}$, and $200 \text{ mA h} \cdot \text{g}^{-1}$ after 2000 cycles at $1 \text{ A} \cdot \text{g}^{-1}$ are obtained in some cases. Post-cycling assessments and preliminary kinetic studies further elucidate the electrochemical response of optimized anodes, highlighting their potential for enhancing LIB efficiency and longevity.

Lignin-Derived Ionic Conducting Membranes for solid-state energy storage devices

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Electrochemical devices, including energy storages and modulators, are expected to play key roles in creating a sustainable future. However, to realize the technological breakthrough in electrochemical technologies, the development of solid electrolytes applicable in various electrochemical devices seems crucial. The electrolyte being an integral part of the energy storage devices (i.e., Li-ion batteries) has been researched extensively, but properties of organic liquid electrolytes such as leakage, instability at elevated temperatures, and inclination to react with active materials seriously limit the development of Li-ion batteries [1,2]. Therefore, solid-state electrolytes are needed as an alternative to commercial liquid electrolytes owing to attributes such as high ionic conductivity, dendrite suppression, and compatibility with high-voltage electrodes in all-solid-state lithium-ion batteries (ASSLIBs) [3]. Here, we developed a polyvinyl alcohol (PVA)-lignin-based composite solid electrolyte, doped with lithium hydroxide (LiOH) salt, for solid-state lithium-ion batteries. The composite membrane exhibits an impressive ionic conductivity of 1.1×10^{-3} S/cm, demonstrating its potential for efficient ion transport. The effect of concentrations of Lignin and lithium salt on ionic conductivity has also been investigated. The obtained all-solid-state polymer electrolyte possessed a wide potential window of 6 V (vs. Li⁺/Li). The ionic conductivity and thermal stability of the membrane were investigated from 25 to 80 °C, and the membrane demonstrated excellent thermal stability and ionic conductivity. The membrane was also tested in devices with hard carbon and hard carbon composites with MoS₂ to investigate its applications in battery and supercapacitor configurations. The device has demonstrated excellent device stability for 5000 cycles and above 95% capacity retentions. The integration of lignin, a renewable and sustainable biomaterial, with PVA creates an eco-friendly and high-performance composite electrolyte for advancing solid-state lithium-ion battery technology while promoting sustainability in energy storage solutions.

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A comparative study of the effect of the active phase (Rh, Ru, Ir and Ni) and catalyst support on CO₂ methanation reaction

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The rapid increase in atmospheric CO₂ levels, due to our continued dependence on fossil fuels (coal, oil and natural gas) for energy production, which intensifies the greenhouse effect and accelerates climate change, imposes the urgent need to review our energy strategies. The global community is now moving in a coordinated manner towards the so-called "energy transition" and the reduction of CO₂ emissions. The capture and reuse of emitted CO₂, in the sense of recycling it by converting it into fuels (e.g. methane, methanol), is currently receiving significant research and technological interest.

In this work, we study the catalytic performance on CO₂ methanation reaction of the noble metals ruthenium (Ru), rhodium (Rh) and iridium (Ir) compared to that of nickel (Ni). These active metals are supported on various metal oxide supports, namely γ -Al₂O₃ (AL), Al₂O₃-CeO₂-ZrO₂ (ACZ), and CeO₂-ZrO₂ (CZ), which exhibit different values of labile lattice oxygen (oxygen storage capacity, OSC), a factor critical for enhancing redox reactions. Our goal is to comparatively evaluate the effectiveness of the various active metal phases in the reaction, but also how the properties of the various supports used affect the catalytic behavior through metal-support interactions. Our findings revealed a clear ranking in the catalytic performance of the active phases, as Ru > Rh > ~ Ni > Ir, regardless of the supports on which they were dispersed. Furthermore, we observed a significant, but not monotonic, effect of the oxygen storage capacity of the support on the CO₂ methanation performance. Interestingly, supports that possess an intermediate oxygen storage capacity, such as ACZ, demonstrated optimal enhancement of the active phase for CO₂ methanation. These insights emphasize the importance of catalyst support properties in the design of efficient methanation catalysts. By carefully tailoring the OSC of the support, metal-support interactions can be optimized and, consequently, the catalytic performance.

Acknowledgments

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Selective Lithium Extraction from Geothermal Brines using Advanced Adsorbent Materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In a world increasingly relying on batteries for energy storage, lithium sourcing has already gone from being a mere matter of technology to a matter of geopolitical relevance. Electric vehicles, smartphones and energy harvesting are just some of the uses of lithium that are gaining more and more importance in our everyday lives in the era of renewable energy.

Since lithium mines and salts are found in just a few regions of the planet (Australia, Andean range, China, US), it is crucial to explore alternative routes of lithium extraction to achieve a more affordable supply. Geothermal fluids are high-temperature aqueous solutions found in geothermal reservoirs, often exploited for energy production. These solutions have a high content of dissolved minerals and may contain lithium salts in non-negligible concentration.

Extracting lithium salts from geothermal brines can represent a solid alternative to mining. Thus, the optimization of materials which can be integrated in processes of selective extraction of lithium from brines is of major importance. Lithium titanate (LTO) and lithium manganese oxide (LMO) are regarded as very promising materials for the task, due to their ability to desorb and adsorb lithium ions multiple times without degrading, by the mutual substitution of Li^+ and H^+ ions in their structure in function of pH.

In this study, some materials and processes for selective lithium removal from a solution are presented: doping LTO and LMO with other transition metals can increase their lithium adsorption capacity and augment their stability in terms of dissolution of the bulk material. Doped LTO and LMO materials show remarkable lithium adsorption/desorption yields, as more than 20mg of lithium can be adsorbed and desorbed from each gram of material for each cycle. In addition to doped LTO and LMO, other materials, including zeolites and novel composite structures, are being investigated. Kinetics and extraction conditions have also been studied to optimize the process, keeping an eye on a reaction scale-up.

The selectivity of extraction of Li^+ ions against competing ones (Mg^{2+} , Na^+ , K^+ , etc.) has been quantified. Pre-treatment strategies are being explored to further enhance the selectivity of lithium extraction. Real geothermal brines from reservoirs on Italian soil have been sampled, characterized and used in laboratory to test the materials.

This study lays the groundwork for the development of a scalable process for lithium recovery from geothermal brines, potentially contributing to a more sustainable and secure lithium supply chain.

ZnSnN₂ films with improved optoelectronic features grown by High-Power Impulse Magnetron Sputtering for next-generation tandem solar cells

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A6_9 - Supercapacitors, Machado Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The pursuit of enhancing photovoltaic (PV) performance while reducing costs has driven towards tandem solar cells, which combine a top cell with an optimized optical band gap (E_{gap}) and a silicon-based bottom cell. These advanced PV systems efficiently harness high-energy photons and, in simulations, show potential beyond 40% efficiency [1], with experimental designs already exceeding 30% [2]. In this context, identifying suitable materials for the top cell of Si-based tandems is crucial. Conventional choices like III-V, CIGS, CdTe, and perovskites, despite their advantages, face limitations such as scarcity, toxicity, high fabrication costs, suboptimal E_{gap}, or stability issues. Therefore, research is targeting towards novel, cost-effective semiconductors with wide E_{gap} (~2 eV), ideal as top cell. Among these, Zinc Tin Nitride (ZnSnN₂, ZTN) emerged due to its tunable E_{gap}, high absorption coefficient, and composition of abundant, non-toxic elements. Additionally, ZTN can be synthesized as thin films via cost-effective methods [3,4].

This study critically compares the synthesis of ZTN using Direct Current Magnetron Sputtering (DCMS) and High-Power Impulse Magnetron Sputtering (HiPIMS). The latter offers improved material quality and tunability due to the more efficient ionization of sputtered species and enhanced gas dissociation. The objective is to assess the role of process parameters in optimizing ZTN. Our methodology involves reactive co-sputtering from Zn and Sn targets in a pure nitrogen atmosphere. The obtained films are analyzed for composition (Zn/(Zn+Sn) ratio), structure, electrical, and optical properties.

Different HiPIMS conditions from the material perspective have been extensively studied (high temperature growth and bipolar pulse applied to the Zn cathode). In particular, this work proves that HiPIMS matches DCMS performed at high temperature, while it is capable of reducing oxygen content below 5% at., incorporating more metallic species due to the possibility to avoid target poisoning and allowing additional structural control through the bipolar pulse. Indeed, carrier density is minimized (10¹⁷-10¹⁸ cm⁻³) by optimizing HiPIMS at room temperature, with bipolar. The fundamental aspect is that high temperature growth is even unnecessary, as it detrimentally increases n-type behavior of ZTN.

Concluding, our results are expected to advance PV technology, paving the way for more efficient and sustainable solar cells.

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The effect of the replacement of La by Sr in $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ perovskite on the catalytic oxidation of light hydrocarbons

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Perovskites, with general formula ABO_3 , are highly promising materials in catalysis due to their excellent redox properties, high lattice oxygen ion mobility, and exceptional thermal stability. Their flexibility in replacing the A-site and/or B-site cations with other elements of the same or different valence (i.e., $\text{A}_{1-x}\text{A}'_x\text{B}_{1-x}\text{B}'_x\text{O}_{3\pm\delta}$) allows them to create oxygen defects (vacancies) and modify the valence state of the transition metals in the B-site. This, in turn, alters (a) the mobility of O_2^- ions within the lattice and (b) their surface redox properties, thereby enhancing their catalytic performance.

In the present study, the catalytic activity of the perovskite $\text{La}_{1-x}\text{Sr}_x\text{MnO}_3$ (LSxM), was comparatively examined for deep oxidation of light hydrocarbons, LHCs, namely CH_4 , C_3H_8 and C_3H_6 , under excess O_2 conditions. The effect of the gradual partial substitution of the A-site of $\text{La}_{1-x}\text{A}'_x\text{MnO}_3$ perovskite, (where $\text{A}' = \text{Sr}$ and $x = 0, 0.3, 0.5$, and 0.7) on the activity and stability of the materials in deep LHCs oxidation. Various characterization techniques such as BET, XRD, and H_2 -TPR were employed to assess their physicochemical properties, correlating them with their catalytic activity. Additionally, different pre-treatment protocols were applied, including (a) pre-reduction, (b) pre-oxidation, and (c) oxidative aging at high temperatures. It turns out that the primary factor affecting the performance of LSxM was the degree of La substitution by strontium (Sr). The catalytic performance of the materials followed an inverted volcano pattern based on the variable x , with the most efficient catalyst being for $x=0$ while the least efficient for $x=0.5$. This observation strongly highlights the impact of x on the total surface area and the reducibility of the materials. Furthermore, complex hysteresis phenomena were recorded for the first time in the catalytic system during heating/cooling cycles, revealing new phenomena and findings that may be of interest to the catalysis under consideration.

Acknowledgments

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Reversible interfacial Li-oxide formation on germanium and silicon anodes revealed by time-resolved microgravimetry

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Germanium has recently garnered attention as a promising candidate for the next generation of Li-ion anodes due to its high capacity, higher conductivity, and faster lithium-ion diffusivity compared to silicon. However, uncertainty regarding the Li-storage mechanism and the formation of a solid electrolyte interface (SEI) has hindered its further development. In this study, operando microgravimetry was conducted on the Ge electrode to determine the SEI mass (irreversibly deposited) and to distinguish it from the reversibly cycled species, and their individual contributions to the total capacity. The time-resolved mass spectra, obtained by correlating gravimetry and charge flux, revealed that Li₂O along with Li is identified as a reversibly cycled species, contributing significantly to the electrochemical capacity. The amount of cycled Li₂O depends on both the cycling rate and the thickness of the anode. Interestingly, the amount of Li₂O decreases if pronounced anode cracking occurs. A direct comparison between Si and Ge indicates that the amount of the reversible Li₂O is predominantly controlled by the diffusivity of lithium into the electrodes. This study provides a general mechanism for balancing the interfacial and bulk storage of Li in the form of an oxide or by alloying, respectively.

Exploring the role of non-metal and metalloid inclusions in transition-metal electrocatalysts for direct seawater splitting

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A6_2 - Hydrogen generation - II, Machado Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Hydrogen, the green and sustainable energy carrier, can be produced through a zero-carbon technology such as water electrolysis without any emission of toxic by-products. As the freshwater sources are very scarce on earth, the utilization of seawater as the feedstock for water electrolysis has become a topic of great interest. However, seawater electrolysis has its own challenges, such as the kinetic competition between chloride oxidation reaction (COR) and oxygen evolution reaction (OER) (+1.36V: COR, +1.23V: OER) at the anode. Currently, the most efficient electrocatalysts for the HER (Hydrogen Evolution Reaction) and OER, are those based on precious metals like Pt, Ir, Ru, etc. But because of their high price and scarcity, they cannot be upscaled. Due to their abundance, low cost, and versatile characteristics, Co and Ni based electrocatalysts exhibit remarkable catalytic activity and stability in challenging seawater conditions and have emerged as one of the most promising bifunctional materials for efficient seawater splitting, offering an environmentally sustainable route to green hydrogen production. In our work, we have explored a series of Co and Ni-based catalysts combined with a non-metal (such as P) or metalloid (such as B) or a combination of both (B and P). The improvement in electrocatalytic activity and selectivity for OER in simulated and natural seawater was investigated. The experimental studies were thoroughly complemented by computational tools to not only assist in materials screening but also gain fundamental understanding of the competing reaction mechanisms over the catalyst surfaces and the role of the non-metal/metalloid in the catalyst. We also explore the degradation mechanism using a combination of transmission electron microscopy and inductively coupled plasma mass spectroscopy, providing information on improving the long-term catalyst stability in seawater-based electrolytes. The present study provides the basis for developing high-performing functional materials for green energy generation through seawater electrolysis that can eventually replace the precious metal catalysts in commercial setups.

Lignin-Derived Hard Carbon-MoS₂ Composite as a Potential Anode Material for High-Performance Energy Storage Devices

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Currently, Li-ion (LIBs) are considered one of the most advanced and dominant energy storage technologies. However, they are still struggling to satisfy the needs of higher and higher energy/power density for large-scale energy storage systems [1-2]. The limitations commonly result from active materials such as graphitic carbon anodes, which have a low theoretical specific capacity and a slow Li⁺ transfer number [3]. The rapid growth of energy storage technologies demands the development of advanced anode materials with high capacity, excellent cyclic stability, and broad operational voltage windows.

In this study, we present a novel lignin-derived hard carbon-MoS₂ (molybdenum disulfide) composite as a potential anode material for energy storage devices. The composite leverages the abundant, renewable nature of lignin as a precursor for hard carbon and combines it with MoS₂ to achieve synergistic electrochemical performance. This hybrid material exhibits a wide operational voltage window of 0–4 V, making it compatible with next-generation high-voltage energy storage systems. Electrochemical testing reveals outstanding cyclic stability over 3000 charge/discharge cycles, with a capacity retention of over 90%, demonstrating its robustness under long-term operation. The enhanced performance can be attributed to the composite's unique structure, which combines the high conductivity and stability of hard carbon with the high theoretical capacity and layered structure of MoS₂. Additionally, the composite displays excellent rate capability, ensuring suitability for fast-charging applications.

The lignin-derived hard carbon-MoS₂ composite represents a sustainable and high-performing anode material, offering a promising pathway toward scalable and environmentally friendly solutions for advanced energy storage devices. Further investigation into its structural optimization and integration into full-cell configurations is ongoing, paving the way for its practical application in lithium-ion and other battery technologies.

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DFT calculations of the electrochemical curve of $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$: influence of the functional and comparison with experiments

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A6_6 - Batteries - II, Machado Room (Level -2), septembre 17, 2025, 10:30 - 13:10

Nickel and manganese spinels are widely studied for their high application potential [1]. The electrochemical behavior of these materials, such as the voltage difference between the $\text{Ni}^{2+}/\text{Ni}^{3+}$ and $\text{Ni}^{3+}/\text{Ni}^{4+}$ redox couples, is influenced by the nickel content and structural defects [2-4]. Detailed characterizations of the lithiated materials, combined with theoretical methods, have provided insight into these defects [2,3]. However, these coupled studies do not fully describe the influence of these defects on the shape of the electrochemical curve of the $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ system ($0 \leq x \leq 1$): either they are limited to the influence on the mean operating voltage [3], or the question is not addressed [2]. A literature review shows that, for the ideal case of the perfectly ordered P432 group structure, only two DFT studies address the description of the electrochemical curve, one with the PBE functional [5] and the other with the same PBE functional with the Hubbard correction [6]. In the first, the curve is qualitatively reproduced with an underestimated mean voltage, whereas in the second, if the mean voltage is like the experiment, the intermediate phase $\text{Li}_{0.5}\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ is not supposed to be unstable and not observed. Thus, before tackling the fine description of the influence of these defects, it is necessary to have a as good as possible reproduction of the galvanostatic curve.

In this communication, we will compare four different functionals to describe the $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ ($0 \leq x \leq 1$) system and check the result with various experimental results. We employed the PBE and PBE+U (adding the Hubbard correction), R²Scan and HSE06 functionals as implemented in VASP [7]. Thus, using a set of experimental/theoretical comparisons, we will describe the $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ ($0 \leq x \leq 1$) system more or less accurately depending on the functional used. At the end of this work, the best functional identified to describe the $\text{Li}_x\text{Mn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ ($0 \leq x \leq 1$) system will be used to study lithium diffusion, the effect of stoichiometry, structural defects, etc.

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High-temperature creep behavior in 8YSZ and 8YSZ-1wt%rGO composites

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

8 mol% yttria-stabilized cubic zirconia (8YSZ) is widely used as electrolyte in solid oxide fuel cells (SOFCs) which function at temperatures between 800 and 1000 °C. This ceramic is chosen due to its optimal combination of affordability, high ionic conductivity, and chemical and mechanical stability across a wide temperature range and in various atmospheres. Also, 8YSZ/graphene composites have been suggested as novel materials for interconnects in SOFC since they fit several requirements to be used in these components, such as high electrical conductivity, chemical, structural and phase stability at operating temperature of 800-1000°C, gas tightness for both oxygen and hydrogen, matching coefficients of thermal expansion (CTE) with 8YSZ-based electrodes and electrolyte for minimizing the thermal stresses during initiation and close-down of SOFC device, as well as moderate mechanical strength combined with outstanding resistance to creep. Studies on creep behavior of polycrystalline 8YSZ are very scarce, besides, the influence of the incorporation of 2D nanomaterials on its creep behavior is completely unexplored until date.

In this work, the high temperature mechanical behavior of 8YSZ and composites of 8YSZ with 1wt% rGO (reduced graphene oxide) were investigated in creep tests between 1200 °C – 1300 °C ($T \sim 0.5 T_m$, absolute melting temperature) at different stress levels using air and Ar atmospheres. The mechanical data were analyzed, considering the microstructural changes observed during testing. These changes were investigated using scanning and transmission electron microscopy. The possibility that the presence of graphene nanosheets at grain boundaries inhibits diffusion processes increasing its creep resistance is investigated.

Understanding electrocatalyst degradation at the atomic scale

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A6_1 - Hydrogen generation - I, Machado Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Climate change has accelerated the demand for cleaner and sustainable fuels. Hydrogen is the most popular candidate for clean energy and its generation through electrochemical water splitting is considered an efficient C-free route. Electrocatalysts play a vital role in reducing the activation energy barrier (1) for the water-splitting reaction for hydrogen and oxygen production. Platinum and iridium (2, 3) (or its oxide) are known for their high catalytic efficiency for hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) respectively. Despite them being the highest-performing catalysts to date, their limited abundance and high cost necessitate greater focus on minimizing their degradation over time.

In this study, we investigate PtIr thin films deposited by physical vapor deposition (4) for OER. Magnetron sputtering and post-heat treatment at temperatures between 700 to 950 °C for 12 hours, allowed for microstructural and local composition variation as investigated by electron channeling contrast imaging and atom probe tomography (APT). During OER, dissolution species are characterized by a scanning flow cell working in conjunction with an inductively coupled plasma mass spectrometer. The as-deposited thin film shows the highest catalytic activity which diminishes by a third after just 50 cycles while the thin film heat treated at 950 °C shows a lower catalytic activity which consistently stays stable. In this regard, we discuss the activity–stability paradox with respect to the role of defects and their local composition for designing better catalysts.

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Improving the Performance of Wood Templated Nanogenerators through Functionalization and Elastomer Impregnation

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A6_10 - Polymers for energy, Machado Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Wood has emerged as a promising material for triboelectric (TEGs) and piezoelectric (PENGs) nanogenerators, offering a sustainable and efficient solution for mechanical energy harvesting. Its natural piezoelectric properties, hierarchical porous structure, and mechanical robustness enhance charge generation and energy conversion. As a renewable, biodegradable, and easily functionalized material, wood presents a compelling alternative for energy harvesting devices, driving the development of greener technologies.

Despite their potential, TEGs and PENGs face challenges in achieving stable, high-output power due to material limitations, structural complexities, and reliance on precious fillers. Impregnating wood templates (WTs) with fillers often leads to poor dispersion, weak interfacial bonding, and dependence on non-sustainable materials, limiting both performance and environmental viability.

To address these issues, this work introduces a scalable method to impregnate cellulose nanocrystals (CNCs) into WTs, leveraging their biodegradability, accessibility, and exceptional mechanical properties to enhance electromechanical performance. By combining delignification with TEMPO-mediated oxidation, porous oxidized WTs were impregnated with eco-friendly fillers composed of CNCs embedded in different elastomer matrixes.

The resulting WT elastomer TEGs, studied across varying CNC concentrations, demonstrated that output performance was influenced by compressive pressure, filler concentration, and surface charge density. CNC incorporation significantly increased surface charge density and charge transfer efficiency, doubling triboelectric performance compared to pure counterparts under identical compression conditions. The enhanced performance is attributed to the improved surface charge retention, increased effective contact area, and optimized charge transfer dynamics facilitated by CNCs impregnation.

These findings introduce an innovative, sustainable methodology to improve wood-based nanogenerators. The CNC-impregnated WT composite offers a scalable and environmentally friendly solution for next-generation energy harvesting, providing a promising pathway toward efficient, self-powered electronic devices.

Lignocellulosic solid-state electrolyte for energy storage devices

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Energy storage devices are essential in modern technology, but their use faces challenges related to sustainability, durability, and safety. Traditional liquid electrolytes present risks such as leakage and flammability, which affect the performance and reliability of batteries and supercapacitors. To develop safer and more sustainable solutions, it is important to replace these electrolytes with durable and environmentally friendly alternatives. Solid electrolytes made from abundant, biodegradable materials offer a promising way to improve electrochemical performance while reducing environmental impact.

In this study, we investigate the use of cellulose and lignin – two abundant, biodegradable and renewable biopolymers – as the basis for solid-state electrolytes. The electrolyte layer is prepared by dissolving lignin and cellulose in water at low temperatures, making the process both economical and sustainable. A neutralization process is then used for the addition of cellulose microfibrils, improving the mechanical properties and ionic transport within the material. Additionally, we conduct a detailed examination of the membrane preparation parameters, focusing on the influence of using different crosslinking agents to optimize the electrolyte's structural integrity and performance.

The resulting solid electrolyte achieved an ionic conductivity of 0.2 mS/cm at room temperature and demonstrated electrochemical stability up to 0.8 V, ensuring reliable performance. We also examined how temperature affects the structure and conductivity of the material, leading to an increase in the ionic conductivity of the electrolyte to 1.16 mS/cm at 80°C. These bio-based materials provide environmental benefits along with flexibility, chemical stability, and adjustable ionic conductivity, making them strong candidates for next-generation energy storage systems. By refining their composition and processing methods, we aim to create a solid electrolyte that is both sustainable and efficient, helping to develop safer and greener energy storage solutions.

To assess the performance of these bio-based solid electrolytes, we conducted a series of tests, including ionic conductivity measurements, electrochemical stability analysis, thermal stability and mechanical characterization. Additionally, we tested different electrode materials to determine the most compatible option for optimal electrochemical performance. By studying the interaction between the electrode and electrolyte, as well as overall cell stability, we aim to determine the best combination for effective energy storage. This study highlights the potential of bio-based solid electrolytes and provides a foundation for further research to improve their performance and applications in sustainable energy storage.

Thermomagnetic properties of multi-principal elements Cu-Fe-Mn-Ni-Sn-Ti alloys for waste heat recovery

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A6_8 - Energy harvesting from heat - II, Machado Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

The study of multi-principal elements alloys (MPEA's) can be a useful approach for the obtention of magnetic materials with tunable properties. A good example of that is the addition of Sn to the CuFeMnNiTi alloy, which increases the magnetic response from an initial paramagnetic to a ferromagnetic behavior with a magnetization saturation of ~15 emu/g at room temperature [1]. Among several magnetic applications, the tunable properties of MPEA's can be applied as thermomagnetic materials in the recovery of low-grade waste heat. The low-grade waste heat is 70% of the energy lost as heat in the transformation industry. Nonetheless, this type of energy source is usually below 230°C, cannot be recovered by conventional methods and requires thermomagnetic materials with Curie temperature near room temperature [2]. In this study, the effects of the Ti content on the microstructural and magnetic properties of CuFeMnNiSnTi alloys were verified using scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray diffraction, thermogravimetric analysis in the presence of a magnetic field, and magnetization measurements at room temperature. The as-cast CuFeMnNiSnTi0.8 alloy was composed of four phases: a Heusler-Ti(Fe, Ni)2Sn phase, a δ -(Cu, Mn)4Sn phase, Fe-fcc, and the Laves Fe2Ti compound. The highest saturation magnetization at room temperature, 44.4 emu/g, was achieved in the CuFeMnNiSn alloy with 74.0 wt.% of δ phase and 5.4 wt.% of an iron solid solution with a bcc structure. Besides that, the Curie temperature was reduced in lower Ti contents from 450 K to 350 K. The reduced phases and a lower Curie temperature are desired in thermomagnetic devices, and these results may be useful for the design of new thermomagnetic materials.

Acknowledgments

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Influence of Chemical Composition of $\text{Fe}_x\text{Zn}_{1-x}\text{S}$ on The Efficiency of Organic-Inorganic Hybrid Solar Cells

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This project aims in development and study of hybrid solar cells based on $\text{Fe}_x\text{Zn}_{1-x}\text{S}$ with P3HT to obtain a solar cell with greater conversion efficiency of energy.

Thin films of $\text{Fe}_x\text{Zn}_{1-x}\text{S}$ were obtained by chronoamperometry in a 3 electrodes cell, where the working electrode was ITO glass, Pt wire as a counter-electrode and Ag/AgCl as reference electrode. The electrochemical bath was prepared with 10 mL of FeSO_4 30 mM, 10 mL of $\text{ZnSO}_4 \cdot 7\text{H}_2\text{O}$ 30 mM and 20 mL of thiourea 30 mM and it was completed to 100 mL with water. pH was adjusted to 2.5 with H_2SO_4 and the reaction was carried out at room temperature for 600 s. The reaction was performed varying the potential (-1.2, -1.5 and -1.7 V) and the molar ratio of Fe:Zn (3:1, 2:1, 1:1).

The chronoamperogram shows the growth mechanism of the thin film on the ITO surface. Three different processes may be observed, the breaking of the double layer, the nucleation process and the growth process. The optical characterization by UV-vis shows absorption at 350-400 nm related to the presence of ZnS and a second absorption at 650 nm attributed to the Fe presence. The Fe content affects the optical properties of the materials, showing higher wavelengths as the Fe content increases. SEM images show a regular deposition with the absence of pores, in addition, when the content of Fe increases, the definition of the morphology and the particle size are better defined.

After the obtention of the ternary material, a solution of P3HT was deposited on top of the semiconductor by the spin coating methods at 4000 RPM. In addition, a solution of PEDOT:PSS 1.3% in water was deposited by spin coating in half of the cells in order to study the influence of a hole transport layer (HTL) on the efficiency of the cell. Finally, a counter electrode of Au was apply by sputtering, in order to close the circuit.

The result shows then increasing the amount of iron on the material produces a higher conductivity, what derivates in a better charge transportation in to the solar cell and a better efficiency, up to 1.5% for 0.25% of Fe. The precense of a HTL did not show an important influence on the efficiency of the solar cell, this indicates that the composition of the ternary, specially the addition of Fe to the crystalline structure determines the performance of the solar cell.

Advanced SiO_x anodes for Li-ion batteries produced by metallothermic reduction of microalgae exoskeletons

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

The development of advanced anode materials for lithium-ion (Li-ion) batteries is essential to meet the growing demand for high-capacity, long-lasting energy storage systems. Understoichiometric silicon oxide (SiO_x) anodes have emerged as a promising alternative to conventional graphite-based anodes due to their higher theoretical capacity and excellent cycling stability. SiO_x anodes are particularly attractive because they exhibit a combination of high capacity, good safety characteristics, and relatively low cost, while maintaining a balance between silicon's volume expansion during cycling and structural integrity. This study explores the synthesis and application of SiO_x anodes produced via metallothermic reduction of silica (SiO₂) sourced from industrially cultured diatoms.

In this work, we utilized the exoskeletons of single-species diatoms, cultured on a large scale in industrial settings, as a sustainable and cost-effective source of SiO₂. Two metallothermic reduction processes, aluminothermic and magnesiothermic reduction reactions, were employed to convert the diatom-derived SiO₂ into SiO_x. These methods were chosen for their efficiency and ability to control the stoichiometry of the silicon oxide phase, yielding a material with enhanced electrochemical properties suitable for Li-ion battery anodes.

The synthesized SiO_x was then incorporated into the negative electrode (anode) materials of Li-ion batteries. A comparative analysis of the electrochemical performance of the SiO_x-based anodes was performed against traditional graphite and pure silicon anodes. The results demonstrated that the SiO_x anodes, derived from diatom-derived SiO₂, exhibited superior cycle stability and high capacity retention. In particular, the SiO_x anodes showed excellent performance in terms of specific capacity, long-cycle life, and rate capability, outperforming pure silicon anodes while avoiding the severe volume expansion issues typically associated with pure silicon. This investigation highlights the promising role of diatom-derived SiO_x as a sustainable and high-performance material for the next generation of Li-ion battery anodes.

The use of industrially cultured diatoms not only provides an environmentally friendly and renewable source of SiO₂ but also underscores the potential of bio-derived materials in advanced energy storage technologies. This study sets the stage for further exploration of metallothermic reduction methods in the production of silicon-based anode materials and opens avenues for more sustainable, high-performance energy storage solutions.

Operando analysis of lead batteries by wavelength-selective neutron imaging

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A6_6 - Batteries - II, Machado Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

We have explored the use of wavelength-selective neutron imaging and Bragg edge analysis to carry out non-destructive studies of working lead batteries fabricated with three commercial electrodes, giving a total battery size of ~15 cm x 10 cm x 1 cm. Due to the high average atomic number of the constituent materials and the large electrode thickness (~3mm), neutron scattering is the only technique that allows the behaviour of these devices to be studied under real operating conditions.

In this technique the concentration of a crystalline phase can be determined by comparing images taken at close neutron wavelengths near a diffraction Bragg edge. This technique offers promising temporal and spatial resolutions and has been applied for the first time to electrochemical storage devices. We will present the first results from experiments carried out at the Paul Scherrer Institut (PSI, Switzerland). These experiments include the analysis of single-phase powders, dry electrodes and operating cells during charge-discharge cycles.

Evaluation of the remaining service life of district heating preinsulated pipes: In-depth study of a method based on the thermogravimetric analysis of the insulating polymeric foam

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

To plan activities aimed at the maintenance and improvement of district heating systems, in a logic of energy efficiency and investment containment, great importance is attributed to the evaluation of the residual service life of the preinsulated bonded pipes in use. A preinsulated pipe is a multi-material system consisting of a steel pipe, in direct contact with the circulating hot water, a rigid polyurethane (PU) foam as thermal insulation, and an outer polyethylene casing. Specific technical-scientific literature suggests that the ageing process of a preinsulated pipe is controlled by the decay of the physical characteristics of the PU foam. In consideration of this, a laboratory testing method based on the thermal analysis of the PU foam has been recently proposed as a promising approach for the estimation of the residual service life of a preinsulated pipe. This method is based on the study of the degradation processes of a PU foam sample collected from a preinsulated pipe, from tests at the thermogravimetric analyser. It allows determining a parameter characteristic of the actual degradation state of the PU foam under investigation, thus enabling an evaluation of the pipe ageing conditions. In this work, this thermogravimetric analysis-based approach is critically reviewed with the final aim of outlining a solid testing protocol that could be used as a reference testing scheme in routine preinsulated pipes condition assessment operations. For this purpose, both the aspects related to the execution of the tests (testing conditions) and those related to data processing are carefully investigated. PU foam samples, collected from preinsulated pipes in service for different periods of time, and taken from areas subject to different levels of thermal load (when in service), are examined. Furthermore, for some pipes, the information obtained from the application of this method is discussed based on the outcomes from other pipe characterization techniques.

COMPOSITE ANODES OF Si/SnS₂ FOR Li-ION BATTERIES: PHASE RELATIONS AND CRYSTAL STRUCTURE INVESTIGATIONS OF THE QUATERNARY SYSTEM

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A6_3 - Batteries - I, Machado Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Li-ion batteries have emerged as a critical technology in energy storage, powering devices from portable electronics to electric vehicles and renewable energy load level systems. This requires the development of novel anode materials, such as silicon and Sn which have high theoretical capacities, in enhancing battery performance and addressing challenges like capacity fading and thermal instability. Silicon (Si) has a very high specific capacity of 3579 mAh g⁻¹ which is about 10 times that of graphite, low cost, and high availability. Recent research shows that Tin (Sn) based materials can be used to increase the reversible capacity of anode by 20% in comparison to the traditional Graphite anodes. The full lithiation of Sn results in the formation of Li₁₇Sn₄ at a theoretical specific capacity of 994 mAh g⁻¹. Although Si and Sn- based materials exhibit high specific capacities, they undergo large volumes of expansion during lithiation. To counter this, we use SnS₂ instead of pure Sn. After intercalation of Li and conversion forming Li₂S and Sn the alloying reaction starts, only the latter is reversible. In a SnS₂/Si composite anode due to the presence of inert Li₂S heterojunction interfaces will be generated to buffer the volume expansions of the Si and Sn nanoparticles, which also inhibit further agglomeration during lithiation. To study and model this process, the main aim is to clarify phase relations and thermodynamics of the quaternary Li-Si-Sn-S system. Samples have been prepared via solid state synthesis in constituent ternary system and analysed using pXRD. Furthermore, some of the known ternary compounds were synthesized phase pure under our scope of work. Thermal analysis and calorimetry were performed to obtain thermochemical information, which will be subsequently used to optimize the Gibbs free energy descriptions of the systems in study. After successful evaluation of the ternaries, the data will be extrapolated into the quaternary, which will subsequently be used for the development of Si/SnS₂ nanocomposite anode materials.

Towards nearly zero energy buildings (nZEBs) with smart optical materials

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A6_5 - Improving Energy in Buildings - II, Machado Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

The transition towards nearly zero energy buildings (nZEBs) requires innovative approaches to enhance energy efficiency and integrate renewable energy sources. In this context, smart optical materials emerge as key enablers of sustainability, as they interact dynamically with their surroundings, providing adaptive responses to environmental demands. This work explores two classes of smart materials and applications: luminescent materials for luminescent solar concentrators (LSCs) [1] and photochromic materials for smart windows [2].

LSCs can be integrated into windows, transforming them into energy-generating elements by capturing and directing solar radiation to photovoltaic cells, thus enhancing energy harvesting and electricity generation in urban environments. Meanwhile, photochromic smart windows dynamically adjust their transparency in response to solar irradiation, reducing heating and cooling demands, improving indoor comfort, and contributing to overall energy savings.

This work explores strategies to enhance LSC performance, including molecular alignment techniques [3] and spectral conversion approaches [1,4]. Furthermore, the potential of hybridizing LSCs with photochromic molecular systems will be discussed. This integration enables the development of multifunctional smart windows that not only regulate light transmission to reduce energy consumption but also generate electricity, creating an innovative solution that simultaneously enhances energy efficiency and sustainability.

The incorporation of these advanced optical materials and devices represents a significant step toward sustainable building design, paving the way for energy-efficient, self-sufficient, and adaptive architectural solutions.

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Poly(vinylidene fluoride) enhanced multisource energy harvesting via Plasma and Vacuum-processed 1D nanoarchitectures.

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A6_10 - Polymers for energy, Machado Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Nanogenerators (NGs) are promising for sustainable energy harvesting, with piezoelectric (PENG) and pyroelectric (PyNG) types converting mechanical energy and temperature changes into electricity. To overcome their limited output, hybrid NGs have been developed to harness multiple energy sources. Ferroelectric polymers like polyvinyl fluoride (PVDF) stand out for their strong pyroelectric response, flexibility, and inherent piezoelectric properties. [1]. The performance of PVDF can be enhanced by incorporating nanofillers, increasing the electroactive phase and the internal strain [2]. Additionally, the implementation of nanoarchitectures multiplies the surface power density yielded on these NGs by increasing the surface area incorporating flexibility to the system, opening the path for permittivity engineering and multifunctional applications.

This communication reports on the first advances in the development of a multisource piezo/pyro NG, consisting of supported 1D organic nanowires as soft templates, conformally covered by either polycrystalline piezoelectric ZnO or amorphous SiO₂ and fully embedded in a PVDF pyroelectric matrix. Our approach integrates flexible commercial PET substrates with 1D nanostructures by combining low-temperature, clean, industrially scalable vacuum and plasma deposition methods.

In previous works, we have reported paper-based piezoelectric NGs and self-powered multidirectional sensors [3] and durable hybrid piezo-triboelectric NGs [4] by embedding surface supported polycrystalline ZnO nanowires into non-piezoelectric organic matrixes. Herein, we advance one step in developing multisource energy harvesters by incorporating the ferroelectric polymer PVDF. Our results show how this multifunctional device can extract energy from vibrations and temperature changes, both individually or concurrently, and how the 1D nanoarchitecture boosts the output power compared with equivalent bulk devices.

ACKNOWLEDGEMENTS

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Optimizing Composite Phase Change Material Thermal Performance via Nanoparticle-Enhanced PCM Properties

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A6_4 - Improving Energy in Buildings - I, Machado Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Thermal Energy Storage (TES) systems, particularly latent heat TES (LHTES), offer a highly effective solution for waste heat recovery, enabling energy conservation and efficiency improvements across industrial and renewable energy applications. Among TES media, phase change materials (PCMs) stand out due to their high energy storage density and nearly isothermal operation. However, their practical implementation is hindered by limitations such as low thermal conductivity, significant volume expansion during phase transitions, and structural instability. To address these challenges, composite phase change materials (CPCMs) have been developed by encapsulating PCMs within porous matrices, which enhance mechanical stability and heat transfer efficiency. Despite these benefits, CPCMs often suffer from complex or costly fabrication processes and a restricted PCM content, typically limited to around 60%, which constrains their energy storage potential.

This study explores the strategic use of SiO₂ nanoparticles (NPs) to enhance CPCMs, achieving an unprecedented PCM content of over 72% through a straightforward mix-sintering approach. Unlike conventional CPCMs, which require intricate processing techniques, our method significantly simplifies fabrication while maintaining high thermal and structural performance. The incorporation of SiO₂ nanoparticles plays a dual role: (1) enhancing the cohesion between PCM and the matrix, thereby improving structural integrity, and (2) modifying the physicochemical properties of the PCM itself, resulting in reduced thermal expansion and increased thermal conductivity.

Experimental results demonstrate that a CPCM containing 72% NaNO₃ exhibits structural stability, surpassing the conventional 60% threshold typically observed in oxide-based matrices. The nano-enhanced CPCM retains 86% of the energy storage density (ESD) of pure NaNO₃ while exhibiting a 28% increase in thermal conductivity. Additionally, the coefficient of thermal expansion (CTE) is significantly lower compared to pure NaNO₃, reducing mechanical stress during thermal cycling. These enhancements are particularly valuable for high-temperature applications where thermal stability and longevity are critical.

By leveraging SiO₂ nanoparticle modifications, this study presents a scalable, cost-effective approach to CPCM fabrication that overcomes long-standing material limitations in LHTES. The findings highlight the potential of nanoparticle-doped CPCMs to enable higher PCM content without compromising stability, opening new pathways for efficient and sustainable thermal energy storage solutions. Further research should focus on optimizing nanoparticle dispersion and exploring alternative high-conductivity matrices to further enhance CPCM performance and industrial applicability.

Half-Heusler thermoelectrics based on $\text{TiFe}_{0.5}\text{Ni}_{0.5}\text{Sb}$ compounds synthesized via mechanical alloying

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Thermoelectric materials with high power factor PF like half-Heusler need optimization in the scattering processes within the material by decoupling the transport phonons and electrons to achieve a better thermoelectric performance. Adjusting dopant concentrations to optimize the carrier concentration and density of states effective mass is one know way to achieve better performance. The other suitable option is to modulate the microstructure and point defects of the material via methods like annealing, thus improving the thermoelectric performance due to the weak electron-acoustic phonon interaction by selective defect reduction. One suitable candidate for investigation is $\text{TiFe}_{0.5}\text{Ni}_{0.5}\text{Sb}$ -based half-Heusler compounds that have an adjustable band structure and intrinsic low thermal conductivity.

This work focuses on the synthesis and characterization of $\text{TiFe}_{0.5}\text{Co}_{0.15}\text{Ni}_{0.35}\text{Sb}$ compounds synthesized via mechanical alloying using a ball milling process. The material characterization included XRD, SEM and EDS analysis and it was done using samples made by hot-press sintering.

Tuning Wetting and Triboelectrical Properties for Water Energy Harvesting

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The evaporation, condensation, precipitation, runoff and wave motion of water during the water cycle provide a great source of energy that is still under-exploited. We present here preliminary results of novel triboelectric devices capable of converting the impact of water droplets and the evaporation and condensation processes into electrical energy, combining techniques such as femtolaser texturing, core-shell nanotube growth and surface functionalisation of rigid, flexible, transparent or porous substrates. In particular, for condensation, we have designed devices that exploit the spontaneous direction of condensation to transport ions induced by the presence of triboelectric nanostructures. For evaporation, porous nanostructured materials that exploit biphilicity to induce ionic currents. For droplet impact, we combined nanostructured surfaces that induce electrification by contact of opposite polarity.

Enhancing Structural Stability and Energy Density in MgO-NaNO₃ Composite Phase Change Materials Through SiO₂ Nanoparticle Incorporation

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Composite Phase Change Materials (CPCMs) offer a promising approach for high-temperature thermal energy storage (TES) applications, combining the high energy density of phase change materials (PCMs) with the structural stability of porous matrices. However, traditional CPCMs often face limitations in achieving high PCM content while maintaining mechanical integrity, particularly in oxide-based matrices like MgO. This study investigates the effects of SiO₂ nanoparticle (NP) doping on the structural and thermal properties of MgO-NaNO₃ CPCMs, comparing two distinct MgO types: Heavy MgO, characterized by larger particle size and lower surface area, and Light MgO, with smaller particle size and higher surface area.

We evaluated CPCMs with a 50% MgO–50% NaNO₃ baseline composition, along with formulations incorporating 5 and 10 wt.% SiO₂, as well as a high-PCM-content 70% NaNO₃ – 10% SiO₂ system. Our findings indicate that SiO₂ nanoparticles significantly enhance CPCM structural stability, irrespective of MgO type. Notably, CPCMs with only 5 wt.% SiO₂ were unable to sustain 70% PCM content, while those with 10 wt.% SiO₂ successfully stabilized this higher PCM concentration. This advancement increased energy storage density while maintaining thermal conductivity at the same level as the base 50-50 composition without SiO₂. The optimized 70% NaNO₃ – 10% SiO₂ CPCM exhibited only an 18% decrease in energy storage density compared to pure NaNO₃, a substantial improvement over conventional MgO-NaNO₃ CPCMs with lower PCM content.

A key observation was the differential effect of MgO type on SiO₂ synergy. Light MgO, due to its smaller particle size and higher surface area, exhibited better interaction with SiO₂ nanoparticles, further enhancing CPCM thermal performance when combined with SiO₂ compared to Heavy MgO. This suggests that finer matrix particles can optimize nanoparticle integration, improving composite integrity.

Overall, this study demonstrates that SiO₂ nanoparticles play a crucial role in enabling high-PCM-content CPCMs while preserving thermal conductivity and mechanical stability. By leveraging nano-enhanced stabilization mechanisms, these findings open new avenues for optimizing MgO-based CPCMs for high-temperature TES applications. Future work should focus on refining matrix-nanoparticle interactions and exploring alternative nanoparticle additives to further enhance CPCM performance.

Eco-friendly tribo- and piezoelectric nanogenerators based on bionanocomposites

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A6_10 - Polymers for energy, Machado Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Circularity and sustainability of energy devices are gaining importance in the face of growing global energy demand, which enlarges the electronics waste as well as increases the scarcity of critical energy materials. Tribo- and piezoelectric nanogenerators have shown great potential in providing renewable energy to IoT and sensing devices, but often lack sustainability as the constituting materials are mostly petrol-based, fluorinated polymers, metals or lead-containing ceramics. Therefore, revalorized biomass like lignocellulosics, agri-food residues and microbial biopolymers are increasingly considered as electro-active components (1).

Here, we present results of eco-friendly nanogenerators based on different bionanocomposites. Biopolymers like cellulose, chitosan, poly-L-lactic acid (PLLA), polyhydroxybutyrate (PHB) and alginate are investigated as matrix with different fillers such as nanocarbons, MXenes, COF, ZnO, potassium sodium niobate and barium titanate particles in order to tune the triboelectric and piezoelectric properties (2,3,4,5,6,7). Special attention is given to the diverse filler-matrix interactions and their impact on the electrical properties of the composites. In addition, the role of porosity is a further parameter under investigation both for the electrical output and complementary properties. Herein, foams are explored for the construction of 3-dimensional triboactive elements with additional insulating and flame retardant behavior, which can be attractive for smart alarm systems, intelligent buildings and other applications. Finally, we will present incipient results of 3D printed PLLA-ZnO bionanocomposites with enhanced piezo-response brought about by the fine adjustment of the 3D printing parameters. Altogether, the results suggest great potential of bio-based polymer nanocomposites for more sustainable nanoenergy harvesting.

Acknowledgements

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The effect of vanadium content on microstructure and magnetic properties of FeSi electrical steels

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Grain-oriented (GO) FeSi steels are widely used as core materials in various types of transformers operating worldwide for the distribution, generation, and consumption of electrical energy. They are characterised by anisotropy of magnetic properties provided by requires a very strong Goss $\{110\}<001>$ texture. The primary magnetic properties of GO electrical steels are magnetic flux density and iron loss. The magnetic flux density is directly associated with the strength of the Goss texture, while iron loss consists of three main components: hysteresis loss, classical eddy current loss, and excess loss. A strong Goss texture is achieved through a technological route first proposed by Goss in 1934 [1], which has remained largely unchanged since then. To develop the Goss texture, inhibitors such as MnS, AlN, and a combination of MnS and AlN play a crucial role in controlling grain growth during primary and secondary recrystallization

In this study, new approaches to grain-oriented steel processing have been explored. The proposed method involves replacing conventional inhibitors, such as AlN and MnS particles, with particles precipitated from the solid solution by introducing vanadium. Typically, vanadium is used as an alloying element, primarily in heat-resistant and tool steels. However, in this work, we propose a novel approach for producing GO steels, utilizing VC nanoparticles as inhibitors in combination with a strain-induced grain boundary motion mechanism and continuous annealing under dynamic conditions during secondary recrystallization. Dynamic (fast-heating) annealing combined with VC particles was applied to grain-oriented steels to achieve abnormal grain growth with the development of Goss crystallographic orientation during secondary recrystallization. This abnormal grain growth resulted in the formation not only of a sufficiently sharp $\{110\}<001>$ Goss texture but also of the cube crystallographic texture $\{100\}<001>$, which is highly desirable for non-oriented electrical steel. Moreover, steels processed using the newly developed method exhibited magnetic properties similar to those of materials subjected to long-duration heat treatments. The coercive field of our steels reached approximately 11 A/m, indicating that the proposed heat treatment, in combination with VC nanoparticles, enables the production of steel with equivalent quality while significantly reducing heat treatment time compared to the conventional GO steel manufacturing process.

This work was carried out within the research project Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I03-03-V04-00314.

Scalable Fabrication of Flexible Perovskite Solar Modules via Roll-to-Roll Two-Step Deposition and Tailored Photonic Annealing

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Perovskite solar cells (PSCs) offer high efficiency and mechanical flexibility, making them strong candidates for next-generation flexible photovoltaics. However, the scalable fabrication of high-quality perovskite layers via roll-to-roll (R2R) processing remains a challenge due to difficulties in controlling crystal growth and drying rates. In this study, we demonstrate a scalable R2R-compatible two-step deposition method—sequentially coating PbI_2 and formamidinium iodide (FAI)—combined with intense pulsed light (IPL) annealing to overcome the limitations of conventional thermal annealing. The rapid, localized energy delivery of IPL enables efficient perovskite crystallization without damaging flexible substrates or requiring prolonged heating. To further enhance the PbI_2 -to-perovskite conversion, cesium formate (CsForm) and cesium iodide (CsI) were incorporated into the PbI_2 precursor solution. This modified composition improved film morphology and facilitated low-hysteresis device operation. Additionally, we developed an IPL-based dual-annealing approach optimized for the R2R process, which significantly reduced device hysteresis and improved overall film quality. Using this method, we successfully fabricated large-area ($10 \times 10 \text{ cm}^2$) flexible PSC modules achieving a power conversion efficiency (PCE) of 11.25%, the highest reported to date using a fully R2R process. Our results highlight the potential of IPL-assisted R2R two-step processing as a scalable and efficient route toward commercial production of flexible PSCs.

Sustainable Thermosets with Dynamic Covalent Bonds: From Lignin-Derived Aldehydes to High-Performance Epoxy Materials

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A7_8 - Catalysis / CAN, U1 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

The escalating urgency of global environmental issues has spurred a transformative shift in chemical research. The widespread use of bisphenol A (BPA), a recognized endocrine disruptor, in conventional petroleum-based epoxy resins has necessitated the exploration of bio-derived alternatives to mitigate potential health and environmental risks [1, 2]. In the pursuit of sustainable and eco-friendly alternatives to traditional epoxy resins, Schiff-based epoxy thermosets have emerged as a promising strategy. These materials leverage the inherent dynamic and reversible nature of imine functional groups, enabling thermal reprocessability and chemical recyclability [3, 4].

This study explores the synthesis of Schiff-based epoxy thermosets using sustainable approaches, starting from lignin-derived aldehydes such as vanillin and syringaldehyde. Starting with these compounds, we synthesized Schiff base monomers which were subsequently glycidylated to create novel epoxy thermosetting resins. A novel self-polymerization strategy is employed, eliminating the need for additional curing agents and resulting in thermosets with high material properties.

The Schiff-based epoxy thermosets developed in this study exhibit impressive performance characteristics. They demonstrate high mechanical properties, with storage moduli at room temperature ranging from 1.5 to 2.2 GPa. The materials also show excellent thermal stability, with glass transition values between 138 °C and 249 °C, significantly higher than traditional DGEBA-based epoxies. Thermogravimetric analysis revealed high thermal stability, with T5% values of 310-350 °C in air [5]. The thermosets also display excellent flame-retardant properties, with Limiting Oxygen Index (LOI) values between 33% and 36%. Notably, these bio-based materials have a lower apparent density (0.74-1.09 g/cm³) compared to DGEBA references, making them suitable for lightweight applications. Additionally, the thermosets demonstrate the ability to be chemically recycled in acidic conditions and thermally reprocessed, highlighting their potential for sustainable and circular material applications.

Keywords:

Bio-based thermosets, Schiff bases, High-performance, Dynamic linkage

Acknowledgements:

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Effect of doping on the structure and mechanical properties of anti-wear TiB₂ coatings

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A7_1 - Synthesis, U1 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

TiB₂-based coatings have been intensively developed due to their physical and mechanical properties, including excellent thermal stability and high hardness with good abrasion and corrosion resistance, which appear to be the most beneficial in industrial application. Previous investigations have shown that doping TiB₂ with Ni and C can significantly reduce residual stresses and improve adhesion, making these coatings ideal on tools to machining aluminum alloys. The aim of this study was to analyze the effect of interlayer on the durability (adhesion) of the deposited Ti_{1-x}M_xB₂ (x = 0; 0.03; 0.06; 0.10) M=W, Cr, Zr coatings and determine the influence of W, Cr and Zr on their microstructure and mechanical properties. The structural characterization of Ti_{1-x}M_xB₂ (M=W, Cr, Zr) coatings was carried out using X-ray diffraction, X-ray photoelectron spectroscopy, transmission electron microscopy and atomic force microscopy. To investigate the mechanical properties, nano-scratch and—hardness tests (NST,NHT) were performed, and fracture toughness of the substrate layer systems was determined. The use of an adhesive layer of pure W, Cr or Zr increased the adhesion of the coatings to the substrate. It is shown that the changes in W, Cr or Zr content not only affect the microstructure, mainly by decreasing the crystallite size (column width), but also the texture (preferred coatings orientation) and phase composition. The addition of W, Cr or Zr also has an effect on the mechanical properties of TiB₂ coating by reducing their hardness and Young's modulus and increasing their fracture toughness (KIC).

Thermomechanical response and microstructural characterization of Nitinol alloy produced by laser powder bed fusion

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A7_9 - AM, U1 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Nitinol (NiTi), a nearly equiatomic nickel-titanium alloy, is the most extensively used shape memory metallic material due to its peculiar smart features, good corrosion resistance and biocompatibility. Thanks to a low temperature phase transformation, known as martensitic transformation, it can exhibit the shape memory effect, which leads to shape recovery after deformation upon heating, or superelasticity, which allows the recovery of large deformations upon stress removal. These properties make it particularly attractive for a wide range of applications, such as in the biomedical, robotics or aerospace fields.

In recent years, several studies have investigated the additive manufacturing (AM) of NiTi to better exploit and expand its application potential, leveraging design freedom and the capability to produce complex shape components offered by these techniques. Laser powder bed fusion (L-PBF) is one of the preferred AM methods due to the finer microstructure and better surface finishing achievable. To optimize the functional properties of L-PBFed NiTi, numerous research efforts are currently focused on developing tailored heat treatments.

In the present work, various aging heat treatments were performed on NiTi samples produced by L-PBF. Specifically, aging treatments were carried out for 15 minutes at 400 °C and 500 °C, both directly after production (direct aging) and after solution annealing. The thermomechanical behavior was examined by performing cyclic compression tests at different temperatures and compression tests up to failure. Temperature-stress diagrams were experimentally determined, establishing the overall behavior of the alloys. Results of mechanical tests were correlated with the transformation temperatures of the alloy, measured by means of differential scanning calorimetry (DSC) analyses, and to the microstructure of the alloy. Precipitates formation was characterized through transmission electron microscopy (TEM) and texture analysis was carried out via electron backscattered diffraction (EBSD).

SELF-HEALING HYDROGELS PRINTED BY PHOTOINDUCED 3D PRINTING TECHNIQUES FOR BIOMEDICAL APPLICATIONS

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A7_9 - AM, U1 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Light-induced 3D printing is becoming increasingly important in various research fields due to its advantages over other additive manufacturing methods, such as higher resolution and printing speed. In this work, we want to exploit light-induced 3D printing and, in particular, Digital Light Processing (DLP) to make a biocompatible and self-healing hydrogel for application in tissue engineering. Self-healing hydrogels (SHHs) with appropriate properties, in fact, can mimic the biomechanical characteristics of biological tissues and self-repair when damaged, acting as ideal three-dimensional scaffolds for cell proliferation and differentiation. So far, such hydrogels have been processed mainly through extrusion-based technologies, limited in design and resolution(1); to obtain more complex objects with better resolution, we will exploit DLP.

Light-induced 3D printing is becoming increasingly important in various research fields due to its advantages over other additive manufacturing methods, such as higher resolution and printing speed¹. In this work, we want to exploit light-induced 3D printing and, in particular, Digital Light Processing (DLP) to make a biocompatible and self-healing hydrogel for application in tissue engineering. Self-healing hydrogels (SHHs) with appropriate properties, in fact, can mimic the biomechanical characteristics of biological tissues and self-repair when damaged(2), acting as ideal three-dimensional scaffolds for cell proliferation and differentiation(3). So far, such hydrogels have been processed mainly through extrusion-based technologies, limited in design and resolution¹; to obtain more complex objects with better resolution, we will exploit DLP.

The hydrogel is fabricated using water-soluble, commercially available materials, such as polyethylene glycol diacrylate (PEGDA), hydroxyethyl methacrylate (HEMA), dithiothreitol (DTT) and borax. We successfully printed complex 3D objects using a commercial DLP printer, and we evaluated the ability of self-repair by cutting the specimens and bringing the two ends together, without any other stimuli: after 72h, the specimen is able to self-standing and resist tension and can be subjected to several cycles of breakage and repair.

We then characterized the hydrogels in terms of chemical, rheological and mechanical properties, and finally we performed cytocompatibility tests to verify applicability in tissue engineering.

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Electrodeposited CuNiCo Ternary Alloy Films as High-Performance Electrocatalysts for Nitrate Reduction

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A7_8 - Catalysis / CAN, U1 Room (Level 0), septiembere 17, 2025, 14:30 - 16:30

Electrodeposition offers a scalable and versatile method for fabricating catalytic surfaces tailored for specific electrochemical applications. This study presents the synthesis of a ternary CuNiCo thin alloy film on a graphite substrate via electrodeposition, optimized for the nitrate reduction reaction (NO_3^- RR). A Hull cell was utilized to gain insights into current density effects, aiming for uniform deposition and improved catalytic performance. Additionally, the influence of precursor concentrations, pH, additives, and current density was systematically analyzed to determine the optimal alloy composition and deposition conditions.

The deposited CuNiCo alloy was characterized using techniques such as scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS), with X-ray absorption near-edge structure (XANES) analysis offering valuable insights into the alloy's chemical composition and electronic structure. Electrochemical performance was evaluated through cyclic voltammetry (CV), linear sweep voltammetry (LSV), and chronopotentiometry in nitrate-containing electrolytes. Preliminary findings suggest that the ternary alloy offers promising activity and selectivity for NO_3^- RR, with indications of higher nitrate conversion rates compared to monometallic and bimetallic counterparts.

Furthermore, the catalyst demonstrated promising potential for CO_2 reduction reactions, highlighting its versatility in various electrochemical applications. This work underscores the synergistic effects of the ternary CuNiCo system, offering a pathway for the development of advanced catalysts for environmentally critical reduction reactions.

Directly Grown CoOx Nanowires Coated with NiOx Nanosheets on Ni foam: A Novel Integrated Electrode for High-Performance Non-Enzymatic Glucose Sensing

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Non-enzymatic glucose sensing is critically important in diverse fields, including medical diagnostics, food quality control, and environmental monitoring, due to its simplicity, robustness, and cost-effectiveness. In this context, nanostructured metal oxide-based electrodes have gained attention as prospective electrode materials, delivering promising electrocatalytic performance.

Addressing this need, this study reports the successful synthesis of a CoOx@NiOx core-shell heterostructure, consisting of CoOx nanowires as the core covered by NiOx nanosheets as the shell, directly grown on nickel foam (NF) to form an integrated electrode for non-enzymatic glucose sensing. The synthesis involved a two-step process: first, the growth of CoOx nanowires on nickel foam via a straightforward hydrothermal method, followed by the chemical bath deposition of NiOx nanosheets to form the CoOx@NiOx core-shell heterostructure.

The morphology, structure, and electrocatalytic performance of the electrode were systematically analyzed using comprehensive physicochemical characterizations. Results confirmed the uniform deposition of the CoOx@NiOx heterostructure on the three-dimensional nickel foam framework. Electrochemical testing revealed that the CoOx@NiOx/NF electrode exhibited exceptional performance, with a high sensitivity of $8700 \mu\text{A} \cdot \text{mM}^{-1} \cdot \text{cm}^{-2}$ and $581.15 \mu\text{A} \cdot \text{mM}^{-1} \cdot \text{cm}^{-2}$ across wide linear ranges of 10–1000 μM and 1000–5000 μM , respectively. This outstanding electrocatalytic performance can be attributed to the unique CoOx@NiOx heterostructure, which provides a large surface area, enhanced exposure of electroactive sites, richer redox reactions, short ion diffusion paths, and rapid electron transfer. Furthermore, the electrode demonstrated excellent selectivity, high reproducibility, and long-term stability, underscoring its suitability for practical applications. In summary, the proposed CoOx@NiOx/NF electrode offers a highly promising platform for continuous non-enzymatic glucose monitoring.

Keywords: Nickel foam, cobalt oxide, nickel oxide, heterostructure, core-shell, non-enzymatic glucose sensor

4D Printable Metamaterial and Terahertz: A Pathway to Next-Generation Devices for 6G Technologies

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A7_2 - Electronics I, U1 Room (Level 0), septembre 15, 2025, 14:30 - 16:30

The next generation of wireless communication (6G), foreseen for the 2030s, will be based on terahertz (THz) radiation. 6G is predicted to aggregate multiple types of resources, becoming a digital ecosystem that connects the digital, physical, and human worlds. [1] To achieve this goal, it is thus necessary to minimize the existing gap between cyber and physical worlds, with distributed and adaptive devices' interactions with THz. Beyond 6G, THz frequencies are also gaining interest in many applications in different areas, such as biomedical, quality control, security, and defense. [2] In this work, the possibility of creating a stimuli-responsive metamaterial that can interact with THz in a programmable and controlled way was investigated to develop 4D printable sensors for 6G technologies or, in general, for THz radiation. This was possible by combining polymeric material characteristics, pattern designs, and responsive dyes.

Despite the pivotal role that this part of the electromagnetic spectrum will play in the next future, the knowledge on matter/radiation interaction is lacking, especially for polymeric materials. To address this, experiments on various photocured (meth)acrylates and thiol-ene resins with different chemical compositions were conducted, evidencing a precise relationship between polymers' chemical composition and THz interaction. The definition of this dataset was the cornerstone to design new formulations that could meet the transparency criteria request for the development of THz-active metastructure, having user-defined interaction with the radiation given by specific pattern designs. For those metamaterials, geometric features of hundreds of microns are necessary due to the high wavelength involved, and those characteristics are perfectly compatible with 3D printing capabilities, particularly with Digital Light Processing (DLP) technology, the one used for this work. [3] Finally, the integration of photoresponsive compounds within the printed formulation allowed the enhancement of the printing resolution and, additionally, the possibility to trigger the THz transmission, resulting in a THz-active 4D printed metamaterial with a light-controlled THz interaction. These findings open new perspectives for the advanced manufacturing of multifunctional materials in strategic fields such as electronics and telecommunications.

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Modifications of furan-based polyesters and copolyesters - a silver bullet for developing novel and sustainable materials

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A7_6 - Environment, U1 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

There is growing interest in preparing new chemicals and materials based on renewable resources, as biomass-derived fuel and chemicals are a promising alternative to fossil-based materials [1]. The 2,5-furan dicarboxylic acid (FDCA) in particular, has been selected as one of the most important building blocks or top value-added chemicals derived from biomass [2]. The promising developments in the FDCA synthesis have led to the lab-scale synthesis of several FDCA-based polyesters including poly(ethylene 2,5-furandicarboxylate) (PEF) and its copolymers and blends. Concerning modification of furan-based materials, the state-of-the-art reports composites based on furan polyesters and copolyesters with carbon nanofiller, mineral fillers, and fibers [1, 3]. In the present work, poly(ethylene 2,5-furandicarboxylate) (PEF)-based copolymers and blends with an elastomer of poly(tetramethylene oxide) (PTMO) or epoxidized natural rubber (epNR) have been studied. Moreover, composites based on PEF-b-PTMO containing plant modifiers such as fenugreek or gentian have been prepared and their impact on flame retardancy has been verified. The molecular structure of the synthesized copolymers has been analyzed by ¹H NMR and FTIR spectroscopies. In order to evaluate phase transition temperatures and the thermal effects in the synthesized series of copolymers and composites, DSC, DMTA, and TGA have been performed. The obtained copolymers and blends exhibited a good combination of mechanical and processing properties, which resulted from high values of limited viscosity number (LVN). The obtained copolymers and blends do not undergo crystallization during cooling from the melt. One confirmed that the addition of PTMO had a significant effect on thermal and thermo-oxidative stability and tensile and cyclic properties. Moreover, it has been clearly demonstrated that the introduction of an elastomeric part during polycondensation is a more effective form of polyester modification than reactive blending with epNR. An increase in hardness and Young's modulus values was demonstrated, with significantly reduced elongation at break values for the samples with the plant additives. Furthermore, flammability analysis revealed that the addition of gentian and fenugreek slightly reduced THR, suggesting the potential of these additives as flame retardants.

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Halide Perovskite Thin Films for Neutron Detection

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A7_5 - Sensing, U1 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

The need for high-efficiency, wide-area coverage radiation detectors is essential in applications related to nuclear medicine, industrial imaging, environmental monitoring, spacecraft applications, and homeland security, among others. In all these applications, the detector material interacts with high-energy particles or photons while operating at high electric fields. The material should also show negligible leakage current, high resistivity, and be able to scale. Cesium lead bromide (CsPbBr_3) is an excellent candidate that needs most of these requirements. CsPbBr_3 has excellent electric, optical, and spectroscopic properties while stable under extreme operating conditions. These properties make CsPbBr_3 an ideal material for high-energy radiation detectors. However, the use of CsPbBr_3 for charged particle and photon sensing is normally limited to single crystals. This is primarily due to the lack of deposition techniques for CsPbBr_3 films, which is necessary for high-energy radiation sensing. To overcome this, thin films were deposited using the close space sublimation (CSS) process, which allows the deposition of stoichiometric and high-quality CsPbBr_3 films with reduced defects, large grains, and high deposition rates. Alpha particles and neutron sensing using a p-n diode are also presented.

Planar $\text{CsPbBr}_3/\text{Ga}_2\text{O}_3$ p-n junction diodes coupled with ^{10}B neutron conversion film have been demonstrated by showing a thermal neutron detection efficiency of 2.5% [1-2]. The theoretical neutron detection efficiency of planar detectors is limited to <4.5% due to the self-absorption of reaction products within the neutron conversion layer. Higher efficiencies (20 % – 35 %) have been demonstrated using micro-structured silicon diodes backfilled with a neutron conversion material [3]. Micro-structured detectors fabricated using thin-film semiconductors can be more easily scaled for large-area applications than detectors using single-crystal semiconductors. Neutron detection efficiency using micro-structured detectors has also been demonstrated recently [4-5].

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Formation Mechanism of J-Aggregates in Two Types of Molecularly-Oriented Bisazo Dye Films

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

[Introduction] We have developed highly-oriented J-aggregates of bisazo dyes.[1-4] In these studies, we found that two compounds differing only in the end group gave completely different results in polarized optical microscopy (POM) images and absorption spectra. These different results are presumably due to the fact that dye 1 is more likely to form J-aggregates, whereas dye 2 is not. In this study, we investigated the formation of J-aggregates by comparing these two compounds.

[Experiment] Bisazo dyes 1 and 2 were vacuum-deposited on the polytetrafluoroethylene (PTFE) alignment layers, resulting in molecularly-oriented films containing J-aggregates. These two films were analyzed by polarized optical microscopy (POM) and atomic force microscopy (AFM). X-ray structure analysis was performed on single crystals of these two compounds, and the molecular packing in their films was investigated using grazing incidence wide-angle X-ray scattering (GIWAXS) measurements.

[Result] Single crystal analysis revealed that the directions of molecules within the unit cell are all parallel for dye 2, but not completely parallel for dye 1. This difference may have affected the formation of J-aggregates because molecular orientation is achieved by trapping along the atomic grooves between adjacent PTFE chains.[2] If all the molecules are parallel and can easily align with the atomic grooves, highly oriented and uniform thin films can form.[1] On the other hand, if the molecules are not parallel within the unit cell, some molecules may be placed across two parallel adjacent atomic grooves, resulting in a reduction in molecular alignment. However, this arrangement could facilitate the formation of J-aggregates because J-aggregates can form under quasi-stable conditions. In fact, when dye 2 was vacuum-deposited onto the glass substrate directly without the PTFE alignment layer, the quantity of J-aggregates formed in the films significantly increased. In summary, a high order parameter is achieved when the molecules fit well into the atomic grooves of PTFE. Conversely, our results suggest that if the molecular arrangement and the atomic grooves are poorly matched, the degree of orientation is reduced and J-aggregates are more likely to form.

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Formation and Emission Properties of J-Aggregates in Molecularly-Oriented Bisazo Dye Films

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A7_3 - Electronics II, U1 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

J-aggregates are known for their unique optical properties and have been studied as various functional materials, including biomedical imaging and phototherapy. We have developed highly oriented J-aggregates of bisazo dyes and investigated their formation mechanisms.[1-4] In this study, we report on the local formation and photophysical properties of J-aggregates in molecularly-oriented bisazo dye films.

A bisazo dye (BZ-5)[4] was vacuum-deposited on polytetrafluoroethylene (PTFE) alignment layers, resulting in molecularly-oriented films containing J-aggregates of BZ-5. When the film was observed by a polarized optical microscope (POM) employing monochromatic light matching the J-band, the regions absorbed by the J-aggregates resembled 'islands'. This observation confirmed that J-aggregates were locally formed in the film. In a comprehensive study using atomic force microscopy (AFM), we found that these J-aggregates are located at quasi-stable branching points between stable crystalline grains.

In general, azo dyes hardly exhibit fluorescence because non-radiative decay due to molecular motion is dominant. However, a sharp peak at 615 nm could be observed in emission spectra for our films. Little emission was actually observed when the crystalline phase was excited in the short-wavelength region. Therefore, the sharp peak must originate from the J-aggregates. In addition, a broad emission peak around 800 nm was also observed, which may originate from a different type of aggregates. However, its intensity is lower than the sharp emission peak at 615 nm, suggesting that energy transfer between different types of aggregates is suppressed. The different types of aggregates are presumably separated by distances exceeding the Förster radius.

In summary, these results show that J-aggregates of the bisazo dye BZ-5 are formed locally in the thin films, and exhibit fluorescence in spite of the azo dye.

[Acknowledgments] JSPS KAKENHI (JP21K04813 and JP23K04885), Iketani Science and Technology Foundation (0361270-A).

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Novel air-jet spinning-assisted 3D printing of porous scaffolds for tissue engineering applications

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A7_9 - AM, U1 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

The fabrication of porous scaffolds with controlled architecture and enhanced bioactivity remains a critical challenge in tissue engineering. Conventional 3D printing techniques, while offering high precision, often struggle to achieve the microporosity and surface topography required for optimal cell attachment, proliferation, and tissue integration. To address these limitations, we introduce a novel air-jet spinning-assisted 3D printing (AJS-3DP) approach for fabricating porous scaffolds with tailored microstructural properties. This hybrid technique combines the advantages of air-jet spinning, which generates ultrafine fibers, with extrusion-based 3D printing, ensuring hierarchical porosity and an interconnected network structure.

In this study, we optimized key processing parameters, including air pressure, polymer solution viscosity, and fiber deposition rate, to achieve uniform and reproducible fiber deposition within the 3D-printed scaffold matrix. The resulting scaffolds were characterized for their morphological, mechanical, and biological properties using scanning electron microscopy (SEM), mechanical compression testing, and in vitro cell studies. The integration of air-jet spun fibers into the printed scaffold significantly enhanced the surface roughness and porosity, promoting cell adhesion and proliferation. Furthermore, the hierarchical porous structure facilitated nutrient and oxygen diffusion, critical for tissue regeneration. In vitro biological assays confirmed superior cell attachment, viability, and spreading on the air-jet spun fiber-enhanced scaffolds. The controlled fiber deposition further enabled the tuning of pore size distribution and scaffold permeability, demonstrating the potential of this technique for designing patient-specific tissue scaffolds.

The novel AJS-3DP method presents a promising strategy for fabricating next-generation biomimetic scaffolds for bone and soft tissue engineering applications. By leveraging the synergistic effects of air-jet spinning and 3D printing, this approach offers a scalable and customizable solution for producing scaffolds with enhanced bioactivity and mechanical performance. This research highlights a significant advancement in scaffold fabrication technology, providing a versatile platform for engineering functional tissue constructs.

Bio-Based Photocatalytic Nanocellulose-based Aerogels: A Sustainable Solution for Microplastic Capture and Degradation

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A7_6 - Environment, U1 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

The utilization of photocatalytic nanoparticles in powder form is frequently linked to considerable additional costs, attributable to the downstream processes necessary for their recovery and reuse post-application, including filtration, sedimentation, or centrifugation. Immobilizing these nanoparticles within a matrix that serves as a structural support material offers a promising solution by significantly reducing the need for such processes, thereby streamlining operations and making particle management and recovery more cost-effective and efficient.

Among the diverse range of options for immobilization, biopolymers, particularly cellulose nanofibers, stand out as a particularly promising solution. These materials exhibit numerous advantageous properties, including biodegradability, renewable origin, non-toxicity, high specific surface area, wide availability, and potential for functionalization. These properties enable the fabrication of composite materials in the form of aerogels with highly porous microstructures, which showcase ease of handling and photoactive surfaces, making them highly suitable for environmental applications.

In this study, C,N-doped TiO₂ photocatalysts with enhanced visible light absorption were incorporated into nanocellulose obtained from agricultural waste using colloidal synthesis routes. The resulting C,N-TiO₂ aerogels offer a dual functionality: they can physically capture microplastics while simultaneously photodegrading them under visible light. This integrated approach offers a sustainable and efficient solution to address microplastic pollution, a critical emerging contaminant in water resources. These findings contribute to the development of environmentally friendly technologies for water purification by exploiting renewable materials and advanced photocatalytic properties.

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Deposition of combinatorial oxide thin films by Spatial Atomic Layer Deposition for optoelectronic applications

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A7_3 - Electronics II, U1 Room (Level 0), septembre 15, 2025, 17:00 - 19:00

Nanoscale films are playing a major role in all modern applications such as photovoltaics and display technologies. Optimization of such films to enhance device performance can be a tedious process. Combinatorial high-throughput (CHT) thin film deposition is an approach for producing films presenting a gradient in at least one property (chemical composition, thickness, etc), for the accelerated optimization of material properties. Although traditional Atomic Layer Deposition (ALD) use have mostly targeted the uniform thin film deposition, several ALD approaches have been developed to perform combinatorial deposition. These procedures take into account the process temperature, non-uniform flow of pulsed gases[1], and saturated/non-saturated cycles[2] to optimize different properties of the films. Spatial-ALD (SALD) is a faster (two orders of magnitude) version of conventional ALD, and is a simpler and affordable approach to obtain high quality nanoscale films at ambient environment[3,4]. Indeed, SALD can be engineered to produce combinatorial films at high deposition rates. It has been implemented to produce ZnO and Al₂O₃ thin films with a thickness gradient for the fast optimisation of metal-insulator-metal diodes (MIM) and perovskite solar cells by using a custom-designed SALD reactor head[5]. The gradients were obtained by the design of the SALD head, with the assistance of computational fluid dynamics (CFD). In this communication, we will present recent CFD results of new reactor-head designs to deposit ZnO and Al₂O₃ films thickness and composition gradients as encapsulation layers of Ag nanowire (AgNW) networks. AgNW networks are alternative indium-free transparent electrodes that present state-of-the art optoelectronic properties but that need to be encapsulated due to AgNW's instabilities (thermal, electrical and chemical)[6]. We will also present experimental results of the impact of oxide encapsulation layer thickness and composition on the stability and properties of AgNW networks. The CHT approach for AgNW networks is intended for low-emissivity coatings[7] in energy-efficient smart windows.

Key words: Combinatorial thin-film deposition, Ag nanowires, SALD, Computational fluid dynamics.

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Synthesis and characterization of polycationic Sn clathrates via ball milling

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Clathrates are defined as inclusion compounds with the guests (atoms or molecules) completely and irreversibly enclosed in the cavities of the framework [1]. Based on the composition of the framework the clathrates classified as clathrate hydrates [2], the framework mainly consists of gas or liquid molecules, and intermetallic clathrates, where the host framework consists of four-bonded Si, Ge or Sn atoms. The intermetallic clathrates, depending on the charge of the framework, can be further classified as polyanionic and as polycationic clathrates. In the polycationic or inverse clathrates, the framework bears a positive charge and in their cavities halogen atoms (I, Br, Cl) are placed as guests. The most common synthesis of polycationic clathrates involves grinding and annealing of the reagents, or alternatively a combination of spark plasma sintering and high-energy ball milling [3].

In this work, we report the mechanochemical synthesis of reverse clathrates with the formula $\text{Sn}_{46-x}\text{M}_x\text{I}_8$, where $\text{M} = \text{Sb, In}$ and $0 < x < 8$. The synthetic route is a combination of planetary ball milling of the reagents and then high-temperature annealing in order to improve the purity and the crystallinity of the resulting products. The polycrystalline compounds are structurally characterized through Powder X-ray Diffraction and Rietveld refinement. The rattling modes of the guest atoms are also investigated through Raman spectroscopy. The thermoelectric properties of the compounds are also discussed in the context of potential device fabrication.

Acknowledgment: The research project is implemented in the framework of H.F.R.I call “Basic research Financing (Horizontal support of all Sciences)” under the National Recovery and Resilience Plan “Greece 2.0” funded by the European Union –NextGenerationEU (H.F.R.I. Project Number:14730).

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Methods of Compound Drug Delivery via Porous Collagen Scaffolds

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This research investigates drug delivery through Porous Collagen Scaffolds (PCSs). Scaffolds that are collagen – based are promising biomaterials, offering significant potential in regenerative medicine. Various studies have explored the use of PCS for peptide – based therapeutics, however only a few focus on the utilization of PCS for controllable long- term delivery of hydrophobic small molecules . Here a PCS Drug Delivery System (DDS) designed for small molecule compounds is presented. The system involves embedded biodegradable polyester microstructures (microrods, fibers, microspheres), incorporated in the PCS during the formation of the scaffold. The microstructures are fabricated via electrospinning/electrospraying. The fabrication of the microstructures was followed by systematic studies that were conducted to evaluate the influence of the type of the embedded matrix (long fibers, spheres etc.), composition (different copolymer blends) and surface characteristics on the diffusion mechanism of the selected drug, BNN27. In addition, the maximum drug loading concentration was studied. The drug release kinetics corresponding to each DDS system was quantified, and the non-toxicity of the polymer grafts was confirmed via bioactivity studies carried out on NIH3T3 cells. Ultimately, the polymeric grafts composition and fabrication techniques were optimized to enhance the DDS's half-life and drug loading capacity, paving the way for improved long-term drug delivery systems.

Metal/polymer nanofluids prepared by nanoparticle-beam deposition for unconventional resistive switching

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A7_2 - Electronics I, U1 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

The growing demand for computational power with lower energy consumption has made the development of novel materials for brain-inspired computing essential. Currently, most artificial neural networks rely on memristors - devices that change their resistance in response to an electric field mimicking biological synapses. However, the top-down fabrication of memristive arrays, typically achieved via techniques like lithography, is approaching limitations due to challenges in miniaturization and wiring complexity. Additionally, the structural organization of these networks diverges significantly from that of biological neuron assemblies, limiting their adaptability, robustness, and learning potential. As a result, the exploration of alternative material systems for brain-inspired computing remains a critical and ongoing research focus.

Gas-phase synthesized metal nanoparticles (NPs) have been utilized to create percolating networks exhibiting neuromorphic functionality. These networks were fabricated by depositing NP beams onto planar substrates equipped with electrodes. Under constant electric fields, the networks produced avalanches of current spikes, displaying scale-free dynamics and long-range spatiotemporal correlations reminiscent of biological neural activity. We advanced beyond the state-of-the-art by creating memristive nanofluids through the deposition of NPs beams into vacuum-compatible dielectric liquids, such as polyethylene glycol (PEG). In an electric field, the NPs underwent electrophoresis and self-organized into long-range conductive paths, growing from anode to cathode. It was demonstrated that the electrophysical properties of the nanofluids and the kinetics of path growth could be finely tuned by modifying the properties of PEG. Fundamental differences in electrical behavior were observed among three types of metal NPs: silver, gold, and nickel. Precious-metal NPs exhibited resistive switching effects during current/voltage cycling, as the voltage applied across electrodes connected by the path revealed memristive behavior. In contrast, nickel-based nanofluids showed no resistive switching, with the resistance matching that of the host liquid, which was attributed to the surface oxidation of the NPs. Detailed analysis of memristive switching in Ag/PEG nanofluids revealed multiple switching events along the path, corresponding to distinct conductivity mechanisms, including Ohmic conduction, tunneling, and space-charge-limited conduction.

Acknowledgments: The work was supported via the grant GACR 23–06925S from the Czech Science Foundation. D.N., K.B. and M.P. acknowledge the support from the Czech German Mobility via the grant number 8J23DE016 from the Ministry of Education, Youth and Sports. A.V., and B.A. would like to acknowledge funding by the German Academic Exchange Service (DAAD), Project ID 57654440.

Advanced multifunctional hybrid carbon nanocomposites

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A7_4 - Composites, U1 Room (Level 0), septiembre 16, 2025, 10:30 - 13:10

This research presents the development of novel hybrid polymer nanocomposites with enhanced multifunctional properties, addressing the growing demand for advanced smart functional materials combined with other advantages of lightweight and easy processability. Hybrid nanocomposites could offer multifunctionality with improved mechanical and electrical properties. However, they have not been explored much. This study focuses on a blend matrix of thermoplastic polyurethane (TPU) and acrylonitrile butadiene styrene (ABS), strategically combining TPU's elasticity with ABS's rigidity to optimize shape memory characteristics and processability. The innovation lies in addressing common challenges in nanoparticle dispersion and agglomeration by the incorporation of both carbon nanotubes (CNTs) and graphene nanoplatelets (GNPs) by solution processing method to create a hybrid reinforcement system. This unique approach exploits the synergistic effects between 1D CNTs and 2D GNPs, resulting in an intercalated hierarchical network forming a co-supporting conductive pathway. The combination of polymer blending and mixed fillers significantly reduces the percolation threshold, thereby improving electrical properties as proved by enhanced conductivity. Our findings demonstrate efficient nanoparticle dispersion without agglomeration as observed by Scanning Electron Microscopy (SEM) imaging. Mechanical properties are also significantly enhanced, with a 50% increase in modulus and tensile strength observed with only 2wt% CNT reinforcement. These nanocomposites exhibit impressive multifunctionality, namely shape memory behaviour and piezoresistivity. Remarkable improvements have been observed in the shape memory properties, with at least 97% shape fixity and 92% shape recovery for only 2wt% GNP composite. Such behaviour is mainly due to increased crystallinity of the hybrid composites, which have been confirmed with X-ray Diffraction (XRD) analysis and Differential Scanning Calorimetry (DSC). The CNT reinforced composite shows good strain sensitivity with a gauge factor as high as 12 at 24% strain, indicating potential for integrated sensing capabilities. Mixed fillers form a more strain susceptible network and offer improved sensitivity. The multifunctional nature of these hybrid nanocomposites makes them ideal candidates for various smart material applications. In aerospace, they could serve as self-sensing, shape-morphing structures for adaptive wings or deployable space structures, or for structural health monitoring. This research represents a significant step forward in the field of smart functional materials, particularly in shape memory polymers. The synergistic effects observed in these hybrid systems not only improve individual properties but also create new possibilities for material responsiveness and adaptability, opening up exciting avenues for further research and development in smart materials.

Multifunctional composites based on covalent adaptable networks modified with recycled carbon fiber

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A7_8 - Catalysis / CAN, U1 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

The development of covalent adaptable networks (CANs) is crucial for advancing composite materials, particularly in enhancing their recyclability and self-healing capabilities. CANs, which incorporate dynamic covalent bonds, allow for the reconfiguration of the polymer network under specific conditions, enabling repair and recycling. This adaptability is essential for extending the lifespan of composite materials and reducing waste.

In parallel, the recycling of carbon fiber composites (CFRPs) is gaining attention due to the high value and performance of carbon fibers which had led to their introduction in several applications such as aerospace industry. This industry makes use of preimpregnated products which cannot be easily recycled, which is a problem due to the large amount of scrap and expired products. Mechanical recycling of this scrap has been previously studied by the research group with extraordinary good results obtaining multifunctional composites with high added value.

In this work the combination of CANs and recycled carbon fibers has led to the development of multifunctional composites with enhanced mechanical properties, self-healing and shape-memory abilities, as well as reduced environmental impact. A commercial imine-based CAN has been modified by the addition of different contents of rCF to reach the percolation threshold and allow Joule effect heating. In this way, the material was heated by Joule effect to temperatures above the T_v and T_g of the material (previously measured) to allow dynamic behaviour of the thermoset resin. Nevertheless, the presence of rCF affected the shape memory behaviour and the capability to change the shape of the materials with temperature. In the same way, rCF affected the flowing capabilities of the material thus affecting the self-healing capabilities, so the rCF content was optimized in the study to allow keeping these functionalities and the capability of reaching the temperature required by Joule effect. Additionally, the self-sensing capabilities and the effect on the mechanical properties of the rCF in the polymer matrix were also studied.

Modified Carbon Aerogels as Fe-N-C catalysts

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A7_8 - Catalysis / CAN, U1 Room (Level 0), septembre 17, 2025, 14:30 - 16:30

Modified Carbon Aerogels as Fe-N-C catalysts

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Carbon aerogels have a great potential to be used in applications like adsorption, catalysis, supercapacitors, fuel cells or batteries based on their unique properties such as well-controlled pore size distribution, high porosity, large specific surface area, high electrical conductivity and low envelope density.[1] They have a three-dimensional, open porous structure and are produced via carbonization of organic aerogels based on e.g. resorcinol-formaldehyde polymers.

Polymer electrolyte membrane fuel cells are a very promising technique for converting hydrogen into electrical energy. But until now, one major problem for large-scale application are the high platinum catalyst costs. A suitable alternative to the critical raw materials are iron-nitrogen (Fe-N_x) complexes embedded in a porous, carbonaceous structure.

For the application as a catalyst, the carbon matrix has to be modified in order to incorporate the active Fe-N_x sites into the carbon structure. Therefore, the carbon is treated with different synthesis steps to introduce nitrogen and iron into the carbon structure.[2] Prior nitrogen doping of the carbon aerogel, oxygen doping was identified as a crucial step. To introduce nitrogen and iron, the oxidized carbon aerogel is mixed with nitrogen and iron precursors and thermally treated to obtain Fe-N-C materials.

The presentation will focus on our recent studies showing different synthesis techniques and the results of physicochemical and electrochemical characterization of the doped carbon aerogels using physisorption measurements, scanning and transmission electron microscopy, X-ray photoelectron spectroscopy, electrical conductivity measurements and rotating ring-disk electrode measurements.[3]

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From local agrifood waste to advanced materials for sensing

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A7_6 - Environment, U1 Room (Level 0), settembre 16, 2025, 17:00 - 19:00

Agri-food waste represents an environmental problem; hence it is important to get in the mindset of the circular economy, using waste in an efficient and sustainable way to reduce the problems related to its disposal.[1,2] In this frame, the aim of the project is to convert fractions of waste into a potential resource for innovative materials.

Herein, cellulose pulp was extracted from Sardinian Olive leaves.

Cellulose pulp has been dispersed with eutectic solvents (ES) [3]; the innovative composition of the ES, using acrylic acid and Zn salt, permits partial dispersion and solubilization, allowing the simultaneous grafting of acrylate functionalities onto the cellulose chain, enabling the production of a “ready-to-use” photocurable formulation in which cellulose acts as a crosslinker. The formulations are suitable as a resin in 3D printing, especially DLP, and present ionic conductivity making them good candidates to produce conformable strain sensors [4].

Some tests have been conducted using aloe vera and olive leaves, which have opened the doors to possible creation of the material using cellulose from various waste sources. Studies are still ongoing.

Acknowledgement

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Composites comprising additively manufactured lattice structures and resorcinol-formaldehyde xerogels

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The ever-growing importance of saving energy implies the use of increasingly efficient insulating materials. Particularly for mobile applications, such materials also have to display light-weight characteristics. Owing to their highly open-porous nature, aerogels and xerogels are excellent insulating materials with low density [1-2]. However, their fragility limits direct applications as structural materials, e.g. in vehicles.

Lattice structures offer high specific strength and can be readily produced using additive manufacturing techniques including selective laser sintering (SLS). Thus, a combination of lattice structures with aerogel materials represents a promising approach for the development of mechanically robust lightweight insulation materials [3-4].

Here, we report on the development of composites comprising polyamide 12 (PA12) lattice structures and resorcinol-formaldehyde xerogels. While the former was accessed using high-speed sintering (HSS) of PA12 powder, the xerogel filling was obtained by sol-gel synthesis followed by ambient-pressure drying.

Specifically, we describe a rational approach of selecting the unit cell geometry of the lattice structure using simulation methods. The production of a variety of composites varying in unit cell dimensions and lattice strut thickness is described. The subsequent characterization of compressive and thermal properties is presented, and the findings are discussed with respect to future applicability.

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Enhancement of Corrosion Resistance of MAO/Polydopamine/Polylactic Acid-Coated AZ31 Magnesium Alloy for Biomedical Applications

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A7_7 - Coatings, U1 Room (Level 0), settembre 17, 2025, 10:30 - 13:10

This paper aimed to investigate the enhancement of the corrosion resistance of a protective system applied on the AZ31 magnesium alloy to be used as an orthopedic biomedical device, composed of three different superimposed layers: (a) magnesium-based oxide, (b) polydopamine, and (c) polylactic acid. Specifically, morphological and chemical analyses, crystallographic, roughness, and micro-hardness were carried out. The electrochemical measurements were performed in Hanks' Balanced Salt solution at 37 °C. The micro arc oxidation (MAO) treatment involved the classic pancake structure of the oxide with a consequent high extension of the real area. The sealing of its pores via the polydopamine was well highlighted through the surface roughness analysis. As expected, the magnesium oxide layer reduced the degradation rate. The presence of polydopamine on the oxide layer improved the corrosion resistance of the alloy, showing a pseudo-passivity range in the potentiodynamic polarization curve, due to the filling of oxide pores. The highest impedance modulus in the electrochemical impedance spectroscopy analysis during the temporal observation of 168 h was observed when all coatings were applied on magnesium substrate, due to a synergetic action. Thus, the multilayers should represent a protective system to control the degradation process.

Keywords: micro-arc oxidation; biodegradable implants magnesium alloy-based; degradation control; polydopamine; polylactic acid; roughness; micro-hardness; potentiodynamic polarization; EIS

A new synthetic route for the production of well-structured PEDOT-MXene hybrid nanoparticles

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A7_4 - Composites, U1 Room (Level 0), septiembre 16, 2025, 10:30 - 13:10

Conductive polymers (CP) are a category of conjugated organic polymers known for their unique features, such as ease of processing, lightweight nature, cost-effective production, and both electrical and ionic conductivity. Moreover, numerous studies have shown that their properties can be tailored and improved by incorporating appropriate organic or inorganic fillers. Among the various inorganic materials utilized as fillers, carbon-based materials like carbon nanotubes, diamond, and graphene are among the most widely used. However, recently, a new class of two-dimensional materials composed of carbides and carbonitrides, known as MXenes, has attracted significant scientific attention for their potential as fillers in CP-based composites. MXenes represent a class of two-dimensional materials with a generic formula of $M_{(n+1)}X_nT_x$ where the symbol "M" indicates the transition metal (such as Sc, Ti, Zr, Hf, V, Nb, Ta, Cr, Mo, and so forth) and "X" denotes the carbon while "Tx" represents a generic terminal surface functional group as -O, -OH, -Cl, or -F. They are typically produced by exfoliation of the corresponding MAX precursor, where A indicates elements belonging to group IIIA or IVA. The unique physical and chemical characteristics of $Ti_3C_2T_x$, such as its hydrophilicity, biocompatibility, high electrical conductivity, large surface area, redox activity, and distinctive optical and electronic properties, make it an ideal material for diverse applications. These include biomedicine, energy storage device fabrication, sensors, and biosensors, as well as batteries and supercapacitors. To harness the established properties of conductive polymers alongside the remarkable characteristics of MXenes, this work presents the synthesis of a composite material composed of poly(3,4-ethylenedioxythiophene) (PEDOT) as the host matrix and MXene as the filler. The nanoparticles were synthesized using sodium dodecyl sulfate (SDS) as a micellar soft template, facilitating control over the shape and size of the PEDOT nanostructures while enhancing their dispersibility in aqueous environments. The morphology and structure of the synthesized nanoparticles were analyzed, along with functional characterizations, to evaluate the properties of the final composite material for potential applications in the optoelectronic sector.

From pure element powders to protective coatings in industrial applications based on thin W-Ta-B films obtained by SPS-HiPIMS method

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 15, 2025, 13:15 - 14:30

The forging of lead-free brass alloys is characterized by low tool durability, presenting a significant challenge in industrial applications. To address this issue, unique magnetron-sputtered coatings based on WB2 alloyed with Tantalum [1], were employed to increase tool life. These coatings were produced from spark plasma sintered (SPS) targets using the high-power impulse magnetron sputtering HiPIMS technology. Initially, the coatings underwent laboratory testing, where their microstructure, adhesion to the substrate, and mechanical properties were tested and evaluated. Those studies shows that proposed material is superhard but also has increased fracture toughness. Additionally, ~ 2 µm thick W0.83Ta0.17B2.5 films are thermally and oxidation resistant at elevated temperatures. The next phase involved testing these coatings on tools used in hot flashless forging processes in an industry conditions. The experiments were conducted on dies that were preliminarily gas-nitrided to provide a suitable substrate for the coating application. The results were compared to those of only nitrided dies. After 102 774 forging cycles with the nitrided tool the wear reaches nearly 0.5 mm, which may represent the maximum acceptable wear limit from the perspective of evaluating the quality of the forged parts. The tool with the nitrided and deposited W0.83Ta0.17B2.5 coating after similar number of forging cycles exhibits less wear, with a depth of approximately 0.15 mm. While this allows for extended service life, it clearly indicates the removal of the protective layer in sensitive areas of tool. The obtained results confirmed the beneficial impact of proposed coatings on enhancing tool durability. In certain cases, the service life of the tools was extended by up to 50%. This study demonstrates that the application of newly developed W0.83Ta0.17B2.5 coating which can significantly improve the durability of tools used in the flashless forging of lead-free brass alloys, offering a promising solution for industrial manufacturing challenges.

[1] C. Fuger, et al., „Influence of Tantalum on phase stability and mechanical properties of WB2,” MRS Communications 9 (1), pp. 375-380, 2019.

This study was founded by National Centre for Research and Development, Poland (NCBR) [grant no. TECHMATSTRATEGIII/0017/2019].

Novel Printable Microwave Metasurfaces for Energy Harvesting Applications

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A7_9 - AM, U1 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Metamaterials are artificially constructed materials, which exhibit tailored interaction with incident electromagnetic radiation, enabling extraordinary functions and properties. Up to now metamaterials and metasurfaces (2D version of metamaterials, consisting of a single plane of meta-atoms) have been realized for a great variety of electromagnetic applications. Among them, metamaterials for energy harvesting gain lately great interest. In this context, most efforts are focusing in the microwave frequency range in the last decade. Reasons for such an attention include the tremendous evolution of wireless communications, resulting to an incredible increment of microwave emitting and receiving, including telecommunication antennas, wi-fi hubs etc.

Conventionally, metasurface units, are constructed employing the printed circuit (PCB) technology, which permits the high printing resolution and the consequent high quality of the produced metamaterial unit. Although PCB technology exhibits some severe drawbacks i.e., it is a multi-step, long-time procedure, complex infrastructure is needed, highly dedicated personnel is required, etc. During the last years, construction of complex objects is being achieved employing additive / subtracting manufacturing technologies. In principle, during an additive / subtractive manufacturing process, a 3D structure is developed by stacking/removing material layers, until the desired object is grown. Such technology exhibits distinct advantages (i.e., it is a quick, cost-effective and user-friendly method) while it allows the large-scale production of objects, reducing their consequent cost and production time.

To date, additive/subtractive manufacturing technology has been successfully used in constructing metasurfaces for applications in the microwave regime. In this context, we hereby present the fabrication of stand - alone metasurface units, of the cut-wire topology, employing the FFF method. In addition, we also employ the CNC engraving method to develop complementary metasurfaces, of toroidal topology. Both metasurfaces were thoroughly studied, regarding their energy harvesting capability in the microwave regime. Experimental results evidently show that they both can effectively absorb electromagnetic energy and transform it to DC electric signal, through a simple rectification circuit. Therefore, they can efficiently be used as energy harvesters, mining energy from surrounding microwave signals.

Nest we present, preliminary results about the combination of metamaterial harvesters with other kind of harvesting devices, such as photovoltaics. Corresponding experimental data show that combination of metasurface with photovoltaic panels could be feasible, resulting in a harvesting system which could continuously provide low -power systems and devices with electrical power.

Corrosion resistance of water borne epoxy/carbon dots coatings on aluminium alloy

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A7_1 - Synthesis, U1 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

The widespread use of various metals, whose degradation produces serious economic losses and environmental pollution, requires continuous solutions to improve their corrosion resistance. Simultaneously, the increasing attention to the sustainability issues has been emphasizing the importance to avoid toxic products. Carbon dots (CDs), as a new zero-dimensional member of the carbon family, possessing the advantages of low toxicity, high solubility, good stability, inhibition properties, are attracting a great attention of researchers in the field of corrosion and protection of metallic materials. In this investigation a low amount of carbon dots was incorporated into a water-based epoxy resin, and then the hybrid coating was used to cover Al 2024-T3 samples. Electrochemical techniques in a 3,5 % by weight of aqueous solution of NaCl, weight loss, surface characterizations are combined to investigate the inhibiting effect and corrosion mechanism.

Controllable Delamination in Multi-Material Multilayer Plastic Packages Using the Addition of oxide particles at the Interface

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A7_10 - Applications, U1 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

Controlling interfacial behaviour is crucial for optimising the performance of multilayer materials, enabling functionalities such as self-healing, self-peeling, and smart bonding. Reversible mechanical interlocking offers a promising strategy for controlling interfacial bonding in these systems.

In this study, oxide particles with optimised structures were applied to polymer surfaces to enhance interfacial bonding. Single lap shear tests were conducted to evaluate shear strength at the interfaces of low surface energy polymers. The results indicate that specific oxide particles with desired geometries significantly improve interfacial shear force. While previous studies have demonstrated an enhanced shear and peeling force by adding oxide particles, a comprehensive understanding of the underlying mechanisms still remains limited. To address this gap, this study further employs modified theories to calculate the interactions between polymers and oxide particles, providing deep insights into interfacial locking mechanisms. The findings can have direct implications for the recyclability of current Multi-Material Multilayer Plastic Packages (MMPPs) applications. During use, different polymer layers can be locked tightly by particles, while after use, the locking can be reversed, facilitating easy delamination of the layers. This approach presents a viable pathway toward sustainable packaging solutions by enhancing both mechanical performance and end-of-life separability.

Rosin-Derived Materials for Active Packaging: A Sustainable Solution for Meat Preservation

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A7_10 - Applications, U1 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

The growing demand for sustainable food packaging solutions has increased interest in bio-based materials and encapsulation technologies. Within the RN21 project, this study explores the use of rosin resin and its derivatives to synthesize limonene-loaded particles and polymeric films with enhanced gas barrier properties. These advancements aim to extend shelf life, improve food safety, and support the transition to circular and sustainable economies.

Rosin, derived from pine trees, presents a renewable alternative to conventional resins. In this work, rosin derivatives were used to develop a sustainable delivery system encapsulating limonene, a natural antimicrobial and antioxidant compound. Flash nanoprecipitation yielded spherical nanoparticles (~150 nm) with a 30% theoretical loading content and 40% production yields. These particles were incorporated into biopolymeric matrices using melt blending, forming functional films for active packaging. The films underwent controlled release studies simulating real-world meat packaging conditions.

Another strategy involved incorporating rosin resin derivatives into biopolymers. A biopolymer was compounded with a rosin-derived resin via twin-screw extrusion, producing composite pellets that were then processed into films through blown film extrusion. The inclusion of gum rosin resin significantly enhanced the barrier properties against water vapor and oxygen, yielding a denser, less permeable matrix. Functional coatings further improved these properties, reducing WVTR and OTR more than 70% when compared to the original substrate.

This work demonstrates the potential of rosin-derived materials as eco-friendly alternatives for active packaging. By integrating renewable resources and advanced encapsulation techniques, these solutions address industry demands for high-performance packaging while contributing to global sustainability goals. Extending shelf life and reducing food waste provides both economic and environmental benefits.

The authors acknowledge the RN21 project, funded by the Environmental Fund through Component 12 – Promotion of Sustainable Bioeconomy (Investment TC-C12-i01 – Sustainable Bioeconomy No. 02/C12-i01.01/2022), of European funds allocated to Portugal by the Recovery and Resilience Plan (PRR), within the European Union (EU) Recovery and Resilience Mechanism, framed within Next Generation EU, for 2021–2026.

Process parameters optimization for L-PBF of a NiTi alloy: a combined analytical and experimental investigation

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A7_9 - AM, U1 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Additive manufacturing (AM) technologies have revolutionized the fabrication of biomedical devices, finding extensive applications in orthopedics, orthodontics and cardiovascular implants. Among the materials employed, Shape Memory Alloys (SMAs), particularly NiTi alloys, are prominent due to their superelastic mechanical properties, functional capabilities and biocompatibility. Their limited machinability through traditional methods has driven increased interest in using AM techniques to address these limitations and enable the production of customized biomedical components.

This study aims to analyze the printability of a Ni50.8Ti49.2 alloy produced through the Laser Powder Bed Fusion (L-PBF) technique. The optimal L-PBF printing conditions were estimated using an analytical model that predicts the temperature field generated by a moving point heat source in steady-state. This model guided the design of an experimental campaign through a full factorial design of experiments (DOE) to determine the printability region to avoid the presence of lack of fusion- or keyhole-induced defects.

Material samples were fabricated using a Renishaw RenAM 500S printer with a maximum laser power of 500 W, operating in continuous or pulsed mode. Based on the insights from the DOE, several printing parameters combinations, including laser power, scanning speed, hatch distance, and scanning strategy, were tested to evaluate the material's feasibility region. Material cubic samples with an edge length of 5 mm were produced and analyzed to correlate the printing conditions with the resulting microstructural characteristics and process-induced defects. Standard microstructural characterization techniques (optical and scanning electron microscopy, OM and SEM) and differential scanning calorimetry (DSC) were employed to assess the microstructural features and transformation temperature ranges (TTRs). The OM and SEM analyses showed that the detected percentage porosity of the samples was consistent with the predictions provided by the analytical model. In terms of the feasibility of the process parameter, ten parameter combinations were identified within the predicted region, which enabled the production of samples with porosity below 0.2 %. The DSC, performed after a solution treatment conducted at 850 °C for 15 min, revealed transition temperatures comparable to those of the virgin powder. These findings suggest that the adopted L-PBF printing parameters did not alter the alloy's chemical composition, preserving its original transition temperatures and confirming its suitability for biomedical applications.

By minimizing porosity and aiming for a defect-free microstructure, this study underscores the potential of L-PBF in overcoming the challenges associated with the traditional machining of NiTi alloys, supporting the production of NiTi-based biomedical components with enhanced functional performance.

A paper-based, gasochromic Pd-WO₃ sensor for hydrogen detection

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

A hydrogen-based society requires secure access to technology, WO₃ gasochromic sensors being promising candidates for integrating new equipment¹. Nonetheless, WO₃ sensors are commonly produced via complex and expensive methodologies. In this work, we report a simple and sustainable strategy to manufacture paper-based WO₃ sensors, thus promoting an environmental-friendly route toward the visual hydrogen detection. WO₃ was prepared via a solvent-based synthesis. Briefly, WCl₆ was dissolved in ethanol (1 mg/mL) for 72 h and freeze-dried. The resultant WO₃ was dissolved in water (40 mg/mL) and an Na₂PdCl₄ aqueous solution (27 mg/mL) was added dropwise. The final Pd-WO₃ particles were obtained by centrifugation and freeze-drying. To prepare the paper-based sensor, bench protective paper (1.0×0.5 cm) was dipped in a Pd-WO₃ aqueous solution (5 mg/mL) for either 5 or 20 min. The gasochromic performances of the sensors (S5 and S20, respectively) were tested in a 10 % H₂/N₂ atmosphere.

The ATR-FTIR analysis of the Pd-WO₃ particles confirmed O–W–O (605 cm⁻¹) and W–O–W (945 cm⁻¹) bands for WO₃, evidencing an efficient conversion of WCl₆ into WO₃. Indeed, Pd-WO₃ was able to change its color ($\Delta E = 30$; $t_{90} = 130$ s) when exposed to a 10 % H₂/N₂ atmosphere. Similarly, both S5 and S20 changed their colors from green to black during the 3 min test. As expected, the longer dipping time of S20 resulted in a more noticeable ($\Delta E = 8$) and faster ($t_{90} = 80$ s) color change comparatively to S5 ($\Delta E = 6$; $t_{90} = 100$ s). Although these gasochromic responses are still far from recently reported Pd-WO₃ sensors, S5 and S20 showed discernible color change (i.e. $\Delta E > 5$) within a competitive timeframe.¹ Such results encourage further studies to validate paper-based WO₃ sensors as suitable hydrogen detectors. Future work will include optimization of the Pd-WO₃ functionalization and, importantly, a detailed chemical, structural and mechanical characterization of the paper/Pd-WO₃ interface.

ACKNOWLEDGMENTS

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Functional All-Cellulose Composites for Innovative Sustainable Textiles

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A7_4 - Composites, U1 Room (Level 0), septiembre 16, 2025, 10:30 - 13:10

Cellulose is the most abundant natural polymer, known for its renewability, biocompatibility, biodegradability, high chemical stability, and good mechanical properties. These attributes have been widely used in the development of various bio-based cellulosic materials, particularly composites.

In recent years, all-cellulose composites (ACCs) have garnered significant research interest. These class of polymer composites consist solely of cellulose (or its derivatives), where the matrix comprises regenerated (or modified) cellulose, and the reinforcement phase is made of high-strength cellulosic (nano)fibers. ACCs present inherent advantages of cellulose, while exhibiting superior mechanical, optical, and barrier properties compared to traditional cellulose-based materials. Their versatility offers a sustainable and innovative approach in several applications, including in sustainable textile.

This work explores the fabrication and characterization of ACCs using different cellulosic substrates (bacterial nanocellulose and cellulose pulp fibers), and following different approaches, and their functionalization with biobased additives for potential application as functional textiles. The developed ACCs presented enhanced properties, namely mechanical performance and water sensitivity, and their renewable and biodegradable nature aligns with circular economy principles, reducing the environmental impact of textile production.

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Acknowledgments:

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Multifunctional oxide coatings with zeolites prepared by plasma electrolytic oxidation

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembere 17, 2025, 13:10 - 14:30

The formation of mixed-oxide coatings by plasma electrolytic oxidation (PEO) proved itself as a valuable tool in many applications. PEO processing enables the incorporation of electrolyte components (including particles) into coatings, providing the pathway for tailoring the properties of such composite coatings. Generally, addition of particles to electrolyte used for PEO processing can act as a sealant making obtained oxide coatings more compact, thus increasing their wear and corrosion resistance. In contrast, highly porous PEO coatings feature an increase of the surface area available for photocatalytic, biomedical and luminescent applications.

Zeolites are porous crystalline materials, characterized by large surface area, exceptional adsorption properties and ion-exchange capacity. Although zeolites are mainly used as absorbers, an innovative immobilization of pure and Me-loaded (Me = Ce, Zn, Eu) zeolites on an inexpensive support using PEO processing proved to be beneficial when photocatalytic, adsorption, photoluminescent and corrosion protection properties are of interest.

Prepared mixed-oxide coatings with immobilized zeolites contain elements originating from the substrate and from the electrolyte. Aside from incorporation of Me-loaded zeolites from electrolyte, an attempt of co-deposited Me-species and corresponding zeolites from the same supporting electrolyte solution is presented. Both types of coatings are thoroughly characterized and tested in different applications. Coatings with incorporated Me-loaded zeolites show slightly better potential for application than those with co-deposited Me-species and zeolites, on the other hand they do require more complicated and time consuming processing procedure.

Smart Polymer Coatings for Safety Applications in Battery Systems: Exploiting Click Chemistry and Diels-Alder Reactions

Daniel Bautista-Anguís, Van-Kien Hoang, Alan Arceta-Lozano, Matthias Kriehuber, Gabriel Ferdigg, Sandra Schlögl

A7_8 - Catalysis / CAN, U1 Room (Level 0), septiembre 17, 2025, 14:30 - 16:30

In the last decade, the production of electric vehicles (EVs) has increased with the aim of reducing CO₂ emissions from traditional internal combustion engine vehicles. The transition to EVs is critical for addressing environmental challenges and promoting sustainable transportation solutions. Therefore, ensuring the optimal functioning of their components is paramount to safeguarding passenger safety. Special attention must be given to monitoring and detecting potential overheating events, particularly within battery systems, to prevent irreversible damage. A promising and cost-effective solution involves the use of temperature-responsive polymers combined with low-cost metal oxide (MOx) gas sensors. When certain critical temperatures are reached, the polymer releases detectable gases, which are captured by MOx sensors connected to an alert system. The use of polymer coatings enables a more thorough and accurate assessment of temperature across the entire surface.

To enable the controlled release of tracer gases at critical temperatures, our work was divided in two different approaches:

In the first approach, short-chain thiols with low boiling points were chosen as tracer gases. Blocked model compounds were synthesized through a click reaction between the short-chain thiols and 4,4'-Methylenebis(phenyl isocyanate) (MDI). The unblocking temperatures of these compounds were determined using different thermal techniques such as differential scanning calorimetry (DSC) or thermogravimetric analysis (TGA) among others. This unblocking reaction, occurring at temperatures above the boiling point of the thiols, results in their release in the gas phase. The released gases were characterized by evolving gas analysis coupled with mass spectrometry (EGA-MS). The most promising thiol, 1-propanethiol, was covalently bonded into a polyurethane matrix made from a polymeric MDI and polyol. The reusability of the polymer coating after releasing the gas was also evaluated, ensuring the reusability of the matrix for different applications or allowing the introduction of more 1-propanethiol.

In the second approach, the focus was on the covalent bonding between thiophene molecules and a thiol-ene network. This method uses the reversibility of the Diels-Alder (DA) reaction between a commercial bismaleimide (BMI-689) and thiophene, also offering a novel strategy for developing functional coatings. The retro Diels-Alder (rDA) reaction enables the recovery of reactants at specific temperatures. The test results proved that the rDA reaction temperature is higher than the boiling point of thiophene, allowing the release of thiophene groups as a tracer gas, easily detected by various sensors. The aforementioned characterization methods for the first approach were used to determine the rDA reaction temperature and identify the released components.

Investigation of the thermoelectric behavior of the ternary composite: Polypyrrole – Ionic liquid – Graphene

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 17, 2025, 13:10 - 14:30

The conversion of waste heat into usable energy has become a significant area of research. Scientists globally are developing novel methodologies to transform residual heat into electricity, a process known as thermoelectricity [1]. The performance of thermoelectric materials is assessed using a dimensionless figure of merit (ZT). This factor relates electrical conductivity (σ), thermal conductivity (κ), the Seebeck coefficient (S), and absolute temperature (T): $ZT = (S^2\sigma/\kappa) \times T$. High ZT values necessitate high electrical conductivity and Seebeck coefficient coupled with low thermal conductivity [2]. Optimizing charge carrier concentration through using new mediums and incorporating carbonic charges is a key strategy for ZT enhancement [3].

The interest aroused by the use of polymeric thermoelectric materials justifies the purpose of this study for the synthesis of a thermoelectric semiconductor polymer, in this case polypyrrole, and emphasize the study of the polypyrrole's thermoelectric properties through:

The use of an ionic liquid 1-ethyl-3-methylimidazolium tetrachloroferrate (Emim-FeCl₄) as a synthesis medium and dopant;

The incorporation of graphene.

A series of physicochemical characterizations were carried out on the obtained products, to determine their chemical structures and their morphologies, by Infrared (FTIR) and Raman spectroscopies (FTIR) and by Scanning Electron Microscopy (SEM).

The thermoelectric properties of the studied products were also evaluated through measurements of electrical (σ) and thermal (κ) conductivities, the Seebeck coefficient (S) for the calculation of the figure of merit (ZT), which reflect the thermoelectric efficiency of the material.

The figure of merit (ZT) value of the developed composite (PPy-LI) is (2.47) time higher than that of the based polymer (PPy).

The ternary composite (PPy-LI-Gr) developed by adding graphene to the (PPy-LI) composition is characterized by the best thermoelectric power and exhibits remarkable physicochemical properties and has a thermoelectric character (2.12×10^3) significantly higher than that of the PPy.

Keywords: Thermoelectricity, Conductive polymers, Thermoelectric composites, Ionic liquids, Graphene.

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Healing effect of nanochitosan, collagen, keratin and hialuronic acid electrospun membranes in a pre-clinical study

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The aim of this study was to produce electrospun membranes made of nanochitosan associated with collagen and keratin, with or without hyaluronic acid, and to evaluate their effectiveness in the healing process of cutaneous wounds in Wistar rats. Solutions of 4% (w/v) nanochitosan diluted in 90% acetic acid were prepared, plus 2% (w/v) collagen; 2% (w/v) collagen and 0.1% (m/m) hyaluronic acid; 2% (w/v) collagen and 12.5% (m/m) keratin; and 2% (w/v) collagen, 12.5% (m/m) keratin and 0.1% (m/m) hyaluronic acid. After homogenizing, the solutions were electrospinning with the following parameters: 12 cm distance between the needle and the collector, 20 kV and a flow of 2.0 mL/h to obtain the membranes. The membranes produced were characterized by scanning electron microscopy (SEM) and their antimicrobial activity was evaluated against the bacteria *Staphylococcus aureus* and *Pseudomonas aeruginosa*. The healing effect was evaluated in a pre-clinical study using Wistar rats, randomly assigned to five experimental groups, one for each type of electrospun membrane and a control with saline solution. The animals were given a surgical wound 2 cm in diameter in the dorsal region and the wounds were cleaned and covered with the electrospun membranes or just cleaned with saline solution (control). The healing of the wounds was monitored on days 3, 7, 14 and 21, when the area of the lesions was examined and the tissue collected for histological analysis. The results were submitted to analysis of variance (ANOVA) and the means were compared using the Tukey test ($p < 0.05$) to determine whether the treatments had a statistically significant reduction in the area of the wounds at each time point compared to the control. The electrospun membranes adhered well to the wound bed and did not require additional covering. The random arrangement of the fibers can be seen by SEM, with visible fragility in the structure of the nanofibers of the membranes containing keratin, which also showed the least adherence to the wound bed. The nanochitosan membranes with collagen were the most effective in the healing process, promoting faster wound contraction, differing statistically from the other treatments and the control group on the 7th and 14th day of evaluation, with greater induction of fibroplasia and epithelialization. It is therefore concluded that these membranes have potential for use as skin dressings, which will be evaluated in a clinical study.

A bespoke atmospheric pressure plasma process for the fabrication of three-dimensional glutathione-silver nanoparticle-polylactic acid composites for skin regenerative applications

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A7_10 - Applications, U1 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

Glutathione (GSH) is an antioxidant which performs anti-inflammatory effects via protecting cells from reactive oxygen species and reactive nitrogen species, making it an ideal candidate to be immobilized on polylactic acid (PLA) for skin regenerative applications including wound dressings. Although PLA shows favourable properties for a wound dressing including being biodegradable, biocompatible and sustainable with good breathability and softness, its poor antibacterial ability and chemically-inert nature leads to the absence of cell recognition sites and increases the difficulty of immobilizing functional groups or materials, such as GSH or silver nanoparticles, resulting in the limitation of its further applications for biomaterials. To tackle these issues with an improved modification efficiency, a bespoke process composed of plasma-induced polymerization, reduction and grafting was developed to fabricate a three-dimensional glutathione-silver nanoparticle-polylactic acid composite. An atmospheric pressure plasma nozzle system utilising an acrylic acid-based hybrid precursor was developed and employed to activate the PLA surface, prepare and deposit silver nanoparticles, then graft GSH to contrive a three-dimensional PLA composite possessing antibacterial and anti-inflammatory properties with improved process efficiency. A comprehensive analysis of the wettability, hydrophilicity stability, surface morphology and depth profiles, elemental composition and biocompatibility of the plasma-fabricated PLA composite was performed. An enduringly stable PLA surface along with the presence of carboxylic acid functional groups, silver nanoparticles and GSH antioxidant was observed, suggesting the potential application of this bespoke process on tailoring functional wound dressings.

LDH synthesis on AZ31 alloy: effect of microstructural modifications of substrate processed by ECAP

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A7_1 - Synthesis, U1 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

The high corrosion rate of Mg alloys in biological fluids limits their use in biomedical applications. Several strategies have been adopted to mitigate this issue, among them many researchers investigated the effects of grain refinement and the deposition of different protective coatings. Layered Double Hydroxide (LDH) coatings not only lead to beneficial effects of the AZ31 corrosion resistance but are also of particular interest due to their tuneable structures and ion-exchange properties, which enable them to load and release drugs.

This work investigates the effect of microstructural modifications of AZ31 alloy substrate caused by Equal Channel Angular Pressing (ECAP) process on LDH nucleation and growth. The LDH deposition process was performed on AZ31 alloy substrate, subjected to 0, 1, 2, and 4 ECAP passes, with two different synthesis times (30 minutes and 12 hours). The samples were analysed using light microscopy (LM), scanning electron microscopy (SEM), and X-ray diffraction (XRD).

The results show that the microstructure of the substrate significantly impacts the LDH deposition process. Nucleation of LDH occurs on screw dislocations at the substrate surface, with a fine and uniform distribution of LDH crystals achieved when surface diffusion takes place, enhanced by particular textures component. For the AZ31 alloy subjected to a single ECAP pass with a synthesis time of 30 minutes, a complete surface coating was formed, and the resulting crystal morphology seems to be promising for medical and biomedical applications.

SELF-HEALING GLASS SEAL FOR HTE/SOFC

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A7_3 - Electronics II, U1 Room (Level 0), septembre 15, 2025, 17:00 - 19:00

A current main challenge in High Temperature Electrolysis and Solid Oxide Fuel Cells (HTE/SOFC) technologies is the glass / metal sealing to prevent gas leak. In the literature, various types of seals are studied including compressed, brazed and glass seals. Glass and glass-ceramics seals appear to be the most promising technologies, provided if the glass / glass-ceramic remains stable over time.

A close matching of the thermal expansion coefficient (TEC) between seal and metal support is essential to prevent crack formation, which can lead to a loose of hermeticity ($10^{-12} \times 10^{-6} \text{ K}^{-1}$). To reach these high TEC values, BaO is often added to the glass composition. The main problem is the reaction between the barium and the environment of the seal at working temperature.

In the present talk, we present our results on a new barium-free glass-ceramic (SCABS) designed for sealing solid oxide fuel cells. Thermal properties, electrical resistivity, thermal ageing, and crystallisation were investigated and related to the glass-ceramic structure, which was characterised by NMR. XRD analyses indicate that crystallisation occurs with the formation of phases such as anorthoclase, feldspar and α -quartz. The SCABS glass-ceramic exhibits thermal and chemical stability under SOFC operating conditions for 960 hours and autonomous self-repair capability at 800°C.

Ultrafast-laser powder bed fusion of Nb₂O₅-TiO₂ mixtures for emerging environmental applications

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A7_9 - AM, U1 Room (Level 0), septiembre 17, 2025, 17:00 - 19:00

Transition metal oxides (TMOs) are materials whose properties can be tuned through their structure and composition. This makes them particularly interesting for energy applications, as battery electrodes [1], and various environmental applications including gas sensing or photocatalysis for water purification and water splitting [2].

Nb₂O₅-based TMOs are interesting candidates for these applications due to their tunable electrical and optical properties. In Nb₂O₅ oxygen content plays a major role in determining its electrical properties. The stoichiometric oxide is insulating, which limits its use in the energy applications. In addition to this low conductivity, Nb₂O₅ has a large bandgap which limits its performance in fields such as photocatalysis, because only ultraviolet light can effectively induce electron-hole pair formation, limiting its utility under visible light. However, the introduction of a metallic doping in the TMO structure allows the formation of shallow levels in the oxide's electronic bandgap, which contribute with carriers to the conductivity and enable the absorption of longer wavelengths, making doping an effective strategy to overcome the inherent limitations of the pure oxide. In the case of Nb₂O₅, conductivity is mediated by oxygen vacancies, but doping also induces oxygen defects that may strongly increase the conductivity of the material [3]. In this context, we have focused our studies on titanium niobates (Ti_xNb_yO_z or TNOs) a class of ternary oxides, with TiNb₂O₇ and Ti₂Nb₁₀O₂₉ being among the most stable ones [4].

Recently, we optimized an ultrafast-laser powder bed processing technique to produce uniform and compact sintered conductive layers of a monoclinic oxygen-deficient Nb₂O₅ phase [5], where the conductivity of the layers was determined by their microstructure and oxygen-deficiency. In this work, we have followed a similar approach, irradiating a mixture of high-purity TiO₂ and Nb₂O₅ powders, to optimize the ultrafast-laser powder bed processing technique to produce continuous TNO layers (with the mentioned targeted stoichiometries). As a result of the optimization process, continuous and compact layers of TNO have been successfully sintered. The effect of the laser processing parameters on the sintering of the layers will be described, as along with the post-processing treatments applied to functionalize them for emerging applications.

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Development of a functional membrane for island and coastal desalination device

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A7_6 - Environment, U1 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

Sustainable desalination methods geared towards geographically isolated and disadvantaged areas (GIDA) are gaining attention. One promising technology is the Passive Solar Driven Membrane (PSDM) desalination system, which possesses key advantages to delivering safe water in rural areas of an archipelagic location. Our research group explores the PSDM multi-stage system to determine the productivity, yield and salinity using simulated seawater, providing valuable insights regarding the system's performance under Philippine atmospheric conditions. Desalination of 3.5% salt solution was conducted on a rooftop setting with PSDM multi-stages. Results show the average productivity of the 1, 2, 4, 7, and 10 stages are 93.84, 328.57, 401.47, 203.701, and 258.15 g/kWh, respectively, showing a 94% - 96% reduction in the salinity of the distilled water at all stages.

Further development on the improvement of this type of desalination system involves modifying its membrane layers. The purpose of this modification is to enhance the productivity and salinity rejection of the desalination device. Such modification was carried out through Polyamide (PA) functionalization of its polyethersulfone (PES) membrane layer. These modified membranes were oven-cured and integrated into PSMDS configured in single, four, and seven-stage setups to evaluate changes in distillate productivity. The presence of polyamide on the surface of PES membrane is confirmed via Fourier Transform Infrared Spectroscopy. The modified PSMDS showed significant increased productivity of 797%, 153%, and 564% for the single, four, and seven-stage configurations, respectively. Water Contact Angle measurements of the PA-PES membranes exhibited an average water contact angle of 17.85° while Scanning Electron Microscopy revealed that the polyamide formed on the PES has corrugated nanostructures. These characteristics enhance the system's hydrophilicity, thereby increasing its productivity. However, only the four-stage configuration achieved 99.9% saline rejection. Such quality water can be used for irrigation for crops, livestock, household use, and potable water.

Ultrafast Laser Functionalization of Doped Zinc Oxide Films

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A7_7 - Coatings, U1 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

Zinc oxide (ZnO) is a large-bandgap semiconductor with n-type conductivity due to natural oxygen vacancies. It has additionally very interesting properties (such as biocompatibility, piezoelectricity or antibacterial activity [1,2]) which makes it a good candidate as active material for photocatalysis, gas sensing and other environmental applications [3]. ZnO can be doped to enhance its conductivity and light absorptance [4] by introducing shallow levels in the bandgap which increase the carrier density at room temperature and reduces the minimum energy required for a photon to be absorbed.

Fs-laser texturing is an excellent functionalization tool for all type of materials. It has already been used to increase silicon absorptance by generating high aspect-ratio structures [5], to generate electrical anisotropies in ITO [6] or to enhance the wettability of marble surfaces [7]. By altering the topography of a material, it is not only possible to increase its active surface, something of primary importance for gas sensing and photocatalysis applications, but also to induce optical and electrical anisotropies while triggering a redshift of its transparency window [8], which can be beneficial for photovoltaics and TICs applications.

In this work, doped ZnO films have been processed with ultrashort laser pulses ($\lambda = 1030$ nm, $\tau = 350$ fs) to generate Laser Induced Periodic Surface Structures (LIPSS) [9]. The films were grown by sputtering or pulsed laser deposition (PLD) using different amounts of Al_2O_3 and Yb_2O_3 as dopants. Coherent LIPSS propagation has been successfully induced for doping levels above a certain threshold. The optimization of the laser conditions for generating morphological, optical and electrical anisotropies in the doped films will be presented while the potential use of the laser generated structures in emerging applications will be discussed.

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3D PRINTABLE IONIC CONDUCTIVE HYDROGELS AND ORGANOHYDROGELS FOR WEARABLE SENSOR APPLICATIONS

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A7_5 - Sensing, U1 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

Smart sensors made from conductive hydrogels have demonstrated significant potential in bridging the gap between the flexible human world and rigid electronics, particularly in fields like wearable technology and soft robotics. However, their widespread use in sensors is hindered by water evaporation, which reduces their durability. In recent years, organohydrogels, hydrogels where part of the water is replaced with a high-boiling-point organic solvent, have emerged as a promising alternative due to their flexibility and long-term stability. Additionally, traditional manufacturing techniques like casting limit the range of achievable shapes, restricting their applications. To overcome these limitations, 3D printing has gained attention as a method for reducing material waste, enabling product customization, and creating complex geometries that enhance sensing performance. However, integrating this technology with hydrogels and organohydrogels remains a challenge.

This study presents a photocurable double-network hydrogel composed of poly(vinyl alcohol)/acrylic acid (PVA/AAC) doped with sodium chloride (NaCl) to enhance ionic conductivity. The resulting PVA/AAC/NaCl hydrogel demonstrated excellent stretchability, electrical responsiveness to strain and pressure, and compatibility with 3D printing. Using Digital Light Processing (DLP) 3D printing, intricate structures were fabricated to improve mechanical stress sensitivity. However, the hydrogel's properties degraded over time due to water evaporation. To address this, a solvent replacement strategy was implemented using a glycerol/water binary solution. The resulting PVA/AAC/NaCl organohydrogel maintained stretchability up to 350%, exhibited stable mechanical and sensing performance for up to three months, reduced hysteresis, and demonstrated high sensitivity to both small and large deformations. The sensor demonstrates an outstanding strain detection limit of 0.05% and a pressure detection limit of 1.5 Pa, enabling the evaluation of micrometric deformations across a wide temperature range, including below room temperature. Notably, its 3D printability remained intact, further enhancing sensing capabilities through structural design. Additionally, the presence of glycerol enabled sensitivity to temperature and humidity. With its versatility, 3D printability, flexibility, and durability, the PVA/AAC/NaCl organohydrogel is a strong candidate for soft sensor applications.

Polarization dependence on the emission of Nd doped bioactive W-TCP coatings on directionally solidified eutectic Calcium Zirconate-Calcium Stabilized Zirconia

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In this work we have developed and characterized coatings of Wollastonite-Tricalcium Phosphate, W-TCP, doped with Nd³⁺ ions on directionally solidified eutectic Calcium Zirconate-Calcium Stabilized Zirconia, CZO-CSZ, ceramics. The bioactive coatings were manufactured by the Laser Floating Zone, LFZ, technique. Before the solidification process, the bioactive coatings, doped with 1 wt%. of Nd₂O₃, were previously placed by dip coating on the CZO-CSZ rod surface. Depending on the thickness of the coating and the applied laser power, an alloying or coating process was achieved.

The optical characterization of these coatings revealed a strong dependence on the polarization direction in which the emission was collected so that both the excitation and emission spectra showed the existence of variations in the morphology depending on the polarization of the electric field.

Micro-Raman characterization was also studied to assess the correlation of this anisotropic emission to the microestructural properties.

Encapsulation of Clove Essential Oil into Sepiolite for Active Food Packaging Applications

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A7_10 - Applications, U1 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

The incorporation of clays as carriers of active substances in polymeric materials is gaining increasing attention. Essential oils (EOs) can provide valuable properties to plastic materials, although their high volatility poses challenges for large-scale industrial applications. This work presents a green, scalable, and versatile method for encapsulating clove essential oil (CO) into food-grade sepiolite clay, which was organo-modified by acid-activation using the food additive E-297 to ensure safety for food packaging applications. The resulting multicomponent nano-materials (MCNMs) enhanced the thermal stability of CO, enabling its incorporation into a low-density polyethylene (LDPE) matrix.

The MCNMs released 10 wt% of CO after 14 days under ambient conditions. Films with different clay loadings (0.5 wt%, 1 wt%, and 2 wt%) were produced by extrusion-blowing, showing optical and thermal properties comparable to pure LDPE. The antimicrobial activity of the films was evaluated against *E. coli*, *Salmonella enterica*, and *Listeria innocua*. Remarkably, the MCNM-films retained 70% of the encapsulated CO after three years of aging at room conditions while still releasing aroma. The films passed the overall migration tests for simulants A and D1, complying with European regulations for food-contact materials.

Additionally, the method was successfully applied to encapsulate other essential oils such as cinnamon, *mentha arvensis*, oregano, citronella, strawberry, thyme, and rosemary. These findings demonstrate the high potential of MCNMs and composite films for applications in active food packaging and agriculture.

Influence of substrate temperature and annealing on the conductivity of ZnO thin films

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A7_5 - Sensing, U1 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

ZnO is highly valued in electronics and optoelectronics because of its wide bandgap, strong exciton binding energy, and natural n-type conductivity. However, controlling its electrical properties is challenging since factors like substrate effects and temperature must be considered. In this study, we explore how the substrate temperature during growth and the use of p-type silicon (p-Si) substrates affect the electrical properties of zinc oxide (ZnO) thin films. ZnO thin films were deposited using Pulsed Laser Deposition (PLD) in a 2×10^{-2} Torr oxygen atmosphere on p-Si substrates. The substrate temperature was adjusted to study its impact on film growth and electrical properties. After deposition, the films were annealed in air at 800°C for three hours to improve crystal quality and reduce defects.

The films were analyzed using X-ray diffraction (XRD), atomic force microscopy (AFM), ellipsometry, UV-VIS absorption and Hall effect measurements. ZnO films showed variable-type conductivity depending on the growth temperature. Our findings suggest the p-Si substrate itself play crucial roles in determining ZnO film conductivity. These results align with existing studies and show that growth conditions and substrate interactions can be used to fine-tune ZnO's electronic properties [1].

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3D-Printed Colorimetric Chemosensors Using Natural Dyes for Sustainable Environmental Monitoring

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A7_6 - Environment, U1 Room (Level 0), settembre 16, 2025, 17:00 - 19:00

The growing interest in sustainable and eco-friendly materials has driven research into natural dyes as viable alternatives to synthetic pigments, which often pose environmental and health concerns. Natural colorants such as anthocyanin and phycocyanin are biodegradable, non-toxic, and renewable, making them promising candidates for applications beyond traditional dyeing. In particular, their intrinsic colorimetric response to environmental stimuli, including pH variations and pollutant exposure, enables their use as chemical sensors. This work explores the integration of anthocyanin and phycocyanin into photopolymerizable resins for Digital Light Processing (DLP) 3D printing to develop functional colorimetric chemosensors. Optimized resin formulations were investigated to ensure both high-resolution printability and reliable sensing performance. The printed materials were characterized through optical spectroscopy to assess their colorimetric response, while photorheology studies evaluated their suitability for 3D printing. Our findings demonstrate that these bio-based dyes enable the fabrication of 3D-printed objects capable of detecting environmental contaminants in both liquid and vapor phases via visible color changes, underscoring the potential of natural dye-based materials for sustainable sensing applications.

Water sorption, conversion rate and fracture toughness of liquid rubber modified dental composites

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A7_10 - Applications, U1 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

Dental composites based on dimethacrylate resins have good aesthetics and mechanical properties, but their brittleness and susceptibility to fracture require modification to improve damage resistance and reduce water sorption and material degradation.

The purpose of this study was to assess the effect of liquid rubber addition on the physicochemical properties of dental composites, particularly water sorption, conversion degree, and fracture toughness. Various types of composites, conventional and flowable, were analyzed, both with and without 5% liquid rubber content (a total of 4 combinations). The composite matrix consisted of a mixture of BisGMA (20 wt.%), BisEMA (30 wt.%), UDMA (30 wt.%), and TEGDMA (20 wt.%). As a modifier, liquid rubber Hypro 2000X168LC VTB was introduced at 5 wt.% relative to the matrix. Both the flowable and conventional materials were microhybrid composites, differing in their component proportions. The filler content in the flowable composite was 50% vol., while in the conventional composite it was 80% vol.

The results showed that the liquid rubber-modified samples exhibited lower water sorption compared to their unmodified counterparts. Average water sorption for the conventional composite decreased by 27.4%, while for the flowable composite, it decreased by 11.8%. The addition of liquid rubber contributed to an increase in the degree of conversion which was confirmed by FTIR studies. A higher degree of conversion indicates a lower amount of residual monomers, which can limit material degradation and improve its longevity in the oral environment. Additionally, a more cross-linked polymer structure can result in increased fracture resistance and reduced susceptibility to wear, which is crucial for the long-term functionality and aesthetics of dental restorations. Fracture toughness analysis revealed positive effects of liquid rubber addition. The fracture toughness coefficient increased by approximately 12% for the conventional composite and by approximately 20% for the flowable composite. It can be assumed that liquid rubber acts as a factor reducing crack propagation within the material structure, enhancing its energy absorption capacity, and improving resistance to mechanical loads.

The findings suggest that the addition of liquid rubber can positively influence dental composites by reducing water sorption, increasing the degree of conversion, and enhancing the fracture toughness. More studies are needed, including long-term stability assessment as well as fatigue behavior under simulated oral conditions.

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Influence of porosity on the electrical and thermal conductivity of sintered metal compacts

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The influence of porosity on the electrical and thermal conductivities of sintered metal compacts is studied in this work. Contrary to what might be thought, the challenge of finding mathematically simple expressions with one or two empirical parameters (which can also be determined by measurement) is still relevant today, when other strategies of massive computing or AI prediction seem to occupy the whole scenario, overriding the traditional ways of acquiring knowledge. However, the advantages of the traditional way are clear, as they lead to a direct and clear understanding of the relationships between microstructure properties. In this paper, some of the expressions put forward by different researchers are confronted, validated and compared with data taken from the literature. The results confirm that this problem cannot yet be considered fully solved.

Development of Doxorubicin Selective Electrochemical Sensors based on Surfactant-Modified ZnO-Nanoparticles

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Electrochemical sensors (ECS) are powerful tools for detecting water pollutants due to their high sensitivity, selectivity, rapid response, and portability. Their performance can be significantly enhanced by modifying bare electrodes with functional materials, such as noble metals, metal oxides, polymers, and carbon-based compounds.

In this study, ZnO-based materials were synthesized and applied as electrode modifiers for the electrochemical detection of doxorubicin (DOX), an anticancer drug that poses environmental and health risks due to its toxicity and accumulation in water systems. ZnO particles, were synthesized in the presence of two different surfactants - cetyltrimethylammonium bromide (CTAB, C₁₉H₄₂BrN, Alfa Aesar, Ward Hill, MA, USA) as a cationic, and triblock copolymer Pluronic® F127 (EO₁₀₆PO₇₀EO₁₀₆, Sigma-Aldrich) as a nonionic surfactant, using a microwave processing of a Zn(OH)₂ precipitate. The synthesized materials were characterized using XRD, Raman, FESEM, UV-Vis DRS, and PL spectroscopy to comprehend their crystal structure, morphology and optical properties, and finally to correlate their physicochemical properties with electrochemical activity for detection of DOX as a pollutant in water. Cyclic voltammetry (CV) was employed to quantify DOX using three types of screen-printed electrodes: Au, Pt, and C. The working ink for screen-printed electrodes modifying was prepared by mixing 10 mg of ZnO materials with 1.5 mg carbon black, 40 µL of 5% Nafion solution, 225 µL ethanol, and 225 µL water. CV was performed in 25 mL of phosphate buffer (0.1 M, pH = 7.0) with the addition of doxorubicin infusion solution (Ebewe Pharma, 50 mg DOX / 25 mL) in a portion of 10 µL to completely 160 µL. All measurements were done in a potential window of -0.4 – 0.6 V at a scan rate of 50 mV/s.

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Functional phosphate glasses for daily applications

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A7_10 - Applications, U1 Room (Level 0), septiembre 18, 2025, 10:30 - 13:10

Phosphate glasses are obtained at lower melting temperatures than silica-based glasses, so their use can have a sustainable advantage in terms of energy consumption. However, their applications are limited due to their hygroscopic properties and high leaching capacity. In this work, controlled leaching phosphate-based glass materials are developed for functional applications that increase sustainability. For this purpose, different formulations and thermal treatments were applied to the designed compositions, so that we were able to adjust the leaching capacity of the glasses to the requirements of the applications. All this thanks to the modification of the short-range order in the microstructure of the glass and this control has allowed different applications:

On the one hand, some phosphate compositions exhibit preservative properties and are suitable for use in contact with food. They are currently used as a bacterial reset due to their rapid dissolution in the presence of moisture. However, in this work, 50% less phosphate than is commonly used in the food industry has been used to achieve antimicrobial properties over time, and not only in the form of a reset.

On the other hand, the doping of such glasses allows them to modulate their radiation absorption properties in different wavelength ranges of the spectrum which, together with the control of the leaching capacity, has allowed them to be used as sustainable inorganic sunscreens in sun creams. The sunscreen currently used is TiO₂ in different particle sizes, leading to the deterioration of the seabed when deposited. Therefore, the application of Fe/Ce doped phosphate glasses is a sustainable solution to the use of TiO₂ in the cosmetics sector.

Oxetanes as a new class of additives for PEDOT:PSS providing high conductivity and water-resistance

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A7_2 - Electronics I, U1 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

Conducting polymers, such as poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS), are very promising for organic electronics, performing as charge transport layers, flexible electrodes, resistive sensors, among others. However, for applications where the devices interface aqueous or humid environments (e.g. in bioelectronics), both high conductivity and water resistance are essential. In this communication, we introduce oxetanes as a novel class of additives that significantly enhance both the electrical conductivity and structural stability in water of PEDOT:PSS films.

We investigated the structural properties of oxetanes responsible for these enhancements. It was discovered that oxetanes undergo polymerization in the acidic medium of PEDOT:PSS, leading to the formation of polyether compounds [1]. Additionally, hydroxyl-substituted oxetanes can create covalent cross-links or hydrogen bond interactions with the negatively charged PSS. These interactions screen the electrostatic forces between PEDOT and PSS, reducing Coulombic interactions and promoting PEDOT segregation and structural rearrangements that enhance charge transport. We demonstrate that PEDOT:PSS ink formulations containing oxetanes, applied through spin-coating or inkjet printing, can produce highly conductive thin films on both rigid (glass) and flexible (PET) substrates. These films can serve as water-resistant electrodes in electronic devices, including photovoltaic cells [2] and electrochemical field-effect transistors operating with aqueous electrolytes [3]. In addition to thin films deposited on substrates, we successfully developed flexible, free-standing PEDOT:PSS films, with enhanced water resistance and conductivity, by incorporating an oxetane compound as an additive. The obtained flexible films demonstrated good potential as health-monitoring electrodes [4].

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In situ monitoring of Ag-BaTiO₃ CerMet sintering process for tuning the metacomposite properties

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A7_7 - Coatings, U1 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

The addition of metal components into dielectric matrices is an interesting way for increasing the effective permittivity. Recently other interesting electromagnetic properties have been reported in such composites, which make them attractive for microwave absorption, electromagnetic shielding, filters, capacitors, etc. [1]. This work investigated Ag-BaTiO₃ composites, in which optimum compositions and phase arrangements are searched to find: (i) giant permittivity in the dielectric state below the percolation, or (ii) metacomposite properties, above the percolation (near-zero or negative permittivity).

To produce different types of microstructures after sintering, Ag-BaTiO₃ composite powders were prepared by mixing BaTiO₃ with Ag micropowders or by precipitation of Ag nanoparticles from AgNO₃ onto BaTiO₃ grains. The composites were sintered in the range of Ag melting temperature (960°C). The resulting ceramics have grain sizes in the range of 350 nm – 3µm and bi-modal distribution of silver filler, with both fine Ag inclusions and large agglomerates embedded into the ceramic matrix. The frequency and temperature dependence of the dielectric, conductive and electromagnetic properties are discussed in function of Ag filler addition and the microstructural characteristics. Different types of microstructures were generated by the interplay between Ag melting/infiltration/recrystallisation processes taking place simultaneous with the ceramic consolidation. In-situ monitoring of these processes allowed to identify the optimum sintering strategy in order to derive different types of microstructures and related properties.

Modeling by 3D finite element calculations (FEM) demonstrated that dielectric, ferro/piezoelectric and tunability properties can be tuned through inhomogeneous field distributions at the interfaces between metal-ferroelectric, thus subjected some regions to higher fields and generating enhanced electrical responses [2]. Three percolation ranges (see Figure) with substantial permittivity increase are found experimentally and described by FEM modeling, as resulted from specific microstructural metallic configurations. As resulted from calculations, the frequency ranges for the metacomposite properties can also be tuned by composition and microstructural design.

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Customizing Luminescence in REPO₄ Nanocrystals via chemical synthesis routes

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

REPO₄ materials (RE= La, Ce, Pr, Nd, Sm, Y, Er, Gd) present interesting properties such as photochemical and thermal stability, high quantum yield, low photobleaching and toxicity, and long lifetime. These features make them promising hosts for up-converting Ln³⁺ ions, which have led to consider them in optoelectronic applications, as well as biomedicine, clean energy, or sensors, among others. Their processing in the nanoscale is key for their incorporation in next generation of smart optoelectronic devices. Controlling the structural and microstructural characteristics of REPO₄ and RE_{1-x}Ln_xPO₄ nanoparticles through the synthesis is essential to tune and enhance their luminescence response. Despite the great interest of these nanostructures and the possibility of crystalizing them in different crystalline structures (hexagonal, monoclinic and tetragonal) and with varied morphologies and particle sizes, there is still a scarce comprehension of the different parameters that interfere during their growth throughout synthesis process. Particularly, Er³⁺ doped and Er³⁺/Yb³⁺ co-doped REPO₄ nanoparticles would be of interest for optical telecommunication applications due to their NIR emissions; however, they have been hardly studied to date.

In this study, we report the synthesis of hexagonal, monoclinic and tetragonal REPO₄ (RE = Eu, Er, Y) and RE_{1-x-y}Er_xY_yPO₄ (RE = Eu, Y; x=Er) nanocrystals using different chemical synthesis routes in order to customize their structural and morphological features and thus their luminescence response from the visible to the NIR range. Special attention is paid to the morphology and particle size, for it, the use of different surfactants, chelating agents and phosphate sources is considered, which determines the growth in certain crystallographic directions and impact on the dispersibility of the nanocrystals. With the aim of successfully evaluating the performance and properties of the nanocrystals, an in-depth structural, microstructural and thermal characterization study is carried out by techniques such as X-ray diffraction (XRD), Raman spectroscopy, scanning electronic microscopy (SEM), Differential Thermal Analysis and Thermogravimetric Analysis (DTA/TGA) and correlated with the photoluminescence response.

These results suggest that REPO₄ hosts are very versatile and promising for the modulation of the luminescent response in nanocrystals, which places them in a privilege position for the fabrication of anti-counterfeiting security markers that emit at specific wavelengths. The tunable emission properties and high stability of these nanoparticles make also them a promising material for future developments in advanced optoelectronic applications, display technologies, and optical sensors.

Synthesis and characterization of thermochromic VxW1-xO2 coatings: A scalable approach using multilayer co-deposition and flash annealing

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A7_1 - Synthesis, U1 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

This work reports on an original and scalable approach to the fabrication of 25 and 50 nm thick W-doped VO₂-based coatings which comprises the initial co-deposition, at glancing angles and in the presence of reactive oxygen, of alternating VO_y/V_{0.85}W_{0.15}O_y multilayers with average W/V ratios between 1/99 and 5/95, and their subsequent rapid thermal annealing in air atmosphere. Exhaustive micro- and nanostructural, compositional, and optical characterizations of samples treated at reaction temperatures of 475 and 550 °C for times below 30 s confirmed the synthesis of homogeneous V_xW_{1-x}O₂-based films with unique thermochromic features strongly dependent on the dopant amounts. In general, a gradual lowering of the critical temperature to 37 °C during heating was achieved for the maximum doping of $x = 0.95$, albeit at the expense of some detriments in optical performances. The best and most balanced results were accomplished in a 50 nm layer doped at $x = 0.97$ (i.e. ~1 at% W) subjected to flash annealing at 550°C, presenting a remarkable light transmittance (63.4%), solar modulation capability (6.2%) and critical temperature drop (44°C). In addition, the hysteresis width and smoothness achieved make this coating potentially suitable for application in glazing exposed to direct solar radiation. The proposed methodologies, involving green-like reactions and single-layer designs, postulate as an attractive, plausible and cost-effective alternative for large-scale manufacturing of VO₂(M)-based smart coatings.

Synthesis of functionalized polyphosphazene-based materials for decontamination of anionic pollutants from wastewater

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¹University of Padova, Padova, , ²University of Oviedo, Oviedo, , ³Ca' Foscari University, Venice, A7_6 - Environment, U1 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

The increasing presence of emerging pollutants in water sources poses a significant environmental and public health challenge. This study presents the synthesis and application of novel anion-exchange polymers designed to efficiently remove anionic contaminants of concern from contaminated water. In particular, anion exchange polyorganophosphazenes are proposed as materials for wastewater treatment. They were synthesized through a multi-step process, involving the functionalization of the polydichlorophosphazene backbone with quaternary ammonium groups, optimizing their ion-exchange capacity and thermal stability.

Polyorganophosphazenes were selected due to the easy and versatile chemical functionalization that allows the development of several structures. The polymer properties were modulated by selecting different molar ratios of side groups introduced by nucleophilic substitution of the chlorine atoms of polydichlorophosphazene, synthesized through cationic polymerization approach.

The material structures were characterized by ¹H, ¹⁹F, ³¹P NMR, 2D HSQC NMR and ATR-FTIR then the thermal and morphological properties were evaluated.

Finally, the ability to bind anionic molecules in solution was investigated through NMR experiments to evaluate the removal efficiency of the synthesized polymers for a range of common anionic pollutants. The results in terms of the sequestration of pharmaceutical and perfluorinated substances in anionic form and highlighting the potential of anion exchange polymers as an effective solution for water purification, offering an alternative to conventional ion-exchange resins.

Functionalization of Phthalocyanines for their use as crosslinkers in 3D-printable photopolymer systems

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Phthalocyanines (Pcs) are a widely investigated class of macrocyclic compounds with remarkable optical, electronic, and thermal properties. These characteristics have led to their widespread application in fields such as organic photovoltaics, sensors, catalysis, and photodynamic therapy. However, their inherently low solubility and processability limit their direct application in polymeric systems. To overcome these challenges, the functionalization of phthalocyanines has been explored as a strategy to improve their compatibility with photopolymerizable formulations while maintaining their intrinsic properties.

In this study, we report the functionalization of metal-centered phthalocyanines via esterification to introduce reactive sites suitable for crosslinking reactions. The functionalized phthalocyanines (f-Pcs) were synthesized and characterized through spectroscopic techniques such as UV-Vis, FTIR, and NMR to confirm successful functionalization. The obtained f-Pcs were then incorporated into photocurable resin formulations to act as crosslinking agents, facilitating their covalent integration into polymer networks. The goal was to transfer the unique electronic and optical properties of Pcs into photopolymer matrices without compromising their stability and dispersion.

The formulated resins containing f-Pcs were subjected to photopolymerization using digital light processing (DLP) 3D printing, a cutting-edge additive manufacturing technique that enables high-resolution fabrication of complex structures with precise control over geometry and material composition. DLP offers several advantages over conventional photopolymerization methods, including faster curing times, improved resolution, and reduced material waste. These benefits make DLP particularly suitable for integrating functional additives like f-Pcs into photopolymerizable systems.

By leveraging the capabilities of DLP 3D printing, this study aims to develop novel polymeric materials with enhanced optical and electronic properties, expanding the application potential of phthalocyanine-based materials. This work provides a new approach to incorporating phthalocyanines into additive manufacturing processes, paving the way for their use in advanced coatings, optoelectronics, and smart material development. Future research will focus on optimizing printing parameters and material formulations to maximize the performance and scalability of these systems.

Solvent-free Remote Plasma Assisted Vacuum Deposition of Organic Nanometric thin films with Tailored Dielectric Properties

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A7_3 - Electronics II, U1 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

Organic high-k dielectric materials have garnered significant attention due to their use as gate dielectrics in flexible organic field-effect transistors (OFETs). Achieving the desired performance requires precise control over the dielectric properties (relative permittivity and dielectric strength) and morphological properties (surface topography and thickness).

Plasma deposition and treatment methods are manufacturing techniques widely present in different industrial sectors, including mass-scale manufacturing in microelectronics and large-area roll-to-roll processing of flexible and wearable materials. The current communication presents the plasma fabrication of high-k organic thin films using a remote plasma-assisted vacuum deposition (RPAVD) technique.[1] This method consists of the vacuum sublimation of functional molecules within the afterglow area of a remote plasma discharge, providing precise control over the fragmentation and poly-recombination processes involved in the plasma polymerization processes. Furthermore, it is a room-temperature and solvent-free procedure compatible with a wide range of flexible and delicate substrates (paper, textiles...).

Previous developments achieved the synthesis of advanced functional plasma-polymer-like thin films that preserve the molecular structure and integrity of complex precursor molecules for: photonics,[2] sensing,[3] lasing,[4] antimicrobial surfaces,[5] conformal protective coatings,[6] and strain engineering of 2D semiconductors.[7] This communication extends this technique to the development of high-k organic thin films for gate dielectrics applications. A luminescent dye with a very high dipole moment, DCM, is used as a precursor molecule. The results of the dielectric characterization show the development of ultra-flat (RMS roughness < 1 nm) nanometric organic thin films (thickness down to a few tens of nm) with controlled relative permittivity, with values between 3.5 and 6.3. The presence of integer dye molecules and the film's optical properties (refractive index) were also studied to determine the origin of this controlled permittivity. Furthermore, dielectric breakdown results confirm the high dielectric strength with breakdown fields in the range of 5 MV/cm.

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Novel Sulfur-rich polymers from inverse vulcanization as functional materials for all-polymer photonic structures and metamaterials

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A7_7 - Coatings, U1 Room (Level 0), septiembre 17, 2025, 10:30 - 13:10

Low materials costs, ease of fabrication and scale-up are making all-polymer photonic structures increasingly researched for light control applications. However, in their transparency region most of processable polymers have relatively low and similar refractive indices, this hindering strong light confinement effects [1]. In this regard, a new class of amorphous polymers with high content of S-S bonds, named inverse vulcanized polymers (IVPs) from the inverse vulcanization (IV) reaction they are obtained [2], promise photonic building blocks with very high refractive index and excellent transparency in the near infrared region (NIR), that is the telecommunication window.

The solvent-free IV process represents indeed an efficient and green method of up-cycling waste elemental Sulfur, abundant and ubiquitous by-product of gas and oil industry, to obtain sustainable polymeric materials with unique functional properties. IV process takes advantage of Sulfur's ring-opening and linear chain-forming tendency at high temperatures to bind hydrocarbon comonomers to the Sulfur radicals being formed. Due to their nature consisting of polysulfide chains cross-linked typically by divinyl moieties, IVPs exhibit dynamic covalent and self-healing behaviour. Moreover, the high content of easily polarizable S-S bonds endows IVPs with high refractive index and excellent NIR transparency.

Here, novel IVPs with outstanding refractive index were prepared from purposely designed cross-linking comonomers, namely isopropenyl aromatics synthesized through a single-step Suzuki-Miyaura cross-coupling reaction [3,4]. Comonomer type and amount were varied to address both the optical behaviour and filmability of the ensuing IVPs, that is the technologically relevant properties for application and industrial scale-up.

Achieved IVPs were employed to fabricate all-polymer photonic structures, such as distributed Bragg reflectors (DBRs) and imprinted metasurfaces. Gathered results open the way to a variety of applications for light emission control, spanning from free-standing, high-reflectance DBRs and microcavities for NIR emitting lasers, to fabrication of metamaterials for advanced nanophotonics.

Acknowledgements

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Synthesis of KNN with tailored morphology to be used as fillers in composite materials for piezoelectric applications

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A7_3 - Electronics II, U1 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

Keywords: KNN, synthesis, composites, biopolymers, 3D printing, PENG

Piezoceramics based on Pb have been used for different electronic devices because of their excellent piezoelectric properties. However, nowadays, advanced materials with low impact on the environment and human health is a priority (1). As a promising substitution, sodium potassium niobate (KNN), $(\text{K}_{0.5}\text{Na}_{0.5})\text{NbO}_3$, has attracted much attention due to good piezoelectric properties and excellent biocompatibility.

KNN ceramics are prepared by sintering of particles obtained by solid-state and hydrothermal synthesis routes. However, ceramic materials have insufficient flexibility for wearable applications like piezoelectric nanogenerators (PENG) and IoT devices. Therefore, ceramic nanoparticles are combined with biopolymers that contribute interesting properties like flexibility, light weight, and even electrical properties (2,3).

In this communication, we present the results of different synthesis methods for KNN particles with tailored morphologies and their combination with the piezoelectric biopolymers poly-L-lactic acid (PLLA) and polyhydroxybutyrate (PHB). Particular attention is given to the filler-matrix interactions by meticulously tailoring the chemical surface properties of KNN through organic surface modification and their impact on the dielectric properties and the piezoelectric response of the composites. The results suggest that precise dielectric coupling together with 3D printing can enhance the performance of energy harvesting and sensing devices.

Acknowledgements

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Influence of Nitride-forming Elements Al, B, and Ti on the Kinetics of Austenite Grain Growth in Microalloyed Steel

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The alloying of aluminum, boron, and titanium significantly influences the microstructure and the mechanical properties of microalloyed steel. Al is used as a deoxidizer in the steel production process, and aluminum nitride (AlN) plays a crucial role in grain size control due to its strong pinning effect [1]. Boron, as segregated at grain boundaries rather than precipitated as boron nitride (BN), acts as an economically very interesting hardenability promoter [2]. Titanium further protects boron from forming BN and facilitates the nucleation of acicular ferrite, enhancing the steel toughness [3]. These elements exhibit a complex interplay, competing for nitrogen, with titanium showing the highest affinity, followed by boron and aluminum [4]. This competition affects the formation and distribution of nitrides, which in turn impacts the microstructural steel characteristics.

The influence of precipitates such as AlN, BN, and TiN on grain growth kinetics in austenite is governed by Zener drag [5], which impedes the movement of grain boundaries. Among these, AlN exhibits the most significant effect in retarding grain growth [1], while fine TiN particles also notably contribute [3]. Moreover, the presence of Ti and B modulates the availability of nitrogen for Al. Thus, especially for B-alloying, it has been reported to significantly increase the austenite grain size [2].

This study investigates the grain growth behavior in high-purity vacuum induction melted alloys with varying fractions of Al, B, and Ti. The resulting microstructures are characterized metallographically by employing light optical microscopy (LOM), scanning electron microscopy (SEM), and electron-backscatter diffraction (EBSD).

By using the present experimental results, we simulate the grain size evolution using a mean-field approach, as implemented in the software package MatCalc [6] and the Calphad-type open-licensed MatCalc database mc_fe_v2.060.tdb.

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Alteration of phase transformation behavior due to elevated tramp element concentrations in a hypoeutectoid steel

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B1_6 - Influence of increased recycling rates, Andalucía II Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

In order to reduce CO₂ emissions, steel industry shifts their production towards the usage of higher scrap amounts. This transformation leads to an elevation of tramp element concentrations, which could alter the steel's behavior during heat treatments. In this work, the phase transformation behavior of a hypoeutectoid steel grade was studied in detail. A reference alloy from the blast furnace route is compared to trial alloys with intentionally increased tramp element concentrations.

Dilatometry experiments were conducted to determine phase transformation temperatures and construct continuous cooling transformation diagrams. Additionally, a detailed exploration of the microstructure was done with hardness measurements, light optical- as well as scanning electron microscopy including electron backscatter diffraction. Moreover, in-situ high-energy X-ray diffraction measurements were done to follow the microstructural evolution during a heat treatment and to give a detailed overview of the evolved phases after cooling. Finally, the prior austenite grain size has been measured with a high-temperature laser scanning confocal microscope and correlated to the results of the phase transformation behaviors.

The results show that tramp elements not only shift the phase fields in the continuous cooling transformation diagrams to longer times, but also decrease the phase transformation temperatures. As a consequence, the evolution of displacive phases, such as martensite and bainite accompanied by retained austenite, is facilitated during cooling. Furthermore, it has been observed that tramp elements impede the growth of prior austenite grains by segregating to the grain boundaries at high temperatures, thereby inducing a solute drag effect, which could influence subsequent phase transformations as well.

Optimal Chemical Composition Ratio of Nb and Ti on the Mechanical Properties of Cold Rolled High Strength Low Alloy Steels

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The balance between Nb (Niobium) and Ti (Titanium) is critical in controlling the recrystallization behavior and mechanical properties of 550 MPa grade cold-rolled (HSLA) High Strength Low Alloys steel. Nb delays recrystallization through solute drag effects and precipitate formation, while Ti not only retards recrystallization but also enhances strength more effectively due to its ability to form fine, stable precipitates. This study aims to determine the optimal Nb/Ti ratio for maximizing yield strength while maintaining ductility.

To achieve this, hot-rolling and cold-rolling processes were simulated, followed by annealing under various temperatures and durations to mimic industrial conditions. The microstructure was analyzed using advanced characterization techniques, including TEM (Transmission Electron Microscopy), SEM (Scanning Electron Microscopy), and EBSD (Electron Backscatter Diffraction), to evaluate the recrystallization kinetics and precipitation behavior in detail. Mechanical properties were assessed through tensile testing, while hole expansion ratio (HER) testing was performed to evaluate the application-specific performance, particularly edge stretchability.

The results show that precise control of the Nb/Ti ratio significantly influences precipitation behavior, grain refinement, and recrystallization delay. Ti-rich compositions demonstrated superior strength due to the formation of finer TiC precipitates, while Nb's role in solute drag contributed to a more uniform microstructure. Annealing conditions were also found to play a crucial role, as longer annealing times at lower temperatures enhanced the formation of desirable precipitates while controlling grain growth.

This comprehensive analysis provides insights into the optimal combination of Nb and Ti to balance high strength, ductility, and application-specific properties. The findings contribute to the development of high-performance precipitation-hardened steels for automotive and structural applications, where both strength and formability are critical.

Toward enhanced tensile and impact properties in low alloy multiphase TRIP-assisted steels

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 15, 2025, 13:15 - 14:30

Multiphase TRIP-assisted steels have emerged as a cost-effective solution offering an exceptional balance of strength and ductility. These steels, characterized by low alloying content (<4 wt.%), consist of ferrite (α), bainite (α_B), retained austenite (γ), and martensite (α'). Their unique microstructure enables enhanced tensile properties through strain partitioning between soft phases (α , γ) and work hardening from hard phases (α_B , α'). Additionally, the deformation-induced martensitic transformation (DIMT) of retained γ delays necking, further improving tensile performance.

While much research has focused on the effects of retained γ fraction and stability on mechanical properties, the impact toughness of multiphase TRIP-assisted steels under high strain rates remains underexplored. These steels are increasingly applied in the automobile industry for their superior formability and high energy absorption potential, improving passenger safety. Furthermore, their low yield ratio and high post-deformation yield strength make them attractive for wire rod applications, where both impact toughness and tensile strength are critical.

This study investigates intercritical annealing (IA) temperature's role in multiphase TRIP-assisted steel's microstructural evolution and mechanical properties. A continuous heat treatment cycle comprising IA, fast cooling, and bainitic isothermal treatment (BIT) was applied. Controlling IA temperature directly influences the phase fraction of α and the stability of retained γ in the final microstructure. Previous research suggests that an intermediate IA temperature $((AC1+AC3)/2+20\text{ }^\circ\text{C})$ maximizes the retained γ fraction. At higher IA temperatures, γ transforms into α and pearlite during cooling, as confirmed through dilatometry analyses.

This research systematically examines the effects of IA temperature on tensile properties and Charpy impact toughness, highlighting the imbalance between ductility and toughness. The findings provide insights into optimizing IA parameters to achieve a desirable combination of microstructural constituents, enhancing formability and impact performance. These results address existing knowledge gaps, advancing the understanding of multiphase TRIP-assisted steels for automotive and wire rod applications.

Multi-Objective Optimization of the Thermo-Mechanical Control Process in HSLA Plate Steels

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B1_5 - Processing and Microstructural Design of Advanced High-Strength Steels, Andalucía II Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The design of the Thermomechanical Control Process (TMCP) of HSLA steels and the identification of the optimum processing parameters constitute a challenging problem in the industrial pipeline applications, especially for heavy plate rolling. The TMCP of an X70 HSLA plate steel consists of a two stage multipass hot rolling in austenite region (roughing and finishing), followed by controlled accelerated cooling during the austenite to ferrite phase transformation. A multi-objective optimization approach is presented for the process design of an X70 HSLA steel using a physically-based mean field (PBMF) model. The PBMF model incorporates an integrated precipitation and recrystallization model to describe the microstructural evolution due to the interaction of strain-induced precipitation of niobium and titanium carbonitrides and static recrystallization of austenite. An integer multi-objective optimization problem is formulated, and the non-dominated sorting genetic algorithm (NSGA-II) is applied on the PBMF model to determine a set of optimal processing routes that meet process design criteria. Aiming to increase the strength of the HSLA plate, a trade-off between the microstructural objectives is obtained, i.e. average ferrite grain size, the niobium content in solution, and the residual strains at the end of the finishing stage. A single processing route was selected, and the microstructural evolution during TMCP was investigated by multi-phase field calculations in conjunction with the PBMF model. Experimental data on the optimized steel via SEM and STEM revealed good agreement with model predictions. The proposed approach can contribute to the process design of HSLA and microalloyed steels.

Phase Stability and Impurity Detection in $\text{TiO}_2(\text{B})$ Synthesized by Soft Chemical Route: Implications for Preparation and Application

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In this study, we investigated the phase stability of $\text{TiO}_2(\text{B})$ synthesized using ion exchange and dehydration with $\text{K}_2\text{Ti}_4\text{O}_9$ as a precursor. The presence of potassium within the material, particularly in $\text{TiO}_2(\text{B})$, remains undetectable by conventional techniques such as X-ray diffraction (XRD) or energy-dispersive spectroscopy (EDS), even at concentrations exceeding those typically classified as "minor impurities." One focus of the research was to evaluate the potential of differential scanning calorimetry (DSC) for detecting residual potassium content. Another focus was the examination of the phase stability of $\text{TiO}_2(\text{B})$ when incorporated into a different metallic systems such as steels.

This work aims to contribute to the production of single-phase, chemically pure TiO_2 nanoparticles, enabling the investigation of their intrinsic properties without interference from secondary phases or impurities. Furthermore, an improved understanding of phase stability can guide the selection of suitable processing methods and facilitate exploration of the material's use in emerging applications.

Selective oxidation in ternary Fe-Al-Mn model alloys

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

In industrial steelmaking process, steel strips undergo several heat treatments during which total surface oxidation or selective oxidation of alloying elements may occur. Under protective atmosphere, Fe-Al-Mn alloys reveal a transition in oxidation mode of the less noble elements, from external to internal with increasing water partial pressure. The formation of external iron particles is often mentioned along with internal oxidation. An experimental study aims to address the oxidation mechanisms based on diffusion and the correlation with the formation of iron particles depending on experimental conditions.

The experimental device consists in a furnace, equipped with three infra-red lamps insuring a rapid heating phase. The particularity of this apparatus resides in the direct connection with an X-rays Photoelectron Spectroscopy equipment, allowing precise in-situ surface characterizations, exempt from air contamination [1].

The study of the oxidation behaviour of a ternary ferritic Fe-Al-Mn model alloy is conducted at 840 °C, in dry conditions ($p_{H_2O} = 1\text{ Pa}$) and humid conditions ($p_{H_2O} = 610\text{ Pa}$). The samples are held for 0; 25; 76 and 150 s at 840 °C. During heat treatment, the native iron oxides are reduced but alloying elements are oxidized. The nature and morphology of surface oxides is analysed by X-rays Photoelectron Spectroscopy and Field Emission Gun Auger microscope. Cross-sections extracted with a Focused Ion Beam are characterized by Energy Dispersive Spectroscopy and electron diffraction in a Transmission Electron Microscope. The surface coverage and the oxidation depth are investigated by Field Emission Gun Scanning Electron Microscope.

In dry conditions, a continuous layer of Al_2O_3 is formed on the surface, the oxidation mode is purely external. In wet atmosphere, external MnO particles are observed while internally, MnO nodules, $MnAl_2O_4$ and a continuous layer of Al_2O_3 at the oxidation front can be found. A variation in internal oxidation depth and nature is observed with increasing holding time, enabling a kinetic approach of the diffusion mechanisms.

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Fundamental study on grain boundary segregation in Fe-Zn system using in-situ heating transmission electron microscopy

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B1_6 - Influence of increased recycling rates, Andalucía II Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The strong need for high-performing materials drives the continuous development of new structural materials. One such example is the next generation galvanized advanced high-strength steels (GI-AHSSs) that excellently combine strength and ductility with a high corrosion resistance. Despite its outstanding performance, this new material class often suffers from ductility degradation due to so-called liquid-metal embrittlement (LME) by Zinc (Zn) during metallurgical joining processes. Under such conditions, the GI coating may melt, allowing Zn to diffuse along grain boundaries (GBs), thereby initiating embrittlement of the matrix. Based on our recent findings using 4D-STEM and thermodynamic calculations, the occurrence of an interfacial decomposition and the subsequent formation of Fe-Zn compounds along high-angle GBs (HAGBs) are sought to be the root cause of LME (Mat. Today Adv. 13 (2022) 100196; Acta Mater. 259 (2023) 119243; Scripta Mater. 238 (2024) 115758). Here we now aim at directly tracking this proposed GB-mechanisms during in-situ TEM experiments. To this end, we capture the microstructural dynamics of Zn-bearing HAGBs. In this talk, we will report the first results of our in-situ heating TEM observation in the temperature regime from 150 °C to 500 °C, which yielded significant alternation of the GB structure due to the presence of Zn upon isothermal heating. The outcome will be discussed in the context of GB segregation and interfacial decomposition in connection to LME of GI-AHSS.

On the mechanism of nucleation of static recrystallization in austenite: a combined experimental and modelling approach

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B1_5 - Processing and Microstructural Design of Advanced High-Strength Steels, Andalucía II Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

In the hot rolling mill, steels undergo static recrystallization (SRX) in the austenite phase. The properties of the new phases formed in the subsequent cooling largely depend on the grain size resulting from this SRX. Consequently, its accurate prediction is key to predicting the final properties of the steel. The grain size after SRX is determined by the density of new grains produced by the SRX. In turn, the nucleation of SRX in hot-deformed austenite is widely known to take place at the boundaries of the deformed grains. SRX nucleation at deformed grain boundaries is directly associated by current models with the event of strain-induced boundary migration (SIBM), or bulging. However, whether SRX nucleation at those sites effectively occurs by SIBM is yet to be experimentally proved. In this view, the present study analyzes in detail the factors determining the nucleation of SRX in a Ni-30%Fe alloy deformed at high temperature, via electron backscatter diffraction (EBSD). Ni-30%Fe has the same stacking fault energy as the austenite in carbon steels, but remains in austenite phase after cooling to room temperature. This makes it possible to access the substructure imparted by the high-temperature deformation. Results show that the number of bulges (SIBM) developed in the deformed microstructure is at least four times larger than the number of SRX grains. Results also demonstrate that significant growth of potential SRX nuclei occurs only when they are fully surrounded by high-angle boundaries (HABs). Therefore, the nucleation of SRX is not determined by SIBM, but by the transformation of their low-angle boundaries into HABs (LAB-HAB transformation). The conclusions of the experimental study are encompassed in a novel physics-based model and criterion for the nucleation of SRX at deformed grain boundaries. This model is based on the migration of dislocations into pre-existing subgrain boundaries, which gradually increases their misorientations. Nucleation then happens whenever the misorientation of a subgrain boundary reaches the HAB misorientation threshold. Finally, the model has been implemented into a 3D-cellular automaton (3D-CA), together with an extensive characterization of the subgrain misorientations in the deformed microstructure of Ni-30%Fe. Predictions of the model display good agreement with experimental results in terms of all nucleation density, SRX kinetics, and SRX grain size. All in all, this study paves the way for a new description of SRX nucleation at deformed grain boundaries, which can give robust predictions of the resultant grain size via models incorporating microstructural topology.

Alloy design strategy for the development of nanostructured bainitic surface layer in gear steels for wind turbines applications

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B1_3 - Investigation in novel processing technologies for special steels - RFCS NanoWinTur and NewAIMS Projects, Andalucía II Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Wind energy is ideally placed to be the European Green Deal's technology of choice since it is the most efficient solution to reduce emissions in the power sector. Europe installed 18.3 GW of new wind power capacity in 2023, a record amount but only half of what it should be building to meet its 2030 climate and energy targets, which requires to install 260 GW of new wind power capacity over 2024-2030. To meet its 2030 climate and energy targets the EU now needs to build 33 GW a year on average. It is well-known that turbine towers are becoming taller to capture more energy. The hub height for utility-scale land-based wind turbines has increased 73% since 1999, to about 100 meters in 2022. The average hub height for offshore wind turbines is projected to grow even taller to about 175-200 meters in 2035. Moreover, the average rotor diameter of newly-installed wind turbines was over 150 meters in 2023. Wind turbines have also increased in maximum power rating, or capacity. Today's new wind power developments have a turbine capacity up to 6 MW range onshore and up to 15 MW offshore.

Gearboxes are a highly loaded part of wind turbines, which is facing numerous challenges the coming years due to upscaling and torque density increase. In this work we will design new ultra-high strength steels for gears, to ensure the increasing gear operating conditions in terms of reliability, performance and compactness that manufacturers demand by wind turbines with higher mechanical torque.

The aim of our alloying design strategy, based on thermodynamic and kinetics data, is to form nanoscale bainitic structures within the carburised layers of medium and large-size gears for on- and offshore wind turbines, by means of alternative heat treatments on propane and plasma carburising in atmospheric pressure furnace limiting at maximum oxide formation during carburising, and a subsequent austempering on low/medium high-silicon steel grades, specially designed as base material.

For that purpose, two digital tools (JMatPro and Mucg83) were extensively validated using phase transformation data of commercial steels for gears manufacturing. Then alloying additions were modified to ensure large austempering windows based on Bs and Ms calculations in carbon carburising profiles, as well as good hardenability, needed to avoid soft phases at the core of the component. Moreover, chemical composition was adjusted to ensure nanoscale bainite formation at the surface in an austempering holding time below 10 hours.

Solid-state phenomena in advanced bainitic steel through in-situ S/TEM observations

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B1_2 - Bainite & Phase Transformations, Andalucía II Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Dynamics in processes and matter observed using in-situ S/TEM microscopy methods provide an outstanding capability for better understanding the complex phenomena in the nanoscale. Solid-state phenomena occurring in steels are mainly observed using a multidimensional approach involving ex-situ conditions. Dynamic microscopy constitutes a research method that supports direct analysis of phenomena that cannot be identified using other research techniques.

Advanced, ultra-fine bainitic steel was designed to stabilize the B2-ordered phase (NiAl)[1]. The chemical composition of tested steel follows Fe-0.4C-8.0Ni-2.8Al-0.8Cu (wt.%), and the design approach was described elsewhere [2,3]. The aim of this study is to understand the precipitation processes of intermetallic during aging processes, the decomposition mechanism of the metastable bainitic structure during reverse transformation [4], and bainite formation during low-temperature transformation. The experiments were performed using the MEMS heating holder and dynamic electron microscopy S/TEM observations. The applied thermal cycles enabled the observation of the precipitation processes of the NiAl intermetallic phase and the reverse transformation of the bainitic structure into austenite. The dynamic precipitation processes of the L12 and B2 phases were evaluated as a function of temperature together with the decomposition mechanisms of the bainitic matrix. Finally, the bainitic transformation at 250 °C was conducted inside the microscope column. The grain boundary and autocatalytic nucleation were observed during bainitic transformation. Moreover, the austenite memory effect was observed. Despite certain limitations of the in-situ S/TEM method, the occurrence of crucial phenomena associated with the bainitic transformation was evidenced.

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Convergence of Pathways to Equilibrium During Tempering of Bainitic and Martensitic Structures in a High-Si Medium Carbon Steel.

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B1_2 - Bainite & Phase Transformations, Andalucía II Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

This research reveals the convergent nature of bainitic and martensitic microstructures during high-temperature tempering in a high-silicon medium carbon steel, while examining their distinct transformation pathways across temperatures ranging from 200°C to 650°C. Despite their different initial states - both containing carbon-saturated tetragonal ferrite matrix and retained austenite - these microstructures follow unique routes to a common equilibrium state. The investigation demonstrates that while retained austenite governs the tempering response in bainitic structures, the highly dislocated, carbon-enriched ferritic matrix controls the transformation in martensitic structures. Through comprehensive analysis utilizing high-resolution dilatometry, scanning electron microscopy, and X-ray diffraction techniques, we establish that both microstructures ultimately achieve identical equilibrium states at elevated tempering temperatures (600-650°C), albeit with significantly different kinetics - bainitic structures exhibiting slower transformation rates. This study maps the critical tempering mechanisms in high-silicon steels and quantifies the transformation pathways to equilibrium. These findings provide fundamental insights for optimizing heat treatment protocols, demonstrating that despite different starting microstructures, carefully controlled tempering can yield convergent final states in advanced steel processing.

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Impact of Steelmaking Route and Rolling Strategy on Nb Solubility in Reinforcement Bars Production

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B1_5 - Processing and Microstructural Design of Advanced High-Strength Steels, Andalucía II Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Traditionally, the use of Nb microalloying has been related to the production of flat products. However, recent innovations have introduced low Nb additions in reinforcing bars production to enhance steel strength and toughness by refining the austenitic structure. Additionally, Nb is being utilized to improve cost efficiency and as an alternative to QST (Quenching and Self-Tempering) processes that do not comply with earthquake safety regulations.

In flat products, Nb is commonly used in low-carbon steels processed through Thermomechanical Controlled Processing (TMCP), where the modification of the austenite structure via strain-induced precipitation enhances mechanical properties. However, in high-carbon long products (>0.20 wt.% C), the role of Nb is less established due to its limited solubility in austenite. In these grades, Nb—whether in solid solution or as precipitates—can help inhibit grain growth during hot rolling, leading to a refined austenitic structure. In this context, understanding the amount of Nb in solid solution at the onset of hot rolling is critical. This is typically estimated through thermodynamic calculations, such as solubility products or commercial software. However, these methods assume equilibrium conditions, whereas industrial reheating processes often deviate from this assumption.

This study proposes an experimental indirect method to evaluate the amount of Nb in solution prior to hot deformation. Nb solubility is analyzed in rebar products coming from different steelmaking routes (BOF and EAF), and various rolling technologies (cold and direct charging), comparing the results with TEM-based precipitation analysis and thermodynamic predictions. The findings suggest that this approach serves as a valuable complementary tool for assessing Nb in solid solution under specific industrial conditions.

Characterization of high-strength medium manganese zinc-coated steels for the automotive industry

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B1_7 - Medium Mn Steels & Processing, Andalucía II Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Advanced high-strength steels (AHSS) continue to evolve in response to the automotive industry's stringent requirements for enhanced environmental sustainability and passenger safety. Within this evolution, medium manganese steels (MMnS), representative of the third generation AHSS, have emerged as exceptional candidates. These steels are characterized by a distinctive compositional range of 3-12 wt.% manganese, up to 0.4 wt.% carbon, complemented by strategic additions of Si, Al, Cr, and microalloying elements (Nb, Ti, and V). Their complex microstructure, comprising ferrite/martensite and retained austenite (>10%), can yield an exceptional combination of high ultimate tensile strength (UTS ~ 1.2-1.6 GPa) and substantial total elongation (TE ~ 15-20%), rendering them particularly suitable for automotive anti-intrusion components and high-energy absorption applications. Moreover, their elevated manganese content facilitates reduced forming temperatures during warm stamping processes while maintaining compatibility with zinc-based corrosion protection coatings, thus addressing historical challenges of liquid metal embrittlement with Zn-coating and associated cracking. This research focused on developing novel medium manganese steels specifically engineered to meet demanding requirements for high-energy absorption (Total Elongation $\geq$ 18%, Ultimate Tensile Strength $\geq$ 1200 MPa) and anti-intrusion (TE $\geq$ 10%, UTS $\geq$ 1500 MPa) components. The alloy design methodology incorporated comprehensive thermodynamic calculations to determine critical transformation temperatures (Ac1, Ac3, Ms) and phase evolution characteristics (volume fraction and chemical composition), using 22MnB5 steel as a benchmark. Based on these calculations, nine distinct steel compositions were formulated varying C, Mn, Al, Cr and B contents, and subsequently produced as 50 kg ingots and processed through sequential hot and cold rolling. The specimens underwent systematic industrial process simulation, encompassing intercritical annealing (700-760°C), hot-dip galvanizing (470°C), hot stamping (700-750°C), and paint baking treatments (170°C, 20 minutes). Through micro-tensile testing, two optimal compositions were identified and subjected to a comprehensive characterization utilizing high-resolution dilatometry, scanning electron microscopy, X-ray diffraction analysis, and hardness measurements. The resultant microstructure consisted of a mixture of ferrite, martensite, and carbon-enriched retained austenite (7-30%), and sometime carbides. The developed materials demonstrated superior mechanical properties, with hardness values ranging from 400 to 500 HV, ultimate tensile strength of 1200-1700 MPa, and total elongation of 10-22%.

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Design of high-strength medium manganese zinc-coated steel for the automotive industry

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The demand for reduced fuel consumption, lower CO₂ emissions, and improved vehicle safety is driving the development of advanced high-strength steels (AHSS). Hot stamping of coated C-Mn-B steels dominates automotive applications due to its ability to produce ultrahigh-strength components. However, these steels exhibit poor elongation, limited crash energy absorption, and require Al-Si coatings with inadequate corrosion resistance. Medium manganese steels (3–12 wt.% Mn), a key material in 3rd generation AHSS, offer superior mechanical properties, lower transformation temperatures, and compatibility with Zn coatings, making them a promising alternative for warm stamping applications.

In this study, new Zn-coated medium manganese steels were developed with the following objectives:
a) Achieving total elongation (TE) $\geq 10\%$ and ultimate tensile strength (UTS) ≥ 1500 MPa for intrusion-resistant components.

b) Achieving TE $\geq 18\%$ and UTS ≥ 1200 MPa (UTS $\times$ TE ≥ 21 GPa%) for energy-absorbing components.

The alloy system consisted of varying amounts of C, Mn, Al, Cr and B.

A total of 72 different variants were identified and analyzed using thermodynamic simulations to evaluate phase volume fractions and chemical compositions. Nine alloys were selected for experimental validation, based on the results of the phase transformation characteristics from the thermodynamic simulations. These alloys were prepared at a laboratory scale, subjected to hot and cold rolling, and subsequently processed through annealing and hot press forming. Based on quasi-static tensile testing, two alloys were identified as promising candidates for pilot scale experiments simulating the industrial heat treatment procedure.

Funding received for this work from the European Research Executive Agency (REA) under the Grant Agreement No. 101112425 is gratefully acknowledged.

Mechanical performance of Al-alloyed medium-Mn steels following IA and QP treatments in the continuous annealing regime

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B1_7 - Medium Mn Steels & Processing, Andalucía II Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The final mechanical properties of construction elements in the automotive industry are often determined in sheet steel stage during heat treatment. For storage, transportation, and technological purposes, steel sheets are often rolled into coils. The heat treatment process of steel coils may be performed using either batch or continuous annealing. A significant drawback of batch annealing is the long processing time and the non-uniform mechanical properties along the coiled steel. In continuous annealing, a single sheet thickness is heat-treated at a time, which shortens production time and enables the use of advanced thermal cycles, leading to multi-phase or two-phase structures.

Recent advancements in automotive steels (AHSS) have led to the development of medium-Mn steels, which may represent an evolutionary step in the automotive steel industry. In this study, a systematic heat treatment optimization process was performed for IA and QP cycles on steel with a composition of 0.17% C, 4.7% Mn, 1.6% Al, 0.2% Si, and 0.2% Mo to achieve the highest possible strength and plasticity product. A wide range of parameters was analyzed, allowing for additional identification of conditions that ensure either maximum strength or plasticity.

The heating and cooling rates, along with the energy-saving annealing time of maximum 120 s (intercritical soaking in IA and partitioning in QP), were selected to enable the heat treatment process using industrially available continuous annealing production lines. The research began with a dilatometric analysis of the material and an investigation of the influence of heat treatment parameters on the thermal stability of austenite (Ms temperature).

For a promising range of process parameters, heat treatment was performed on subsize tensile samples using a dilatometer. In the IA process, the maximum UTS × TEI of 38 GPa% was obtained for a sample with a total elongation (TEI) of 38%. In the QP process, the maximum value was 29 GPa% for samples with a yield strength (YS) of 850 MPa.

Additive Manufacturing of low alloyed 90MnCrV8 tool steel

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B1_3 - Investigation in novel processing technologies for special steels - RFCS NanoWinTur and NewAIMS Projects, Andalucía II Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

The development of an electron beam powder bed fusion (PBF-EB) process for 90MnCrV8 aims to leverage the advantages of additive manufacturing (AM) for producing high-performance tool steels. In PBF-EB, it is possible to utilize microstructural engineering, and the aim is to develop such hardening mechanisms to increase the performance of low alloyed steels, to compete with less environmentally friendly alloys in terms of performance. This study takes a new approach for heating the feedstock powder, where a polar-hexagonal spot heating is used rather than the standard linear rastering. The polar-hexagonal heating and melting strategy were developed and used to produce solid samples from gas atomized 90MnCrV8 feedstock. The optimized EB-PBF process demonstrated the ability to produce fully dense parts which were analyzed using scanning electron microscopy (SEM) and X-ray diffraction (XRD).

Role of cementite precipitation in lath martensite revealed by rapid tempering and conventional tempering treatments of medium-carbon steel

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B1_4 - Advanced Characterization of Phase Transformations and Microstructural Evolution in Steels, Andalucía II Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Rapid tempering offers an energy saving process similar to induction heating and generates wide opportunity for the achievement of desired mechanical properties in several fields, for example in the automotive sector. Since the introduction of the tempering parameter, it has been successfully applied to a variety of steel alloys across a wide range of time–temperature combinations. The present study reveals promising mechanical properties with rapid tempering (20 s) as compared to conventional tempering treatment (1 h) of as quenched C45E martensitic steel, for the same tempering parameters. FESEM reveals that nanometer sized finer cementite is more evenly distributed in rapid tempered samples as compared to the conventional tempering. Fracture mechanisms and percentage elongation stood compliment to the cementite precipitation occurred in the tempered martensite under various tempering regimes (from 250 °C to 700 °C).

Deformation-Induced Microstructural Evolution in a High-Nitrogen Stainless Steel: A Detailed EBSD Study

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B1_4 - Advanced Characterization of Phase Transformations and Microstructural Evolution in Steels, Andalucía II Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Due to upcoming regulatory changes, the use of medical devices containing cobalt will be severely restricted. As a consequence, it is urgent to find alternatives to cobalt-chromium alloys, widely used to produce dental prosthetic structures. As a promising alternative, the BioDur 108® alloy, a nickel-free high-nitrogen austenitic stainless steel (HNSS) has been investigated in this work. In addition to its excellent biocompatibility and good corrosion resistance, it presents favorable mechanical properties which can even be further improved through cold-working for specific demanding applications. While already commercial for some specific applications, only limited information is available on the microstructure-property relationships. Therefore, in this work, an extensive microstructural investigation including the impact of prior deformation on its final mechanical properties has been completed. For this purpose, cold-rolling, as well as classic and SEM-EBSD in-situ tensile testing were conducted, allowing the monitoring of the evolution of mechanical properties and microstructure during deformation. The results showed that deformation is mainly based on dislocation glide, and mechanical twinning appears beyond a certain threshold. Furthermore, with increasing deformation, the twin boundaries interact with dislocations, improving the material's strength and causing the reorientation of thermal twins. It is worth noting that this alloy has a significant strain-hardening capacity while maintaining good ductility, and it does not form martensite even under high stress, thus remaining non-magnetic and MRI-compatible. These findings suggest that BioDur 108® is a highly promising candidate for replacing Co-Cr alloys.

A New Carburizing Steel Grade for Aeronautical Transmission: Design and Modelling

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

To achieve carbon neutrality by 2050, the air transport sector is implementing new technical solutions related to synthetic fuel, but also to aircraft engine technology. The evolution of aircraft engines tends to considerably reduce polluting emissions and fuel consumption. To meet these needs, new technologies have recently emerged such as the power gear box and ceramic ball bearings. These new technologies highlight several metallurgical challenges and request the development of new grades or processes.

The purpose of this presentation is to review current metallurgical solutions and to present the latest developments in case-hardening grades aiming at increasing surface hardness levels, while maintaining the right balance between mechanical strength and toughness, focusing on a new carburizing grade developed by Aubert et Duval, the C65NiL®.

In recent years, to meet the demand for improved performance compared with M50NiL, new grades have appeared, such as FERRIUMC64® developed by Questek, or ARCTIC 15® developed by SKF whose metallurgical design and performance will be described. We will highlight the design criteria and the technical difficulties to increase the level of surface hardness. Details on a new carburizing grade, C65NiL®, developed by Aubert et Duval will be given. This grade has an original metallurgical design that enables to achieve a hardness level of more than 825 HV (about 65 HRC) after thermochemical and heat treatments with a toughness level comparable to M50NiL.

the interest of artificial intelligence, in particular machine learning, to predict a hardness profile after carburizing and quality heat treatment with C65NiL, will be shown. We will see how these new digital design tools can accelerate metallurgical design, speed up the thermochemical processes or analytical balancing, while highlighting the limitations.

Design of QP heat treatments for plastically-deformed and undeformed austenite in medium-Mn steels alloyed with Mo and Cu

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B1_7 - Medium Mn Steels & Processing, Andalucía II Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

High strength steels (yield strength >700 MPa and tensile strength >900 MPa) are widely used for automotive forgings, which should withstand high stresses under different load conditions. The 42CrMo4 steel meets the requirements concerning a combination of high strength and fracture resistance; however, due to the increased chromium content and the need for applying high-temperature energy-consuming heat treatment after the forging process, the use of this type of steel associated with a high environmental impact. A promising alternative to 42CrMo4 steel are medium manganese steels containing 3-5 wt.% of Mn. This type of steel has a multiphase microstructure composed of ferritic/bainitic or martensitic matrix providing high strength and 10-15% of ductile retained austenite (RA) preventing the formation of microcracks.

Ultra-high strength (yield strength >900 MPa and tensile strength >1300 MPa) Quenching and Partitioning QP steels have been originally developed for hot/cold rolled automotive sheets. Such beneficial mechanical properties can be achieved for medium-Mn QP steels mainly through proper designing of martensite-austenite (a quenching step) ratio and a tailored stability of RA (a partitioning step). The adaptation of QP treatment for products with increased thickness requires different approaches for designing their thermal processing routes. The challenge is to ensure a uniform microstructure throughout the entire cross-section of the forging.

The aim of this study is to characterize the phase transformation kinetics of plastically-deformed and undeformed austenite during the isothermal holding step and to design optimal time-temperature parameters of QP treatment of medium-Mn steels (4 wt.% of Mn) containing Cu and/or Mo additions with a potential application for automotive forgings. The critical temperatures as well as phase transition phenomena during isothermal holding were theoretically determined using Thermo-Calc and JMatPro softwares. The experimental time-temperature-transformation (TTT) and deformation-time-temperature-transformation (DTTT) diagrams were determined in dilatometric investigations, which were the basis for designing quenching and partitioning parameters of the QP treatment. Due to the increased Mn addition, only the formation of martensite and bainite were recorded during the isothermal holding step, while the formation of undesired ferrite and pearlite was eliminated both in the plastically-deformed and undeformed states. The quenching temperatures in a range of 270-290°C were applied to determine the optimal martensite-austenite ratio. The partitioning step was carried out at temperatures from 400 to 450°C and times from 120 to 900s to obtain lath-type microstructures composed of carbide-free martensite and about 10-15% of RA with a tailored stability.

Thermal Stability of Nanostructured Bainitic Steels: Investigating the Microstructural Changes and Mechanical Properties After Reheating

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B1_2 - Bainite & Phase Transformations, Andalucía II Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Nanostructured bainitic steel, also known as super bainite, represents a significant advancement in third-generation AHSS, combining high strength, ductility, and toughness properties. Exceptional strength and ductility properties result from a unique microstructure consisting of nanoscale bainitic ferrites and austenite films in bainitic sheaves, separated with austenite blocks. It is essential to study the thermal stability of the microstructure and resultant mechanical properties at temperatures higher than that of the bainite forms. This is particularly important for high-temperature applications or in scenarios where the temperature of an engineering component increases during service. This study investigates the microstructural variations and corresponding changes in mechanical properties in super bainite achieved by isothermal bainite heat treatment at 250 and 300 °C after reheating to the temperature range of 300-700 °C. Microstructural features were characterized using field emission gun scanning electron microscope and X-ray diffraction methods, and consequently, hardness, tensile and Charpy impact tests were carried out to study the resultant strength and ductility combination. It has been shown that reheating the originally achieved super bainite up to 400 °C didn't affect the microstructure and mechanical properties, indicating considerable thermal stability. However, cementite precipitation, austenite decomposition to pearlite, cementite spheroidization and complete decomposition of the microstructure to spherical cementite particles distributed within a ferritic matrix occurred at elevated temperatures. While yield strength, ultimate tensile strength, elongation and impact energy of the super bainite remained unchanged until heating to 400 °C, different strength-ductility combinations and impact toughness energy values were achieved at different heating temperatures depending on the corresponding microstructural variations. It has been shown that, big austenite microblocks are susceptible to decomposition to pearlite, despite the austenite films that are thermally more stable. Cementite precipitation was more pronounced in nanobainite with higher dislocation density, as dislocations acted as potential diffusion paths for carbon, accelerating the cementite precipitations. Finally, results approved that the tempering behavior of the same steels with martensite in their microstructure was different from that of austempered materials, indicating the higher tempering resistance of nanostructured bainite compared to that of martensite.

An in-situ analysis of the kinetics of κ -carbide precipitation in Fe-Mn-Al-C low density steels

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B1_4 - Advanced Characterization of Phase Transformations and Microstructural Evolution in Steels, Andalucía II Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The reduction of energy consumption is together with improving safety standards paramount in modern transportation. In this regard, the development of strong, tough, and ductile steels for automotive applications is an essential part in steel research. Low density Fe–Mn–Al–C steels are promising candidates for structural forged parts owing to their capability to contribute in reducing the vehicle weight mainly achieved through alloying with aluminium (Al) (~1.3% density reduction per 1 wt.% Al). The alloying elements not only promote the formation of austenite but also of carbides such as κ . The κ -phase is particularly important for enhancing strength due to its hardening effect. However, to effectively manage the precipitation, namely the size and distribution of the κ -phase within these alloys, poses the challenge of understanding the phase transformation kinetics during quenching and subsequent aging.

In this study, time-resolved analysis of κ -phase precipitation is conducted during heat treatments using in-situ high-energy synchrotron X-ray diffraction (HEXRD), enabling for real-time observation of phase transformations. After solution treatment of the Fe–Mn–Al–C alloy, the kinetics of κ are investigated as a function of the cooling rate and aging conditions. The obtained samples are then characterized using both optical and scanning electron microscopy (SEM), as well as hardness testing. Results from in-situ HEXRD indicate that slow cooling (<1°C/s) promotes local κ -phase growth along austenitic grain boundaries, whereas rapid cooling (>21°C/s) leads to a dispersed formation of the κ -phase. The results are contrasted with the diffusion-controlled mechanisms of κ -phase precipitation. The findings cannot be acquired through conventional post-mortem characterization and offer novel information for optimizing the thermal treatment conditions of low density steels.

Bimodal 316L austenitic steel: Enhancing mechanical performance through ODS strengthening

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Achieving an optimal balance between strength and ductility remains a critical challenge in materials engineering. This study explores a novel bimodal microstructural approach to enhance the mechanical properties of 316L austenitic stainless steel by integrating a fine-grained oxide dispersion-strengthened (ODS) matrix with a coarse-grained austenitic phase. Unlike conventional strengthening strategies, the use of ODS steel provides enhanced stability against grain growth and contributes to improved mechanical performance.

Bimodal microstructures were fabricated by mixing mechanically alloyed fine ODS 316L steel powder with coarse austenitic powder, followed by spark plasma sintering (SPS). Three bimodal compositions with 70%, 75%, and 80% fine-grained ODS steel were investigated alongside unimodal coarse and fine-grained variants. Microstructural characterization, including electron backscatter diffraction (EBSD) and transmission electron microscopy (TEM), confirmed the forming of a distinct bimodal grain structure with an aspect ratio of ~10 between coarse and fine grains.

Mechanical testing revealed that bimodal structures significantly improved the strength-ductility balance compared to unimodal counterparts. Hardness measurements showed a non-linear increase with the fraction of fine ODS grains, aligning with predictions between the Voigt and Reuss bounds, suggesting a non-negligible coupling between coarse- and fine-grained regions. The highest hardness of 2.96 GPa was achieved for the ODS80 composition, compared to 1.46 GPa for the unimodal coarse-grained steel.

Tensile tests substantially enhanced yield strength (YS) and ultimate tensile strength (UTS) while maintaining acceptable ductility. The ODS70 and ODS75 compositions exhibited YS of 605 MPa and 673 MPa, respectively, surpassing the 260 MPa of unimodal coarse steel. The UTS of the bimodal variants reached up to 908 MPa, significantly higher than the 605 MPa of coarse-grained steel. Despite the increase in strength, bimodal samples retained uniform elongation between 18.5% and 22.3%, deviating from the conventional Hall-Petch trend.

Comparisons with literature on bimodal steels prepared by alternative methods, such as bimodal or high-energy ball milling, indicate that the proposed approach offers a simple yet effective route to achieving superior mechanical properties. The results demonstrate that tailoring the volume fraction of ODS fine grains enables optimized mechanical performance, making this strategy highly promising for applications requiring a strong yet ductile material.

Effects of silicon addition on the microstructure and mechanical properties of austenitic stainless steel

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Austenitic stainless steel is a kind of promising fuel cladding structural material for the lead-based fast reactor (LFR). Recent studies show that silicon addition is an effective way to improve the corrosion resistance of stainless steels in the lead-bismuth eutectic alloy. However, effects of silicon on the mechanical properties of austenitic stainless steels have not been systematically studied yet. Basing on the composition of 15-15Ti, the authors designed and fabricated a silicon-bearing austenitic stainless steel named as 15-15TiSi, and investigated its microstructure and mechanical properties through the methods of thermal-calc calculation, microstructural observation, and uniaxial tensile and creep tests.

Silicon addition decreases the solidus and liquidus temperature of alloy and leads to the precipitation of δ during the solidification of the 15-15TiSi stainless steel with 2.5wt.% silicon. In contrast, δ is absent when the silicon addition is 2.0wt.%.

For the 20% cold-worked 15-15TiSi stainless steel plates, a better strength-ductility combination can be achieved at room temperature by silicon addition. Since silicon has the effect of reducing the stacking fault energy of alloy, during cold work it promotes the formation of deformation twins, which are beneficial for the work hardening behavior of material.

During the creep tests of 15-15TiSi stainless steel, silicon addition causes an intergranular precipitation of σ -phase, which affects the mechanical property of alloy differently at various temperatures. At 550°C, σ particles are fine and discrete and beneficial for the intergranular creeping deformation resistance of 15-15TiSi. At 650°C, however, σ precipitates massively and causes an evident drop in the creep rupture life of alloy.

Briefly, to avoid the precipitation of δ , the silicon content of LFR cladding used austenitic stainless steels should be limited to 2.5 wt.%. In addition, at the temperatures no higher than 550°C, there is no undesirable effect of silicon on the mechanical properties of 15-15TiSi.

Experimental and simulation study of the mechanical behaviour of high-strength steel processed by friction stir welding

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B1_5 - Processing and Microstructural Design of Advanced High-Strength Steels, Andalucía II Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The welding of high performance materials such as high strength steel is recognised as a challenge for the development of new structural components within the European production industry. Maximising material performance and hence material efficiency requires improved joining technologies to overcome the limitations of conventional welding methods applied to high strength steels. In this scenario, the friction stir welding process (FSW) arises as a candidate solution. FSW is a solid-state joining process in which the materials are joined without reaching their respective melting temperature. Hence, most of the quality issues (e.g voids) associated to conventional welding methods are avoided. For its introduction in load-bearing applications, it is required to control the weld seam properties and orientation, as they have a critical influence on the material properties, and on any subsequent forming operation that takes place. In this work, FSW-joints performed on high strength structural steels (Docol S700MC and Docol S960MC) provided by the Swedish steel manufacturer SSAB in 6 mm thick sheet format are tested at coupon scale under quasi-static tensile and bending loads, as well as impact toughness testing, following relevant standards (ISO 4136, ISO 5173, ISO 6892). Different positions of the weld's root are considered to assess its impact on the bending behaviour. Metallographic analysis and microhardness measurements are carried out as a means of linking the microstructure of the weld seam with the macroscopic behaviour of the material. Besides, microstructural evaluation allows identifying the main regions of the weld (Weld Nugget, Thermo-Mechanical Affected, Heat Affected Zone), as well as detecting the presence of any kind of defect that may influence the performance at the macroscale. The data obtained during the tests are used to feed a Finite Element model of the material in its base and welded conditions, including the Heat Affected Zone. This model is then employed to carry out a parametric study of the influence of the weld seam positioning and properties on the forming behaviour of the welded steel joints. Finally, the potential application of this solution in strategically placed reinforcement plates of a loader crane is explored, as a lighter and customizable substitute of conventional plate-on-plate construction methods.

Phase transformation behaviour in a laser powder bed fusion produced maraging steel

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B1_2 - Bainite & Phase Transformations, Andalucía II Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

In conventional manufacturing, maraging steels present a martensitic structure hardened by precipitation during ageing at a specific temperature and time period. In contrast, Laser Powder Bed Fusion (LPBF) produced maraging steels consist of mainly martensite and some retained austenite with intrinsic thermal cycles promoting early stages of precipitation for a given set of parameters. As a result, the two manufacturing routes produce distinct microstructures. Understanding how these phase transformation differences affect the microstructure is essential for its control, strategic use and to avoid compromising the mechanical integrity of the final part.

This work investigates how changes in the layer thickness and laser emission mode affect the metallurgical phenomena (i.e., the martensite-to-austenite transformation and precipitation of intermetallic phases) during printing—melting, rapid solidification, and repeated heating and cooling. Microstructural characterisation techniques and multiscale chemical analyses were performed to examine as-built samples and those aged at 480 °C and 540 °C.

Scanning Electron Microscopy allowed to identify layer thickness as a key parameter influencing the solidification cell size in as-built samples. For all conditions, X-ray diffraction results showed that the tetragonality of martensite remained consistent across layers despite successive reheating cycles. Retained austenite was found both at and away from melt pool boundaries at the mesoscale in the as-built structure and its volume fraction increased with ageing temperature. Electron Probe Micro Analysis results showed that mesoscale Cr segregation and Ni and Ti depletion caused by competing mechanisms during printing, persists even after ageing. No significant impact of the printing parameters on microstructural evolution during ageing was observed. However, nanoscale clustering and precipitation in aged samples differ from those found in conventionally processed materials. Finally, hardness values of aged LPBF-maraging steel samples were found to be comparable to those achieved in samples processed by conventional manufacturing methods, highlighting the potential of this technique to produce end-use parts.

Microstructural constituents influencing toughness in maraging steels

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B1_1 - Alloy Design & Mechanical Properties, Andalucía II Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Maraging steels are one of the most versatile high-performance materials due to their excellent combination of strength and toughness. They are used for many demanding applications, such as aircraft wheel suspensions and plastic mold materials. The microstructure of these steels consists of uniformly distributed, nanometer-sized, intermetallic precipitates embedded in a Ni-rich martensitic matrix. Depending on the alloy composition and the heat treatment applied, different types of precipitates can form during the ageing process. The investigated steel belongs to the group of PH 13-8 Mo grades and obtains its strength increase during ageing through the precipitation of intermetallic β -NiAl particles. Furthermore, so-called reverted austenite forms during aging, which has a significant influence on the toughness properties.

In this study, particular attention was paid to the presence of δ -ferrite and its influence on toughness. An increase in the proportion of this phase led to a drastic decrease in impact toughness. When examining the microstructure, it was found that the embrittlement is caused by cracks originating from delta ferrite.

In addition to the use of high-resolution methods such as transmission electron microscopy and atom probe tomography to characterize the intermetallic precipitates, in-situ methods such as high-temperature X-ray diffraction and the use of high-energy synchrotron radiation have proven to be beneficial for understanding the microstructural development during heat treatment. For example, the occurrence of the austenite memory effect and recrystallization without prior cold working in PH 13-8 Mo steels could be demonstrated by cross-scale in-situ methods [1]. The latter effect leads to a significant refinement of the microstructure, which has a positive effect on the mechanical properties. Another part of the investigations was dedicated to intercritical annealing prior to ageing. Targeted analysis of the microstructure using atom probe tomography and transmission electron microscopy showed that this annealing step creates zones enriched with Ni, which promote the formation of reverted austenite during the subsequent ageing process. In-situ high-energy X-ray diffraction tensile tests also showed that this phase exhibits high mechanical stability [2].

In addition to the negative influence of the δ -ferrite, it was shown that the phase fraction of transformed austenite has the greatest influence on toughness, while that of the martensite block sizes is negligible.

[1] A. Rosenauer, et al., Materials Characterization, 2024, 208, 113554.

[2] A. Rosenauer, et al., Material Science & Engineering A, 2024, 895, 14622.

Decomposition of carbide-free bainite during prolonged holding at bainite transformation temperatures

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B1_2 - Bainite & Phase Transformations, Andalucía II Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

TRIP-assisted steels rely on retained austenite in their microstructure, which enables the so called TRIP-effect. Alloying with sufficient amounts of Si or Al is employed to suppress carbide formation during the bainite transformation to allow for enrichment of austenite with carbon during bainite formation and thereby stabilizing it down to room temperature. While Si or Al can suppress carbide formation in carbide-free bainite for durations typically employed for bainite transformation (e.g., several minutes), prolonged holding at the transformation temperature eventually leads to carbide formation in the austenite areas. These precipitates reduce the carbon concentration in austenite, destabilizing it and promoting martensite formation upon quenching. To understand this decomposition process is crucial to optimize large-scale production of TRIP steels, where steel often cools down in large coils and therefore the time to reach room temperature can be up to several hours, leading to a reduced TRIP-effect.

To investigate this behaviour, samples of a steel containing 0.4 wt% C, 1.5 wt% Mn, and 1.5 wt% Si were austenitized at 950 °C and then quenched with 50 K/s to bainite transformation temperatures ranging from 450 to 350 °C. The samples were held at these temperatures for up to 10 hours. The heat-treatment was done on a Dilatometer Baehr Type 805. A combination of XRD and EBSD investigations was used to examine the decomposition process.

Advanced High-Strength Steels: Fundamental Insights and Industrial Applications

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B1_5 - Processing and Microstructural Design of Advanced High-Strength Steels, Andalucía II Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Martensitic PHS 1500 steel has been the dominant choice in the automotive industry for over two decades, offering a tensile strength of 1.5 GPa and an elongation of 6–8%. To achieve an optimal balance between strength and ductility, a sustainable approach combining press hardening with subsequent bake hardening is employed. Enhancing the steel's properties requires a thorough fundamental understanding and precise control of its microstructure after these processes. To understand microstructural changes at the atomic scale during press hardening and bake hardening, a micro-alloyed, fully bainitic steel with low dislocation density than martensite was selected as a laboratory alloy.

The mechanical properties of PHS 1500 steel were evaluated through tensile, bending, and fracture toughness tests. The samples exhibited excellent tensile properties, with an ultimate tensile strength of 1542 ± 7 MPa, a yield strength of 1147 ± 3 MPa, and a total elongation of $8.86 \pm 0.16\%$. While bake hardening led to an increase in yield strength, it had no significant effect on bending properties. Fracture surface analysis revealed ductile dimpling, indicating high fracture toughness.

The laboratory alloy after deformation simulating press hardening condition and aging simulation bake-hardening treatment was studied using transmission electron microscopy and atom probe tomography and tensile testing. The microstructure consisted of fine bainitic structures with a lower dislocation density than martensite, enabling atomic-scale characterization. Notably, the yield strength of laboratory alloy increased significantly under different strain aging conditions, reaching up to 790 MPa, compared to 630 MPa after initial processing. The experimental results showed the formation of carbon Cottrell atmospheres around dislocations and the formation of carbon clusters/fine carbides in the bainite during aging. It is proposed that this is associated with the high dislocation density of bainite (martensite in industrial steel) with formation of a complex dislocation substructure after deformation and its high average carbon content. The segregation of carbon and substitutional elements such as Mn to the bainitic lath boundaries was observed by atom probe tomography.

Revealing the history of white etching layer formation by correlative multiphysical characterization

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B1_4 - Advanced Characterization of Phase Transformations and Microstructural Evolution in Steels, Andalucía II Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The surface of a railway track is exposed to harsh conditions: compressive load, severe plastic deformation, frictional heat, and rapid cooling. Such a complex thermomechanical loading can lead to the formation of so-called white etching layers (WELs) – hard and brittle near-surface regions, that can induce surface damage or even rail failure. The exact mechanisms responsible for appearance of WELs is still a matter of debate since multiple kinetic phenomena are acting simultaneously, rapidly, and spatially localized.

To take a closer look at the WEL formation mechanisms, we applied multiple characterization approaches in a correlative manner, covering different length scales and different measurement principles. A single WEL and its interface to the bulk was first characterized by nanoindentation mapping followed by electron microscopy, high-energy XRD as well as atom probe tomography to pinpoint the exact structural changes, which are responsible for the specific morphology and properties of the WEL.

It is proved that austenitic transformation has occurred within the WEL, suggesting that its microstructure is, at least partially, martensitic. At the same time, the WEL is characterized by normally distributed circular grains with the average grain size of about 400 nm. Such microstructure is not typical for a martensite. Atom probe tomography reveals a very sharp transition between the WEL with fully dissolved cementite and deformed pearlite with fully undissolved (though mechanically fractured) cementite. This observation contradicts with the model of progressive WEL development over large number of cycles. Based on the correlative characterization data we formulate a model suggesting that WELs can be formed through a single event of substantial wheel slippage. In this scenario, high temperatures required for material austenitization are reached not only due to the frictional heat generated on the rail surface, but also due to the volumetric heat caused by severe plastic deformation with high strain rate.

Although the developed model does not pretend to be the only mechanism of WEL formation, it is crucial to understand whether WELs appear as a results of multiple loading cycles or due to a single event as well as whether shear plastic deformation or frictional heat is a dominant factor responsible for WEL formation. The mitigation strategy should be then adjusted according to the active WEL formation mechanism, e.g. prevention of a fatigue-based effect requires different measures than prevention of single slip events.

High-throughput method for steel development using directed energy deposition

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B1_1 - Alloy Design & Mechanical Properties, Andalucía II Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

The advancement of research methods is critical for developing novel steels for demanding applications. Conventional materials research requires significant human effort and time, making it slow and expensive. The Materials Acceleration Platform (MAP) concept aims to revolutionize the field by utilizing high-throughput experiments and characterization combined with data informatics to create automated research cycles. This research explores a high-throughput methodology for stainless steel development, employing state-of-the-art Directed Energy Deposition (DED) equipment with the capability of in-situ mixing of up to six elemental powders.

The use of DED enables the rapid creation of extensive alloy families. Samples are designed to minimize the processing time while utilizing the full potential of automated characterization. This approach significantly accelerates the discovery and optimization of new alloys by allowing learning, rapid iteration and testing. The integration of advanced characterization techniques, such as high-throughput microscopy and spectroscopy, facilitates detailed analysis of the synthesized alloys. The combination of high-throughput synthesis and automated characterization represents a significant development leap in alloy research, promising to deliver novel materials with enhanced performance for a variety of industrial applications.

In this research iron, nickel, chromium, and molybdenum are used as alloying elements to demonstrate MAP concept for stainless steels. These elements were chosen to validate the methodology, as they are common elements in stainless steels and facilitate different phase structures (Ni: austenite; Cr, Mo: ferrite). In the work, DED parameters are optimized, to achieve a homogeneous structure. Therefore, characterization of homogeneity of the samples is done by X-ray diffraction (XRD) and microscopy techniques. For high-throughput determination of mechanical properties, an indentation method is utilized. The used characterization methods are semi-automated, creating grounds for full automation. By streamlining the research process, MAP not only reduces costs and time but also opens new avenues for innovation in materials science. This research is the first step towards MAP, creating foundations for future research. When combined with data informatics and computational modeling, the methodology has a huge potential for developing novel steels for challenging applications, such as hydrogen production, storage and transport.

Impurities in Recycling Steels - Challenge and Potential for the Fatigue Resistance of Steels

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B1_6 - Influence of increased recycling rates, Andalucía II Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Representing more than 20% of the industrial CO₂ emissions, the steel value chain provides a powerful lever to substantially contribute to the goal of eliminating the net CO₂ emissions by 2050. The transformation towards direct reduced iron (DRI) that can be gradually mixed with scrap and melted in the electric arc furnace (EAF) allows climate-neutral production of steel grades. However, the change in metallurgical refinement by the DRI route and contamination of post-consumer scrap, lead to variations and gradual accumulation of detrimental impurities, like Cu, Sn or N. Accordingly, the respective recycling steel grades are not sufficient to fulfil the demanding specifications of modern steel grades. During hot forming, selective oxidation of Fe leads to a near-surface enrichment in Cu that may segregate at the prior austenite grain boundaries, eventually leading to the problem of hot shortness, i.e., massive embrittlement of hot-formed steel products. Increasing nitrogen contents lead to the risk of coarse TiN inclusions, acting as fatigue crack initiation sites in high strength steels. In the present study, various low- and medium-C lab-scale steel grades were enriched with 0.5 to 2 wt.% Cu and tested with respect to hot shortness susceptibility and fatigue behaviour in the solution-annealed and aged state. In the case of aged Cu-containing steel grades, an improvement of the fatigue strength and damage tolerance is associated with the precipitation of nano-sized, semi coherent Cu precipitates that were identified by high resolution transmission electron microscopy (TEM) and atom probe tomography (APT). The results are discussed in terms of future recycling steel grades with higher degrees of impurities and inclusions but nevertheless, having fatigue-resistant microstructures for successful application in a circular economy.

Exploring G91 Steel in Laser Powder Bed Fusion: Powder, Parameters and Microstructure

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B1_5 - Processing and Microstructural Design of Advanced High-Strength Steels, Andalucía II Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

G91 grade is a ferritic-martensitic steel extensively used in the manufacturing of components for high temperature applications within the energy sector due to its excellent mechanical and thermal properties, as well as its affordability. Consequently, it is employed for the production of structural components in power plants. However, traditional manufacturing methods commonly employed to produce these components hold back the creation of complex geometries. Laser Powder Bed Fusion (LPBF), an Additive Manufacturing (AM) technique, has been brought in to fabricate components in various alloys. Nevertheless, the feasibility of producing G91 steel components using LPBF is still being investigated.

This study focuses on the fabrication of G91 steel samples using Laser Powder Bed Fusion (LPBF). A comprehensive characterization of the G91 steel powders ($D_{50} = 44.4 \mu\text{m}$), produced via gas-argon atomization, was performed. The chemical composition of the G91 steel was confirmed using ICP-OES and XRF, while the initial crystallographic phase in the powder was identified as α -Fe through XRD analysis. Additionally, microstructural observations were carried out using both Light Optical Microscopy (LOM) and Scanning Electron Microscopy (SEM), revealing the absence of oxides and impurities. Moreover, the presence of minimal porosity and homogeneous spherical particles was observed, which correlates with the excellent flowability behavior demonstrated in the rheological tests.

Following an extensive optimization process aimed at reducing porosity to values between 0.035% and 0.2%, the optimal printing parameters were determined: 150-200 W, 750-1000 mm/s, a hatch distance of 0.05 mm, and a layer thickness of 0.03 mm. The resulting microstructures were examined in both as-built and normalized conditions. XRD analysis revealed the formation of retained γ -Fe, coexisting with α -Fe. Consequently, detailed metallographic observations were conducted using LOM and SEM. The results displayed a complex mix of morphologies, dependent on the printing conditions. However, no evidence of microsegregation was found, in line with the results from EPMA analysis. Finally, the mechanical properties were assessed through Small Punch and compression tests.

Making High Mn Steel by Sustainable Ferromanganese Pre-alloy for Cryogenic Applications

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B1_6 - Influence of increased recycling rates, Andalucía II Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Driving toward net-zero CO₂ emissions in steel industry, a more sustainable approach should be adopted in both iron-making and steel-making processes. While the sustainability of iron making is supported by the prospering hydrogen-based direct reduction technology [1], research on the sustainability of alloying ingredients used in steel making has been limited.

In this study, we utilized three Mn alloying ingredients to produce three high Mn steels with similar composition. The first one is electrolytic Mn (hereafter referred to as “EMn”), which is a high purity form of metallic Mn; the second one is a conventional medium carbon ferromanganese pre-alloy (FeMn), which has been used in the steel making industry; and the third one is a “green” FeMn pre-alloy produced by a novel “HAIMan” process, which ensures lower energy consumption during the production of FeMn pre-alloy [2]. These three steels were named as EMn steel, MCFEMn steel and HAIMan steel. The chemical composition is designed with the aid of thermodynamic calculation, aiming for cryogenic applications of high Mn steel.

All three steels are produced by a lab-scale vacuum induction melting furnace, and underwent identical thermomechanical processing. Comparability between these steels were demonstrated by a thorough microstructure characterization, and mechanical testing at either room temperature or cryogenic temperature. From the testing results, all three steels exhibited similar microstructure, similar grade of tensile properties and impact toughness, which demonstrated the feasibility of making high Mn steel by the HAIMan “green” FeMn pre-alloy.

In summary, the HAIMan steel showcases similar grade of high Mn steel performance as EMn steel and MCFEMn steel while utilizing a more sustainable alloying ingredient. This research effort aims to reduce the overall energy consumption of steel making without compromising steel performance, contributing to a more sustainable future in the steel industry.

References:

[1] D. Raabe Chemical reviews, 2023, 123, pp.2436-2608.

[2] J. Safarian Conference of Metallurgists. Cham: Springer Nature Switzerland, 2023, pp.749-756.

Microstructural optimization and mechanical behavior of SS-QP treated 30CrNiMo8 steel

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B1_4 - Advanced Characterization of Phase Transformations and Microstructural Evolution in Steels, Andalucía II Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The quenching and partitioning (QP) process aims to achieve superior mechanical properties and enhanced toughness by developing a microstructure consisting of martensite and retained austenite. In this study, single-step QP treatments (SS-QP) were applied to the commercial 30CrNiMo8 steel, a material widely used in industrial high-strength applications but not specifically engineered for this process. Preliminary studies on the initial microstructure are performed through the application of different routes for intercritical treatments. Microstructure evolution was examined using XRD and SEM/EBSD, while tensile tests were conducted to evaluate the impact of the treatment on the final properties of the material. SS-QP treatments were successfully implemented, delivering high tensile strength and improved ductility. Strain hardening behavior was analyzed and compared with specimens treated using conventional quenching and tempering treatments. The results demonstrate the feasibility of applying the QP process to 30CrNiMo8 steel and highlight the importance of initial microstructural control and treatment design in achieving desired mechanical performance.

Effect of Mo and Cu on hot deformation behavior, recrystallization kinetics and thermomechanical processing of QP-treated medium-Mn steels

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B1_7 - Medium Mn Steels & Processing, Andalucía II Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The evolution of Quenching and Partitioning (QP) steels was from 0.2C-1.5Mn-1.5Si to higher strength levels using increased C and/or Mn contents. Especially promising results were achieved in lean medium-Mn sheet steels like: 0.2C-(3-5)Mn alloyed with different Si and/or Al additions. Microalloying was also applied, although it should be noted that the effects of Nb and Ti (sometimes V) are different than that known in HSLA steels. Finally, recycling induced impurity elements (like Cu, Cr, Mo, Ni) need to be consider for new steel designs.

The high hardenability of Mn and its effective use makes sense in high-thickness products like plates for structural applications or forgings for automotive or machine industries. The hot deformability of three 4Mn steels alloyed with silicon and aluminum were investigated in the present study. Mo alone (0.3wt.%) or together with Cu (1wt.%) were added to investigate the effects of the elements on hot deformability compared to the 0.17C-4Mn-0.5Si-0.8Al reference steel. The continuous compression tests were performed at 900, 1000 and 1100°C at different strain rates of 0.05, 0.5 and 5 s⁻¹ in the Gleeble 3800 simulator. The registered compression curves allowed to assess values of flow stress and to determine the activation energy of plastic deformation, which was above 420 kJ/mol. Double-hit compression tests were applied to determine the kinetics of austenite recrystallization. Finally, the steels were subjected to different quenching and partitioning treatments following the deformation to identify the effect of the QP parameters on microstructure, retained austenite amount and sub-sized mechanical properties.

Acknowledgement

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Understanding the effect of laser powder bed fusion thermal cycles on the microstructure of a tool steel

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B1_3 - Investigation in novel processing technologies for special steels - RFCS NanoWinTur and NewAIMS Projects, Andalucía II Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Laser Powder Bed Fusion (LPBF) is an advanced additive manufacturing technique used to produce complex components layer-by-layer by scanning the cross-sections of a 3D CAD model with a high-intensity laser. During the LPBF process, materials are exposed to extreme and rapid thermal cycles, characterized by high heating and cooling rates, as well as localized melting and solidification. These unique temperature profiles differ significantly from those encountered in conventional manufacturing methods, resulting in highly heterogeneous microstructures in the additively manufactured parts.

To simulate the thermal behaviour of the LPBF process and its impact on microstructural evolution, an ultra-fast heating experiment was conducted using a dilatometer on a conventional tool steel sample. This approach aimed to replicate the thermal cycles experienced during LPBF by achieving comparable peak temperatures and rapid temperature transitions. The microstructural analysis focused on a two-layer printed steel model to understand changes in phase distribution, grain refinement, and thermal-induced transformations such as carbide precipitation and variations in dislocation density.

These findings provide valuable insights into the thermal response of tool steels during additive manufacturing processes and propose methods for reproducing LPBF-like thermal cycles, enhancing material design and performance optimization in advanced manufacturing contexts.

Optimizing Tool Steel Performance through Additive Manufacturing: Exploring PBF-EB and PBF-L Technologies

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B1_3 - Investigation in novel processing technologies for special steels - RFCS NanoWinTur and NewAIMS Projects, Andalucía II Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Additive manufacturing, particularly 3D printing, offers significant potential for design optimization and the production of limited series components, aligning well with several industrial and economic sectors. However, the technology is currently constrained by a limited selection of available materials. In the case of tool steels, the choice is often restricted to costly superalloys or high-alloy steels, such as Maraging grades. Despite their higher cost, these materials fall short of conventional tool steels in terms of durability and performance. This study aims to explore and demonstrate strategies using two 3D printing technologies—PBF-EB (Powder Bed Fusion-Electron Beam) and PBF-L (Powder Bed Fusion-Laser)—to produce cost-effective, high-performance steel based on the high-carbon grade 1.2842 (90MnV8). LPBF was conducted using a high-temperature module to achieve powder bed conditions comparable to those in EBM. The increased temperature helped prevent cracking and enabled in-situ heat treatment of the material. Both techniques demonstrated promising results in terms of manufacturing efficiency and the development of unique microstructural features. Additionally, samples from both technologies underwent distinct heat treatment processes. Microstructural phase changes were analyzed using scanning electron microscopy (SEM) and X-ray diffraction (XRD).

Additive Manufacturing of Fe-Mo-W-C high thermal conductivity steel by electron beam and laser powder bed fusion

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B1_3 - Investigation in novel processing technologies for special steels - RFCS NanoWinTur and NewAIMS Projects, Andalucía II Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Metal forming tools are subjected to harsh conditions, including fluctuating temperatures and repeated wear. Additively Manufactured (AM) carbide-reinforced steels have demonstrated significant advantages in such applications, as the added geometrical freedom enables optimized tool design while reducing both production complexity and lead time. This study evaluates a novel high thermal conductivity steel (HTCS) developed using alloying and processing methods patented and pioneered by the Spanish company ROVALMA, aiming for short cycle times and long tool lifetimes in processes such as hot stamping, die casting, and forging. HTCS powder was atomized by INNOMAQ21 and fabricated using two additive manufacturing techniques: Electron Beam Powder Bed Fusion (PBF-EB) and Laser Powder Bed Fusion (LPBF). Samples were produced across a wide range of process parameters and analyzed using microscopy, microindentation, and spectroscopy. For PBF-EB, the as-built microstructure exhibited a hardness of approximately 390 HV, with elongated grains oriented along the build direction and separated by boundaries containing Mo precipitates. The optimal process window for PBF-EB was found to be above 2 J/mm², with no balling observed even at 1200 W and 6000 mm/s, indicating excellent potential for high throughput. LPBF was conducted using high-temperature module to obtain comparable conditions of powder bed as in EBM. Temperature increase allowed to avoid cracking and perform in-situ heat treatment of the material during LPBF. As-build samples presented comparable hardness, while after the post heat-treatment in the dilatometry furnace they featured various changes in the hardness. Both techniques yielded promising results in terms of manufacturing efficiency and unique microstructure features.

Atom-scale insights on the influence of B in preventing liquid metal embrittlement (LME) of third-generation advanced high-strength steels (AHSS)

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B1_7 - Medium Mn Steels & Processing, Andalucía II Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The 3rd generation advanced high strength steels (AHSS) are developed to optimize strength and ductility combinations majorly for automotive structural application. Examples of such steels include enhanced dual-phase (DP) steels, modified transformation induced plasticity (TRIP) steels, medium-Mn TRIP steels, ultrafine bainitic steels and, quenching and partitioning (Q&P) steels.

Some AHSS grades are alloyed with high Si to prevent detrimental cementite precipitation. Moreover, the automobile AHSS parts undergo sacrificial Zn or Zn-Fe coating to prevent corrosion. However, The presence of Si enhances Zn-assisted liquid metal embrittlement (LME) behavior during resistance spot welding, a common welding process for automobile parts.

The LME is an embrittlement phenomenon that occurs because of molten Zn diffusion into steel prior austenite grain boundaries (PAGBs) during welding. The diffused Zn reduces PAGBs cohesive strength and thus causes intergranular cracking in the presence of tensile stresses.

The mitigation of LME is possible through 10-50 wt.ppm B addition to the steel's chemistry. The significant reduction of crack lengths was conclusively verified using an LME-specific resistance spot welding test. The theory is that B segregates to PAGBs, mitigates Zn diffusion, and thus regulates LME cracking by decreasing grain boundary energy. Recent investigations through hot-tensile tests also displayed B effectiveness except for the tests performed at 900 °C. Here, the ductility loss of the boron steel appears higher, which suggests a shift in the state of B and its behavior regarding LME.

In the current work, we use site-specific atom-probe tomography (APT) investigations to unravel the mechanisms causing ductility loss in a B-added AHSS heat-treated at 900 °C. The APT results show that all the B is confined in grain boundary nano-carbides network along PAGBs instead of segregating at PAGBs. Thus, B is no longer playing the role in decreasing the grain boundary energy through segregation. Moreover, the generated precipitate-matrix interfaces are supposedly weaker than PAGBs. This further resulted in adverse performance at 900 °C than in no-B condition.

Calibrating a TRIP crystal plasticity material model from in-situ high-energy X-ray diffraction data considering the uniaxial load direction

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Transformation induced plasticity (TRIP) steels stand out for their high strain hardening and high formability. Their mechanical properties and performance largely depend on the processing history and resulting microstructural attributes. To optimize application-specific TRIP components, engineering of the microstructure is crucial. Simulation tools capable of predicting the impact of forming conditions and strain path on the mechanical response and resulting part behaviour are becoming inevitable for inexpensive optimization of the related forming processes. Describing the material behaviour under these complex industrial deformation conditions, necessitates constitutive models that define the material response based on microstructural characteristics, such as grain/crystallite sizes of austenite and martensite, dislocation densities etc. Calibration and validation of these models benefit from detailed reference data, such as datasets from in-situ experiments probing multiple scales at the same time.

In this work, we explore the calibration of a physics-based crystal plasticity-based TRIP constitutive material within the DAMASK [1] simulation framework for a metastable austenitic stainless steel. A comprehensive dataset [2] recorded via in-situ high-energy X-ray diffraction at beamline P07 at DESY, giving access to phase fractions, transformation kinetics, crystallographic texture, lattice strains, load partitioning, and dislocation densities next to the macroscopic stress-strain response, served as reference for the model calibration. The model parameters, describing dislocation motion and saturation, initiation and evolution of martensitic phase transformation were calibrated by multi-objective Bayesian optimization while comparing simulation results with experimental observations depending on direction of uniaxial loading. The optimized parameters will be discussed with respect to the identification approach and compared with results of similar models in the literature. The results indicate that the employed crystal plasticity model (although popular among the crystal plasticity community) cannot fully capture martensite evolution and strain hardening when comparing simulations with the in-situ measured local material behaviour. As such, this work stimulates and suggests further work in the near future that would eventually help improve the robustness and comprehensiveness of load direction sensitive models.

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Atom probe tomography investigation of the impact of tramp elements from steel scrap recycling on the embrittlement of 51CrV4 quenched and tempered steel

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B1_6 - Influence of increased recycling rates, Andalucía II Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

To mitigate CO₂ emissions, the steel industry increasingly relies on recycling steel scrap using the electric arc furnace. However, this practice introduces increased amounts of tramp elements such as Ni, Cr, Mo, Cu, Sn, Sb, and As into steels, some of which, unless already used as alloying elements, can significantly degrade mechanical properties. Sn, Sb, and As are particularly detrimental among the tramp elements, potentially causing severe embrittlement.

This study investigates the effects of tramp elements on an industrial 51CrV4 steel subjected to quenching and tempering. Small-scale laboratory alloys were produced with controlled additions of Sn, Sb, Cu, and Ni to simulate increased levels that may occur due to recycling in the future, ranging from 0.01 – 0.2 wt.%. Hardening at 840 °C and tempering at 450 °C, 550 °C, and 650 °C with subsequent furnace cooling was applied to assess the susceptibility to reversible temper embrittlement. Mechanical properties were evaluated using tensile and Charpy V-notch impact tests, while multiple microstructural characterisation methods were employed to identify the cause of the embrittlement. The results revealed no significant change in tensile strength or elongation, consistent with the absence of detectable microstructural changes in scanning electron microscopy and electron backscatter diffraction analyses. However, impact toughness decreased by half with increasing amounts of Sn, Sb, and Cu. In combination with advanced site-specific sample preparation methods using femtosecond laser ablation and focused ion beam techniques, atom probe tomography (APT) was used to identify nanostructural changes. APT revealed nm-sized Cu clusters and precipitates along grain boundaries and significant segregation of Sn and Sb to high-angle grain boundaries. Furthermore, the difference in segregation to various types of high-angle grain boundaries, specifically martensitic and prior austenitic grain boundaries, is discussed. These findings suggest that embrittlement is primarily driven by the segregation of Sn and Sb and nanoscale precipitation of Cu at high-angle grain boundaries rather than bulk microstructural changes.

This work highlights the critical role of tramp elements, particularly Cu, Sn, and Sb, in the embrittlement of 51CrV4 steel during tempering. It underscores the importance of advanced characterisation techniques, such as APT, for uncovering the nanoscale mechanisms behind mechanical property degradation.

FATIGUE CRACK INITIATION AND GROWTH IN ADVANCED BAINITIC STEELS: NOTCH AND MICROSTRUCTURAL EFFECTS

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B1_1 - Alloy Design & Mechanical Properties, Andalucía II Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Knowing the effect of the microstructural features such as interfaces on the fatigue re-sponse of bainitic steels containing retained austenite, is a topic of high interest for, among others, bearing applications. The up-scaling in the development and use of such complex advanced steels in actual components requires a comprehensive study of both microstructural and notchs effects, aspects often treated in isolation.

New results from studies based on scanning electron microscopy and electron backscat-ter diffraction over the crack path, in correlation with the crack growth rate, will be pre-sented, revealing the twofold effect of the retained austenite.

Acknowledgements:

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The Influence of Mo and Cu on Microstructure and Mechanical Properties of Air-hardening Ductile Forging Steels

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Air-hardening ductile forging steels are gaining industrial interest due to their potential to reduce the global warming impact of steel forgings. To investigate their robustness against recycling-induced impurities, the effect of Cu and Mo needs to be investigated. For this matter, three alloy variants were produced: reference steel without Mo or Cu, Mo-alloyed steel, and Mo+Cu-alloyed steel. The microstructural evaluation is supported by X-ray diffraction and experimental continuous cooling-transformation (CCT) diagrams. Mechanical properties are characterized by tensile and hardness testing. The results show that the reference and Mo-alloyed steels consist of bainite and martensite. While reference steel primarily exhibits bainite with 6.2% retained austenite (RA), the bainite fraction decreases in Mo-alloyed steel along with RA to 5%. On the other hand, in Mo+Cu-alloyed steel, the critical cooling rate to form martensite further decreases, resulting in a fully martensitic microstructure with 2.8% RA after air cooling. While Mo alloying enhances strength compared to the reference steel but leads to the lowest ductility, Mo+Cu alloying results in the highest strength without significant ductility loss. The further assessment of mechanical properties will be completed with instrumented Charpy impact tests and fractographic analysis for deeper understanding.

Microstructure development in case-carburized bearing steels for wind turbines

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Large-sized main shaft steel bearings are crucial components in wind turbines. Malfunction of these critical parts can lead to complete gearbox failure and prolonged downtime. To withstand the high loads, shaft bearings need high fatigue strength, toughness, and wear resistance. These combinations of properties can be achieved through case-carburization, which is a heat treatment process that enriches the surface of steel with carbon, creating a hard, wear-resistant outer layer while maintaining a tough core. After case-carburization, the processing of these steels is followed by annealing, hardening and tempering, leading to a complex microstructural evolution that eventually determines the performance of these gigantic components. This work examines the microstructural evolution of case-carburized steels during annealing, hardening and tempering, for two different annealing routes: bainitic and pearlitic. Investigations combine microstructural characterization by optical and electron microscopy, electron backscatter diffraction and X-ray diffraction with thermodynamic and kinetics simulations. It will be shown that the evolution of the microstructures is not only affected by the carbon gradient after case-carburization, but also, and very strongly, by the inherent segregation bands of substitutional elements present from solidification. Bainitic annealing produces alloy-rich regions with twice the fraction of martensite-austenite islands compared to alloy-lean areas, leading to a bimodal grain distribution and carbide-dense bands after hardening. In contrast, pearlitic annealing results in three distinct regions: a pearlitic case, a sharp transition zone, and a martensitic-ferritic core, with hardening producing a uniform distribution of retained austenite. After tempering, these microstructural variations lead to significant hardness differences even in areas with constant carbon concentration. This study highlights the importance of understanding microstructural development during shaft bearing processing to design microstructures for maximum performance.

Habit plane induced anisotropy of lath martensite micro-plasticity in dual-phase steel

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Among the Dual-Phase (DP) steel microstructure constituents, lath martensite is generally considered to be the hard and brittle phase that determines strength and restricts ductility. However, recent studies have shown that lath martensite islands can deform in a considerable ductile manner in DP steels. These observations have been related to recent studies on fully lath martensitic steels, in which strong plasticity preferentially occurred over the habit plane through various competing micromechanical deformation mechanisms. However, it has been unclear to what degree these insights can be extended towards DP steel microstructures. Therefore, this paper presents a study in which the lath martensite plastic anisotropy in DP steel is correlated to the habit plane orientation. To this end, a series of advanced micromechanical measurement and identification methods are employed, ranging in scale and complexity, to unravel the individual mechanisms and to assess the statistics of the influence of the habit plane orientation. On well-defined "1D" and "2D" specimens, microstructure-correlated strain mapping and identification of micro-plasticity shows that the habit plane determines how plasticity percolates through the lath morphology in cases of a favorably oriented habit plane. Through a "3D" bulk experiment, a more comprehensive and statistical study on a large number of coarse martensite islands, embedded in a ferrite matrix, reveals that strong plasticity occurs most frequently over the habit plane, even when it has relatively unfavorable orientations.

Advancing of mechanical and exploitation behaviors of steel grinding balls by industrial-scale “Quenching and Partitioning”-based processing

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A “Quenching and Partitioning” (Q&P)-based heat treatment has been developed and successfully implemented on an industrial scale for 104 mm diameter rolled grinding steel balls (0.75 wt.%C-1 wt.%M-0.5 wt.%Cr). This innovative approach aims to enhance both surface and bulk hardness, improve impact resistance, and, crucially, prevent cracking during heat treatment, a common issue with conventionally processed high-hardenability steel balls. Traditional manufacturing of steel balls involves rolling, followed by direct water quenching interrupted at an average bulk temperature of 220-250°C, and subsequent self-tempering. This conventional method is effective only when the martensitic transformation is limited to a depth of 5-10 mm from the surface. However, with high-hardenability steels, martensitic transformation occurs throughout the entire ball volume leading to surface cracking due to the significant volume change associated with martensite formation in the core. To address this critical limitation, the Q&P principle has been strategically adapted. The modified Q&P process involves two key steps: (a) controlling the quenching duration to ensure that the ball's core temperature falls below the martensite start (Ms) temperature, and (b) replacing the self-tempering stage with a controlled furnace tempering process. The optimal bulk temperature at which the water quench is interrupted has been determined to be within the range of 125-170°C. This specific temperature range ensures a balanced “Martensite/Retained Austenite” ratio within the ball at the moment of quenching interruption. Following the quench, a tempering at 200-250°C is implemented to relieve stresses and facilitate carbon partitioning from the martensite to the austenite. The resulting microstructure exhibits a gradient from tempered martensite in the outer “shell” layers to a “Martensite/Bainite/Retained Austenite” microstructure in the core. Notably, the retained austenite content in the core is significantly increased, reaching 25-30 vol.%, due to carbon enrichment resulting from the partitioning process from martensite (and bainitic alpha-phase) to the gamma-phase (austenite). This controlled increase in retained austenite content from the surface towards the core effectively balances stresses and prevents the formation of cracks. The Q&P-based heat treatment has been successfully implemented on an industrial scale. The Q&P-treated grinding balls achieved a remarkably uniform hardness of approximately 55 HRC throughout their cross-section, and, importantly, no hardening cracks were observed. Furthermore, these Q&P-treated balls demonstrated exceptional fracture resistance under repetitive impacts of 6.8 kJ each, a critical requirement for their demanding operational conditions. This improved performance makes the Q&P process a highly promising route for manufacturing high-performance grinding media.

Iron oxidation simulation on IF-Ti steel: kinetics and diffusion mechanisms

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B1_8 - Tailoring Steel Microstructures, Andalucía II Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Advanced High Strength Steels (AHSS) are high-alloyed steels presenting enhanced mechanical properties. Their growing use in the automotive industry makes their galvanizing process a key operation that enables their systematic use in exposed parts. Galvanizing operations involve a thermal annealing followed by a coating step to protect the steel sheets against corrosion. The annealing takes place in a reducing atmosphere (typically N₂-5 vol.%H₂). However, this atmosphere reducing towards iron is oxidizing for most alloying elements such as Si, Mn, Al, and Cr because of water traces in the atmosphere. The high amounts of these elements in AHSS promote selective oxidation during annealing, leading to coating defects.

A solution is the pre-oxidation technique, also called total oxidation, to avoid these defects. It implies the controlled formation of an iron oxide scale in an oxidizing atmosphere, followed by a reduction step where the previously formed minor elements oxides get covered under the newly reduced iron oxide layer. This way, a metallic surface can be obtained for the hot-dip galvanizing [1,2].

Because the gas-metal reactions happening during pre-oxidation are complex, this paper focuses on the pre-oxidation of an IF-Ti (low-alloyed steel, Interstitial Free Titanium) to first elucidate the basic behavior of an industrial “almost pure” iron material. Thus, an overview of the oxidation of an IF-Ti steel in various oxidizing atmospheres at 600 °C is presented. The annealing tests are performed in a resistance-heated furnace in which the gases are injected at 300 °C, assuming to allow a direct thermodynamical equilibrium with the sample. The targeted oxidizing powers are set by the oxygen-to-gas ratio as in industrial DFF (Direct Fired Furnace using gas burners).

Thickness measurements of oxidation layers will allow to draw iron oxidation kinetical laws. The measurements are performed by Secondary Ion Mass Spectrometry for extremely thin oxidation layers (thinner than 50 nm). SEM images of samples' cross-sections allow the measurement of thicker layers and morphological observations of the oxidized layers, the substrate underneath and the interface between them. Iron oxide phases are identified by Raman spectroscopy and X-ray diffraction. An interpretation of these results will be proposed to determine the diffusion mechanisms occurring during thermal oxidation in a low-alloyed steel substrate.

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Carburizability and transformation kinetics of new high silicon steel alloys for nanostructured bainitic surface layer in wind turbines applications

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B1_3 - Investigation in novel processing technologies for special steels - RFCS NanoWinTur and NewAIMS Projects, Andalucía II Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Wind energy is a key enabler of the European Green Deal, offering the most effective means of reducing emissions in the electricity sector. In 2023, Europe set a record by installing 18.3 GW of new wind power capacity. However, this falls short of the pace required to achieve the 2030 climate and energy objectives. To stay on track, Europe must add 260 GW of new wind capacity between 2024 and 2030, requiring an annual installation rate of 33 GW on average.

Wind turbines are becoming progressively larger and taller, with power ratings reaching 5-6 MW for onshore installations and 14-15 MW for offshore systems. As a result, gearbox design faces growing challenges, as larger gears push the limits of traditional case-hardened gear steels. Additionally, the need for lightweight designs is gaining importance to minimize static loads on the tower and nacelle.

Within the project framework of NanoWinTur new gear steels are to be developed for the demanding application in future gear boxes. The talk will address the overall carburisability of six different newly developed case hardening alloys containing high amounts of silicon to achieve carbide free bainite. The carburisability was investigated especially against the background of high silicon content reducing the carbon activity in steels and significantly hampering the carburization. Both gas carburizing and low pressure carburization were tested.

For certain carbon contents the transformation behaviour into martensite and austempering kinetics are investigated in dilatometer. The results of the analyses are presented and discussed.

Quenched and Partitioned Steel for Advanced Engineering Applications: Insights into Microstructure and Properties

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The third-generation advanced high-strength steel, Quenched and partitioned steel (Q&P), is a promising grade for advanced high-performance structural applications. It promotes the production of lighter and stronger parts with improved performance, which minimizes the need for additional reinforcement. Consequently, high energy efficiency, saving of resources and costs during the production processes, and industrial applications can be achieved. This is due to its outstanding mechanical characteristics compared to imitative high-strength steels. Q&P steel is more appropriate for the automotive, aerospace, and construction sectors, where performance and safety are essential. Its continued development and application are crucial to cope with the challenges of a rapidly evolving industrial and environmental requirements.

This article presents a detailed examination of the evolution of quenched and partitioned (Q&P) steel, focusing on processing techniques and their influence on mechanical properties. It displays the impact of processing conditions on the resultant phase transformations and the microstructure, particularly the formation and stabilization of retained austenite. Also, the effect of chemical composition and heat treatment parameters on mechanical characteristics such as strength, ductility, and toughness to optimize its performance for specific applications. The weldability and the change in the structure in the heat-affected zone of this steel will be discussed. This study strives to be a foundational resource for researchers and steel producers to increase their understanding of the microstructure and properties of Q&P steel for advanced engineering applications.

Exploring Different Replacement Rates of Recycled Construction and Demolition Waste in Building Applications

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B10_5, Z1 Room (Level -3), settembre 16, 2025, 10:30 - 13:10

The construction industry faces an urgent need to address the depletion of natural resources and the environmental impact of material extraction. In this context, Construction and Demolition Waste (CDW) emerges as a promising resource, accounting for nearly 40% of the total waste produced annually in Europe. While traditional recycling practices have leveraged CDW for applications such as road base materials, these strategies only address a small fraction of the waste generated, emphasizing the necessity for more comprehensive solutions. Recent studies explored CDW as an aggregate and cement substitute in structural mortars, have shown promising results. In this work, virgin aggregates were replaced with processed CDW in varying proportions (25%, 50%, 75%, and 100%) and using fine CDW powder as a partial Portland cement substitute (5%, 10%, 15%, and 20%). This dual substitution approach not only enhances CDW valorization but also aligns with circular economy principles, reducing dependency on virgin materials and promoting sustainable construction practices. Such innovations are essential for advancing the construction sector's sustainability and reducing its environmental footprint.

After 7 and 28 days, all specimens were tested following the UNI-EN 196-1 standard. The specimens generally exhibited similar or slightly lower performance compared to the control mixture. The improvement in mechanical properties of mortars made with Construction and Demolition Waste (CdW) can be attributed to the porous nature of CdW aggregates, which absorb free water in the mixture, reducing the effective water-to-cement ratio and enhancing mechanical performance. At 28 days, the compressive strength of the CdW mortars was approximately 6% higher than the control mixture. The fine fraction obtained during the sieving process was used as a partial replacement for Portland Cement at 5%, 10%, 15%, and 20% (CdWF). Flexural strength decreased as the fine fraction increased, with a notable 30% reduction at 10% substitution compared to OPC. However, compressive strength remained promising up to a 10% substitution, after which it declined from 50 MPa to around 43 MPa. This loss of more than 10% in compressive strength is expected, as the reduction in cement content directly affects the binding capacity of the mixture, with cement acting as the primary binder.

Surface Quality Analysis of Thermally Treated Wood by Advanced Techniques

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Developing innovative solutions for the thermally surface treatment of wood is a current research topic. In this regard, the flame-charring of wood boards [1,2] represents a good compromise, allowing sufficient protection of the wood surface. The disadvantage of this technique is the low consistency of the process. An alternative option is the use of the contact hot plate method, which shows that the correct application of wood pyrolysis can provide reasonably good effects of wood protection while maintaining sufficient mechanical properties [3,4].

In the presented contribution, an innovative technique utilising arc plasma discharge was investigated. The main motivation for this study is to develop in-depth knowledge and introduce new possibilities that will allow the replacement of the above-mentioned techniques. The structure and roughness of thermally treated wood surfaces were analysed using microscopy techniques. Additionally, the samples were investigated in cross-section to determine and characterise changes in the depth profile. Mechanical properties at the microstructural level were evaluated through nanoindentation, while Fourier-transform infrared spectroscopy was employed to analyse changes in chemical composition after the treatment.

The obtained data provide valuable insights into the structural changes optimising wood conservation and treatment technological processes.

Acknowledgements

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Impact of the interparticle forces in the rheology and particle size of binary blended cements.

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B10_3, Z1 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

The interest of the cement community towards limestone-calcined clay cements (LC³) has increased in recent times because of their lower carbon emissions and suitable hardened properties. However, they also have very high water demands that can be compensated by the use of superplasticizers. These chemical admixtures decrease the initial yield stress of LC³ cements although they still suffered a fast flow loss, whereby the mechanisms remain unknown. This study aims to gain a deeper understanding of the parameters controlling the rheology of LC³ cements. For this purpose, rheological properties, polymer adsorption and evolution of the particle size distribution of binary blends of the main components of LC³ cements, ordinary Portland cement (OPC), limestone (LS) and metakaolin (MK), were investigated. These results together with the zeta potential values of the individual components, in absence and presence of superplasticizers, were used to calculate the interparticle forces in binary blends by using the open access software Hamaker (<http://hamaker.epfl.ch/>).

In absence of superplasticizers, initial particle agglomeration was observed in all studied systems, pure OPC, limestone-blended cements with limestone contents up to 30% and in metakaolin-blended cements with metakaolin contents up to 50%. These results can be explained by the interparticle forces calculation (Hamaker simulation), where very high absolute values of the secondary potential minimum were calculated for all mixes which correlates with strong attractive forces and agglomeration. With time, particle size decreases due to both, particle deagglomeration and OPC dissolution.

When PCE superplasticizer is added to the systems, interparticle forces calculations show a strong repulsive potential barrier up to distances equal to the adsorbed layer thickness of the polymer, which leads to the particle deagglomeration experimentally observed. At initial hydration times, higher dosages of PCE are required to induce particle deagglomeration in OPC-MK systems, with respect to OPC-LS blends. This is attributed to the higher specific surface area of metakaolin particles and thus the higher dosages needed to reach a certain polymer surface coverage. Over time, particle agglomeration is observed which could be related to the formation of hydrates able to also adsorb polymer.

Thermal treatment of beech wood under controlled conditions: Physico-chemical characterisation.

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The long-term durability of wood, especially for outdoor applications, depends significantly on effective surface treatments. Among various preservation techniques, thermal treatment is considered an environmentally sustainable alternative. However, to achieve optimal thermal treatment without weakening the structural integrity remains a major challenge [1][2]. Nowadays, various techniques are available, and e.g. plasma-induced surface carbonisation offers a promising approach leading to surface protection with minimal internal degradation [3].

This work is aimed to investigation of the progressive thermal degradation of wood constituents, providing a detailed baseline for future studies focused on carbonisation of solid wood surfaces. Powdered beech wood (*Fagus sylvatica* L.) was thermally treated in a sealed conditions. This approach allowed to get the control over the pyrolysis process, limiting the ignition and combustion. Based on the thermogravimetric analysis (TGA) results, several temperature values were selected within the range of 110°C to 600°C. The physico-chemical properties of the thermally treated samples were subsequently characterised using advanced analytical techniques, including Fourier-transform infrared spectroscopy (FTIR), ultraviolet-visible spectroscopy (UV-VIS), colorimetry, X-ray diffraction (XRD) and scanning electron microscopy (SEM).

The findings showed that the color change could be used as a reliable indicator of the temperature of applied thermal treatments and, thus, may pinpoint out expected changes in the physico-chemical properties of thermally treated beech-based samples. The knowledge obtained for controlled themally treated samples may find utilization for the complex characterisations of the role of thermal treatments on wood properties and may help in the development of optimised wood preservation techniques that enhance its durability, improve weather resistance, and preserve the structural integrity leading to long term sustainability of wood constructions.

Acknowledgment

This research has been supported by the Czech Science Foundation (GAČR), project No. 24-10430S.

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Scalable Cement-Based Thermoelectric Systems for Sustainable Energy Harvesting in Outdoor Environments

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Thermoelectric (TE) materials offer a promising pathway for converting waste heat into sustainable energy. While conventional TE materials typically exhibit low Seebeck coefficients (<1 mV/K), ionic TE materials achieve higher values but are limited by scalability and cost challenges. Cement-based TE materials emerge as a practical alternative, offering scalability, affordability, and durability. This study explores the potential of engineered cement composites for outdoor photo-thermoelectric energy harvesting. By leveraging cement types arranged to enhance light absorption and temperature gradients, a system of interconnected TE cells demonstrated a Seebeck coefficient exceeding 9 mV/K. Additionally, different strategies were employed to maximize the energy harvesting potential, achieving significant energy output. The intrinsic ability of the cement composite to absorb atmospheric humidity after drying further mitigated issues of evaporation common in ionic TE systems. These findings highlight the feasibility of cement-based TE systems as a scalable and sustainable solution for efficient energy conversion, paving the way for innovative approaches to renewable energy.

Mechanism of Alkali-Activated Cements Retardation by Zinc Addition

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B10_1, Z1 Room (Level -3), septembre 15, 2025, 9:20 - 10:20

The incorporation of zinc into cementitious materials has been explored both for heavy metal stabilization and its retardant properties on initial setting. However, its role in regulating rheological fresh properties and its compatibility with superplasticizers remain unclear. This study aims to review and investigate the mechanism by which Zn influences the properties of fresh alkali-activated cements. The control of its retardant effect in the presence of polymer-based admixtures will allow the monitoring of cement paste workability.

The composition and microstructure of zinc-doped cement paste, and the zinc mechanism of action during the hydration process remain subjects of ongoing debate. The hydration of cement paste during the induction period is a highly complex system involving interconnected reactions that are modified in presence of zinc. The specific impact varies depending on the chemical form of zinc, whether as ions (together with their counter-ions) or oxides. These effects have been predominantly reported for OPC-type materials(1). Several mechanisms of zinc action have been proposed in literature: 1- formation of a metastable coating that impedes ion transport, 2- inhibition of C-S-H nucleation through the precipitation of calcium-zinc hydrates on grain surfaces, 3- pH reduction caused by zinc precipitate formation, and 4- complexation of Zn^{2+} with silanol and aluminol groups on surfaces. For low-Ca-content materials, such as alkali-activated systems like blast furnace slags, the situation is less clear due to interplay of Zn with the activator(2).

This work focuses on the fate of zinc in the presence of other admixtures that also help control the initial rheological properties, such as superplasticizers. The behavior of zinc in activated solutions of various types and pH, both with and without the addition of polymers, has been studied. Various Zn-doped alkali-activated paste preparation protocols were examined, resulting in different zinc precipitate products and corresponding variations in the rheological behavior of fresh paste. These results contribute to a deeper understanding of the zinc action mechanism in alkali-activated materials, depending on the activated solution, as well as the interaction and potential competition between the retardant and superplasticizer effects to control the fresh cement properties.

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Innovative Geopolymer Composite for Buildings Thermoregulation

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The construction industry contributes 40 % of global greenhouse gas emissions (GHGE), of which 80 % is generated during energy consumption for the heating and cooling of buildings. To limit climate change and reduce CO₂ emissions from the construction and building sectors, numerous research teams have concentrated on creating highly energy-efficient and sustainable materials with minimal carbon footprints. Geopolymers have emerged as eco-friendly alternatives to conventional Portland cement, with the aim of reducing manufacturing expenses by repurposing industrial waste. In recent years, thermal energy storage materials (e.g., inorganic salts) have attracted increasing interest because of their ability to absorb and release energy at high and low temperatures. This research seeks to develop novel sustainable thermoregulator building materials using a zero-carbon-emission-composite-based geopolymer. Herein, we present a physicochemical analysis of the behaviour of an innovative geopolymer composite containing Calcium L-lactate (CaL), an organic salt hydrate that enhances the thermochemical energy-storage capacity of the material. CaL was incorporated into the geopolymer matrix at various weight percentages (wt. %), promising new thermochemical material exhibiting good thermal stability (150 °C) and complete hydration-dehydration reversibility cycles. Moreover, owing to the macroporous structure of the composite, which facilitates water vapor flow during the expansion and contraction of the organic salt, the heat storage and release capacities of the composite material were determined to be 301-441 kJ/kg of the composite material. This study provides valuable insights into the development of sustainable and energy-efficient building materials that can contribute to mitigating climate change within the construction sector.

Investigating the micro-structure of calcium carbonate precipitated during bio-cementation of sand

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B10_5, Z1 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Bio-cementation of sand is a new, environmentally friendly process gaining traction for soil reinforcement, material fabrication, and for the preservation of buildings and monuments. This process uses bacterial activity to precipitate calcite (calcium carbonate, CaCO_3) crystals in the sand (quartz, SiO_2) matrix. This calcite acts as a binder between the sand particles. This process can be used as an alternative to other, hazardous materials that are commonly used in construction, such as cement. However, there is still a lack of information on the microstructure of these crystals and how it changes under mechanical load. Understanding this could be crucial for optimizing the process and improving the material's strength.

In this study, two samples were studied using x-ray tomography (CT), 3D X-ray Diffraction (3DXRD) and Dark Field X-ray Microscopy (DFXM) on ID03 at the ESRF. One sample was a single grain covered with calcite crystals. The other was a pair of sand grains bonded by the calcite crystals. For both samples, the orientation maps obtained with 3DXRD for the calcite phase showed a visible texture, indicating a preferential growth orientation of the crystals. Some crystals visible in CT appear as stacks of multiple grains, each with different orientations, resulting in polycrystalline structures. The 3DXRD strain tensor revealed mostly undeformed crystals, with the presence of some hydrostatic strain due to impurities. Using DFXM to 'zoom-in' on Bragg reflections in two different lattice planes, we were able to observe the local misorientation and strain in one individual calcite crystal. The computed mosaicity maps show distinct sub-domains. In particular zones of the grain, the elastic strain was coupled with misorientation, which also shows that the crystals indeed grow in a certain preferential orientation. A comparison of DFXM measurements showed that calcite crystals bridging two sand grains had a relatively 'pristine' microstructure, whereas calcite crystals attached to only one sand grain showed significant strain, indicating that they might have undergone fracture. Furthermore, applying mechanical load was found to significantly alter the calcite microstructure, leading to increased elastic strain in the grains.

In conclusion, we employed a multimodal approach to investigate the microstructure of bio-precipitated calcite in sand, providing insights critical for optimizing bio-cementation processes. Future work will explore calcite growth mechanisms during cementation cycles and the behavior of the calcite grains under shear loading, aiming to enhance material performance for sustainable construction and soil reinforcement.

Machine Learning to Predict the Thermomechanical Properties of Reinforced Polymeric Composites Manufactured with Thermoplastic or Thermosetting Matrices – A Review for Civil Construction Applications

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

This review explores the potential of using machine learning (ML) to predict the thermomechanical properties (TMP) of polymeric composites (RPC's), which are made with reinforced thermoplastic or thermosetting matrices for civil construction applications. The typical ML workflow includes several steps: Data Collection and Preprocessing: Gathering data on TMP of RPC's, covering composition, processing parameters, and environmental conditions. This step also involves preprocessing the data to handle missing values, outliers, and scaling; Feature Selection and Engineering: Identifying relevant features and creating new ones, if needed, to enhance model performance. This may require domain knowledge and statistical techniques to pinpoint key predictors for TMP; Model Selection: Choosing suitable ML models such as regression, neural networks, or decision trees for prediction tasks; Training and Evaluation: Splitting data into training and testing sets to train models and evaluate their performance using metrics like mean squared error, mean absolute error, or R-squared; Hyperparameter Tuning – Optimizing model hyperparameters through grid search or random search techniques; Cross-Validation – Evaluating model generalization and preventing overfitting; Model Interpretation – Analyzing feature importance and relationships between input variables and TMP to derive insights. To support this approach, the authors compiled recent scientific literature, including their own research, primarily focusing on RPC's TMP. It is well established that achieving optimal TMP depends on a proper combination of multiple material families—often two or even three in hybrid materials. These composites exhibit favorable performance under harsh environmental conditions (e.g., saline or corrosive atmospheres) and provide durability and permeability suited to specific applications. However, achieving the ideal material combination is rarely accomplished on the first attempt. Multiple experimental iterations are necessary to refine the formulation, ensuring optimal TMP without significantly compromising individual material properties. Any misalignment in composition adjustments can negatively impact the final desired TMP of the RPC's. In this context, ML serves as a valuable tool to fine-tune material compositions and predict desired TMP, ultimately reducing experimental costs while improving efficiency. By leveraging ML, researchers and manufacturers can streamline the material selection process, enhance performance predictions, and optimize RPC's formulations tailored for various structural applications. This topic is still under development and has emerged to meet the increasingly complex demands of the civil construction sector in the search for new construction materials capable of meeting a variety of applications.

Effect of PCE superplasticizers on the control of the rheology of low clinker cements

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B10_3, Z1 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Understanding the rheological properties of cementitious materials is essential to control their properties in the fresh state and to improve their practical applications. Clinker replacement by supplementary cementitious materials (SCMs) is currently the most feasible strategy to reduce cement and concrete carbon footprint. However, the SCMs availability and their slow reactivity have limited the level of clinker replacement in recent years. Limestone calcined clay cements (LC3) are cements with clinker contents even above 50% which contain widely available SCMs. In general, mortars and concrete prepared with LC3 have suitable hardened properties but rheological properties still need to be improved to facilitate its application onsite, while keeping low water/binder ratios. In this research, the effect of superplasticizers on the rheology of LC3 pastes and mortars have been investigated and compared to zeolite-blended cements. These rheological properties have been also correlated with the polymer adsorption on the cements and its impact on the cement hydration.

The obtained results concluded that, compared to zeolite-blended cement, LC3 cement pastes required a double dosage of superplasticizer to reach a similar initial yield stress, despite the similar clinker replacement of both blended cements (53% clinker substitution) and the similar specific surface area of the zeolite and calcined clay used. In particular, a dosage of 0.4% of PCE superplasticizer was needed to obtain LC3 pastes with an initial yield stress of around 5 Pa, while 0.2% of PCE was needed for zeolite-blended cements. This can be explained by the higher polymer adsorption of PCE measured for LC3 pastes. In contrast, a faster increase of the yield stress over time was observed for the admixed zeolite-containing cements.

Study on the Reinforcement of Eco-Friendly Basalt/Epoxy Composites with Varying CNT/Graphene Content

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Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Basalt fiber is a naturally abundant material distributed worldwide and is increasingly recognized as a next-generation eco-friendly inorganic fiber that can replace conventional organic fibers. Compared to traditional fibers, it exhibits low toxicity to humans, excellent mechanical strength, and outstanding chemical resistance, leading to extensive research on its applications in composite materials.

Previous studies have shown that Basalt/PET composites outperform glass fiber composites in terms of flexural and tensile strength. Additionally, research indicates that the mechanical properties of epoxy composites improve significantly after the surface treatment of multi-walled carbon nanotubes (MWCNTs). These findings suggest that basalt fiber has great potential as a reinforcement material for high-performance composites.

The objective of this study is to enhance the mechanical properties of basalt fiber composites while maintaining their inherent thermal stability and durability. To achieve this, carbon nanotubes (CNTs) and graphene were incorporated to analyze their effects on composite performance. Both CNTs and graphene are advanced materials with a hexagonal carbon lattice structure and sp^2 bonding, known for their lightweight nature and exceptional strength.

In the fabrication process, basalt fiber was mixed with epoxy resin and a curing agent, followed by the addition of CNTs and graphene to ensure uniform dispersion. The mixture was then compression-molded using a hot press to create standardized test specimens. These specimens were subsequently subjected to mechanical tests, including tensile testing and wear resistance evaluation.

Experimental results revealed that the basalt fiber composites containing CNTs and graphene exhibited a 50% increase in flexural strength and a 25% improvement in wear resistance compared to composites without these nanomaterials. This indicates that the addition of CNTs and graphene plays a crucial role in enhancing the mechanical performance and durability of basalt-based composites.

In conclusion, this study highlights the potential of basalt fiber as a sustainable and high-performance composite material for various industrial applications. Given its durability, lightweight nature, and thermal stability, basalt fiber-reinforced composites present a promising alternative for industries requiring advanced materials, with significant potential for future applications.

Recycling of gypsum based binding materials

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B10_5, Z1 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Gypsum is one of the most used building materials. Because of the energy transition a large raw material source, FGD-Gypsum, will be lost. Gypsum is $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$, but to use it as a binding material the better soluble Hemihydrate $\text{CaSO}_4 \cdot 0.5\text{H}_2\text{O}$ or Anhydrite CaSO_4 is produced by heating or in an autoclave process. This subhydrate will react back with water to gypsum. This process is predestined for recycling. It is well known from other recycling processes, like glass, paper or polymers, that the quality may change during the recycling process. The normal raw material for gypsum recycling at the moment is plaster board. That plaster board is not pure gypsum, it contains cardboard, fibres and several organic additives like retarders, super plasticizers, surfactants and some more. The fibres and the cardboard are collected nowadays very accurately, but there is a lack in research for the organic additives.

During the research presented in this paper a stepwise project was done. During the first step, larger self-grown gypsum crystals were recycled by heating up to 140°C to produce hemihydrate and followed by rehydration with water. This process was done for several cycles. As the next step gypsum crystals, produced in presence of single additives, were cycled. This part is more academic to understand the basics. The obvious upcoming step was to use technical gypsum for the recycling process with and without additives. To do that, hemihydrate was hydrated with or without additives and then cycled also at 140°C .

During any recycling step several analyses were done. The morphology of the gypsum was investigated by scanning electron microscopy, the heat of hydration was measured by heat flow calorimetry and the phase composition was examined by simultaneous thermal analysis and x-ray powder diffraction. It is shown, that during the recycling process the particle size of the gypsum particles change. The gypsum crystals become smaller till a limit is reached, hence influencing also the product properties. The other challenge is the remaining of the additives during the cycling, because those additives are changing the morphology of the gypsum crystals and the properties, too. Most of the additives stay inside of the recycling material and can cause side effects in the later use of the recycling materials. As particle size shrinks in recycling, the effect of the additives lowers to a certain extent. Gypsum recycling is possible, but may be tricky.

Simulation-Driven Optimization of Multifunctional Sandwich Panels for Energy-Efficient Buildings

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

In recent years, the building sector has made great progress in developing advanced materials and technologies that enable the practical adoption of near-zero, or even energy-positive, energy/emission buildings. These innovations aim to balance and reduce the energy costs of the building industry through innovative and more efficient materials and components that adapt to the environment [1]. Multifunctional composite sandwich panels have a layered design which has the advantage of being able to couple different materials with specific functions to offer advanced multifunctional features [2]. Moreover, the use of innovative materials, which have a specific thermal response, has been increasing. Among these innovations, Phase Change Materials (PCM) stand out due to their capacity to accumulate energy, and mortars combined with aerogel provides high thermal insulation performance. These advanced materials beyond SOA can be integrated into composite sandwich panels to help providing the desired thermal response.

Given the possibilities offered by multifunctional composite panels in terms of geometry and material design, computer simulation plays a key role in optimizing thicknesses and selecting materials to meet specific requirements. Thus, this work aims to develop and validate simulation models that reproduce the mechanical and thermal behaviour of sandwich panels, optimizing thicknesses based on the thermal and mechanical loads they are subjected to. To experimentally evaluate the performance of the sandwich panels mechanical (compression and 3-point bending) and thermal (static and dynamic) tests in heat flow meter apparatus were carried out. The experimental results were used to calibrate thermal and mechanical Finite Element (FE) models of the composite sandwich panels. Design of Experiments (DoE) approach was applied to generate simulations adopting such models, which were then used to generate metamodels capable of predicting thermal and mechanical responses of the panel under various load cases and thicknesses. Finally, a digital tool, based on these metamodels, was developed, providing a user-friendly application applicable to various façades types and environments. This methodology offers a powerful virtual engineering tool for predicting the behaviour of intelligent multifunctional composite panels.

This research has received funding from the European Union's Horizon 2020 research and innovation programme iclimabuilt, under Grant Agreement No 952886.

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Ceramic 3D printing of constructive systems of façades. Pros and Cons

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Ceramic is a material with a large tradition in Spain due to the abundance of clay materials in most of the Peninsula. This circumstance together with the appropriateness of the material are some of the reasons for its proliferation. In addition, their inorganic nature, strength and chemical resistance made them suitable and justify its durability, in such a way that examples of centuries of history could be found in a perfect state of conservation.

Against their vision as a traditional and obsolescence material, ceramic industry has driven a complete renewal and change of perception in which 3D printing has arisen as an alternative for the implementation of a new image.

Indeed, in the last decades, 3D printing with ceramics had arisen because of its high potential in terms of the versatility in the design of complex shapes without a specific tool, but also, manufacturing 3D printing is aligned with the reduction of waste during the fabrication and the control processes to optimize them.

Taking advantage of this tool, there is still a huge field to research in terms of ceramic compositions, designs not only as a single piece but as part of a constructive systems, especially in façades. Indeed, ceramic printing has a huge potential in the development of constructive systems in new buildings but also for renovation purposes, in which the optimization of the design could be achieved attending to the final properties in terms of appearance but also to control lighting or shadowing, among others. On the contrary, the extrapolation of printing of single parts to the manufacturing of large quantities requires high throughput.

In this paper, a review of the literature regarding the use of this technology for 3D printing on constructive systems of façades is performed attending to their requirements, final performance and difficulties found in the application to large manufacturing processes.

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FUNCTIONALIZED CARBON MATERIALS IN CEMENT BASED COMPOSITES, A MULTIVARIATE APPROACH

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B10_5, Z1 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

This study focuses on optimizing mechanical performance in cement-based composites reinforced with functionalized carbon allotropes: carbon nanotubes (CNTs), graphene nanoplatelets (GNPs), and carbon fibers (CFs). Functionalization was achieved via acid treatment to introduce carboxylic (-COOH) and hydroxyl (-OH) groups, enhancing dispersion and matrix interaction. A face-centered central composite design (FCCD) was employed to vary the amounts of CNTs, GNPs, and CFs, ensuring the total content did not exceed 0.2% by cement weight. The study aimed to determine how these variables influence flexural strength, fracture energy, and compressive strength. Response surface methodology (RSM) was used to analyze the data, identify optimal conditions, and maximize mechanical responses. RSM revealed that fracture energy increased with higher carbon allotrope concentrations, while compressive strength showed more complex behavior. This multivariate approach identified optimal amounts of carbon allotropes for maximizing the responses within the chosen domain. The optimized composite achieved a 27% increase in compressive strength and a 690% increase in fracture energy compared to the reference.

Development of new glass frits for melting via sustainable electrification systems

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

There exists an increasing trend towards glass materials and enamels to create decorative, durable, and highly resistant architectural solutions. Nevertheless, the common processes to produce glass implies high energy consumption and pollution and therefore, environmentally friendly processes with a view on electrification of the glass industry is now pursued.

With an aim to determine the ultimate relationships between the structural characteristic of a glass composition and its electrical characteristics, there have been prepared several glasses with different Zn contents. The structural characteristics of the glasses were studied by spectroscopic techniques which allowed determining the effect of the Zn in the glass matrix in terms of altering the proportion of bonding and non-bonding oxygens. Zn enters in the network as a network former and induced the formation of BO₄ units, as deduced from the increase of the band centered at about 910 cm⁻¹. These results have been correlated with the viscosity of the glasses, their thermal behavior as the electrical conductivity high temperature.

The complete characterization of the glasses will set up the basis for the development of new glass compositions with selected electrical conductivities to be used in newly developed electrified glass melting technologies.

Cement-based sorption thermal energy storage materials for applications in the energy and construction sector

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B10_4, Z1 Room (Level -3), settembre 15, 2025, 17:00 - 19:00

Thermal energy storage is crucial for exploiting sustainable and renewable energy sources by bridging the gap between supply and demand, particularly in the field of buildings, where local availability of low-temperature heat would reduce consumption of fossil resources. The fundamental operating principle of sorption-based thermal energy storage (STES) relies on reversible physical or chemical reactions, respectively absorption or adsorption, to store and release heat.

In literature, STES materials are classified into two main categories. Physically porous sorbents (e.g. zeolites) offer good stability but typically exhibit low energy densities. In contrast, salt hydrates provide higher energy densities but suffer from deliquescence, and bulking, which compromise stability and heat and mass transfer performance. Composite materials incorporate salt hydrates within a porous matrix, mitigating these issues while maintaining satisfactory energy densities.

This study uses an innovative approach to synthesise cost-effective composites by employing cement as a host matrix for various salt hydrates. Cement is chosen for its relatively low cost and wide availability and use in the construction sector. The composites were synthesised via the 'in situ' method by using Portland cement. A sequential learning algorithm is employed for material screening, evaluating 11 salt hydrates, saline solution concentration, water-to-cement ratio, and anti-settling agent concentration. Multiple objective functions are optimised during the screening targeting energy density and economic Key Performance Indicators (e.g. material cost divided by stored kWh).

Following the screening, the most promising composites are analysed in detail, including material characterisation (using SEM and optical imaging), and assessment of heat and mass transfer properties. Thermal conductivity was evaluated by Hot Disk[®] analysis, while adsorption properties, such as kinetics, energy density, isosteric heat of adsorption, and water uptake, were investigated using a water dynamic vapour sorption (DVS) analyser by proUmid.

The synthesised composites matured for 7 days in a glovebox at 100% relative humidity. After maturation, samples were pelletised, sieved (1 mm to 2 mm range), and dehydrated in an oven at 90 °C for 24 hours. Experimental water vapour adsorption isotherms were measured at 20 °C and 40 °C using the DVS analyser. Experimental data are thus fitted using the three-parameter BET equation to derive the isotherms. Finally, Polanyi's potential theory is applied to predict isotherms at additional temperatures, enabling the construction of isosteric curves on a Clapeyron chart, which are essential for defining the thermodynamic cycle and evaluating composites' performance in STES systems with promising applications in the building sector.

Sustainable Concretes Containing Red Mud And Slag: Mechanical Characterisation, Radioactivity and Heavy Metal Leaching

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B10_5, Z1 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

The cement manufacturing for the concrete production accounts for a high percentage of the global CO₂ emissions (6-8%), and therefore in the current climate change scenario it is imperative to enforce mitigation measures to reduce the environmental impact in the construction industry. One of these measures is the partial or total replacement of cement with supplementary cementitious materials (SCM's), such as copper slag (S) and red mud (RM), an industrial by-product of copper manufacturing and an unexplored waste derived from bauxite processing for alumina and aluminium production, respectively. However, these materials are known to have high concentrations of heavy metals, as well as being classified as Naturally Occurring Radioactive Materials (NORM), and as a result of this, their use might represent health and environmental risks. Other materials typically used in the construction sector are granites, which, although they do not have high concentrations of heavy metals, are considered also as NORM due to its high concentration of natural radionuclides. For this reason, research studies besides evaluating the mechanical properties of the produced concretes, should also assess their suitability from a radiological protection point of view and the potential leaching of heavy metals when exposed to different operating conditions.

With that purpose, in this work different concrete mixtures were designed, according to the composition of the cementitious fraction: i) concrete made with 100% of an ordinary Portland Cement (OPC), ii) blended concrete with 70% OPC and 30% RM and, iii) alkaline activated concrete with 70% S and 30% RM. The mixes were prepared in duplicate, using in each case 100% siliceous aggregate (SA) or 100% granitic aggregate (GA). Specimens with dimensions of 15 cm x 7.5 cm were prepared and their compressive strength was characterised at ages of 2 and 28 days, in addition to the radionuclide activity concentration by gamma spectrometry. Finally, leaching tests were performed on concrete samples by varying the following parameters: 1) the samples geometry (bulk and powdered) and 2) the leaching environment (water and acid water). Preliminary results revealed optimum compressive strengths at 28 days ages and a radionuclide content suitable from a radiological protection point of view. The heavy metals concentration released into the environment was compared to the limit values established by the European regulation for inert wastes, showing that the leaching values can be controlled by proper mix design.

Mechanisms involved in the flow evolution in superplasticized limestone-blended cements

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B10_3, Z1 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Limestone is a globally accessible Supplementary Cementitious Material (SCM) widely used to replace clinker and decrease the carbon footprint of cement and concrete. However, clinker replacements above 10% leads to a reduction of the mechanical properties due to the almost “inert” nature of limestone. Superplasticizers play a crucial role to decrease the water demand in limestone-blended concrete to compensate the loss of strength. The rheology of admixed limestone blended cements is complex and controlled by different mechanisms that simultaneously occur. In particular, rheology depends on particle packing, polymer adsorption and cement hydration. The main focus of this research is to understand the flow loss in limestone blended cements (OPC-LS) containing polycarboxylate-ether superplasticizers (PCE) and its correlation with polymer adsorption and the new hydrates formed. The main outcomes have been compared with the flow loss in pure OPC systems. Results concluded that at the same solid volume fraction, OPC pastes required higher dosages of PCE than OPC-LS pastes to reach a similar initial yield stress. This is related to the higher amount of ettringite initial formed in admixed OPC pastes, as measured by 27Al MAS NMR, since ettringite has a high affinity to adsorb polymer. In general, a good correlation between the evolution of the yield stress and hydration kinetics have been observed. The onset of the flow loss occurs at the end of the induction period when the higher increase of the specific surface area due to precipitation of hydration products has been measured. An increase of the charge density of the PCEs leads to greater delays of the onset of the flow loss.

Comparing pastes with the same initial yield stress, a faster flow loss is observed in admixed OPC-LS pastes than in OPC pastes. This can be explained by the lower initial PCE dosages used in OPC-LS blends, leaving less free PCE to adsorb over time onto the new surfaces formed as concluded from the analysis of the organic carbon content of the pore solution.

When PCEs are added a few minutes after mixing the binder and water, lower dosages of polymer are required to reach a certain value of yield stress with respect to when PCE is added directly into the mixing water. This is explained by the adsorption of PCE on ettringite nuclei in direct addition. Furthermore, a faster flow loss is measured in pastes when PCE was added in delayed mode.

CaCl₂/MgCl₂/Silica Gel Sorbent Material for Thermal Energy Storage

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B10_4, Z1 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

This study assessed a novel CaCl₂/MgCl₂/silica gel composite sorbent for low-grade thermal energy storage (TES) application to reduce the scientific and technological gap for promoting sorption TES in building heating applications. Low-temperature dehydration/hydration salt hydrates are widely investigated for TES applications. Nevertheless, the use of pure salts as sorbents presents critical issues, such as deliquescence and agglomeration, which reduce their efficiency over cycling. Recently, CaCl₂ was encapsulated in silica gel to prevent salt spillage during its use caused by the deliquescence. However, the amount of salt that can be embedded in the matrix effectively reducing the deliquescence is still a limiting aspect. To this aim, a mix of CaCl₂/MgCl₂ was investigated in this study. Indeed, although MgCl₂ has a much lower heat storage and sorption capacity than CaCl₂ as a pure salt, it exhibits significantly less deliquescence, which is related to its higher deliquescence relative humidity (DRH%). Indeed, the DRH at 25 °C is 33% for MgCl₂ and 28.5% for CaCl₂. Hence, a synergic effect is expected from their mixture. The CaCl₂/MgCl₂ ratio was investigated between 1:1, 2:1 and 5:1. The salts mixture load into silica gel was fixed to 30% wt. The mixture was impregnated in mesoporous silica gel spheres and assessed structurally, morphologically, and thermochemically. Remarkably, the 1:1 CaCl₂/MgCl₂ mixture exhibited a significantly reduced deliquescence phenomenon without a sensible reduction in heat storage and sorption capacities. Furthermore, the TES potential of these composites was assessed under conditions relevant to residential buildings, and the sorption/desorption kinetic was investigated using the Thermal Large Temperature Jump (T-LTJ) method. This method measures the temperature difference at the inlet and outlet of the adsorber due to a sudden inlet temperature drop or jump, triggering the sorption or desorption step, respectively. The 1:1 CaCl₂/MgCl₂- silica gel composite was tested under the boundary conditions of real adsorption storage cycles. Specifically, two different evaporation temperatures were considered for the sorption, namely 10 and 15 °C. The investigated temperature drops are 85 → 35 °C, and 74 → 32 °C. The results highlight that the 1:1 CaCl₂/MgCl₂ mixture exhibits a high specific heat storage/release capacity (~850 kJ/kg) with fast sorption/desorption kinetics. To conclude, the approach of mixing two salts with different DRH effectively limits the deliquescence issues without sacrificing the heat storage capacity promoting its potential use in sorption-based thermal energy storage (TES) for building heating applications.

Fresh and hardened properties of concrete formulated with enforced carbonated recycled aggregates

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In agreement with the objectives of the European Green Deal, concrete and cement sector aims at reaching zero emissions by 2050 by applying different technologies including carbon capture, utilization and storage. The present research is focused on quantifying the effects of enforced carbonation of recycled concrete aggregates on the rheology and hardened properties of concrete with the final aim at maximizing the level of natural aggregates by recycled one without affecting the technological properties of the material. For this purpose, recycled concrete aggregates of different size ranges were initially characterised and afterwards enforced carbonated by direct injection of 20% CO₂, using different carbonation times and relative humidity.

Concrete specimens were prepared by maintaining the w/c ratio and searching for and target slump. Properties of new concrete in the fresh and hardened state were evaluated using replacements of natural aggregates by recycled aggregates (carbonated and non-carbonated) in the range between 0 and 75%.

The results of this preliminary study established that the ideal exposure time to enforced carbonation of the aggregates was 6 h, and RH was optimized to maximize carbonation. Carbonation treatment improved the rheological properties of the concrete containing recycled aggregates. Different replacements of uncarbonated and carbonated recycled concrete aggregates showed promising results at fresh concrete properties and 7 days compressive strengths

Competitive low-carbon cements prepared with low-grade kaolinitic clays as SCMs: enhancing strength through C-S-H gel nucleation seeding

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In this study, we expand the potential of LC3-50 binders (52 wt% Portland cement (PC-52.5), 30 wt% calcined clay, 15 wt% limestone and 3 wt% gypsum) by using low-grade kaolinite clays and C-S-H gel nucleation seeding. Different commercially available kaolinite clays, each containing approximately 20 wt% kaolinite, were initially characterised. After thermal activation and milling ($D_{v,50}=11 \pm 2 \mu\text{m}$), the R3-test (ASTM C1897-20) confirmed that their low pozzolanic reactivity was characteristic of this type of clay, as indicated by heat flow values of approximately 200 J/g SCM.

The pozzolanic reactivity and the effect of seeding were evaluated in LC3-50 (water-to-cement ratio, w/c, of 0.4) pastes through calorimetry, Rietveld Quantitative Phase Analysis (RQPA), thermal analysis, and porosimetry, as well as in mortars through mechanical strength tests. While LC3 mortars exhibited relatively low compressive strengths, particularly at one day, seeding significantly enhanced the early-age strength (>60%), reaching values of up to 20 MPa. Although the strength gains from seeding at 28 days were less pronounced, they remained significant (>10%), achieving mortars with compressive values up to 57 MPa. Consequently, after one day, LC3-50 mortars exhibit higher environmental performance (EP) values compared to plain PC52.5. However, as hydration time progresses, EP values reduce significantly due to the corresponding increase in compressive strength for the same level of CO₂ emissions. Additionally, a competitive LC3-50 concrete was developed using seeding and a w/c=0.5, achieving compressive strengths of approximately 20 MPa at one day and 40 MPa at 28 days. The quantitative analysis of the pastes provided deeper insights into the pozzolanic reactions and the role of C-S-H seeding. Further details will be provided and discussed at the congress.

Unveiling the Link: Correlation Between R3 Test Results and Compressive Strength in Five SCM Families

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B10_3, Z1 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Incorporating locally available supplementary cementitious materials (SCMs) into cement blends is essential for reducing the building materials industry environmental footprint. The pozzolanic activity of SCMs is typically assessed using two standardized methods: ASTM C1897 (R³ test, which measures continuous heat release at 40°C) and ASTM C311 (Strength Activity Index, SAI, evaluated at 20°C after 28 days). However, previous studies have reported weak correlations between these two approaches. To address this inconsistency, this study examines the elemental composition, mineralogy, texture, and pozzolanic behavior of 22 different SCMs.

While the ASTM C1897 procedure was followed precisely, the ASTM C311 methodology was modified in two key ways: (1) maintaining a constant water-to-binder ratio and (2) introducing an additional mix alongside the conventional 80% Portland cement (PC) and 20% SCM blend. This new formulation—comprising 68% PC, 20% SCM, 10% limestone, and 2% gypsum—was designed to minimize filler effects and better reflect real-world applications.

Results aligned with known pozzolanic kinetics, revealing a general trend: kaolinite-rich calcined clays $\gtrsim$ silica fume > smectite-rich calcined clays > natural pozzolans $\gtrsim$ class-F fly ashes. In the standard 80/20 series, the SAI at 20°C after 28 days (SAI_{20°C_{28d}}) exhibited two distinct correlation patterns with heat release at 40°C after 12 hours (Heat_{40°C_{0.5d}}), separating kaolinitic calcined clays from other pozzolans. Conversely, in the 68/20/10/2 series, correlations were notably stronger, as the influence of filler materials was reduced. The SAI_{20°C_{28d}} demonstrated a robust relationship with Heat_{40°C_{3d}}, forming two well-defined clusters indicative of broader material behavior.

These findings suggest that the modified mix design provides a more reliable basis for SAI evaluation. Furthermore, additional insights into pozzolanic kinetics and SCM performance contribute to a deeper understanding of their role in sustainable construction.

Carbon-negative concrete by using biochar

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B10_5, Z1 Room (Level -3), settembre 16, 2025, 10:30 - 13:10

Biochar is a carbon-containing material obtained as the solid residuum of the pyrolysis of vegetable feedstocks. Its current main interest resides in the fact that it fixes carbon coming from the atmosphere in solid form. Thus biochar can help to compensate the carbon emitted during the cement and concrete production and transport. Biochar is typically obtained by pyrolysis between 200 and 1000 °C, and the main vegetal sources are wood, food, and agricultural wastes, with a particular interest in silica-rich ones (i.e. from rice). Biochar contains mainly carbon, and present high specific surface area. If carbonization is not complete, oxygen, nitrogen, and hydrogen are still found in biochar, together with Ca, Mg, Si, Al, Fe, Na, K, depending on the vegetal feedstock.

In this work we report the preparation of mortar and concrete containing biochar, where the amount of biochar was selected in order to reach first zero-carbon and then carbon negative conditions. In literature it is known that the addition of biochar can lower the mechanical strength of mortar and concrete, save in the case of silica-rich biochar. In this work, however, by conveniently choosing the vegetal feedstock and thus the properties of biochar, and by suitably selecting the biochar grain size distribution, the mechanical properties were not reduced, even at rather high biochar content. Thus, we could prepare carbon neutral or carbon negative mortar and concrete, with the same or higher compression strength than reference samples. The addition of biochar, however, caused the worsening of the workability of the mortar/concrete paste, so that a superplasticizer additive was added. The lower workability was due to the adsorption of water by the biochar, as shown by water adsorption isotherms. Biochar seemed also to retard the mortar setting. The main parameters influencing mortar strength were deemed to be porosity, water absorption, chemical composition, and powder size distribution of the biochar. Porosity measurement performed on mortar samples containing biochar helped to elucidate the mechanism governing the development of significant mechanical properties, notwithstanding the biochar insertion inside the mortar/concrete.

The calculated emissions of standard concrete were 0.33 tCO₂/m³. With 10%wt substitution of cement and 5%wt substitution of aggregate it was possible to obtain a carbon neutral concrete (-0.08 tCO₂/m³) with slightly improved compressive strength with respect to the reference, while with 10%wt substitution of both cement and aggregate the concrete was carbon negative (-0.35 tCO₂/m³), with comparable strength.

Alginate biopolymers for sorption technologies in building and industrial applications

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B10_4, Z1 Room (Level -3), settembre 15, 2025, 17:00 - 19:00

The water affinity of adsorbent materials can be exploited for many building and industrial applications: air humidification, water desalination, atmospheric water harvesting, industrial chilling, thermal storage (L. Lavagna et al, 2020). Recently, biopolymeric hydrogels have been studied as an option for such applications requiring adsorbent materials: compared to other common sorbents such as zeolites and silica gels, calcium-alginate (CaAlg) hydrogels show higher water uptake capacity and faster sorption kinetics, and their properties can be controlled by varying the material composition (V. Gentile et al, 2024). By properly adjusting the manufacturing process, CaAlg can be integrated within structural host matrixes, e.g. cements or plasters (V. Gentile et al, 2023), significantly increasing their moisture buffering value (MBV). This research aims at understanding whether CaAlg remains a suitable option when repetitively cycled in a real industrial sorption machine, at various temperatures and in more severe stressing conditions, such as under non-environmental pressure.

In this study, 700 grams of CaAlg are produced and tested in an industrial prototype for water desalination, to investigate the water uptake performance and stability of the material over time. The sorbent undergoes a cycle consisting of an adsorption followed by a desorption multiple times, while the desorbed water is condensed in a dedicated tank. After 0, 20, 30 and 40 cycles, a sample of material is removed from the machine and tested in a gravimetric machine to evaluate the uptake performance.

The first results show a significant amount of water processed per unit of time in the prototype. With an adsorption at 35°C for 45 minutes and a desorption at 70°C for 45 minutes, the prototype filled with CaAlg was able to condense ~126 mL/cycle (meaning a clean water production of 120 mL per hour and per kg of dry material), compared to the ~56 mL/cycle condensed under the same test conditions and with the same machine previously filled with 700 g of a common Silica Gel. The adsorption curves derived with the gravimetric machine on the material after 0, 20, 30 and 40 cycles do not show significant differences: the uptake capacity and kinetics after cycling the material are comparable to the ones of the non-cycled material.

Given the shown performance, integrating CaAlg in structural matrixes in place of other common sorbents may indeed be considered as an option: such a choice would reduce the size of an adsorption-based solution, decreasing production costs and design complexity.

Integrating AI and Image Processing for Microstructural Analysis and Strength Forecasting in Cement-Based Materials

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The development of high-performance cementitious materials relies on accurately predicting mechanical properties and understanding their microstructural composition. This study employs two distinct yet complementary approaches: Computer Vision (CV) to analyze cement microstructure from Scanning Electron Microscopy (SEM) images, and machine learning (ML) to predict compressive strength. In the ML framework, various predictive models, including polynomial regression, Support Vector Machines (SVM), random forests, and neural networks, are trained on a dataset where input features characterizing the material composition and elaboration conditions are used. Here, the target variable is the compressive strength. A comparative analysis of the model's output is done. In parallel, we explore several techniques of deep clustering to segment cement SEM images at different stages. A Convolutional Neural Network (CNN)-based approach is proposed to analyze these images, identifying and segmenting cement phases such as clinkers, hydrates and pores. This automated microstructural characterization enables a deeper understanding of phase distributions, which can further support material optimization. By integrating data-driven strength prediction with AI-powered microstructural analysis, this research provides a scalable, cost-effective framework for cement design and optimization. The results highlight the potential of machine learning and computer vision in accelerating material science research and enhancing the performance of cementitious materials. This study is conducted as part of the MatCHMaker project.

Experimental analysis and optimization of sorption thermal energy storage systems

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B10_4, Z1 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Thermal energy storage (TES) systems based on sorption materials enable long-term energy storage, promoting the use of renewable energy for building air conditioning. This technology can therefore contribute to the decarbonization of the sector and the achievement of carbon neutrality by 2050. To widespread this technology, the sorption materials used must be low-cost, exhibit high adsorption capacity, and ensure safety and long-term stability.

Research focuses on thermal energy storage systems based on innovative sorption materials, including cement-based and mesoporous silica gel impregnated with salts. Through a detailed experimental analysis supported by numerical simulations, the study highlights the advantages of the proposed technology and its potential applications in HVAC systems. In particular, system performance is experimentally analyzed under operating conditions representative of real use, and the results are used to assess the benefits at the building scale.

Microstructural Analysis of Fractures in Cementitious Materials: From the Matrix to the Concrete Scale

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The mechanical behavior of cementitious materials is directly related to their microstructure and the fracture mechanisms that develop under load. This study conducts a detailed microscopic analysis of fracture surfaces in specimens of cementitious matrix, mortar, and concrete using high-resolution optical microscopy and trinocular microscopy.

The primary objective is to characterize fracture patterns and assess the impact of partially replacing Portland cement with wind turbine waste (RAG) and oxy-combustion ashes (OXI). Phenomena such as the formation of interfacial cracks in the paste-aggregate transition zone, the propagation of microcracks within the matrix, and the morphology of hydration products were identified.

The obtained images reveal significant differences between the studied materials. In the cementitious matrix, dispersed microcracks with intragranular propagation predominate. In mortar, an increase in interfacial porosity is observed, affecting the cohesion between the aggregates and the cementitious matrix. In concrete, fractures tend to be more tortuous, with energy absorption zones and plastic deformation areas suggesting optimized mechanical behavior.

The results confirm that incorporating waste materials influences the adhesion between the cementitious paste and the aggregates, modifying fracture energy and material ductility. It is concluded that microstructural analysis is essential to understand the relationship between material composition and mechanical performance, allowing for the design of stronger and more sustainable cementitious materials.

Preliminary Research on the Incorporation of Wind Turbine Blades Wastes into Clay Materials

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The increasing demand for renewable energy has led to the widespread use of wind turbines, resulting in significant quantities of waste materials, particularly from the sanding and finishing processes of turbine blades, thus promoting sustainable practices in the wind energy and ceramics industries. This study investigates the potential of using sanding dust from wind turbine blades as an additive in the formulation of clay ceramics, specifically focusing on its incorporation into kaolin and clays from the Zamora area. Green densities were determined, the sinterability curves of new materials were plotted, the evolution of porosity was analyzed, and the phases present were characterized using X-ray Diffraction (XRD) for a composition with 30% sanding dust addition. The sanding dust, primarily composed of epoxy resins, fiberglass, and to a lesser extent balsa wood, presents unique challenges and opportunities when integrated into clay matrices. Preliminary results indicate that the addition of sanding dust significantly influences the plasticity, shrinkage, and behavior during the firing of clay mixtures. Samples with a 30% addition show greater shrinkage than the base materials, and some temperatures exhibit a certain conical deformation. Regarding the optimal sintering temperature, there are hardly any variations compared to the base materials, although density decreases due to the incorporation of lower density materials like fiberglass. This preliminary study demonstrates the feasibility of using sanding dust from wind turbine blades in conjunction with clay ceramics, creating a new composite material.

Kinetic feature in Calcium Chloride-Impregnated Mesoporous Silica Gel Composites for Thermochemical Energy Storage

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B10_4, Z1 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

The development of advanced materials for efficient energy storage is essential for supporting the transition to renewable energy sources. This study investigates the adsorption and desorption kinetics of composite materials made from mesoporous silica gel impregnated with calcium chloride (CaCl_2). The first part of the study focused on determining the optimal salt content to balance storage capacity with the material's chemical-physical stability, specifically addressing issues related to swelling and deliquescence. Characterization tests, including TG/DSC analysis and thermogravimetric measurements, were conducted to assess the material's maximum water uptake and heat storage capacity. The results indicated that a 25 wt.% calcium chloride content provided the best compromise, improving the material's stability and performance. The maximum value of water uptake (41.60 wt.%) and heat flow ($1199.10 \pm 59.95 \text{ J/g}$) were evaluated in a range of temperature comprises between 120°C and 25°C with a scan rate of 5°C/min under a isobaric condition (17 mbar).

Then, the kinetic properties of the composite material were evaluated using a Large Temperature Jump (LTJ) apparatus during both adsorption and desorption processes under varying boundary conditions. LTJ experiments were conducted using a heat exchanger with dimensions of $120 \times 80 \times 22 \text{ mm}$ and a fin pitch of 4.6 mm, filled with pure microporous silica gel, the composite sorbent, or a 50/50 in weight mixture of silica gel and composite sorbent. The boundary conditions tested were $P_{\text{ev}}/\text{cond}$ values of 12.3 mbar and 23.4 mbar, with an adsorption/desorption temperature set to 30°C . The high temperature source was fixed in the range between 50°C and 80°C .

The results showed that the composite material exhibited enhanced water adsorption performance compared to pure microporous silica gel, while the hybrid mixture displayed intermediate behaviour. Additionally, the heat exchanger filled with the composite/microporous silica gel mixture demonstrated slower adsorption/desorption kinetics compared to exchangers filled with single materials. This comparative approach allowed for a thorough analysis of how the composition of the sorption material affects kinetic parameters, such as the mechanisms governing adsorption/desorption and heat transfer between grains of the same or different sorbent materials.

In conclusion, the findings of this study will enable the optimization of composite materials for large-scale thermal energy storage systems, improving their efficiency and performance.

Machine Learning and High-Throughput Experimentation in Sustainable Infrastructural Materials Research

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B10_2, Z1 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Innovation in materials science has long been a catalyst for technological advancement. Historically, these advancements relied on costly and time-consuming trial-and-error experimentation. Depending on traditional development protocols and legacy laboratory technologies often introduces complexity and unpredictability, as these approaches often demand the screening of millions of candidates, incurring substantial costs and requiring extended timeframes. However, recent advances in computational screening, industrial automation, and artificial intelligence (AI) have transformed this landscape. By integrating machine learning (ML) and deep learning (DL) with high-throughput experimentation (HTE), AI-driven platforms are revolutionising polymer discovery—predicting properties, optimising formulations, and generating novel structures with unprecedented efficiency.

This project aims to develop a novel, reduced-temperature mastic asphalt for infrastructural applications, addressing the energy-intensive and often toxic nature of traditional asphalt. By leveraging AI-informed data analytics, molecular dynamics (MD) simulations, density functional theory (DFT), and quantum chemistry models, researchers can accelerate the identification of sustainable materials in parallel with the optimisation of mechanical, electrical, and thermal properties. Previous efforts have shown progress in reducing application temperatures, but further innovation is needed to minimise the embodied energy of the installed technology.

By combining AI-driven predictive modelling, object-based material synthesis, and real-time optimisation, this research seeks to redefine the future of mastic asphalt. The project not only advances sustainable infrastructure but also exemplifies how AI and advanced synthetics can transform materials science—reducing development time, costs, and environmental impact while pioneering next-generation polymer systems for the pavement industry.

Advancements and open challenges in sorption-based thermal energy storage for industrial and building applications: The LOBSTER project perspective

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B10_4, Z1 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Thermal energy storage (TES) is a pivotal technology for mitigating the temporal mismatch between renewable energy supply and energy demand across both building and industrial sectors. Building heating and cooling account for a significant portion of global energy consumption, while industrial processes similarly demand efficient thermal management. Among the various TES technologies, sorption-based systems offer promising advantages by utilizing adsorption or absorption processes to store and release latent heat effectively, enabling long-term thermal energy retention with minimal losses.

In this presentation, we will provide a comprehensive overview of the state-of-the-art in sorption-based TES, highlight the open challenges that impede its broader adoption, and outline the advancements achieved within the LOBSTER project. Although the project primarily focuses on enhancing energy performance in nearly zero energy buildings, its innovations have implications for industrial applications as well, particularly in processes requiring low-temperature heat recovery and loss-free long-duration storage.

The LOBSTER project is a multidisciplinary research initiative that bridges expertise in thermal engineering, multi-scale material simulations, building physics, and material science to develop advanced sorption-based TES solutions. Our work focuses on optimizing two principal TES configurations. Closed systems, which employ evacuated tanks and optimized heat exchangers, are designed to achieve high energy density with minimal external influence, offering stable performance independent of ambient conditions. In contrast, open systems present a more straightforward and scalable technological approach, but their effectiveness is inherently tied to ambient air properties such as humidity and temperature, necessitating optimized sorbent materials.

A key aspect of the project is the development of multi-scale models and the systematic optimization of composite sorbents, enabling the selection of materials with tailored thermophysical properties for seasonal TES applications. Complementing this digital toolset, we have established innovative in-house synthesis protocols—including wet-impregnation of salt solutions into porous matrices and one-pot synthesis methods—to produce novel composite sorption materials. These materials are engineered to overcome existing limitations in storage capacity, cyclic stability, and degradation, while addressing key concerns such as cost, toxicity, and corrosiveness.

Beyond material and system development, the project integrates a techno-economic assessment to evaluate the scalability, market potential, and overall sustainability of these TES technologies. Thanks to the advanced material engineering and system-level optimization, LOBSTER contributes to the transition toward more efficient, renewable-based thermal energy solutions for both the building and industrial sectors.

Recycling of oil bleaching earths and mine tailings as a precursors in alkaline one-part cements activated with a sodium silicate based on spent diatomaceous earth residues.

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B10_1, Z1 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

The search for sustainable cementitious materials has driven the development of alkali-activated cements (AACs) using industrial by-products. This study explores the valorization potential of spent bleaching earth (SBE) from the oil refining industry as a precursor for one-part AACs. An alternative sodium silicate, derived from the thermal treatment of NaOH and spent diatomaceous earth (a by-product of the brewing industry), is employed as the activator.

The use of alternative sodium silicate derived from waste materials offers several advantages over commercial sodium silicate. Firstly, it significantly reduces the environmental impact associated with conventional sodium silicate production, which involves energy-intensive processes and the consumption of natural resources such as silica sand and sodium carbonate. Secondly, it promotes industrial waste valorization, fostering a circular economy and reducing landfill disposal. Moreover, by utilizing alternative feedstocks and less energy-intensive processes, this approach presents a more cost-effective and sustainable solution for AAC production.

The study first examines the influence of the Na₂O content in the alternative activator on the activation of SBE, assessing the technological properties of the resulting cements. Subsequently, the effect of partially substituting SBE with mine tailings is investigated to optimize the cementitious system's composition and enhance its mechanical performance.

Results indicate that the Na₂O content in the activator significantly influences the technological properties of AACs based on SBE. Furthermore, the partial incorporation of mine tailings enhances the mechanical properties of the final product. These findings provide a deeper understanding of the potential of these industrial by-products as raw materials for alternative cement production, contributing to waste valorization and the development of materials with a lower environmental footprint.

This research aligns with the principles of the circular economy and green transition by offering a viable and sustainable alternative to conventional cements, advancing the use of industrial by-products in the construction sector.

Incorporation of Mine Tailings into diverse industrial waste for the production of Alkali-Activated Cements in Sustainable Construction

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The sustainable utilization of industrial waste in construction materials is essential for reducing environmental impact and promoting circular economy principles. Alkali-activated cements (AACs) have emerged as a viable alternative to conventional binders, enabling the valorization of industrial by-products while minimizing the consumption of natural resources. This study evaluates the effect of mine tailings (MT) as precursor in AACs formulated with various industrial residues, including Aldebarán bottom ash (CFA), construction and demolition waste (CDW), and bleaching earth waste from the oil industry (TDCoosur). The primary objective is to assess the impact of MT incorporation on the mechanical performance of AACs and identify optimal precursor-activator combinations to enhance compressive strength.

Two types of activators were employed: a commercial activator and an alternative activator, the latter synthesized through the thermal treatment of NaOH and spent diatomaceous earth, a by-product of the brewing industry. Cementitious mixtures were prepared by incorporating 10% and 40% MT by weight into the selected precursors, and compressive strength tests were conducted to evaluate mechanical properties.

The results indicate that the incorporation of 40% MT into CDW, activated with the alternative activator, led to the highest compressive strength improvement, demonstrating the synergistic interaction between these materials. Similarly, the addition of 10% MT to TDCoosur using the alternative activator resulted in even greater compressive strength values, highlighting its potential as a precursor. Conversely, when 10% or 40% MT was added to CFA with the alternative activator, a decline in compressive strength was observed, suggesting a less favorable interaction under the tested conditions.

These findings underscore the potential of mine tailings and industrial waste as sustainable raw materials for AAC production, provided that the appropriate precursor-activator pairings are selected. The study highlights the importance of optimizing AAC formulations to enhance mechanical performance and expand the applicability of waste-derived binders in sustainable construction. Further research should focus on long-term durability assessments and microstructural analyses to deepen the understanding of these alternative cementitious systems.

Synthetic precursors as efficient SCMs

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B10_1, Z1 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

Synthetic precursors as efficient SCMs

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Abstract

In this work, the feasibility of synthesizing materials with excellent pozzolanic properties has been studied. Different precursors with a composition like a type C fly ash, have been synthesized. More specifically, the reactivity of the precursors has been analyzed by studying the influence of the incorporation of several fluxing agents to the raw meals, as well as by changing the synthesis temperature (1000 and 1250°C). The precursors manufactured have been characterized by XRD and ²⁹Si and ²⁷Al MAS NMR. The reactivity of the different precursors has been checked according to the R3 test and the saturated lime dissolution test. Two precursors have been selected to produce hybrid alkaline cements (HAC), also known as Ultra-Low Clinker Cements (clinker < 30%). The mechanical strengths were determined. Characterization of the reaction products (by XRD, TG, NMR and BSEM) revealed the formation of a (N)-C-A-S-H gel responsible for the good mechanical behavior of the cements. Precipitation of portlandite, calcite and ettringite as secondary hydration products was observed.

Valorization of phosphate mining waste: Dolomite sand application in durable self-compacting mortar systems

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Phosphate mining operations generate vast quantities of mixed-type by-products that accumulate and deposit on mine surfaces without proper management, creating severe environmental concerns. Simultaneously, the construction industry faces sustainability challenges due to extensive extraction of virgin materials and diminishing natural resources. This research investigates the durability properties of self-compacting mortar (SCM) incorporating dolomite, a phosphate mining by-product, as a replacement for natural sand at 0%, 50%, and 100% substitution levels.

Durability was assessed through acoustic and thermal property measurements, capillary water absorption, shrinkage, and alkali-aggregate reaction tests. The alkali-carbonate reaction of dolomite aggregates was specifically investigated by subjecting samples to tetramethylammonium hydroxide (TMAH). Resistance to aggressive environments was evaluated by immersing specimens in 5% HCl and H₂SO₄ solutions, with residual mass loss and compressive strength monitored at 7, 28, 56, and 90 days of acid exposure. Microstructural analysis of acid attack mechanisms employed XRD and SEM techniques.

Results demonstrate that dolomite-based SCM exhibits enhanced performance with lower thermal conductivity, reduced capillary water uptake, and decreased shrinkage, with no evidence of alkali-aggregate reaction in either mortar type. The minimal amount of brucite produced further confirms that dolomite aggregates are non-reactive. Notably, in acidic environments, conventional mortar lost 26.2% and 46% of mass in HCl and H₂SO₄ respectively, with corresponding compressive strength reductions of 97.3% and 86.6%. In contrast, dolomite-based mortar lost only 8.7% and 10.9% of mass, with strength reductions of just 31.5% and 41.3%. These findings indicate that dolomite from phosphate by-products represents a promising sustainable alternative for durable construction materials.

Acknowledgements:

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Titanium matrix composites produced by Electro-Sinter Forging

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B2_6, U2 Room (Level 0), septembre 16, 2025, 14:30 - 16:30

Electro-sinter-forging (ESF) is a novel ultrafast field-assisted sintering process developed by EPOS Technologies SA that combines the dual application of a mechanical pulse and an electromagnetic pulse to drive densification. This technology ensures a sintering at full density, in a sample obtained in a few seconds, and is highly suited for the production of unique metal matrix composite structures.

We explore in this work the production of titanium matrix composites using ESF process capabilities. This comprises the design and production of new materials, the in-depth study of their microstructural development, and their characterization for mechanical behaviour. General goals of the project are to design novel, high-performance titanium metal matrix composites for structural applications, and to contribute to our understanding of the links between composition and process parameters on one hand, and resulting microstructures and mechanical properties on the other hand, of metal matrix composite materials produced by the electro-sinter-forging process. This presentation will focus on in-situ Ti/TiC composites and their mechanical properties including their tensile behavior and elastic properties.

Microstructural Investigation of β - and π -type Fe-rich phases in Al-Si cast alloys

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B2_3, U2 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

Primary-based A356 casting alloys with increased transition metal concentrations were produced to represent the use of increased amounts of scrap in primary-based alloys, as this production approach requires higher Fe and Cu contents to maximize the proportion of scrap types that can be used. This leads, inter alia, to a pronounced phase proportion of Fe-rich phases, which are often also referred to as AlFeSi phases. These phases usually have a detrimental effect on the mechanical properties due to their undesirable platelet-shaped morphology.

The fabricated alloys were analyzed in the as-cast and annealed state using scanning electron microscopy methods (EBSD, EDS) to determine the transformation of Mg- and Fe-rich π -type phases to Fe-rich β -type phases during annealing. The shape change of the phases during this transformation and the crystallographic properties are described, supported by thermodynamic calculations using Thermo-Calc Software package.

The major finding was the shape change of AlFeSi phases caused by a π - to β -phase transformation during annealing. This results in the formation of a more rounded AlFeSi phase morphology revealing a potential method to cover for the detrimental effect of transition elements regarding mechanical properties in recycling-based materials.

A new Al-Si casting alloy with high elastic modulus

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B2_3, U2 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

Elastic modulus, a.k.a. Young's modulus is a measure of the stiffness or rigidity of a solid material, determined by the interatomic bonds. Pure aluminium has an elastic modulus in the reign of ~ 70 GPa and there have been extensive attempts to increase the modulus of aluminium alloys by introducing either ceramic particles or intermetallic phases having relatively higher elastic modulus than that of the aluminium matrix. We have recently developed new Al-Si based casting alloys with high elastic modulus in the range of 90-100 GPa and low density less than 3.0 g/cm³, by alloy design and microstructural refinement approaches. Based on the preliminary study of alloying elements on the elastic modulus, microstructure and castability, we have selected new candidate alloys, hypereutectic Al-Si alloys with Ni additions, where large volume fractions (~ 40 vol.%) of hard primary Si and primary Al₃Ni phases were present. However, coarse primary Si and primary Al₃Ni formed upon solidification can interfere with the melt flow, reducing the castability and also were deleterious to elongation. By the assessments of the crystallographic misfit between a nucleant substrate and a nucleated solid, therefore, we discovered modifying elements to refine such coarse and brittle primary phases, particularly Al₃Ni. More importantly, along with the improved elastic modulus, an elongation of about 1% was achieved alongside advantageous yield strength of over 230MPa. Candidate application fields where the new high modulus aluminium casting alloys can be utilised are also suggested.

Simulation of the Extrusion of high purity aluminum wires

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Aluminum wires play a crucial role in nearly all power and control electronics. Being used to connect different materials, aluminum wires are not just subject to high electrical energies but also thermal and mechanical stresses. To enhance the efficiency of named aluminum wires and simultaneously reduce costs in production, new materials and production technologies are investigated by a project at Hochschule Bonn-Rhein-Sieg in cooperation with an industrial partner. As a material, ultra-high purity aluminum is investigated due to its high electrical conductivity. As one part of the manufacturing process, hot extrusion of cast material is investigated. Through hot extrusion, semi-finished products are generated, which will be pulled to the final wire in a later manufacturing step.

To gain deeper insights into the extrusion of aluminum wires, simulations are performed with the software Inspire Extrude Metal. For these simulations, the knowledge of the temperature- and strain-rate-dependent flow stress is of great importance. A suitable constitutive model is fitted to describe the flow stress as a function of temperature and strain rate. Due to a lack of literature data on the investigated material, high-temperature tensile tests are performed at different strain rates and temperatures ranging from 20 degrees Celsius to 500 degrees Celsius.

With the data on flow stress obtained from the performed tensile tests and other thermomechanical properties gained from the software JMatPro, the simulation and optimization of the extrusion process of the aluminum wires are performed. The influence of the process temperature, the extrusion speed, and the wire thickness on the extrusion process are investigated with the aid of simulation in virtual experiments. The results of the research and simulations carried out by this paper can help the industrial partner understand and optimize the real-world manufacturing process.

Acknowledgment

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Effect of Zn content on tensile properties and fracture toughness in Al-Zn-Mg-Cu alloy

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B2_2, U2 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

To investigate the effect of zinc (Zn) content on the yield strength and fracture toughness of high-strength Al-Zn-Mg-Cu alloys, systematic investigation was conducted using three alloys with Zn contents increasing. The yield strength increased from approximately 500 MPa to 600 MPa as the Zn content increased from 5.6 to 7.8 wt.%. However, the fracture toughness decreased from 28.1 MPa√m to 23.0 MPa√m with the same increase in Zn content.

Optical microscopy observations showed that the fraction of secondary phases was similar across the three alloys. Microstructural analysis performed using EBSD revealed that the grain size, recrystallization fraction, and texture were also comparable among the alloys. Furthermore, XRD analysis of dislocation density indicated that the three alloys had a similar dislocation density of approximately $3.8 \times 10^{14} \text{ m}^{-2}$. The increase in yield strength with higher Zn content was attributed to the precipitation strengthening effect of the additional Zn. Regarding fracture toughness, the increase in Zn content, which enhanced the yield strength, resulted in a reduced Stretch Zone Width (SZW) and an increased presence of cleavage facets on the fracture surface, leading to decreased fracture toughness. Fractographic analysis conducted after fracture toughness testing showed a reduction in the Plastic Zone Size (PZS). According to the Arrhenius equation, the reduction in PZS contributed to the observed decrease in fracture toughness.

In summary, while the increase in Zn content in Al-Zn-Mg-Cu alloys has minimal influence on factors such as the fraction of secondary phases, grain size, recrystallization fraction, and texture, it significantly enhances yield strength through the precipitation strengthening effect. However, this increased yield strength reduces the SZW at the pre-fatigue crack tip during fracture toughness testing, resulting in a lower crack initiation fracture toughness value (KIC). This study demonstrates that while increasing Zn content in Al-Zn-Mg-Cu alloys can improve tensile strength via precipitation strengthening, it simultaneously reduces fracture toughness.

Optimizing Over-Aging Resistance in Al-Mg-Si-Cu Alloys through the Addition of Trace Elements

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B2_2, U2 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

This study focuses on enhancing the thermal stability of Al-Mg-Si-Cu alloys by incorporating trace elements such as silver (Ag) and scandium (Sc), while carefully controlling copper (Cu) content. The primary strengthening phase in these alloys, β'' (Mg_5Si_6), is prone to over-aging at elevated temperatures, leading to a loss of strength and reliability. Microalloying with Ag and Sc improves thermal stability by preventing the coarsening of precipitates and delaying hardness degradation. Ag promotes the formation of disordered atomic structures and stabilizes the alloy during over-aging, while Sc prevents the growth of the β'' and β' phases, maintaining high hardness. The combined effects of Ag and Sc, along with an optimized Cu content, result in a synergistic enhancement of thermal stability, particularly in alloys subjected to prolonged thermal exposure. This novel approach offers promising improvements in the high-temperature performance of Al-Mg-Si-Cu alloys, making them suitable for demanding applications such as electric vehicle battery enclosures.

Microstructure and Mechanical Properties of AZ91-MXene Composites Fabricated by Spark Plasma Sintering Near Solidus Temperature

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B2_7, U2 Room (Level 0), septembre 16, 2025, 17:00 - 19:00

MXenes, a novel class of two-dimensional (2D) metal carbides, are emerging as promising materials for reinforcing lightweight alloys due to their exceptional properties. In this study, we explore the mechanical properties and microstructure of composites composed of a magnesium alloy (AZ91) and varying concentrations of MXene, ranging from 0.1 to 10 wt%.

To achieve homogeneous distribution of MXene within the AZ91 matrix, we employed an optimized powder metallurgy process. Key steps included synthesizing the MAX phase, the precursor of MXene, followed by etching to obtain the desired 2D structure and subsequent integration into the composite matrix. Each stage of the process was carefully analyzed, with particular attention to parameters critical for achieving high-quality, dense MXene-AZ91 composites.

The synthesis was conducted near the solidus temperature of the AZ91 alloy not only to maximize densification during powder metallurgy but also to enhance interaction between MXene and AZ91. This approach enabled us to produce samples with near-full density, a crucial factor for ensuring mechanical reliability. The homogeneity and compactness of the composites were validated using advanced microstructural characterization techniques.

To evaluate the performance of these composites, we conducted friction and compressive tests, revealing significant insights into their mechanical behavior. The results suggest that MXene-AZ91 composites could be valuable in applications where a combination of lightweight properties and mechanical durability is essential, such as in aerospace and automotive industries.

Exploring the Quenching and Partitioning Heat Treatment in a Fe-alloyed Titanium Alloy: An in-situ and ex-situ approach

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B2_5, U2 Room (Level 0), septiembre 16, 2025, 10:30 - 13:10

Titanium alloys and steels, although chemically rather different, share some similarities in their metallurgical behavior. For example, the interplay of martensitic structures within a ductile matrix phase, such as austenite in steels or the β -phase in titanium, leads to the overlapping applicability of some rules and treatments for both metals. These structural similarities motivate the exploration of the effects that quenching and partitioning (Q&P) heat treatments have in the realm of titanium alloys. The Q&P process was initially developed to enhance the mechanical properties of advanced high strength steels by stabilizing the retained austenite matrix through the redistribution of interstitially dissolved carbon from the martensite phase into the austenite. In comparison to conventional Quenching and Tempering treatments and dual phase steels, this results in an increase in strength with consistently high elongation or, conversely, an increase in elongation with consistently high strength. This achieves a balance between high strength and good ductility.

With this heat treatment being well established in steels, the question arises, if such a primary phase transformation would also be applicable to Ti-alloys. As it is equally conceivable to induce martensite upon solution heat treatment and subsequent quenching and decompose it in a partitioning step, where β -stabilizing elements redistribute into the softer β -matrix. Especially, additive manufacturing (AM) could benefit strongly from such a heat treatment, as many Ti-alloys face the issue of relying on thermo-mechanical treatments for a good strength-to-ductility balance. In the AM context this means that plastic deformation must be introduced already during manufacturing in every individual layer, which hence increases complexity and costs. The application of Q&P could finally balance out the tense relationship between high strength and good ductility in AM Ti-alloys without relying on traditional thermomechanical treatments.

To investigate the feasibility and impact of Q&P treatments in titanium alloys, a series of experiments were conducted. These include synchrotron X-ray diffraction to track the phase transformations during the Q&P treatment and dilatometer compression tests on untreated and Q&P-treated material with microhardness measurements to evaluate its effects on the mechanical properties. Further, scanning electron microscopy was used to characterize the undeformed microstructures. The combination of these techniques provides detailed insights into the phase evolution and microstructure, clarifying the occurrence and exploitation potential of the Q&P effect in Ti-alloys.

Lightweight Alloys for Material Circularity and Manufacturing Sustainability

Prof. Alan Luo¹

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B2_3, U2 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

A significant portion of our carbon footprint comes from production of light metals such as aluminum, magnesium and titanium. Increasing the circularity of these nonrenewable metals and reducing energy consumption in their manufacturing activities would significantly contribute to a carbon-neutral society and a circular economy. This presentation reviews some of new light alloys and manufacturing technologies being developed towards material circularity and manufacturing sustainability in the automotive industry. Examples are given on aluminum and magnesium sustainability. While aluminum is increasingly used for lightweighting applications in the transportation industries to reduce energy consumption and carbon footprint, primary production of aluminum is energy-intensive with extensive CO₂ emission. However, recycling aluminum scrap only uses ~5% of the energy and has 95% reduced emission compared to primary aluminum extraction from bauxite ore. The wide use of recycled aluminum in structural applications will improve the sustainability of the supply chain in aluminum and manufacturing industries. Magnesium, as the lightest structural metal and one of the most abundant metallic elements on earth, has been used for lightweighting in the transportation and electronics industries. However, the primary production of magnesium, especially the carbothermal (Pidgeon) process, is also a climate liability due to its large carbon emissions. The future of magnesium industry and applications will largely depend on how we address this sustainability challenge. For structural applications, research is needed to improve the mechanical and corrosion properties, manufacturing processes, and integrated computational materials engineering (ICME) tools.

For manufacturing processes, the development and evolution of energy-efficient large thin-wall die casting (also called mega/giga casting) will enhance the sustainability of automotive manufacturing. The alternative energy vehicles tend to have more simplified body structures, enabling the use of large and consolidated castings which significantly reduce welding, joining and assembly. The development of large thin-wall die casting, using solidification-based ICME tools, will improve the sustainability of transportation manufacturing. Microstructure models for light alloys have been developed based on computational thermodynamics and kinetics, coupled with manufacturing process models. These ICME models are integrated to predict location-specific mechanical properties, based on location-specific microstructure of solidification (casting, welding and additive manufacturing) products, for lightweight and sustainable applications. Ultimately, the combination of recycled/renewable materials and energy-efficient manufacturing processes will drive the automotive industry towards circularity and sustainability.

Thermal properties of Aluminum Matrix Composites reinforced with pitch carbon fibers fabricated via hot pressing

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B2_4, U2 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

Aluminium matrix composites (Al-MMCs) reinforced with pitch-based carbon fibers have gained significant attention due to their exceptional thermal properties, making them suitable for advanced thermal management applications. This study investigates the thermal behavior of Al-MMCs reinforced with various types of pitch carbon fibers fabricated via hot pressing. The parameters of the hot-pressing process were tailored in order to achieve full densification. Detailed microstructural analyses were conducted on the fabricated samples to understand the material characteristics. The influence of fiber type, volume fraction, and interfacial bonding on thermal conductivity, and thermal expansion, was systematically analyzed. Experimental results establish a clear relationship between the type and volume fraction of carbon fibers and the resulting thermal performance of the composites. Furthermore, the incorporation of pitch-based carbon fibers significantly reduced the coefficient of thermal expansion (CTE) of the Al-MMCs, enhancing their dimensional stability during thermal cycling. These findings highlight the potential of tailored pitch carbon fiber-reinforced Al-MMCs for aerospace, electronics, and automotive applications requiring advanced thermal performance.

Eco-friendly anodic colouring of titanium alloys

Mrs. Itziar Hidalgo-González¹, Mr. Jaime Martínez-Cabrerizo¹, Prof. M. Isabel Barrena¹, Prof. Raúl Arrabal¹, Prof. Endzhe Matykina¹

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B2_5, U2 Room (Level 0), septiembre 16, 2025, 10:30 - 13:10

Titanium alloys are widely used in several sectors of the aerospace and biomedical industries due to their exceptional in-service properties. The anodization of titanium promotes the formation of a nanometric oxide titanium film (TiO₂), which provides an improved corrosion resistance in aggressive environments, facilitates the adsorption of lubricants and helps to prevent galling. Additionally, light interference of the passive film (<350 nm) is of great utility for colour-coding of biomedical devices and aesthetics in jewellery. The variation in the passive film thickness, and consequently the colour, is influenced by the applied voltage (ranging from 10 to 100 V) and surface pre-treatment. EN 2808 standard recommends surface pre-treatment in an aqueous mixture of HF and HNO₃ and anodizing in concentrated H₂SO₄, which are extremely aggressive and present severe health-and-safety risks. In this study, a commercial alkaline surface pre-treatment (BONDERITE C-AK 4181 L AERO) and an alternative alkaline anodizing process at different voltages were assessed for Ti6Al4V alloy. The resulting colours were characterized using the CIELAB colour space and compared to those obtained in H₂SO₄. Other characterization techniques included scanning electron microscopy (SEM), Rutherford backscattering spectrometry (RBS), contact angle measurements, and optical profilometry. Corrosion resistance was evaluated using electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) tests in Harrison's (acid rain) solution and Hanks' solution at 25°C and 37°C, respectively. Pitting and crevice corrosion resistance were examined in selected samples according to the ASTM F 746-87 standard.

It may be concluded that for aerospace and biomedical applications, as well as for colour-coding systems, eco-friendly alkaline surface pre-treatment and anodizing are suitable alternatives to acidic industry-approved procedures.

Electropulsing-Assisted Deep Drawing: Challenges and Key Results

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Electropulsing is an innovative approach for improving formability in sheet metal forming. Direct current pulses are employed to influence forming forces and improve material properties during forming, for example in deep drawing. The process holds significant potential for sustainable manufacturing, as it may reduce energy consumption compared to hot forming. However, despite the promising possibilities, electro-pulsing-assisted deep drawing faces significant technological challenges that need to be solved in order to achieve consistent and scalable results.

One of the biggest obstacles is ensuring effective electrical contact between the forming tools and the workpiece. Reliable contact is essential to deliver high current densities evenly across the forming area. Another significant hurdle is reaching the required current densities to produce a beneficial electroplastic effect. Precise control of the pulse parameters, including amplitude, frequency and duration, is key. These parameters must be optimized with regards to the material properties and the specific geometries of the forming process.

We developed an electrically assisted deep drawing setup, capable of delivering high-current pulses with amplitudes in the kiloampere range and millisecond-scale durations. Aluminum alloy EN AW-5083, known for its excellent corrosion resistance and moderate strength, was selected for the experiments. The selected geometry was successfully formed at different depths. The results show that pulsed electric currents significantly influence the forming forces compared to conventional methods. These improvements are attributed to local thermal and electroplastic effects.

Our research demonstrates the feasibility of electropulsing-assisted deep drawing. Future research will focus on further optimizing the process, scaling it up for industrial applications and investigating its feasibility for other materials.

Influence of cooling rate and Mo/Fe-ratio on solidification path in a secondary Al7Si-alloy with focus on structural appearance of phases.

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Iron (Fe) is a detrimental impurity element in secondary (i.e., recycled) Al-Si alloys, as it adversely affects their castability and mechanical integrity. Its presence promotes the formation of Fe-containing intermetallic phases, particularly the brittle, plate-like β -Al_{4.5}FeSi phase, which significantly increases the susceptibility to cracking. Secondary aluminum alloys typically contain additional elements introduced either as residuals or intentional additives to refine the microstructure. Among these, manganese (Mn) and chromium (Cr) have been extensively studied and are commonly employed as effective modifiers to mitigate the adverse effects of Fe by the formation of harmless α -Al-(Fe,Mn,Cr)-Si phase.

Molybdenum (Mo) is also commonly found in recycled aluminum alloys. Although Mo is claimed to have similar effects as Mn and Cr in promoting the formation of α -Al-(Fe,Mo)-Si over β -Al_{4.5}FeSi, detailed research on its role in forming and partitioning of these phases is limited. Moreover, the possibility of Al₁₂Mo and (Al,Si)₂Mo phase formation must be carefully considered. This knowledge gap emphasizes the need for further research to better understand the effects of Mo on the microstructure and mechanical properties of recycled aluminum alloys.

In the present study, the formation of intermetallic phases in Al_{7.1}Si(1.5-x)Fe(x)Mo alloys (in at%), with x = 0.3, 0.45, 0.6, and 0.75 at%, was investigated under cooling rates spanning the orders of 0.01 to 100 K/s. The alloys were synthesized by arc melting pure elements and subsequently remelted at 950°C in an Ar atmosphere using Al₂O₃ crucibles, prior to defined cooling. The resulting microstructures were analyzed in detail using scanning electron microscopy (SEM) including energy-dispersive x-ray spectroscopy (EDS) and electron backscatter diffraction (EBSD).

The study highlights the significant influence of cooling rate and Mo/Fe ratio on the phase formation in a secondary, Fe-containing Al7Si alloy during solidification. Faster cooling rates effectively refined the microstructure, reducing the size and altering the morphology of Fe-rich intermetallic phases. The addition of Mo, particularly at higher Mo/Fe ratios, promotes the formation of compact or dendritic α -Al-(Fe,Mo)-Si particles instead of plate-like β -Al_{4.5}FeSi particles. Thereby, Mo partitions mainly in the α -Al-(Fe,Mo)-Si phase competing with formation of Al₁₂Mo and (Al,Si)₂Mo while it is almost not solved in the β -Al_{4.5}FeSi phase. These findings underline the critical role of process parameters and alloy composition in tailoring the microstructure and improving the performance of secondary aluminum alloys.

Recrystallization Mechanisms in an AA2024 Sheet Alloy

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B2_2, U2 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

The mechanical properties of the aluminum alloy AA2024, which is commonly used in the aerospace industry, depend heavily on the microstructure e.g., grain shape and crystallographic texture. During industrial processing, the material is subjected to various thermomechanical treatments that determine the grain properties due to mechanisms such as recrystallization. Recrystallization itself is a complex transformation that depends on several influencing parameters such as the degree of deformation, secondary phases, precipitation kinetics, dispersoids, etc.

In situ electron backscatter diffraction (EBSD) was used to investigate the recrystallization process. With this technique, it is possible to study the entire transformation on a sample by recording scans during the annealing process. The correlation of the initial crystallographic microstructure and precipitation state with the fully recrystallized state after annealing is also determined. Three samples with different degrees of deformation were prepared and in-situ heating experiments were carried out with different heating rates from 1 K/min to 70 K/min. These experiments were used to determine the dependence of recrystallization on mechanical deformation and annealing heating rate. After annealing, a strong recrystallization texture was observed, consisting mainly of Cube and S grains and a smaller fraction of Goss grains. The in situ experiments showed an inconsistent growth behavior of recrystallized grains, with some showing strong growth while others remained almost unchanged after nucleation. Regarding the texture components, no obvious advantage of the cube over the other texture components was found. In addition to studying the microstructure and texture evolution, the behavior of secondary phases during the annealing treatments was investigated using scanning differential calorimetry (DSC). It was found that the S phase shows a change in the temperature window of recrystallization. The work described provided a detailed picture of the recrystallization mechanisms in AA2024, which will help to further improve the microstructure and thus the mechanical properties.

MICROSTRUCTURAL AND MECHANICAL CHARACTERIZATION OF A NOVEL SECONDARY ALUMINUM ALLOY FOR AUTOMOTIVE INDUSTRY

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B2_1, U2 Room (Level 0), settembre 15, 2025, 9:20 - 10:20

Up to 95 % of aluminum currently used in the automotive industry can be recycled and, considering the multiple harmful by-products created during its production from ore, this recycling practice needs to be strongly encouraged. Aluminum recycling consumes only about 5 % of electricity and produces lower amounts of CO₂ compared to the amount generated during primary aluminum production. However, the use of secondary aluminum certainly has some disadvantages, mostly due to undesirable levels of metal impurities that often occur in the melt; among them, iron is the worst due to its detrimental effects on the mechanical properties of aluminum castings.

This work aims to evaluate the microstructural and mechanical properties of a novel AlSiMgCu secondary aluminum alloy specifically tuned for the automotive industry, with the iron content controlled by the addition of manganese and poured in permanent mold casting. The equivalent primary alloy was also considered for comparison purposes. The chemical composition of both alloys was determined by optical emission spectroscopy, whereas the microstructural features in the as-cast condition, i.e., secondary dendritic arm spacing (SDAS), eutectic Si morphology, mean average grain size and intermetallic phases were evaluated by optical microscopy and scanning electron microscopy equipped with energy dispersive spectroscopy (SEM/EDS). The mechanical properties were investigated on samples drawn from the castings in as-cast and T6 heat-treatment conditions by tensile and impact tests, and Brinell hardness measurements. Impact tests were carried out through a 50 J instrumented Charpy pendulum to calculate the total impact energy (Wt), the maximum load (Fm), the energy at maximum load (Wm) and the crack propagation energy (Wp). At the same time, the energy absorption was estimated through the measurement of the pendulum's angle of rise (CV). After tensile and impact tests, the fractured specimens were observed by scanning electron microscopy to identify the main failure mechanisms. The results emphasized that the microstructural features and tensile properties of primary and secondary alloys, in the same metallurgical state, were almost comparable. The impact properties of the secondary alloy were slightly lower than those of the primary alloy. In any case, the morphology of the fractured surfaces suggested a ductile fracture mechanism even with different amounts of fractured intermetallics phases according to the different iron contents.

Multi-scale microstructure characterization of ultrafine Ti-Fe-based eutectics for additive manufacturing

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B2_6, U2 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

Ti alloys are useful in applications that require a high strength-to-weight ratio, such as aerospace or structural applications. However, Ti parts are often costly and difficult to manufacture. Ti alloys can be particularly difficult to machine which increases their cost and limits their use outside of specialized applications. The development of additive manufacturing (AM) has provided an opportunity to manufacture Ti parts in near-net shapes, reducing the need for costly machining processes.

AM techniques like selective laser melting (SLM) use a laser to selectively melt metal powder in desired locations to build up a final shape layer by layer. This process involves melting and cooling the metal at timescales much faster than in traditional manufacturing. Investigators have taken advantage of this unique temperature environment to create alloys and microstructures that were not previously possible. For the first time eutectic and near-eutectic Ti-Fe alloys with ultrafine hierarchical eutectic microstructures were created using SLM techniques, and exhibited high strengths and enhanced compressive ductilities at room-to-intermediate temperatures. These alloys still pose challenges, though, as the extreme temperature gradients during melting and cooling induces significant thermal stress, causing the Ti-Fe alloys to crack during the printing process. High baseplate temperatures (approximately 790C) have been used to successfully prevent cracking during printing and solidification, but most commercial SLM systems are not equipped to reach such elevated temperatures which could limit the adoption of these alloys in industry.

Previous work has identified Ti-26Fe-4Sn-2.5Nb(wt%) as an alloy with potential to successfully print at temperatures below 790C [1]. In this study we investigated Ti-26Fe-4Sn-2.5Nb(wt%) using synchrotron x-ray imaging to determine how laser power, scan speed, and baseplate temperature affected the generation of defects such as cracks during the printing process. Laser power and scan speed affect the laser energy density, which is known to affect the formation of defects during SLM. Further multi-scale characterization was performed to determine the microstructure of the Ti-26Fe-4Sn-2.5Nb(wt%). Using the in-situ experiments along with the post-mortem characterization, the processing-microstructure relationships of Ti-26Fe-4Sn-2.5Nb(wt%) were explored.

The results from this work are expected to advance the knowledge of the fundamental mechanisms of SLM techniques in alloys sensitive to residual stresses and cracking during or after solidification. Using the in-situ experiments, we hope to help close the gap between information from process monitoring systems used in commercial AM machines and post-mortem characterization by standard laboratory techniques.

[1] Gussone, et al. <https://doi.org/10.1016/j.apmt.2020.100767>

Novel aluminium-carbon nanomaterials fabricated by means of friction stir processing and plasma welding

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The electrical conductivity of a material plays a significant role in many areas including energy transfer, electronics, and electric vehicles. Improvements in conductivity translate into reduced energy losses and, therefore, represent an important focus in materials research for modern society. Yet, for many applications, conductor materials also require a high mechanical strength, and resistance to aging as well as elevated temperatures. Since in many classic alloys these requirements, i.e. high electrical conductivity and high strength, are in conflict to each other, this work investigates novel aluminium-carbon nanomaterials on the basis of alloy Al-6061 and activated carbon nanopowder (nC), which show great potential for simultaneous improvements in both properties. The aim is to create special crystallographic structures by the application of different processes.

Friction stir processing (FSP) and plasma welding were combined to achieve these promising microstructures and, thus, material properties. In a first step, FSP was used to produce a homogeneous pre-material by introducing 3 wt.% nC powder into the Al-6061 base material. To this purpose, the nC powder was mixed with ethanol and subsequently applied to grooves in Al-6061 sheets. Upon closing the filled grooves in a pin-less FSP setup, metal-matrix composites (MMCs) were created in a multi-pass FSP process. Different groove geometries and process parameters were tested to ensure high homogeneity in terms of carbon distribution. In a second step, the MMCs were remelted by plasma welding. During plasma welding, the melt pool is subjected to an electric current, which exerts an influence on the crystallographic structure of the nanocarbon within the aluminium matrix. Different welding parameters were investigated and correlated with the resulting microstructures and material properties. A comparative analysis between the properties of the new aluminium-carbon nanomaterials and the initial, untreated Al-6061 sheet material finally evaluates the potential of the created material as well as of the suggested unconventional, yet reproducible and resource-efficient fabrication route.

A new approach on TWIP titanium alloys design: oxygen segregation through grain boundaries engineering

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B2_5, U2 Room (Level 0), septembre 16, 2025, 10:30 - 13:10

In the context of global warming, titanium alloys play an increasingly crucial role in the transportation sector due to their lightness and unique properties. Among these, TWIP (Twinning Induced Plasticity) titanium alloys stand out. They offer an excellent combination of mechanical properties and strain-hardening ability, along with inherent titanium characteristics such as lightness and corrosion resistance.

However, titanium's sensitivity to interstitial elements like oxygen in solid solution makes these alloys vulnerable during the fabrication process, especially during heat treatments or when using lower-grade materials, such as recycled materials that contain more impurities than commercially pure elements.

Oxygen has two main effects on TWIP alloys. High oxygen levels prevent the formation of twins during deformation, favouring dislocation slip, which degrades mechanical properties (through embrittlement effect) [1]. Additionally, oxygen naturally segregates at grain boundaries [2].

The aim of this study is to optimize oxygen distribution in a β -metastable alloy through grain boundary engineering. This approach aims to maintain the TWIP mechanism, ensuring excellent mechanical properties, while developing strategies to mitigate the effects of impurities in these alloys. By optimizing microstructural control, impurities could even be leveraged to enhance the material's mechanical properties.

To achieve this goal, a Ti-15Mo-0.2O (wt%) alloy was investigated in different states. Following a simple fabrication process primarily based on heat treatments, a fully recrystallized microstructure was characterized and used as a reference state for comparison with the segregated state. EBSD mapping and in situ tensile tests were conducted to observe twin behaviour near grain boundaries and conditions of plasticity transfer. A quantitative analysis highlighted the impact of such impurities on mechanical properties, such as yield strength.

[1] MIN, Xiaohua, BAI, Pengfei, EMURA, Satoshi, et al. Effect of oxygen content on deformation mode and corrosion behaviour in β -type Ti-Mo alloy. *Materials Science and Engineering: A*, 2017, vol. 684, p. 534-541.

[2] PRITHIV, T. S., KLOENNE, Zachary, LI, Dian, et al. Grain boundary segregation and its implications regarding the formation of the grain boundary α phase in the metastable β -Titanium Ti-5Al-5Mo-5V-3Cr alloy. *Scripta Materialia*, 2022, vol. 207, p. 114320.

Upcycling Secondary Al-Si Casting Alloys: Unlocking the Potential of Rare Earth Elements Microalloying to Mitigate Fe Contamination

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The global transition to electric vehicles, alongside policies phasing out fossil-fuel-powered cars by 2030, is set to reduce the demand for conventional casting alloys, such as those used in engine blocks. By 2040, this transition could lead to a surplus of up to 8.7 million tons of scrap metal, with 3.6 million tons potentially becoming "dead metal" if innovative recycling methods are not developed. Secondary aluminium alloys (SAAs), derived from mixing different alloy scraps, exhibit inferior mechanical properties due to contamination. In Al-Si casting alloys, contaminants such as Fe and oxides significantly reduce mechanical performance compared to primary alloys. The precipitation of brittle intermetallic phases further deteriorates properties, mainly ductility. Phases such as β -AlFeSi, α -Al(FeMn)Si, or π -AlFeMgSi can form depending on the alloy composition. Some studies have investigated the effect of Mn, Cr, or Mg on morphology optimisation and phase transition. Despite these challenges, the automotive industry must maintain its competitive advantage by minimising raw materials and manufacturing costs. Researching upcycling methods to modify Fe-rich phases is crucial for enhancing the properties of SAAs, ensuring their economic competitiveness with primary alloys. To address these challenges, this research focused on adding rare earth elements (REEs) in SAAs to enhance their overall quality and mechanical properties. REEs additions, typically limited to less than 1 wt.% to avoid the formation of excessive Al-REE phases that can deteriorate mechanical properties, are referred to as "REEs microalloying." Elements such as lanthanum, cerium, and erbium have been shown to refine α -Al grains, modify the morphology of eutectic Si, and improve fluidity. These advancements offer promising pathways for upcycling SAAs.

This study aimed to evaluate the impact of microalloying with La, Ce, and Mischmetal (a 50% mixture of La and 50% Ce) at concentrations of 0.05, 0.10, and 0.15 wt.% on a highly Fe-contaminated AlSi7Mg0.3 alloy, about 3.8 wt.% Fe. The evaluation was conducted on castings with and without T6 heat treatment. Samples were extracted from castings and prepared using conventional metallographic techniques. Optical and scanning electron microscopy with energy dispersive spectroscopy were used to analyse the microstructures and identify the phases. Subsequently, tensile and hardness tests were conducted to evaluate the influence of REE microalloying on the mechanical properties of the alloy. Even a minimal addition of 0.05 wt.% of REEs showed significant potential in refining β -AlFeSi needles, partly transforming them into irregular star-shaped α -AlFeSi. Additionally, the T6 temper enhanced the breakdown of the needle structures.

Influence of Fe concentrations on the improvement of the recycling content of Al-Mg-Si wrought alloys.

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B2_3, U2 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

The recycling capability of Al-Mg-Si wrought alloys is limited by the contents of some alloying elements. Increased Fe concentrations, particularly, have an adverse effect on the mechanical properties of the alloy. To better comprehend this, CALPHAD simulations using Thermo-Calc were conducted on multiple Al-Mg-Si alloys with varying Fe contents. Casting samples at laboratory scale were fabricated to corroborate the obtained simulation results. Standard microstructure investigation methods were used to analyse phase formation in the castings. The effects of homogenization on phase transformation were also examined, followed by mechanical analysis. The results specifically focus on having a better understanding of the relation between Fe concentrations, parameters influencing the alloy microstructure and the alloy mechanical properties through a preliminary study. Through these findings, the recycling strategies in the aluminium industry can be positively informed.

Tailored Nanocrystalline Aluminium Grain Size in a Nanolaminated Architecture: New Horizons

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B2_3, U2 Room (Level 0), septiembre 15, 2025, 14:30 - 16:30

Grain growth limits the applicability of engineering metals alike Aluminium (Al) alloys. Coarse-grained Al microstructures usually result in reduced mechanical properties – risking catastrophic failure [1,2]. In this work, we are reporting interface-engineered AlNi - AlOH (25 – 1 nm) thin films with tailored impediment to Al grain growth in two dimensions - expanding the application of engineering Al alloys. The thin films were deposited by means of combined hybrid physical vapour (PVD) and atomic layer deposition (ALD) in a SwissCluster AG SC-1 cluster deposition chamber. Mechanical testing was conducted by Nanoindentation with a Berkovich tip. High-resolution analysis of the microstructure was performed by means of combined transmission electron microscopy and atom probe tomography. As-deposited Al95Ni5 – AlOH (25 – 1 nm) thin films are reported to possess a lateral FCC Al grain size of only 10 nm with fine 1 nm Ni-rich segregations and roughly 1 nm AlOH interlayers. This unique microstructure is set to explain the > 5 GPa Nanoindentation hardness of the thin film stack. Vacuum annealing at various temperatures is gradually lowering the hardness until reaching 2.6 GPa for vacuum annealing at 450°C for 1 h, where interlayers set to broaden and Al-Ni phase separation completes. AlNi - AlOH (25 – 1 nm) thin films with > 5 GPa as-deposited hardness show superior mechanical response, even at elevated temperatures. Thus, the system serves as blueprint for further developing Al-based engineering materials towards higher strength and thermal stability with novel combination of deformation mechanisms.

[1] Q. Li, J. Wang, H. Wang, X. Zhang, Achieving strong and stable nanocrystalline Al alloys through compositional design, *J. Mater. Res.* 37 (2022) 183–207.

[2] Z. Chen, F. Liu, H.F. Wang, W. Yang, G.C. Yang, Y.H. Zhou, A thermokinetic description for grain growth in nanocrystalline materials, *Acta Mater.* 57 (2009) 1466 – 1475.

Microalloying Strategy: How Small Additions of Alloying Elements Can Significantly Boost the Strength of Titanium Alloys

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B2_5, U2 Room (Level 0), septembre 16, 2025, 10:30 - 13:10

Due to their low density, high corrosion resistance, and biocompatibility, titanium and titanium alloys are highly attractive for many industries, including notably aeronautics and biomedical fields. However, the mechanical strength of Ti-based materials can be too limited for certain applications at room temperature, and even more so at high temperatures. In an original approach, this study aims to investigate the impact of adding small amounts of alloying elements on the microstructure and mechanical properties of titanium. Among various beta-stabilizing elements, the effect of microalloying with rhenium is particularly investigated. The results obtained highlight that a limited addition, < 1 wt.% of Re, can more than double the mechanical strength while maintaining a high reserve of ductility. The associated microstructural analysis shows that the addition of Re induces the presence of nanometric beta-phase particles (both intra- and inter-granular) as well as a significant refinement of the grain size.

Novel Heterogeneous Structure Design and Performance Tailoring of Ultrahigh Strength-Toughness Titanium Alloy

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B2_5, U2 Room (Level 0), septiembre 16, 2025, 10:30 - 13:10

To address the urgent demand for titanium alloys with superior strength-ductility synergy in aerospace structural lightweighting, this study innovatively proposes a heterogeneous lamellar structured titanium matrix composite (TMC) fabricated from high-strength β titanium alloy powder and Si powder via low-energy ball milling, reactive hot pressing sintering, and controlled hot extrusion. By dual regulation of reinforcement configuration and matrix structure, the TMC exhibits a 10% increase in tensile strength and an 8-fold enhancement in uniform elongation compared to extruded titanium alloys. The strengthening mechanism is mainly heterogeneous deformation induced (HDI) strengthening and multi-stage strengthening mechanisms are sequentially activated: heterogeneous deformation-induced work hardening at initial deformation, Si-enhanced cross-slip in the middle stage of deformation, stress-induced ω -phase transformation and dislocation pinning by submicron Ti₅Si₃ particles at intermediate stages. This hierarchical activation sustains high strain hardening rates even under large deformations.

Based on the above research, a grain boundary-engineered aging treatment was developed to fabricate ultra-high strength hetero-cellular structured TMC. The optimized microstructure comprises $\sim 5\ \mu\text{m}$ cellular grains formed by nano-scale Widmanstätten α -phase grain boundaries (αWGB), with cell interiors containing hierarchical nano-graded α -phase (αHS) and pyramidal α -phase ($\alpha\text{pyramid}$) near Ti₅Si₃ particles. The HCS Ti-Si composite achieves a yield strength of 1720 MPa, ultimate tensile strength of 1839 MPa, and ductility of 5.5%, demonstrating simultaneous improvements in strength and plasticity over aged titanium alloys.

What's more, In-situ TEM heating revealed the dynamic phase evolution, while SEM-based digital image correlation (DIC) elucidated micro-deformation mechanisms, confirming the critical roles of hetero-interfaces and stress partitioning in enhancing mechanical performance.

Effects of Creep in Titanium at Room Temperature during Tensile and Profilometry-based Indentation Plastometry Testing

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B2_6, U2 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

Titanium alloys at room temperature are often observed to exhibit a dependence on strain rates within the 'quasi-static' regime. Three titanium alloys have been tested at a range of strain rates via conventional tensile testing and by Profilometry-based Indentation Plastometry (PIP) with a range of penetration velocities. In addition, they have been creep tested at fixed loads corresponding to nominal stresses in the vicinity of the yield stress. It is shown that the dependence of these materials on strain rate can be explained by simply considering the results of room temperature creep tests near the yield stress.

A numerical model has been developed, combining analytical equations for quasi-static plasticity and creep. Good overall consistency is observed and the procedures described here are thought to have wide potential for understanding and characterising titanium alloys which show a dependence on strain rate during tensile testing. These effects should have a large impact when designing protocols for materials testing certain alloys.

The Effect of Si Additions to an Industrial 7xxx Aluminium Alloy in the Context of Recycling

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B2_1, U2 Room (Level 0), septiembre 15, 2025, 9:20 - 10:20

Using post-consumer scrap in the manufacturing of industrial aluminium alloys is becoming increasingly attractive for the implementation of a circular economy due to decreased energy consumption, lower CO₂ emissions and lower production costs. However, this practice leads to accumulation of unwanted elements which may degrade the performance of such alloys, especially if sorting of scrap is not done properly. In the case of industrial 7xxx alloys the main alloying elements are Mg and Zn, and the most likely pollutant is Si, a major solute element in the composition of 6xxx Al-Mg-Si alloys. In the present work it was investigated the effect of 0.3 wt% Si addition to an industrial Cu-free 7xxx alloy with composition 0.90Mg, 5.70Zn, 0.20Fe and 0.15Zr (wt%) on hardness evolution during artificial aging and connection with the precipitate microstructure. It was found that the Si added alloy had slower precipitation kinetics, achieving a lower peak hardness after a longer aging time than the base alloy. While the base alloy in the peak hardness condition contained the expected metastable η precipitates, two types of precipitates were observed in the Si added alloy. The first type was metastable η phases forming a coarser microstructure, while the second type was L laths with $\langle 100 \rangle_{\text{Al}}$ growth directions present in the volume in-between the η precipitates, with a dense microstructure. The L-phase is a thermally resistant precipitate observed in Mg-rich Al-Mg-Si-Cu alloys. High angle annular dark field scanning transmission electron microscopy imaging showed bright contrast atomic columns in the composition of the L-phase, and atom probe tomography confirmed the presence of Zn. It was therefore concluded that the decreased performance of the Si-added alloy was caused by Si binding with Mg to form L-phase, stabilized by the presence of Zn in its structure. Accumulation of Si in Al-Mg-Zn alloys is therefore detrimental to their mechanical properties and must be avoided. Another interesting observation of this study was the presence of up to 10 at% Zn, Si and Mg in the composition of Al₃Zr dispersoids.

Grain size and texture effects on twinning in magnesium alloys

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B2_7, U2 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

Twinning is a significant plasticity mechanism in magnesium alloys, influencing their mechanical properties. Despite the long-term effort, it is still not fully understood. Analyzing twinning is challenging because it initiates a process on the atomic level but rapidly propagates to a grain size scale. The presented study analyses local stress-strain conditions inside the polycrystalline magnesium alloy and assesses the effects of grain size and crystallographic orientation on twin nucleation and propagation. The impact of existing twins on further twin evolution is particularly considered. The analysis is performed using the finite element method and crystal plasticity framework and compared with experimental observations. The results provide insight into the evolution of plasticity and twinning at the local scale.

Corrosion Behaviour in NaCl and PBS Solutions of the Magnesium Alloy ZK60 after High Pressure Torsion Extrusion

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B2_7, U2 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

Magnesium alloys are promising materials for implants. Not only because their mechanical properties are comparable to those of bones, which helps to prevent the stress shielding effect. Also, their high corrosion activity can be used to create bioresorbable implants – implants that degrade in the body over time to be replaced with the regrowing bone. Thus, making implant removal surgeries obsolete.

To be used for bioresorbable implants, the alloy should be non-toxic to the body, its mechanical strength should be adequate to support the healing bone, and the corrosion rate should be slow enough for the bone to be able to regrow. The main constituents of the magnesium alloy ZK60, Mg, Zn and Zr, are not toxic to the human body, making this alloy an interesting candidate for the manufacturing of implants. The corrosion rate can be modified, among other options, by refining the grain size. This can be straightforwardly done by Severe Plastic Deformation methods such as High Pressure Torsion Extrusion (HPTE).

In the present study, specimens of ZK60 are subjected to HPTE at two different temperatures. The resulting specimens, which show a significantly refined grain size, are subsequently tested for their corrosion activities in NaCl solution and Phosphate Buffered Saline (PBS) solution. The results are compared to the corrosion activity of the initial state before HPTE to determine whether the changes in the microstructure lead to different corrosion behaviours.

Tensile instabilities in 6xxx series aluminium alloys

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B2_2, U2 Room (Level 0), septembre 15, 2025, 10:50 - 13:10

Tensile instabilities are well known within the 5xxx (Al-Mg) series of aluminium alloys, giving rise to serrated tensile, namely the Portevin – Le Chatelier (PLC) effect. High Mg content, typical for this series, is responsible for blocking the dislocations in the Cottrell atmospheres increasing strength until the dislocation is released and the strength is lowered. 6xxx (Al-Mg-Si) series alloys, with lower Mg contents than most 5xxx alloys, are generally considered to be insensitive to this phenomenon. Yet, at high strains, instabilities of tensile curves have been reported [1,2]. Presence of such serrations is an indication of potential for premature cracking at stamping linked to strain localisation. Additionally, surface aspect and quality can be degraded. 6xxx alloys widely used in the automotive industry for both outer and inner panels could be impacted by this neglected phenomenon.

A focus on detection and understanding of tensile serrations was made in this study at both laboratory and industrial data. It has been noted that the occurrence of instabilities results in high scatter of elongation measurements, up to +/-8% absolute for total elongation and up to +/-5% for uniform elongation. Elongation measurement scatter was chosen as an appropriate parameter to analyse at both laboratory and industrial scales. Various 6xxx alloys, with Si/Mg ratios between 1 and 4, were tensile tested 1 to 10 days after quench. Three major findings were observed: 1) Elongation scatter decreases with natural ageing, reaching the typical measurement scatter within a few days; the scatter is reduced as the solid solution is depleted of Mg atoms by clustering and precipitation. 2) Increased ratio Si/Mg accelerates the stabilisation of the tensile curves and decreases the observed scatter of elongation. For particularly high Si contents (Si/Mg > 4) the serrations and elongation scattering are nearly absent. 3) The tensile instabilities are present despite a pre-ageing treatment.

Clear relation between Mg content and the occurrence tensile serrations was observed in various 6xxx alloys suggesting that the mechanism responsible for these instabilities is of the same nature as in 5xxx alloys.

[1] Influence of natural aging on the precipitation hardening of an AlMgSi alloy. Cuniberti, A., et al. 527, 2010, Materials Science and Engineering , Vol. A, pp. 5307-5311

[2] Propagative instabilities: an experimental view. Ling, C.P., Venkadesan, S. et McCormick, P.G. 1993, Scripta Metallurgica et Materialia, Vol. 29, pp. 1159-1164.

Modeling Strain Hardening in Al Alloys: Effects of Solutes and Microstructure Across Binary and Technical Alloy Systems

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B2_4, U2 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

Understanding the influence of microstructure on the evolution of dislocations is fundamental for accurately simulating material behavior during plastic deformation. This study investigates the effects of solutes, clusters and precipitates on the strain hardening behavior of aluminum alloys. Compression tests are performed on the aluminum alloys 6016 and 6061 after various artificial and natural aging treatments, as well as on two binary systems, AlSi and AlMg, which are solutionized to evaluate their fundamental microstructural properties. This approach assesses how changes in solute concentration and microstructural states affect dislocation dynamics, particularly focusing on dislocation generation and annihilation processes critical for work-hardening and dynamic recovery.

Measured flow curves are modeled using the thermo-kinetic software package MatCalc and an extended Kocks-Mecking approach to evaluate the dependency of model parameters on the material state. The study specifically examines the roles of silicon (Si) and magnesium (Mg) solutes on the dislocation behavior, emphasizing their impact on the mechanical response in aluminum. The findings are cross-referenced with state-of-the-art constitutive modeling theories, offering enhanced insights into the interaction between microstructure and deformation behavior. This work contributes to a deeper understanding of how tailored microstructural engineering can improve formability and overall performance in aluminum alloys.

In-situ synthesis of Metal Matrix Composite (MMC) by Laser Powder Bed Fusion

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B2_4, U2 Room (Level 0), septembre 15, 2025, 17:00 - 19:00

The in-situ synthesis of Aluminium Matrix Composites (AMC) via the Global Reactive Synthesis (GRS) has already been demonstrated as a promising approach to control reinforcement size and distribution, as well as to obtain sharp matrix/reinforcement interface. Based on the use of chemical precursors, the GRS is driven by controlled reactivity and thermodynamics enabling the in-situ formation of both the matrix and the reinforcement under basic geometries (cylinders or plates). It has been applied successfully to conventional AMCs like Al-TiC [1] and Al-TiB₂. It has also paved the way to a new class of AMCs and the most advanced studies have been focused on Al-Tau3 AMC, where Tau3 is a ternary borocarbide (Al₃B₄₈C₂) [2,3]. Nowadays the challenge is to combine both the GRS and novel Additive Manufacturing techniques in order to get near-net shape pieces of AMC with complex geometries, where both the matrix and the reinforcements are formed in-situ during the manufacturing process.

The synthesis of AMC via GRS was studied with the Laser Powder Bed Fusion (LPBF) and focused especially on the Al-B-C ternary system. In this talk, we will present the interesting and complex microstructures so obtained and we will discuss the different process parameters, such as precursor composition, high heating and cooling rate, laser speed and power that influence the phases formed, their sizes and distributions as well as their morphologies. Two main AMC will be presented: Al-AlB₂ AMC from a precursor mixture of 98 %wtAlB₂-2%wtC and the Al-Tau3 AMC from a 90 %wtAl-9.8 %wtAlB₂-0.2%wt C mixture.

References

- [1] N. Samer et al., Composites Part A: Applied Science and Manufacturing, 2015, 72, 50-57.
- [2] Samer, Nassim. PhD thesis (French), Materials. Lyon, 2016.
- [3] O. Dezellus et al., Patent FR1556859, 2017

Laser-ultrasonic characterization of additively manufactured TiNb alloys with low elastic moduli

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B2_6, U2 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

TiNb-based alloys are highly promising for biomedical applications, such as hip implants. Their key property is a low elastic modulus, which prevents stress shielding caused by a mismatch between the elastic moduli of bone and the implant. Metastable Ti alloys achieve the lowest elastic moduli while having complex multi-phase structures containing alpha, beta, and omega-Ti phases. Various alloying elements strongly influence the phase composition and the resulting elastic moduli, where even slight changes in the element combinations can lead to significant changes in material properties. Additive manufacturing is particularly advantageous in this context, as it enables the production of a diverse range of alloys from elemental powders. In this contribution, we used laser-ultrasonic techniques to study the elastic properties of additively manufactured TiNbZrO and TiNbSnFe alloys with varying compositions. By laser resonant ultrasound spectroscopy, we determined elastic moduli and the level of elastic anisotropy from resonant spectra of millimeter-sized samples. Besides that, scanning acoustic microscopy and transient grating spectroscopy were used to reveal the local variations in elastic properties. It was found that the lowest elastic moduli are achieved in the alloys with a low amount of the stiff omega phase, which simultaneously have a composition near the stability limit of the parent beta phase.

Investigation on the interactions between nucleation, grain growth, and particle dispersion in magnesium-SiC nanowhiskers composites

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B2_7, U2 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

Magnesium and its alloys reinforced with SiC nanowhiskers are promising candidates for lightweight, high-strength metal matrix composites, particularly in structural applications within the aeronautics, aerospace, and lightweight vehicle industries. Despite their potential, achieving a uniform dispersion of reinforcing particles within the metal matrix and understanding the interphase between the components remains a significant challenge. Factors such as nanoparticle agglomeration, dispersion techniques, interfacial secondary phases, and nucleation and solidification dynamics all play critical roles.

This research focuses on achieving well dispersed SiC nanowhiskers particle in Magnesium using melt stirring and die casting method. Since the as-received SiC nanowhiskers are heavily agglomerated, a particle loosening pre-treatment is essential. This optimised process can significantly reduce the agglomerate size, promoting much better dispersion during composite manufacture. Metallography and SEM-EDX analyses reveal that the particle loosening pre-treatment successfully minimise the nanoparticle agglomerates, breaking them down into individual particles and thereby improving their dispersion. With smaller particle sizes, there still has a tendency for those nanoparticles to be swept toward grain boundaries during the metal solidification, which is not desired in the composite microstructure design as the nanoparticles won't act as effective reinforcements at grain boundaries. A good understanding of the interaction between the nanoparticles and the metal melt solidification front is therefore needed to further guide the material microstructure design.

Synchrotron-based techniques, such as Diffraction Contrast Tomography (DCT) and Phase Contrast Tomography (PCT), are therefore employed in this study to observe particle distribution and position relative to grain and grain boundaries. These analyses indicated that particle distribution was predominantly concentrated at grain boundaries in both pure Mg and AZ91 alloys, which may be explained by the effect of Al element additional to the interface formation in the composites. Furthermore, TEM analysis is also conducted to observe the atomic level of the interface between the SiC nanowhiskers with the metal matrix, both inside the grains and at the grain boundaries.

Aging of ZA63 alloy containing stable quasicrystal phase

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B2_7, U2 Room (Level 0), septiembre 16, 2025, 17:00 - 19:00

The stability of the quasicrystalline i-phase in the Mg-6Zn-3Al (wt%, ZA63) magnesium alloy presents an exciting opportunity to develop cost-effective quasicrystal-strengthened magnesium alloys. In this presentation, we highlight the growth behavior of the i-phase during aging and its effects, as revealed through various characterization techniques, including microhardness measurements, electron microscopy, small-angle X-ray scattering (SAXS), laser-based resonant ultrasound spectroscopy (RUS), and X-ray microscopy. Additionally, the fatigue crack growth rate and fracture toughness of this alloy are investigated, with crack propagation analyzed using scanning electron microscopy (SEM), X-ray microscopy, and electron backscatter diffraction (EBSD). Cracks resulting from the anisotropy of thermal expansion during quenching are also examined to identify potential weaknesses that may impact the industrial application of this alloy.

Microalloying Al-Mg-Si alloy with indium as a new approach to control precipitation processes

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B2_2, U2 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

Microalloying has been proven to be an effective method for modifying conventional precipitation hardening in aluminium alloys. The constant quest for novel compositions accelerates the development of alloys with an improved strength-to-density ratio. This study specifically focuses on the addition of indium to a commercially available 6082 alloy. The manufacturing procedure involves melting the master alloy with the addition of new alloying elements, a process that is straightforward and applicable, for instance, during recycling processes.

The 6082 alloy has been remelted with various amount of indium and then casted into copper moulds. The heat treatment process, crucial for precipitation hardening, revealed that indium does not significantly affect hardness following direct aging compared to the original alloy. However, an alternative treatment, including room temperature storage (common in industrial practice), indicated that for a certain indium content, it is possible to restore the peak hardness level typical of the non-alloyed 6082 alloy with a simple one-stage aging process. This unexpected effect was thoroughly investigated using techniques such as differential scanning calorimetry and atomic resolution scanning electron microscopy. The study demonstrated that the properties of indium, including its melting point, vacancy binding energy, and solubility in aluminium, have a critical impact on the nucleation and growth of strengthening phases in the AlMgSi system. The overall precipitation sequence depends on the diffusion efficiency of the indium which binding energy to vacancies is the highest within alloying elements. Two factors influence tendencies to form indium clusters and deplete solid solution from vacancies – indium content and room temperature storage time. It has been shown that the former should be kept small when direct ageing is required but the latter enable to mitigate unwanted natural ageing hardness loss. The tendency to form clusters with other alloying elements and vacancies appears to be a potent tool for the development of new alloys and heat treatment procedures aimed at achieving controllable precipitation strengthening

Effect of iron on the crystallographic texture and mechanical properties of extruded 6xxx aluminium alloys

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B2_2, U2 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

This study examined the effect of three different iron (Fe) levels on the grain structure and texture of AA6xxx extrusion alloys. Microstructural analysis was carried out to measure the micro texture and the results were correlated with tensile and bending properties. Results demonstrated that the fragmented intermetallic particles after extrusion were found to act as the nucleation sites of new grain refinement changing the dominant texture from standard deformation and/or recrystallisation textures both at the centre of thickness and peripheral grains. In alloys with dispersoid-forming elements such as Mn, fibre texture components were dominant with a small fraction of Cube recrystallisation that increased from 7 to 10% by increasing iron content from 0.2 to 0.5 wt.%. In the recrystallized alloys the Cube texture was dominant at the centre of profile thickness accompanied by a fraction of Rotated Cube texture, which increased with Fe content. The thickness of the peripheral grain surface layer decreased with increased Fe content in the fibrous alloy due to increased amount of dispersoid precipitation which prevents grain growth. The tensile properties of both alloys were reduced by increased Fe content due to consumption of Si in Fe-based intermetallic compounds which led to reduced free Si required for precipitation hardening.

Microstructure evolution via 3D printing parameter development of Scamallo/SiC metals matrix composite

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B2_4, U2 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

Lightweighting has long been a critical focus in industries like aerospace, automotive, and healthcare. Two common approaches to achieving this are using materials with higher specific strength and employing well-ordered porous structures. Among metallic materials, aluminium alloys play a key role due to their light weight, strength, heat dissipation, corrosion resistance, and ease of processing. Composite material development holds significant potential in meeting lightweighting goals. Silicon carbide (SiC), a third-generation semiconductor, is often chosen as the reinforcing phase for its high strength, thermal conductivity, and resistance to high temperature and pressure. Building on prior research in developing aluminium-magnesium-scandium alloys, this study incorporates SiC to enhance both mechanical and thermal properties. However, manufacturing these composites poses challenges. Traditional processes are costly and struggle with structural complexity. Layer-based manufacturing technologies, particularly Powder Bed Fusion (PBF) in metal additive manufacturing, address these limitations and have become essential in lightweight metal applications. Compared to traditional methods, adding SiC to aluminium-magnesium-scandium alloys through additive manufacturing enables more uniform SiC distribution in the matrix, improving reinforcement effects. However, issues with aluminium-silicon carbide intermetallic compounds can weaken material strength and elongation. To address this, the study will optimize printing parameters for aluminium-magnesium-scandium-SiC composites using Selective Laser Melting (SLM) technology. A key objective is to minimize intermetallic compound formation by identifying optimal printing parameters. The mechanical properties—including strength, Young's modulus, energy absorption, and thermal conductivity—will be evaluated through tensile, compression, and thermal conductivity tests on all samples. This work aims to enhance the performance of lightweight Aluminium-SiC composites and expand their application potential in advanced industries. And moreover we also look forward to find out the relationship between the printing paramerter amd mechanical properties and microstuctrue

Tailoring strength, ductility and directionality in laser powder bed fusion processed Ti-6Al-2Sn-4Zr-2Mo-Si and Ti-6Al-4V via post-process heat treatments

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B2_6, U2 Room (Level 0), septiembre 16, 2025, 14:30 - 16:30

Laser Powder Bed Fusion (LPBF) of the titanium alloys Ti-6Al-2Sn-4Zr-2Mo-Si (Ti-6242) and Ti-6Al-4V (Ti-64) results in an unfavorable as-built microstructure, necessitating post-process heat treatment to tailor mechanical properties for specific technological applications. For Ti-6242, which is designed for high-temperature applications up to 540 °C, research on suitable post-LPBF heat treatments remains limited. Furthermore, in additive manufacturing, variations in processing parameters and feedstock materials complicate the comparison of studies and literature, including a direct comparison of both alloys regarding their heat treatment response, is lacking.

At this point the present work picks up. This study aims to evaluate promising post-LPBF heat treatment strategies for each alloy and enable a direct comparison of their microstructural and mechanical response, particularly in terms of strength, ductility, and anisotropy. Therefore, various heat treatments were selected based on literature and applied to LPBF-processed samples. More precisely, the alloys were produced using alloy-specific processing parameters, and a selection of heat treatments following different approaches (stress relief, $\alpha+\beta$ annealing, α -globularization, subsequent ageing) were conducted in a vertical furnace flushed with argon gas. The as-built material as well as 14 heat treated material states were characterized. Microstructural characterization was performed using scanning electron microscopy (SEM) and high-energy X-ray diffraction (HEXRD). Mechanical properties were assessed through hardness and tensile testing, with tensile tests conducted in two loading directions to evaluate the directional dependence of mechanical properties.

The study revealed that heat treatments decomposed the initial fully martensitic microstructure, forming $\alpha+\beta$ microstructures. A broad spectrum of mechanical properties could be achieved through various heat treatments in both alloys. Coarser microstructures tended to be more ductile but less strong, following a general strength-ductility trade-off. Ti-6242 showed a greater variation of the uniform elongation and elongation at fracture for a given change in strength compared to Ti-64. Ti-6242 exhibited a highly elongated β -grain structure that persisted after all heat treatments. This resulted in a significant anisotropy of the ultimate tensile strength and yield strength. In contrast, Ti-64 did not show strong directionality.

Overall, the study enables a direct comparison of the heat treatment response of Ti-6242 and Ti-64, showing similar trends in both alloys. Specialized heat treatments enable the microstructure and mechanical properties to be tailored towards application specific requirements.

The effect of deformation on Al-Mg-Si(-Cu) alloys

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 15, 2025, 13:15 - 14:30

By studying the microstructure of aluminium alloys, we aim to optimize thermomechanical processing, possibly allowing for better performance while maintaining their recyclability. Al-Mg-Si(-Cu) alloys are commonly used in automotive, aerospace and construction due to their combination of lightweight properties, strength and corrosion resistance. These alloys strengthen via precipitate hardening, where fine particles hinder dislocation movement. Small additions of alloying elements like zinc and iron can drastically alter the precipitation in a material, changing the performance. This is a common challenge when it comes to recycling of aluminium. Higher recycling rates require broader compositional windows and tolerance for impurities, and it can be crucial to find thermomechanical processing routes optimized for high scrap content.

Plastic deformation improves the tensile strength by introducing dislocations and changing the precipitate formation, but the mechanisms behind are not yet fully understood. In this study we look at two different processing routes, involving plastic deformation after extrusion; the first involves cold rolling before heat treatment and the second has an additional heat treatment before the rolling. We use transmission electron microscopy (TEM) techniques such as conventional bright-field and dark-field TEM along with high-angle annular dark-field scanning TEM (HAADF-STEM) to quantify precipitate size, density and type. The aim is to link the mechanical properties to the microstructure, with an emphasis on sustainable alloy design.

SiC nanowhisker reinforced lightweight metal composites: a detailed study of the interface

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B2_4, U2 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

The interest to use nanoparticles and nanocarbon to reinforce light metals has attracted attention in recent years due to their potential application as lightweight high performance materials for both environmental and economical benefit, in applications including aeronautics and automotive. Challenges in successfully producing lightweight metal composites are to achieve a homogenous dispersion of nanoparticles in the metal matrix and to build a suitable interface between those nanoparticles and lightweight metals.

Nano- β -SiC is a promising reinforcement for Mg-Al alloy matrices. However, past research paid less attention to the interfacial behaviours between β -SiC and Mg-Al matrix, with most reports stating the interfaces were 'clear' and exhibited an 'absence of interfacial reactions'.

In this study, β -SiC nanowhiskers were introduced into Mg AZ91 matrix. The interfacial behaviours in this nanocomposite were thoroughly investigated using multiscale characterisation techniques including X-ray phase contrast tomography (X-PCT), scanning transmission X-ray microscope (STXM) and advanced electron microscopy. The analysis identified a less commonly reported ternary carbide, T2-Al₂MgC₂, adjacent to the nano-SiC, providing strong evidence of interfacial reactions during manufacturing. The effects of this ternary carbide on the composite microstructure, e.g. phase distributions and interfacial texture were also investigated. This comprehensive understanding of the interface of the β -SiC reinforced Mg and its correlation to nanocomposite properties is crucial for optimising manufacture and provides key inputs for modelling studies on interfacial mechanics.

Impact of microstructure heterogeneities and casting defects on the very high cycle fatigue of Aluminium components

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B2_2, U2 Room (Level 0), septiembre 15, 2025, 10:50 - 13:10

Aluminium cast components play a key role in achieving sustainability goals and CO₂ emission targets due to their low specific weight. However, this great potential remains partially untapped, as the limited fatigue strength of cast aluminium components shortens their service life and requires high safety reserves in component design. The main reasons for early failure of cast aluminium components in the very high cycle fatigue (VHCF) regime are casting defects and microstructural heterogeneities, including secondary dendrite arm spacing (SDAS), eutectic silicon, and porosity. The inhomogeneous cooling conditions in complex industrial components lead to locally different characteristics of these inhomogeneities, as could be shown using the example of cylinder heads and engine blocks for automotive engineering. Pores were identified as particularly critical, as they can serve as crack initiation sites and can lead to early failure, especially in the case of large, fissured shrinkage pores. Avoiding shrinkage pores through sufficient feeding is usually not possible with technical components due to multidirectional solidification. Therefore, a targeted modification of the pore shape and size was carried out by hydrogen up-gassing of the melt prior to casting, aiming to reduce large fissured shrinkage pores by small spherical hydrogen pores.

Ultrasonic fatigue testing and resonance bending crack propagation tests were performed on cast aluminium specimens with different alloy composition, cooling conditions and pore modifications in order to investigate correlations between microstructure and fatigue performance. High resolution analysis, including μ -CT, STEM and EBSD mapping, revealed that cracks are likely to initiate at near-surface fissured pores and propagate along {111} slip planes. Large α -aluminium cells as well as a short SDAS have a positive impact on crack propagation. Spherical hydrogen pores are beneficial compared to fissured shrinkage pores, as they can retard crack propagation by crack deflection, crack splitting and crack tip blunting. The insights provide a deeper understanding on fatigue mechanisms in cast aluminium alloys and demonstrate the potential of future microstructure optimization for improved fatigue life.

The effect of Zn on grain boundary segregation and IGC in Al-Mg-Si-Cu alloys

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), september 15, 2025, 13:15 - 14:30

The inclusion of Cu and Zn impurities are often unavoidable in the recycling process of 6xxx aluminium alloys, both of which may result in a decrease of the corrosion resistance of the alloy. Corrosion experiments have however found that the addition of Zn to alloys already containing Cu may in some cases improve IGC resistance. In this study a series of Al-Mg-Si-Cu alloys with varying amounts of added Zn were investigated, with a particular focus on the influences of the impurity element on the solute segregation at grain boundaries as well as the atomic structure and chemistry of age hardening precipitates.

The alloys were investigated using a combination of APT and various (S)TEM techniques, including conventional bright field/dark field, STEM-EDS and HAADF-STEM. To produce site specific APT samples a Xe-Plasma FIB equipped with an EBSD detector was utilized, which allowed high angle grain boundaries to be targeted and analyzed. The results of the characterization experiments were then linked to the results of corrosion tests. The underlying mechanism on the influences of Cu and Zn on the intergranular corrosion (IGC) behaviors are discussed.

Elimination of stretcher strain marks in high-Mg Al-Mg alloys: deformation behavior and microstructural insights in H16 temper

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The occurrence of stretcher strain marks (SSMs), also known as Portevin–Le Chatelier (PLC) bands, presents a challenge in high Mg content Al-Mg alloys, affecting both surface quality and mechanical properties. This study investigates the effect of Mg content on the deformation behaviour of Al-6Mg, Al-7.5Mg, and Al-8.5Mg alloys in H16 temper (60% cold rolled condition). The alloys were produced using Eco-Al processing, where Mg was alloyed with a Mg+Al₂Ca master alloy to enhance melt stability. Tensile testing and Digital Image Correlation (DIC) analysis reveal a direct correlation between Mg content and SSM formation. Al-6Mg exhibited early SSM initiation, while Al-7.5Mg showed a delayed onset with localized strain concentration. In contrast, Al-8.5Mg exhibited no evidence of SSMs, demonstrating uniform deformation, enhanced strength, and greater elongation than Al-6Mg and Al-7.5Mg. This novel finding suggests that the formation of SSMs can be eliminated in high Mg alloys processed to H16 temper, significantly improving mechanical stability and surface quality. X-ray Diffraction (XRD) and Full Width at Half Maximum (FWHM) analysis indicate that dislocation density increases with Mg content. Electron Backscatter Diffraction (EBSD) provides insights into texture evolution, while Transmission Electron Microscopy (TEM) examines dislocation morphology. These findings offer valuable insights into strain localization and strengthening mechanisms in high Mg Al-Mg alloys, contributing to developing materials with superior mechanical performance and surface integrity for industrial applications.

Structural application focused characterization of Continuous Fibre based Aluminium MMCs

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B2_4, U2 Room (Level 0), septiembre 15, 2025, 17:00 - 19:00

Metal Matrix Composites (MMC) are viewed as a better recyclable alternative to Polymer Composites, however established manufacturing methods are not comparable with the time and process efficiency of the latter. and remains a challenge. Over the past decades Continuous fibre based Metal Matrix MMCs have been intermittently used for bespoke structural applications in the aerospace and automotive industries, alongside Particulate MMC. Along the route to establishment of better standardized production methods lie several challenges including the definition of befitting applications. While Aluminium MMCs offer the advantage of weight and relative sustainability when compared with Titanium MMCs, there is little published data for Continuous Fibre based Aluminium MMC from the perspective of structural application at an end-user. A discussion focused upon salient observations from testing of two approaches to this type of MMC is presented. The approaches in focus are: (1) Solid-state processed Silicon Carbide fiber based in Al-Mg-Si (6061 type) alloy. (2) Liquid state processed Alumina fibre in Al-Mg-Si alloy and primary Aluminium. Initially targeted applications, resultant microstructure, select material properties and expectations for maintainability in-service are focused upon.

Creep resistance of metal-ceramic composites based on austenitic stainless steel and recycled magnesia particles

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B3_1 - Novel Materials, Z1 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

In this study, creep properties of potential materials for carbon-free electrodes used in the fused-salt electrolysis of primary aluminium are investigated. The examined metal-ceramic composites feature an austenitic stainless-steel matrix (60 vol.%) reinforced with coarse-grained recycled magnesia particles (40 vol.%) sourced from spent MgO-C refractory lining bricks. These composites were produced using the field-assisted sintering technique (FAST), as this processing route results in a low porosity. A pre-oxidation of the composites at 900 °C was found to promote the formation of a protective MgO-FeO solid solution surface layer, enhancing corrosion resistance against both molten aluminium and molten cryolite [1,2].

Creep experiments under compressive loading conditions were conducted at 900 °C to compare composites reinforced with recycled magnesia to reference composites reinforced with fresh-fused magnesia. Results indicate that the recycled nature of the particles does not impair creep resistance. On the contrary, composites containing recycled magnesia particles demonstrated superior creep strength due to their smaller, more uniform particle size distribution within a given size fraction. This is the result of mechanical crushing steps during the recycling process. The influence of a pre-oxidation on the creep resistance was examined. Furthermore, variations in the volume fractions of steel and magnesia were evaluated for their impact on creep strength. Microstructural deformation mechanisms were characterized using back-scattered electron imaging and electron backscatter diffraction measurements in a scanning electron microscope.

In summary, this study compares the creep properties of coarse-grained steel-ceramic composites reinforced with either fresh-fused or recycled magnesia particles and examines how the narrower and more homogeneous particle size distribution of the recycled reinforcements enhances creep resistance.

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Modeling of precipitation processes in multicomponent alloys

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B3_1 - Novel Materials, Z1 Room (Level -3), septembre 17, 2025, 10:30 - 13:10

The time evolution of a precipitate population under non-isothermal conditions in a multicomponent alloy is presented. The tracking of this population is carried out using a particle size distribution model, and calibrated with experimental measurements performed by Atom Probe Tomography reported in the literature.

The model incorporates the thermodynamic properties of the alloy extracted from a database. Local equilibrium at the interface is considered, including the curvature effect. The analytical solution of the unsteady diffusion problem for a non-diagonal diffusion matrix, previously validated by a numerical solution for an isolated precipitate, is employed to determine the growth kinetics.

A new iterative algorithm is proposed to fix the interfacial operating point. This point is defined by (i) the equilibrium tie-line between phases and (ii) the solute diffusion flux balance on each side of the interface. An approximation related to the diffusion flux for species of large diffusion coefficients is applied to overcome the difficulties associated to uniform solute profile. It enables an efficient computation of the solution.

The model is applied to the growth of gamma prime phase precipitates in a gamma phase matrix for the Inconel 738 superalloy. This application highlights the impact of common simplifications found in the literature, such as assuming a diagonal diffusion matrix or a steady-state diffusion regime. The potential applications of the model will also be discussed, including the tracking of solid-state precipitation kinetics in direct coupling with an additive manufacturing process. The presented model is integrated into the PhysalurgY software library developed at CEMEF.

Optimizing the strength of Ni-based superalloy Udimet 720Li through tailored heat treatments

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B3_4 - Nickel based superalloys II, Z1 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

The outstanding mechanical properties of superalloys are largely influenced by their microstructure, such as grain size, volume fraction, morphology, and size distribution of the γ' precipitates. The microstructure is determined by the heat treatment, e.g. solution annealing, quenching, and subsequent aging. To study the effect of the heat treatment process, four different solution annealing temperatures, four different cooling rates, and two different aging steps were used to produce diverse microstructures in the polycrystalline, cast-and-wrought disc alloy Udimet 720Li. Characterization of the microstructures is carried out by scanning electron microscopy and transmission electron microscopy investigations. The mechanical properties were evaluated using Vickers hardness testing and compression tests at room temperature. A sub-solvus solution annealing temperature and an intermediate cooling rate led to the highest yield strength. The super-solvus solution annealing temperature led overall to the lowest yield strength at any cooling rate. This research resulted in a better understanding of the effects of the heat treatment process on the mechanical properties and microstructure, which will be useful for designing optimal heat treatment processes.

Effect of rhenium on rotating bending fatigue properties of single crystal superalloys

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B3_3 - Single crystals, Z1 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Aero-engine blades undergo fatigue damage due to cyclic stress-strain deformation during service. Rhenium (Re) is an important strengthening element for superalloys. However, there is limited information in the literature regarding the influence of Re on the rotating bending fatigue behavior of single crystal (SX) superalloys, and the associated damage mechanism remains unclear. In this study, a SX superalloy without Re (referred to as the 0Re alloy) and a SX superalloy with 2 wt.% Re (referred to as the 2Re alloy) were used for comparison. The rotating bending fatigue behaviors of both alloys were evaluated at 800 °C and 900 °C. Detailed microstructure characterization was performed using scanning electron microscopy (SEM) and transmission electron microscopy (TEM).

It was found that most of the fatigue crack initiation sites were pores near the surface at 800 °C, and the rotating bending fatigue strength of the 2Re alloy increased from 380 MPa to 410 MPa compared to the 0Re alloy. In the 0Re alloy, γ' precipitates sheared by stacking faults were observed, while dislocations moved through the γ channel by bowing and cross-slip in the 2Re alloy. The addition of Re increased the misfit in the superalloy and hindered dislocation movement in the γ matrix, leading to improved rotating bending fatigue performance of the alloy. As the fatigue testing temperature increased, the fatigue crack initiation sites gradually shifted from pores to the surface, indicating that oxidation damage became dominant during fatigue. It can be seen that oxidation cracks of both alloys were lower at 800 °C. However, oxidation cracks on the surface of the 2Re alloy significantly increased compared to those in the 0Re alloy at 900 °C, due to the detrimental effect of Re on the oxidation resistance of superalloys, which led to a decrease in rotating bending fatigue strength.

Keywords: Ni-based single crystal superalloy; Rhenium; Rotating bending fatigue; Deformation mechanism

Development and enhancement of a physics-based mean-field creep model for martensitic 9-12% Cr steels with application to Grade 91

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

"Creep deformation poses a significant challenge to the durability of components in high-temperature applications, with martensitic 9% Cr steels, such as Grade 91 (9Cr-1Mo), serving as a widely used standard material in industry due to its excellent high-temperature strength, manufacturability, and creep resistance. At our institute, a physics-based mean-field creep model was developed based on data for pipe material P91 at 650°C under a constant stress of 70 MPa. This model was subsequently extended to other martensitic 9-12% Cr steels, including pipe material P92 (9Cr-2W-Mo), rotor material FB2 (9Cr-1Mo-1Co), and another novel Cr steel, resulting in further optimization, enhancement, and validation of its predictive capabilities. These advancements are now being specifically adapted for P91, including a refined description of diffusion mechanisms and an improved model for Zener pinning, which increases the accuracy of simulated subgrain coarsening. Precipitate data stem from re-evaluated thermo-kinetic simulations in software MatCalc. Additionally, the model is being extended to simulate creep behaviour at temperatures below 650°C, as these are more relevant for practical applications compared to higher temperatures. The enhanced model enables accurate predictions of creep curves, microstructural evolution, and time-to-rupture behaviour, demonstrating excellent agreement with experimental data. This framework not only advances the understanding of creep mechanisms in P91 and related steels but also serves as a powerful tool for optimizing high-temperature materials and supporting material design in both research and industrial applications. Implementation of the model into the developed creep behaviour software CreeSo is planned.

Research Progress in High-Temperature Titanium Matrix Composites and Their Precision Thermoforming Technology

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B3_5 - Titanium alloys, Z1 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Titanium matrix composites (TMCs) have low density, high specific strength, excellent corrosion resistance, as well as superior oxidation resistance at higher temperatures, which can effectively compensate for shortcomings of existing high-temperature alloys, such as their high density or low service limit temperature, and show broad application prospects in aerospace, automobile manufacturing, weapon equipment, and biomedicine. However, due to its unique properties, the thermoforming process faces many challenges. For example, casting defects such as interface reactions, shrinkage porosity, and misrun are easily formed during the investment casting process because of the low fluidity, significant solidification shrinkage, and high chemical reactivity. Additionally, the addition of reinforcements will increase the difficulty of the thermal processing of TMCs, so it is extremely challenging to prepare a large-size thin sheet.

In this work, an in-situ particle-reinforced high-temperature TMCs resistant to 700 °C were effectively developed by optimizing the composition design on the basis of a 650 °C short-time high-temperature titanium alloy. A specific kind of aerospace cabin and skeleton were developed using investment casting technology. After heat treatment, the tensile strength of the part at room temperature is 1200 MPa, with a 7% elongation. At 700 °C, the tensile strength is 650 MPa, and it is 560 MPa at 750 °C. Furthermore, the TMCs thin sheets of 2060 × 680 × 2 mm were prepared by the pack ply-rolling technique, which is the largest size of TMCs sheets reported. Notably, the tensile strength of the sheet at 700 °C is 592 MPa following multi-step heat treatment, which can effectively satisfy the service requirements. In the near future, we have additionally prepared 2150×650×0.8 mm sheets, which will better meet the real engineering demands. More importantly, this work provides novel guidance for future materials design and production to satisfy specific engineering requirements.

Hybrid Reinforced Ferritic Alloy Fabricated by Mechanical Alloying and Spark Plasma Sintering: Preparation and Selected Properties

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Oxide dispersion-strengthened (ODS) ferritic steels are advanced materials characterized by outstanding high-temperature strength, creep resistance, and corrosion resistance. Their primary method of production is powder metallurgy, which includes mechanical alloying (MA) followed by consolidation, most commonly through hot isostatic pressing (HIP) or hot extrusion (HE). ODS steels are typically reinforced with Y_2O_3 , which dissolves into the ferritic matrix during MA and facilitates the formation of ultrafine complex oxides containing Y and Ti, which provide remarkable functional properties and make them highly suitable e.g., for advanced nuclear energy applications. In this study, the reinforcement strategy was modified to a hybrid approach by incorporating both conventional Y_2O_3 and additional Al_2O_3 nanoparticles to enhance material performance. A production method was developed for Hybrid Reinforced Ferritic Alloys (HRFAs) with a fixed Y_2O_3 content and varying amounts of Al_2O_3 , using MA for powder preparation and an alternative consolidation method - spark plasma sintering (SPS). The aim was to explore whether this hybrid reinforcement approach could further boost the already exceptional characteristics. The fundamental properties of the alloys were investigated, focusing on microstructure and surface characteristics through techniques such as SEM, EDX/EDS, AES, and XPS. Additionally, their corrosion behavior in chloride-ion-containing environments was analyzed using open circuit potential (OCP), linear sweep voltammetry (LSV), and electrochemical impedance spectroscopy (EIS).

Influence of cobalt content on the grain growth and recrystallization kinetics of VDM Alloy 780

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B3_2 - Nickel based superalloys I, Z1 Room (Level -3), septembre 17, 2025, 14:30 - 16:30

VDM Alloy 780 is a newly developed Ni-Based superalloy aiming service temperatures up to 750°C. This alloy is a derivative of Alloy 718, where cobalt content is raised at the expense of iron and the Al/Ti ratio is modified to increase its microstructural stability at higher temperatures while maintaining its mechanical properties in this temperature range.

Raising cobalt is expected to reduce the stacking fault energy (SFE). Low values of SFE may affect the movement of dislocations during deformation by modifying mechanisms like dislocation dissociation, cross-slip, dislocation climb and deformation twinning. This is expected to directly affect the dynamic and post-dynamic recrystallization kinetics of the alloy. Also, alloying elements in solid solution may also influence the grain boundary mobility, affecting the grain growth behavior of the alloy.

The presented work aims to study the dynamic (DRX) and post-dynamic (PDRX) recrystallization, and grain growth (GG) kinetics in supersolvus domain varying the cobalt content in VDM Alloy 780. Cobalt contents from 0 to 25 %wt. have been investigated, where cobalt is replaced by nickel in the weight balance.

To analyze the microstructure evolution as a function of heating time, annealing tests have been carried out at 1050°C with different holding times followed by water quenching. The mean equivalent grain size of a statistically significant population of grains has been calculated and compared. Initial experimental observations exhibit that GG seems to be impacted by the changes in chemical composition, being slower for higher cobalt contents.

To analyze the recrystallization kinetics, cylindrical samples have been compressed up to various strain levels and using different strain rates at 1050°C. Immediate water quenching after deformation was performed to study DRX. Alternatively, samples were left after deformation at the test temperature for different holding times to study PDRX. According to the first experimental results, DRX kinetics seem to be relatively slower for materials with higher cobalt contents. However, their PDRX behavior is observed to be relatively fast.

Here we will discuss the effects of Co content on the microstructure mechanisms during recrystallization process in VDM Alloy 780.

Effect of withdrawal rate and wall thickness on the microstructure of LEKv – 94 single crystal nickel-based superalloy

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B3_3 - Single crystals, Z1 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

LEKv – 94 is a variant of the single crystal (SX) nickel-based superalloy LEK-94, which has different concentration of refractory elements Re, W and Ta to the original. Due this modification, its SX castability is previously checked through Bridgman technique. Furthermore, process parameters that affect the solidification rate and temperature gradient, as withdrawal rate and wall thickness are changed and their influence on the microstructure and microsegregation of elements are observed. Thin-walled and cylindrical samples are casted under withdrawal speed (V) of 1 to 10 mm·min⁻¹ and single crystals were obtained between 1 and 5 mm·min⁻¹. Crystallographic orientation [001] was obtained for all SX, and the maximal crystal deviation related to it was 15°. The primary dendrite arm spacing (PDAS) has remained under 450 µm for both SX geometries. Tertiary dendrite arms were observed between 3 and 7 mm·min⁻¹ and the lowest primary dendrite arm spacing (PDAS) was found for 5 mm·min⁻¹. The thin-walled areas (0.4 mm and 2.0 mm) showed a reduction of PDAS values compared to cylindric geometry Ø 15 mm. In all combinations, microsegregation analysis showed that elements Co, Re, and W segregate to the dendrite core with Al, Ni, Cr, Mo, Ta, and Ti partitioning to the interdendritic regions.

The influence of spark plasma sintering parameters on the structure and properties of NiAl based materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 17, 2025, 13:10 - 14:30

Sintering is a thermally activated process that depends on many technological factors, such as temperature, time, external pressure, atmosphere, etc. [1]. The progress of sintering, measured by an increase in the cross-sectional area of the intergrain neck and a decrease in the distance between the centres of two adjacent grains, leads to an increase in the density of the material. A great increase in interest in field assisted sintering techniques has been evident in recent years. The main advantage of the Spark Plasma Sintering technique is the direct resistive heating of graphite elements and electrically conductive powders [2]. Due to the high heating rates (up to 1000°C/min) and short dwelling time at the sintering temperature, the limitation of undesirable material reactions and structural transformations can be obtained.

The goal of the presented work was to investigate the changes in the microscopic and macroscopic parameters related to the microstructure of the NiAl and NiAl-Al₂O₃ composites and its dependence on the sintering parameters (temperature and pressure). The materials were densified using Spark Plasma Sintering method. The applying of diversified sintering parameters allowed to obtain a materials with different relative density (from 70.0 to 97.5%). The analyses included SEM investigations by electron backscatter diffraction to evaluate the crystallographic orientation of NiAl grains and microcomputed tomography to visualize the grain evolution at different stages of sintering, especially the grain size, shape and boundary contact features. The application of the electric current resulting in high temperature and the additional external loading leads to the significant changes in the structure of sintered materials, such as the occurrence of lattice reorientation resulting in grain growth, increase in the grain neighbors, or the evolution of grain ellipticity, circularity, grain boundary length, and fraction.

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High temperature oxidation behaviour of Ti-nitrides and O or N-enriched Ti model materials

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B3_5 - Titanium alloys, Z1 Room (Level -3), septembre 18, 2025, 14:30 - 16:30

Titanium-based alloys are widely used in the aeronautic industry for their high strength-to-weight ratio. However, their use is limited below 650 °C, due to issues like environmental embrittlement and poor creep resistance [1]. In high-temperature oxidizing environments, alongside TiO₂ scale formation, significant oxygen dissolution could occur in the alloy and lead to reduced ductility [2]. Nitrogen, from air, plays also an important role in the oxidation of Ti alloys [3,4,5,6]. Recent works suggested its beneficial effect on the oxidation resistance of some Ti alloys, due to the formation of nitrides and/or oxynitrides at the oxide/alloy interface [4,5,6], acting as diffusion barrier for oxygen. However, the formation mechanism of these nitrides/oxynitrides is unclear and the oxidation behaviour of Ti₂N is also unknown.

In order to shed some light on these phenomena, two sets of experiments were conducted. First, the oxidation behaviour in air of TiN and Ti samples enriched in O (concentrations from 0 up to 20 at. %) or N (5 at. %) was studied at 650 °C, for durations up to 1000 hours. The mass variation of each sample was recorded with time, during the oxidation tests. However, it was not possible to obtain a sufficiently pure Ti₂N sample to study in these conditions. So, a Ti-TiN diffusion couple (DC) was prepared by spark plasma sintering and was subjected to a heat treatment at 800 °C, under vacuum, for two months, to promote the formation of a Ti₂N layer (approximately 30 µm thick) at the Ti/TiN interface. The DC was then oxidized in air at 650 °C for 500 hours to evaluate the oxidation behaviour of all phases (Ti, Ti₂N and TiN). The oxidized samples were then characterized using X-ray diffraction, Raman spectroscopy and scanning electron microscopy with energy dispersive spectroscopy.

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A new model for particle pinning in 2d polycrystals

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B3_2 - Nickel based superalloys I, Z1 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Grain growth control is a critical factor in optimising the microstructure and properties of polycrystalline materials. This study presents a novel analytical model for predicting the effects of second-phase particle pinning on grain growth in a two-dimensional polycrystalline system. Unlike classical models on Smith Zener pinning, that focus mainly on limiting grain size, our approach also accounts for grain size heterogeneity, improving our understanding of microstructure stabilisation. Our findings reveal that particle pinning not only restricts grain expansion but also prevents the complete disappearance of smaller grains, resulting in bimodal grain size distributions. The model quantifies the interaction between grain boundaries and particles at equilibrium, predicting both the sizes and the fraction of large and small grains in the final pinned microstructure. Furthermore, the model highlights the significant influence of initial grain size on the final stabilized grain size, challenging conventional assumptions that limiting grain size is governed solely by particle size and volume fraction. Validation against full-field level-set simulations demonstrates very good agreement, confirming the model's predictive accuracy. The possible extension of this 2D model to 3D microstructures is explored. The ability of this approach to provide a simple yet robust framework for designing materials with tailored grain size distributions and improved performance is discussed.

Additive manufacturing of a high-temperature coating for aero-engine applications

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B3_2 - Nickel based superalloys I, Z1 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Traditionally, the production of metallic overlay and bond coatings for high temperature applications such as nickel-based superalloy blades in aero-engines is achieved by thermal spraying processes. In this study, we investigate the potential to produce such coatings by additive manufacturing processes that will allow the repair of such components on- or near-wing. In particular, the well-known overlay coating Ni-25Cr-6Al-0.4Y (at.%) was deposited by a laser-based directed energy deposition (DED) process directly on a nickel-based superalloy substrate. The primary aim is to investigate the microstructure in the as-built condition after the deposition. As such coatings are not traditionally produced by additive manufacturing processes, a multi-scale analysis was deployed to investigate the as-built microstructure. Electron backscatter diffraction (EBSD) revealed columnar grains consisting of columnar dendrites along the building direction. Scanning electron microscopy (SEM) and electron probe microanalysis (EPMA) revealed the presence of micro-segregation of Y and Al between the dendritic and interdendritic regions. Besides, no cracks were observed between the deposited coating and the superalloy substrate. Finally, atom probe tomography (APT) provided compositional information at near-atomic scale for various phases formed during the DED processing. The Y-rich regions observed by EPMA were further confirmed by APT, while other phases were also measured which revealed significant compositional differences at the nano-scale. These observations will be presented in detail and potential future steps for processing coatings by additive manufacturing techniques will be discussed.

Effects of laser parameter on the recrystallization temperature of additively manufactured IN718

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B3_2 - Nickel based superalloys I, Z1 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Recently, research on additive manufacturing (AM) technology has been actively pursued in high-value-added industries due to its potential to overcome the design limitations of conventional manufacturing methods, enabling a significant reduction in manufacturing time and a remarkable enhancement in performance. Manufacturing high-temperature gas turbine components represents one of the most effective fields for harnessing the advantages of AM technology, with active research primarily focusing on Ni-based, Co-based, and Ti-alloys. However, challenges arise in addressing property degradation such as crack formation, ductility reduction, and anisotropy before/after heat treatment, which must be overcome to expand their applications. In this study, IN718 specimens were fabricated using laser-based powder bed fusion (L-PBF) by varying laser power, laser scan speed, layer thickness, and hatch distance. The changes in recrystallization temperature according to each laser parameter were investigated after applying various solution heat treatment temperatures. Furthermore, the residual stresses and microstructure analysis of as-built specimens were performed to understand the driving force for recrystallization according to the laser parameters. The specimens were manufactured within a volumetric energy density (VED) range of 61.7 J/mm³ to 260 J/mm³ by varying laser power (370W, 380W, 390W), laser scan speed (600mm/s, 800mm/s, 1000mm/s), layer thickness (25 μ m, 37 μ m, 50 μ m), and hatch distance (0.1mm, 0.11mm, 0.12mm). Solution heat treatment was carried out at 1,065°C, 1,080°C, and 1,095°C with a 90-minute interval while aging heat treatment was performed using AMS standard conditions. The volume fraction of recrystallized grain was determined using the Grain Orientation Spread (GOS) value obtained from Electron Backscatter Diffraction (EBSD), and areas with GOS values below 1 degree were considered as recrystallized grains. Additionally, the occurrence of recrystallization was identified when the volume fraction of recrystallized grains after heat treatment exceeded 50% of the observed area. Within the experimental range, the recrystallization temperature of L-PBF IN718 decreased with increasing laser power, scan speed, and layer thickness. As a result, the variation in recrystallization temperature showed minimal correlation with VED and mainly depends on the cooling rate of the melt pool, which is influenced by the volume of the melt pool and the heat dissipation of the melt pool.

Precipitation and microstructure features affecting the mechanical properties of a newly developed Ni-Based Superalloy

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B3_2 - Nickel based superalloys I, Z1 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Ni based superalloys are prominent candidate for aerospace applications to be employed under demanding conditions. Emerging new technologies to improve engine efficiency and reduce environments footprints require alloys to withstand severe conditions and higher temperatures. VDM Alloy 780 offers a diversity of properties namely microstructure uniformity, high oxidation resistance and good mechanical properties up to 700°C as well as weldability and good hot workability making it a suitable candidate for aerospace applications.

Depending on the application, grain size following forging process should be controlled to meet the required mechanical properties and in-service requirements. Grain size and precipitation of gamma' and eta/delta precipitations during and following hot deformation is the direct consequence of the thermally activated microstructure mechanisms like recrystallization, grain growth and precipitation kinetics. These could be tuned through multi-stage heat treatment including solution treatment and aging processes.

In this work, the influence of forging temperature and the subsequent heat treatment process on the microstructure and tensile properties are studied. Two different forging temperatures, namely 950°C and 1050°C, are used to study the microstructure development in subsolvus and supersolvus domains, respectively, giving rise to full recrystallization and grain coarsening in supersolvus domain. The subsolvus hot deformation, however, adds to the complexity of dislocations multiplication and dynamic recrystallization in the presence of gamma' particles. The following heat treatment assists completing the recrystallization process and obtaining uniform distribution of gamma' precipitates, at which delta phases appear not to be present at high amount. This defines the mechanical properties particularly the tensile strength and elongation at rupture. It appears that the following heat treatment could eliminate the effects of the deformation temperature on the tensile properties through the microstructure modifications. Tuning the grain size and the amount of gamma' precipitations with a unique processing route could improve the mechanical properties of the VDM Alloy 780 making it appropriate for high performance applications.

Stress relaxation and analysis of activation volumes in 9% Cr-steel: insights into dislocation glide

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This work investigates the stress relaxation behavior of martensitic 9% Cr steel P91, a material of key interest in high-temperature applications. We focus on determining the activation volume, a critical parameter for calculating the glide velocity of mobile dislocations. To achieve this, data from repeated stress relaxation tests were analyzed, obtained from experiments in a deformation dilatometer at 650°C under a compressive stress of 200 MPa. The established logarithmic relaxation law was compared to a new analytical solution, derived by combining the Orowan equation with Hooke's law. This new approach, which accounts for the material's microstructural condition, provides a potential improvement over traditional methods. In the new method, the activation volume is found to depend on the dislocation density. This characteristic was determined using transmission electron microscopy (TEM) for different relaxation conditions. Additionally, synchrotron data from the same samples were complementarily evaluated using a modified Williamson-Hall approach. The findings contribute to the calibration of the dislocation glide velocity and are essential for improving the predictive accuracy of mean-field creep models in the primary creep regime. The close relationship between relaxation and creep behavior is also discussed, offering insights that could enhance the performance and longevity of high-temperature materials.

Modeling of the thermodynamic and diffusivity properties of the Ti-N system

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B3_5 - Titanium alloys, Z1 Room (Level -3), septembre 18, 2025, 14:30 - 16:30

Titanium alloys are excellent materials for aeronautic engines, thanks to their high strength-to-weight ratio. However, their current use is limited below 650 °C, due to issues like environmental embrittlement and poor creep resistance at higher temperatures. When titanium alloys are exposed to oxidizing environments at high temperatures, a TiO₂ scale forms, accompanied by significant oxygen dissolution (up to ~33 at.%) into the alloy [1]. This oxygen-rich layer is approximately three times thicker than the oxide itself and is responsible for a loss of ductility [2-3]. Nitrogen plays an important role [3-6]. For many titanium alloys, oxidation kinetics are slower in air than nitrogen-free atmospheres [3], [5]. This effect has been attributed to (1) the formation of oxynitride/nitrides between the oxide and the metal and (2) competition between oxygen and nitrogen dissolution [5]. Nitrogen has effects similar to those of oxygen on the mechanical properties of titanium; however, it diffuses more slowly, thereby reducing the depth of the affected zone [7]. Consequently, both the (oxy)nitride and the nitrogen-rich zone act as diffusion barriers for oxygen [5], with beneficial effects on oxidation resistance [3].

To predict these complex equilibria and guide the design of new alloys, a comprehensive understanding of the thermodynamic and kinetic properties of the Ti-N-O system is essential. Current thermodynamic databases fail to reproduce our experimental observations [5]. Therefore, as a first step, we conducted an extensive study of the thermodynamic and kinetic properties of the Ti-N system by experimental investigations, DFT, and CALPHAD modeling. Diffusion couples experiments between Ti and TiN have been performed and completed by accurate characterizations, including EPMA, EBSD and TEM. The new data have been adopted to improve the previous CALPHAD thermodynamic assessments of the Ti-N system [8-9]. A diffusivity database is being developed using diffusion coefficients from experiments and DFT calculations.

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Development of a novel Method for repairing Crack-like Structures in Ni-based Superalloys

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B3_4 - Nickel based superalloys II, Z1 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Single-crystal (SX-) turbine blades made of Ni-based superalloys are used in high-pressure stages of jet engines. The harsh operating conditions result in wear and the formation of cracks which impair the engine lifetime. Currently, the repair of SX blades is limited as conventional repair methods are not capable of regenerating the required SX microstructure in the applied region.

In previous investigations, the high potential of the additive manufacturing technique laser- and powder-based directed energy deposition (DED-LB/P) for repairing SX blades has already been demonstrated. By using a two-step approach of deposition and a subsequent remelting of the material, the regeneration of a directionally solidified microstructure was achieved. This two-step approach was developed in baseline investigations using substrate sheet material and then transferred to the tip of high-pressure turbine blades.

In this study, the repair of crack-like structures with different width-to-depth ratios in two different SX Ni-based superalloys has been investigated. The goal of this contribution is to examine a broad range of artificially introduced defects and evaluate their repairability by DED-LB/P. The required SX-microstructure in the substrate material is achieved by the Bridgman-method with a subsequent heat treatment. In order to simulate a broad range of defect dimensions, an ultrashort pulse laser process was utilized to intentionally introduce notches (crack-like structures) into the substrate. The investigated widths range from 0,1 to 0,4 mm with depth from 0,25 to 0,4 mm. For a profound analysis of the interrelations between defect geometry, process parameters and resulting microstructure, a central-composite experimental design was used. The design of experiment includes the process parameters laser power, traversal speed and powder feed rate as well as the area fraction of SX area with the repaired section and degree of closing of the crack-like structure.

This study demonstrates that closing the crack-like structures is possible for depths up to 300 µm. The experiments show that a greater depth of crack-like structures is challenging regarding the closure of the whole volume and with respect to its resulting microstructure. This contribution highlights the conflict of applying a high line energy to achieve greater melting depths and the use of a low line energy, which is required to achieve single crystallinity in the resulting microstructure. In general, high thermal gradient and high solidification rates are required to maintain SX directional solidification. Furthermore, this study highlights the effect of a prior remelting of the crack-like structure before applying material by DED-LB/P.

Misfit strains and deformation behavior of lamellar (α_2 + γ) colonies in-Ti-42Al-8.5Nb

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B3_5 - Titanium alloys, Z1 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Conventionally used γ -titanium aluminides consist of lamellar colonies formed by the Al-rich γ -phase (tetragonal) and the Ti-rich α_2 -phase (hexagonal). In Nb-containing γ -alloys the α_2 -phase can transform to the orthorhombic O-phase during slow cooling or during annealing between 480 und 650 °C. The transformation is observed if the Nb content exceeds a threshold between 5-7.5 at-%. It is accomplished by stretching the hexagonal lattice along three equivalent α_2 - $\langle 11\text{-}20 \rangle$ directions. The orientation relationship between α_2 and O-phase is $(0001)\alpha_2 // (001)\text{O-phase}$ and $[11\text{-}20]\alpha_2 // [100]\text{O-phase}$.

The initially formed O-phase has the identical composition as the α_2 parent phase, Ti-38Al-9Nb. With prolonged annealing time, this metastable phase separates into a mixture of hexagonal α_2 and orthorhombic O-phase. The compositions of the newly formed phases are Ti-37Al-6Nb (α_2 -phase) and Ti-36Al-12Nb (O-phase).

The replacement of α_2 -phase by (α_2 + O)-phases introduces strains to the lattice of the former α_2 -phase lamellae. These can be seen by high resolution imaging where the crystal lattice is continuous but deformed across the α_2 -O-phase boundaries.

Internal stresses resulting from small differences in lattice parameters can be measured conveniently by high-energy X-ray diffraction (HEXRD), giving average results over a large volume. These measurements show that the lattice parameter of γ -phase stays constant after different annealing times, while the lattice spacings in the O-phase vary.

In the TEM, microstructural characteristics can be traced on a more localized scale. We monitor the relative strains between (α_2 /O)-phase lamellae and γ -lamellae in different annealing states by precession diffraction using the Nanomegas® system in a Talos F200i Transmission Electron Microscope. The measurements show an increase in the mismatch between (α_2 /O)-phase lamellae and γ -lamellae with annealing time.

In a second experiment we evaluate the effect of the O-phase on the mechanical properties of the alloy. Micro-pillars of lamellar colonies in selected orientations were milled in an FEI Nova 200 dualbeam FIB/SEM microscope and were deformed at room temperature at constant strain rate in a Hysitron TI 980 Nanoindenter. The results of these experiments show a higher yield stress in the annealed alloy than in the alloy without O-phase. Furthermore, the yield stress strongly depends on orientation.

Finally, dislocations and twinning activities in the deformed microstructures were observed by Transmission electron microscopy using cross-sections that were excised from the deformed pillars by focused ion beam milling.

Role of Intermetallic Phases in Fe-based Shape-Memory Alloys

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B3_1 - Novel Materials, Z1 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Shape-memory alloys (SMAs) based on the Fe–Mn–Al–Ni system provide promising advantages over conventional NiTi-based alloys in terms of materials costs and cold workability. The shape-memory effect in these alloys proceeds quite unusually between a bcc-type parent phase (Stukturbericht designation A2) and a martensitic fcc-type phase (A1). Thereby, coherent nano-sized precipitates (B2) inside the parent matrix are necessary to suppress dislocation-driven plasticity, which would interfere with the martensitic transformation and thus deteriorate the superelastic properties. The B2 precipitates are based on the intermetallic phase AlNi and their size, volume fraction and the chemical composition strongly influence the transformation temperature, superelastic strain, critical stress to induce the martensitic transformation and stress hysteresis. To understand energetic contributions of the intermetallic B2 precipitates to the parent phase in order to initiate the martensitic transformation, thermodynamic calculations were performed using a quaternary Al–Fe–Mn–Ni CalPhaD (Calculation of Phase Diagrams) database. With the aid of extrapolated T_0 temperatures for the B2 precipitates and energetic considerations (EAM potentials) of the differences between B2 and $L1_0$, both adopted from literature data, the thermodynamic stability of the B2 phase was approximated.

Calorimetric studies are essential for SMAs to describe thermodynamic properties over a wide temperature range, because e.g., the T_0 temperatures fall below ambient temperatures in these systems. Therefore, specific heat capacity functions of various intermetallic phases in the binary system Al–Ni and the ternary system Fe–Ni–Ti were measured using the classical three-step method in heat-flux and power-compensated differential-scanning calorimeters. Moreover, enthalpy increment measurements were performed using a Calvet-type calorimeter in transposed drop calorimetry mode. In order to verify the applicability of thermodynamic calculations for a target-oriented alloy design of Fe-based SMAs, several samples with varying fractions of B2 particles and different stabilities against the martensitic transformation were prepared, annealed, subsequently tested using nanoindentation, and analyzed using electron-backscatter diffraction (EBSD). In order to describe the deformation behavior and to assess the reversibility of the martensitic transformation upon loading and unloading, the work-recovery ratio was determined from indentation curves. Since the martensitic transformation behavior is strongly dependent on the crystal orientation, the nanoindentation and EBSD measurements were performed on numerous differently oriented grains. It is shown that the volume fraction and the stability of the intermetallic B2 precipitates against the transformation towards an $L1_0$ -like state severely influence the overall stability of the parent state in Fe–Mn–Al–Ni SMAs and consequently, the reversibility of the martensitic transformation.

Corrosion mechanisms under phosphate-rich deposits during (co)-incineration of sewage sludge and mitigation strategies for sustainable waste management

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B3_4 - Nickel based superalloys II, Z1 Room (Level -3), septiembere 18, 2025, 10:30 - 13:10

Sewage sludge (SeS) needs to undergo thermal treatment in the European Union due to recent legislation changes targeting sustainable waste management. This thermal treatment results in the formation of sewage sludge ash (SSA), which offers great potential for phosphorus recovery. Approximately half of this process occurs through mono-incineration. The remaining half involves co-incineration, predominantly taking place in coal-fired power plants. Therefore, the influence of such phosphate-rich ash deposits on the corrosion of superheater tubes of power plants needs to be thoroughly investigated since such systems were never designed for this purpose. While (co-)firing of biomass increases corrosion rates significantly due to the formation of low-melting deposits and the superimposition of active oxidation and sulfidation, little is known about the corrosion mechanisms under phosphate-rich deposits.

This study investigated the corrosion mechanisms during the mono-incineration of SeS at 500°C and its co-incineration with bituminous coal at 625°C. Quasi-isothermal corrosion tests up to 7000 h were undertaken for various steels ranging from 9% Cr steels, e.g. P92, to high alloyed steels such as AC66. The samples were exposed in alumina crucibles to gas atmospheres including H₂O, CO₂, HCl, SO₂, representing the mono- and co-incineration of SeS while being embedded into simulated SSA containing Ca₃(PO₄)₂ or FePO₄ and Ca₅(PO₄)₃ among other sulfate and chloride species. Thereafter, water-free metallographic preparation of cross-sections, wall-thickness measurements, SEM and EPMA investigations were used to characterize the corrosion attack. Even though the attack is significantly aggravated when compared to coal ash in the case of co-firing at 625°C, possibly due to the formation of additional low-melting eutectic deposits, the results suggest that balanced Ni/Cr content can provide sufficient protection against both, chlorine-induced corrosion and sulfidation. In the case of mono-incineration of SeS at 500°C, higher PO₄-content in the SSA led to the formation of a dense Fe₃PO₇ outer scale on low Cr-steels, which improved the corrosion resistance compared to the PO₄-lean ash compositions. Cr-Si slurry coatings and Cr-rich alloy claddings substantially elongate the corrosion lifetime in mono-incineration and co-incineration. Their application can enable low-Cr-steel superheater tubes as structural materials in the co-incineration.

Enhancing Creep Strength of Co-based Superalloys Utilizing Local Phase Transformation Strengthening and CALPHAD Based Design

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B3_6 - Refractory, Z1 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

Deformation in the intermediate temperature creep regime of Co- and Ni-based superalloys (~700-850 °C) is dominated by shear of planar defects, e.g. stacking faults and microtwins, whereby diffusion and reordering drive shearing processes. Local Phase Transformation (LPT) to η or χ occurs at these defects (χ -SISFs/microtwins and η -SESFs) and prevents rapid strain accumulation by halting further shearing partial dislocations. A CALPHAD-based design approach has been implemented leveraging the LPT strengthening effect; for Ni-based systems this has proven to enhance a polycrystalline alloy to the performance of traditionally used single crystals. This was accomplished by increasing the propensity for only η -LPT. Here, new Co-based superalloys were created by aggressively promoting both η as well as χ -LPT, the latter having shown extremely effective in preventing microtwin thickening and stacking fault ribbon formation, with the goal of creating an optimized alloy for polycrystalline response. Single crystalline analogs of several alloys were also cast to study fundamental deformation and effectiveness of LPT under specific compressive loading conditions, namely along [001] (enabling SESF/microtwinning) and [011] (enabling SISF and SF ribbons) crystallographic directions, which allowed for alloy performance to be mapped as a function of loading conditions. Comparing these to the optimized polycrystalline alloy provided insight on which LPT dominates polycrystalline response; they were also compared to several benchmark Ni-based LPT alloys. HR-STEM observations, including atomic resolution energy dispersive spectroscopy (EDS), of deformation substructures allowed analysis of LPT and its effectiveness; these observations ultimately informed design of an optimal creep-resistant polycrystalline alloy and refined the CALPHAD-based multi-criteria optimization algorithm PyMultOpt.

Revealing the influence of temperature, stress and strain rate on deformation mechanisms of the Ni-based superalloy Udimet 720Li

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B3_3 - Single crystals, Z1 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Udimet 720 is a Ni-based superalloy, which was developed more than 40 years ago. Its derivative alloy Udimet 720Li exhibits slight differences in the carbon, boron and chromium content. Although this alloy has already been investigated, there is no systematic parameter study regarding the creep properties and the related deformation mechanisms at various temperatures and stresses or strain rates, respectively. As it is known e.g. that the deformation mechanisms can vary from APB-coupled dislocations to stacking fault shearing and microtwinning at different temperature-stress or temperature-strain rates combinations, respectively, this study was performed. Those different mechanisms have a major influence on the performance of superalloys, which can be used for alloy development and creating new material models. Before investigating the creep behavior, the fully heat-treated condition of Udimet 720Li was analyzed via scanning and transmission electron microscopy to present the status quo condition. For the purpose of analyzing the creep performance, tensile tests and tensile creep tests at temperatures between 650 °C and 750 °C with resulting deformation rates between 10^{-3} s^{-1} and 10^{-7} s^{-1} were performed and analyzed via transmission electron microscopy. The occurring dominant deformation mechanisms regarding the different test parameters will be compared and categorized in trends. The importance of the deformation mechanisms for alloy development and material models will be discussed.

Effect of Laser Treatment on the High-Temperature Oxidation of Titanium Alloys Through Surface Nitrogen Enhancement

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

High-temperature corrosion of Ti-based alloys remains a challenge in applications operated above 600 °C. Recent experimental studies have shown that atmospheric nitrogen significantly influences the oxidation of Ti and its alloys in an air atmosphere [1-3], with a synergistic interaction between nitrogen and alloying elements [1,2]. The interaction of nitrogen with alloying elements contributes to the formation of a compact oxide scale and reduces the mass gain during high-temperature tests.

Therefore, this work's main aim is to intentionally introduce nitrogen into the surface region of the near- α Ti alloy using laser surface treatment (LST) and to evaluate its resistance to high-temperature oxidation. LSTs were performed using the Brilliant laser (nanosecond, 1064 nm) on the multi-component Ti-alloy Timetal 834 (Ti-Al-Sn-Zr-Nb-Mo-Si-C). Treatments were performed in the air atmosphere with varying laser settings to modify the nitrogen content in the surface layer, producing samples with distinct surface colors, including yellow, purple, and blue. Oxidation tests at 650 °C for 100 hours in an air atmosphere revealed a significant improvement in the high-temperature oxidation resistance of LST-treated samples. To explain the observed phenomenon, the modified Ti834 samples (both unoxidized and oxidized) were analyzed in terms of morphology, roughness, chemical composition, and phase composition. Particular emphasis was placed on examining the microstructure and chemical composition of cross-sections after laser treatment.

A systematic comparison of surface conditions after LST and their oxidation resistance enabled the identification of key factors responsible for enhancing high-temperature oxidation resistance. LST modification, through microstructure refinement and presence of the nitrogen in the surface region, causes changes in the oxidation behavior of Ti834 alloy.

These findings are especially significant as they can facilitate the development of surface treatments tailored for applications in the aerospace, automotive, and gas turbine industries.

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Influence of the oxygen partial pressure on the oxidation mechanism of rutile-type oxide-forming refractory high entropy alloys

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B3_1 - Novel Materials, Z1 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

The lack of intrinsically protective oxides inhibits most refractory-based alloys from being used as high temperature structural materials. The catastrophic oxidation of most refractory metals, resulting in the formation of volatile or voluminous oxides, begins as low as 500 °C. Recent investigations found potential refractory compositionally complex, or high entropy alloys (HEAs), offer improved oxidation resistance at temperatures as high as 1500 °C. Additionally, high entropy alloys have been shown to be capable of exhibiting greater strengths than conventional alloys.

The Cr-Ta-Ti-Al-Mo HEA system is potentially oxidation resistant through the formation of a thin and continuous CrTaO₄ at the interface between the substrate and a mixed outer oxide scale. CrTaO₄ has been shown to play a role in the oxidation resistance of other high temperature oxidation resistant alloys, including some Ni-based superalloys. High temperature oxidation experiments of Cr-Ta-Ti-Al-Mo were performed at 1000°C in Ar-O₂ atmospheres with varying oxygen partial pressures to clarify the dominant defect structure(s) and formation mechanism(s) of CrTaO₄. As rutile-type oxides are known to be very susceptible to doping, small additions of elements with varying oxide valences were added to investigate a potential doping effect. Higher valence doping of Cr-Ta-Ti-Al-Mo was successful in showing reduced oxygen diffusion through the oxide and thus better oxidation performance.

Live presentation of CreeSo - Creep Software

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B3_3 - Single crystals, Z1 Room (Level -3), septiembere 17, 2025, 17:00 - 19:00

“CreeSo” is short for “Creep Software”. This application is currently developed at the Institute for Engineering Materials – Metals and Alloys at the JKU Linz, Austria. The institute works on different models for the simulation of creep and other material properties utilizing descriptions of the microstructure for the materials in question. The resulting systems of differential equations cannot be solved analytically and numerical methods have to be applied. CreeSo provides a GUI (Graphical User Interface) for the creation of the model and the simulations. It enhances the speed of the simulation by a factor of approximately 10 compared to MatLab. CreeSo also contains a variety of tools for e.g. creation of time-to-rupture (TTR) diagrams, comparison to creep curves, parameter finding, and data export. Although it still is a prototype, CreeSo is built as a desktop and online version so that researchers outside our institute can also access our models and carry out simulations. A subset of the functionality can even be tried out publicly under <https://imk.jku.at/creeso>.

Data-driven study of the enthalpy of mixing in liquid alloys

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B3_1 - Novel Materials, Z1 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

The enthalpy of mixing in the liquid phase is a key input in Calphad and machine learning [1] models for predicting the melting temperature range of alloys. As a result, it is an important property for the design of a variety of alloys, such as brazing alloys, cast alloys, or phase change materials for thermal energy storage. In multicomponent liquids, the main contribution to the enthalpy of mixing comes from the pairwise interactions, yet, this property has only been measured in at most a third of the binary systems. Therefore, predicting the enthalpy of mixing in binary liquids remains highly important, and to this day, Miedema's semi-empirical model [2] has been regarded as the most reliable for this task.

This presentation will focus on using machine learning to predict the enthalpy of mixing in binary liquids formed by 70 elements. To achieve this, we collected enthalpy of mixing data from the literature in more than 400 binary systems. By using active learning and clustering models, we identified the need for new data for liquids with a refractory metal, which we obtained in 29 binary systems using ab initio molecular dynamics simulations. This led to improvements to our machine learning model [3], which was already performing better than Miedema's model. We will also discuss the temperature dependence of the enthalpy of mixing, and the reliability of its extrapolation from the binary systems in multicomponent liquids. Through this presentation, we will outline directions for further research on this property, which is essential for predicting phase equilibria.

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[3] G. Deffrennes, B. Hallstedt, T. Abe, Q. Bizot, E. Fischer, J.-M. Joubert, K. Terayama, R. Tamura, Data-driven study of the enthalpy of mixing in the liquid phase, *Calphad* 87 (2024) 102745. <https://doi.org/10.1016/j.calphad.2024.102745>.

In-Situ Precipitation of Secondary Phases for the Strengthening of AISI 316L Austenitic Steel

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The reinforcement of materials for demanding applications, such as high temperatures and extreme mechanical loads, can be achieved by incorporating fine oxide particles or other secondary phases into the matrix. This study explores the development of dispersion-strengthened austenitic steel AISI 316L, where secondary phase particles are formed directly during processing. Powder metallurgy techniques, specifically mechanical alloying (MA) and spark plasma sintering (SPS), are employed to fabricate ODS 316L steel with tailored properties. Reinforcement precursors, including yttrium hydride (YH₂), boric acid (H₃BO₃), and titanium (Ti), are introduced into the austenitic steel powders to enable the controlled formation of stable dispersoids during sintering. The ability of these elements to dissolve in a solid solution and subsequently precipitate as fine particles is systematically investigated. Spark plasma sintering is utilized for powder consolidation, offering precise control over temperature and densification while minimizing grain growth. The resulting materials are subjected to comprehensive microstructural and mechanical characterization, including scanning electron microscopy (SEM), transmission electron microscopy (TEM), and electron backscatter diffraction (EBSD). Additionally, mechanical testing, such as tensile and creep tests, evaluates the strengthening effects of the in-situ formed dispersoids.

This study aims to develop a reliable approach for producing ODS 316L steel with enhanced strength and thermal stability while maintaining good workability. The findings contribute to advancing ODS steel technology and provide insights for future applications in the energy, aerospace, and nuclear industries.

This research was funded by the Czech Science Foundation (project No. 22-04227L).

Bridging Alloy Design and Processing: Microstructure, Mechanics, and Additive Manufacturing of Hf-Mo-Nb-Ti RMPEAs

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B3_6 - Refractory, Z1 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

Refractory multi-principal element alloys (RMPEAs) within the Hf-Mo-Nb-Ti system exhibit excellent mechanical properties, high-temperature stability, and thermal resistance, making them strong candidates for structural applications in extreme environments. However, the composition-dependent mechanical behavior of these alloys remains insufficiently understood, necessitating systematic experimental validation. Additionally, conventional processing methods introduce challenges such as elemental segregation and coarse grain formation, which compromise microstructural uniformity and mechanical reliability. Additive manufacturing (AM) offers a promising alternative by enabling rapid solidification, refined microstructures, and near-net-shape fabrication, potentially overcoming these limitations and expanding the processing window for RMPEAs.

This study investigates the mechanical response of RMPEAs through micropillar compression and nanoindentation under controlled loading conditions, correlating experimental results with computational modeling. Thermal stability was assessed via in situ high-temperature X-ray diffraction (XRD), confirming a predominantly body-centered cubic (BCC) phase with minor secondary precipitates. As-cast alloys exhibited a dendritic microstructure with elemental partitioning, while annealing at 1600°C for 10 h followed by furnace cooling led to the formation of Hf-rich precipitates within a solid solution matrix. Yield strength and hardness varied with composition, with Mo- and Nb-rich alloys demonstrating increased mechanical strength due to solid solution strengthening.

To address processing challenges, laser-based techniques were employed to evaluate the feasibility of AM for RMPEAs. Laser surface scanning reduced elemental segregation and refined the microstructure, mitigating coarse grain formation as confirmed by electron backscatter diffraction (EBSD) analysis. This approach enhanced manufacturability by minimizing the need for extensive post-processing, such as homogenization heat treatments. By integrating experimental characterization with computational validation, this study establishes a framework for designing RMPEAs with tailored mechanical properties, improved thermal stability, and enhanced processability for extreme environments.

Microstructural characterization of GTA and EB welded Inconel 718®, subjected to prolonged high-temperature aging conditions.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Inconel 718 is a precipitation-hardened nickel-based superalloy consisting of nickel, chromium and niobium which enables it to maintain structural integrity under severe thermal and mechanical stress, even at elevated temperatures.

In the present study, Inconel 718 specimens were welded using two different techniques: Electron Beam Welding (EBW) and Gas Tungsten Arc Welding (GTAW). They were then subjected to Post Weld Heat Treatments (PWHT), according to AMS 5662 SAE Standards. After the PWHT, all samples were exposed to the following heat treatments: aging at 700 and 800°C for 24 up to 500 hours in order to investigate their microstructural characteristics and correlate them to the attained mechanical properties. Scanning Electron Microscopy and X-Ray Diffraction were employed for the microstructure characterization, and revealed the precipitation of gamma prime & gamma double prime phases and a significant amount of carbides. Specimens subjected to aging for 500 hours contained delta phase dendritic grains along with smaller volume fractions of gamma prime & gamma double prime phases. Additionally, uniaxial tensile and Vickers microhardness tests were conducted. An increase in mechanical strength of all specimens that were heat-treated was revealed. Finally, the welded zones exhibited excellent mechanical properties ,after aging for over 24 hours at 700 and 800°C. That makes them suitable for components such as turbine blades, jet engine parts, and pressure vessels.

Effect of long-term thermal aging on microstructure and tensile properties of a highly-molybdenum nickel alloy

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B3_6 - Refractory, Z1 Room (Level -3), septembre 18, 2025, 17:00 - 19:00

Highly-molybdenum nickel alloys exhibit exceptional corrosion resistance in chloride-bearing solutions. For this reason, they are promising candidates for structural materials in molten chloride salt environments, especially for the future Molten Salt Reactors (MSR). However, the effect of thermal aging on the microstructure and mechanical behavior of the high-molybdenum nickel alloy have not yet been investigated and well documented. So the objective of this work is to study the effects of thermal aging on the microstructure of Ni alloys and their possible consequences on the mechanical properties of these alloys. In this study, the microstructural evolution of a high-molybdenum nickel alloy, the Hastelloy B3, was investigated after thermal aging at 600 °C and 650 °C for 1 000, 4 000 and 10 000 hours using complementary techniques such as SEM (Scanning Electron Microscopy), EDX-SEM (Energy Dispersive X-ray), SEM-EBSD (Electron Backscatter Diffraction), and X-ray diffraction. Small punch tests and tensile tests were carried out to study the mechanical behavior of the material at room temperature and at 500°C. Fracture surfaces were characterized by SEM to determine the rupture mechanism. The influence of pre-rolling of the material is also studied. The Inconel 625 was also studied under the same conditions for comparison. The study was supported by France 2030 and BPIFrance in the ISAC (Innovative System for Actinides Conversion) project of the France Relance initiative.

Evolution of the microstructure and mechanical properties of TiNbAl (beta+O) alloys with additions of Ta, Mo or W

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B3_5 - Titanium alloys, Z1 Room (Level -3), septembre 18, 2025, 14:30 - 16:30

Ti- Nb-Al ternary system with the precipitation of stable orthorhombic phase in the bcc matrix are potential candidates to replace nickel or TiAl alloys for high temperature application in aircraft engines, between 800°C and 1000°C. These alloys, with a Nb/Ti ratio = 1 and 15%Al present good mechanical properties, combining rather good resistance to damage at room temperature and high resistance at high temperature. In order to increase the service temperature of such alloys, the effects of a partial substitution of Nb by refractory elements such as Ta, Mo and W, on the precipitation of the O-phase have been investigated by scanning and transmission electron microscopy.

The evolution of the mechanical properties with the chemical composition and heat treatments has been followed by hardness measurements and compression tests at 800°C, and discussed in relation with the observed microstructures.

Control of impurity elements in molten Ni-based superalloy

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B3_2 - Nickel based superalloys I, Z1 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Nickel-based superalloys are special alloys that enhance heat resistance through the addition of various alloying elements. In particular, aluminum plays an important role in the formation of Ni₃Al and securing high-temperature strength. However, the presence of impurities such as O, N, S, and H in superalloys can lead to the formation of brittle phases by reacting with the alloying elements added for the desired properties, which critically affects the mechanical properties of the superalloy. Therefore, controlling these impurities is crucial. When produced solely through Vacuum Induction Melting without additional refining processes such as Electro Slag Remelting or Vacuum Arc Remelting, the use of slag is limited due to the vacuum conditions, making effective removal largely dependent on vacuum control.

In this study, various experiments were conducted to establish fundamental data for controlling the formation of three non-metallic inclusions (O, S, H) in molten nickel-based superalloys. First, for sulfur, desulfurization experiments were carried out to investigate the desulfurization capacity based on the types of desulfurizers and their addition methods. Inclusions were analyzed to elucidate the desulfurization mechanism and derive optimal desulfurization conditions based on the predicted changes in sulfur concentration during ceramic filtering.

For oxygen, equilibrium deoxidation experiments were conducted using the equilibrium reaction between Al and Al₂O₃, varying the aluminum content in nickel. The equilibrium solubility of oxygen in Ni-Al alloys with compositions ranging from 0.0005 wt% to 15 wt% was measured, and equilibrium constants and interaction coefficients were derived using interaction coefficient models such as WIPF (Wagner's Interaction Parameter Formalism) and Redlich-Kister type polynomial. Evaluations of deoxidation equilibrium were conducted for each model.

For hydrogen, equilibrium experiments of H₂ gas were conducted at three temperature ranges (1773 K, 1823 K, 1873 K) using Sievert's law to derive the equilibrium constant for the reaction of hydrogen dissolving in pure nickel as a function of temperature. At 1873 K, the equilibrium hydrogen solubility of Ni-Al alloys with hydrogen concentrations ranging from 1 to 6 wt% was measured, deriving the equilibrium constant for the hydrogen dissolution reaction in Ni-Al alloys. The interaction coefficient between aluminum and hydrogen was also derived through changes in the activity coefficient of hydrogen with increasing aluminum concentration.

Development of Ca-based coatings for vanadium alloys used in high temperature corrosive environments

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B3_5 - Titanium alloys, Z1 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

The constant aim to increase gas turbine efficiencies is strongly coupled to an increase in service temperature. For that purpose, the materials must retain their mechanical properties at high temperatures and simultaneously be oxidation resistant. As an alternative to state-of-the-art Ni-based superalloys, vanadium alloys are interesting due to their lower density and high strength. They were recently investigated based on the intermetallic-reinforced Mo-Si-B alloying concept with V instead of Mo. Still, the V solid solution matrix is prone to oxidation, making the material unusable for most technical applications due to the melting point (~680 °C), toxicity and corrosiveness of vanadium oxide. The classical alloying elements that form a protective external scale, Cr and Al, are non-protective against molten vanadate corrosion. Alkaline earth metal oxides can suppress this V₂O₅ corrosion as they can form higher melting, more stable vanadates. Ca was found to form more stable compounds than Mg and is interesting due to its low cost and availability. In this work, Ca-based coating systems were developed and tested for V alloys. The composition and morphology were validated via optical microscopy, XRD, Raman spectroscopy, and SEM. Oxidation experiments of the coated V alloys were performed at 600-800 °C to investigate the oxidation resistance of the new material system.

Advanced Polycrystalline γ' -Strengthened CoNiCr-Based Superalloys

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B3_6 - Refractory, Z1 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

Novel complex concentrated CoNiCr-based superalloys with excellent mechanical properties have been developed, which combine the multiprincipal element nature of high-entropy alloys with the precipitation strengthening in superalloys.

A series of advanced polycrystalline γ' -strengthened CoNiCr-based superalloys, called CoWAlloys, with varying contents of Al, W, Ti, Ta, Mo, and Nb are investigated in terms of microstructure, thermophysical properties, yield, and creep strength. The microstructure of all CoWAlloys consists of an fcc solid solution matrix phase (approximate γ composition in at. pct: 50Co–20Ni–20Cr–10X (X = other alloying elements)), which is strengthened by a multicomponent γ' (Ni,Co)₃(Al,Ti,Ta,W,Nb)-based precipitate phase with a very high-volume fraction of around 60 vol pct (approximate γ' composition in at. pct: 45Ni–30Co–25X). These alloys have high solidus temperatures above 1300 °C and moderate γ' solvus temperature between 985 °C and 1080 °C leading to a large processing window. The increasing content of γ' -forming elements Ti, Ta, W, and Nb decreases this window, but increases the γ/γ' lattice misfit and the anti-phase boundary energy, which contribute to a significantly higher yield and creep strength. In another series, the effect of substituting Fe for Co was investigated. Despite a decrease in creep strength with higher Fe content, the alloys still demonstrate comparatively good creep properties.

In order to better classify the properties of these CoNiCr-based superalloys, they are also discussed in comparison with conventional polycrystalline Ni-base superalloys and so-called L1₂-strengthened high-entropy alloys, revealing that the creep strengths of the CoWAlloys are significantly higher. This is due to the reduced strain rate sensitivity of the CoWAlloys due to different underlying deformation mechanisms: By increasing the anti-phase boundary energy, a transition to stacking fault shearing and microtwinning occurs. Additionally, high-resolution scanning transmission electron microscopy coupled with energy dispersive spectroscopy measurements reveal that solute segregation towards these planar defects occur and that the stacking faults locally transformed into the ordered hexagonal χ and η phases. This significantly enhances the creep strengths of superalloys during high-temperature deformation. Additionally, this study discusses the kinetic aspects of solute segregation and subsequent local phase transformations at the stacking faults. Based on these results, guidelines and strategies for the design of next-generation advanced high-temperature polycrystalline superalloys are proposed.

Evolution of deformation micro-mechanism in thermally exposed Superalloy 625: Tracing strain hardening characteristic using a physics-based model

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The Ni-based superalloy 625 possesses an outstanding set of creep resistance, high strength, corrosion resistance, and superior fatigue strength at elevated temperatures, making it suitable for high-temperature applications in the range of 650-750°C. Understanding the influence of lattice defects on secondary phase transformation during service and its impact on plastic deformation micromechanisms is crucial. This study establishes the microstructure-deformation micromechanisms correlation for Superalloy 625 alloy (Indian grade) during tensile deformation. It includes aging treatments of both solution-treated and solution-treated + cold-rolled alloys at 700°C for up to 1000 hours. Microstructural assessments are carried out on heat-treated alloys using scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), and high-resolution electron microscopy (HREM). Additionally, uniaxial tensile tests of the aged samples are conducted at room temperature, followed by fracture and microstructural analysis to observe dislocation activity and deformation features. A physics-based model is used to predict flow stress curves, accounting for the effects of grain structure, secondary phases, and evolving deformation micromechanisms.

Influence of the fabrication process on the oxidation behavior of a eutectic high-entropy alloy

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B3_1 - Novel Materials, Z1 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

High entropy alloys are considered a promising option for high-temperature applications due to the possibility to achieve excellent oxidation resistance. However, processing conditions play a crucial role in determining the final microstructure and, consequently, the material's properties. This study examines the impact of various fabrication methods on the microstructure, mechanical properties, and high-temperature oxidation behavior of a non-equiatom AlCrCoFeNi_{2.1} eutectic high-entropy alloy (EHEA). The alloy was fabricated using traditional arc-melting and a powder metallurgy (PM) technique, spark plasma sintering (SPS), using gas-atomized powders as starting materials. While the fabrication method had a minimal effect on the primary phases present, it significantly impacted the microstructure morphology. Additionally, differences in mechanical properties were observed. All samples primarily consisted of a body-centered cubic (BCC) phase and a face-centered cubic (FCC) phase. However, the arc-melted alloy exhibited a typical lamellar structure, whereas the SPS-ed alloy displayed also globular structures in certain regions. The powder metallurgical method of SPS significantly refined the grain size. Powder metallurgy routes enabled the microstructure of the samples to be tailored to improve mechanical properties and oxidation resistance. During oxidation tests, samples fabricated by SPS exhibited more homogeneous oxide layers.

High Temperature Intergranular Oxidation of Nickel Based Superalloy Inconel 718 and Stainless Steel 316L

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B3_4 - Nickel based superalloys II, Z1 Room (Level -3), septembre 18, 2025, 10:30 - 13:10

Keywords: Inconel 718, 316L, Intergranular oxidation, Wagner's theory.

In polycrystalline alloys, grain boundaries (GBs) can undergo preferential oxidation [1]: this phenomenon is known as Intergranular Oxidation (IGO). Oxidized GBs can act as initiation sites for cracks, resulting in premature failure. Therefore, in order to predict the behaviour of alloys in harsh environments, it is important to understand IGO. Although there are several works that deal with experimental characterization of IGO [1-3], there is no recognized model for it.

Sanviemvongsak et al. studied the IGO of the Ni-based IN718 superalloy at 850°C [2]. In these conditions, even if forming a Cr₂O₃ external scale, the alloy is subject to IGO: oxides rich in Al and Ti are observed in the GBs. The IGO penetration depth was found to follow a parabolic kinetics. An analytical model was derived to describe the parabolic rate for the evolution of IGO penetration depth, based on Wagner's theory for internal oxidation. The proposed IGO mechanism involves two competing processes. The first one is the inward diffusion of oxygen to the tip of the oxidation front, along the incoherent interfaces between the intergranular oxide and the alloy matrix; the second one is the outward diffusion of Al and Ti.

The objective of the present work is to verify the validity of this model for the IGO of IN718 and the stainless steel 316L. To this aim, oxidation experiments on these alloys were performed at two temperatures, 650°C and 700°C, for durations up to 10,000 hours. Samples were removed periodically and weighed. Then, X-ray diffraction (XRD) and Scanning Electron Microscopy (SEM) characterizations were performed on the samples. These characterizations were performed at three intermediate durations: 1000 h, 3000 h and 5000h. New IGO data were obtained by systematic microscopic characterizations. These data are herein compared to the model described by Sanviemvongsak et al. [2].

Références

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Dynamic recrystallization during hot deformation of an oxide-dispersion-strengthened ferritic steel

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B3_1 - Novel Materials, Z1 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Future technologies for green energy production strongly rely on high-temperature alloys in order to maximize their efficiency. Among many candidate alloy systems, oxide dispersion strengthening (ODS) has shown its potential regarding creep resistance many times, but production via powder metallurgy is still challenging. Moreover, the alloy contains only a low amount of critical raw materials. To support the establishment of this alloy class, the dynamic recrystallization behavior of a novel ODS alloy during hot-rolling was simulated by using Gleeble compression testing. The hereby achieved microstructure was investigated by scanning electron microscopy and correlated with a finite-element model to obtain the local deformation and deformation rate. These coupled methods led to a set of material data that was further used for the modeling of the recrystallization behavior of this novel ferritic ODS alloy.

Oxidation of additively manufactured Ni-base alloy IN625: mechanism of intergranular oxidation

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B3_4 - Nickel based superalloys II, Z1 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Ni-base superalloys are state-of-the-art structural materials for high-temperature applications requiring both high creep strength and environmental resistance, e.g., in power generation, jet-engine technology, petrochemical industry, nuclear technologies, heat processing, etc. Additive manufacturing (AM) of high-temperature alloys has been booming in the past decade, especially in aeronautics, where AM offers a significant flexibility of shaping components as well as decreasing material waste

Additively manufactured (AM) LB-PBF Ni-base alloy IN625 suffers from intergranular oxidation (IGO) during air exposure at 900 °C in contrast to the conventionally manufactured (CM) forged alloy. IGO is triggered by oxide buckling over the grain boundaries (GBs) in the alloy followed by oxidation of the open intergranular voids. The Cr₂O₃ scales thermally grown on the AM and CM alloy specimens were analyzed with SEM/EDX, EBSD, GD-OES, TEM and APT. A new mechanism of IGO in AM alloys highlighting the role of oxide scale adhesion is proposed and experimentally validated.

Hot tensile behavior of cold worked XH43 superalloy at 650 °C - Role of η phase.

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B3_3 - Single crystals, Z1 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

XH43, a wrought Ni-Fe-based superalloy, is widely used in aerospace applications due to its excellent mechanical properties and high-temperature corrosion resistance. The strength of this alloy is primarily derived from the precipitation of γ' (Ni_3Ti) and γ'' (Ni_3Nb) phases through a conventional dual aging process. The evolution of these strengthening phases is significantly influenced by prior thermomechanical processing, particularly cold working. In this study, the effects of cold rolling followed by two-step and three-step aging on the microstructural and textural evolution of XH43 superalloy were investigated using scanning electron microscopy (SEM), transmission electron microscopy (TEM) and electron backscattered diffraction (EBSD) techniques. Microstructural characterization reveals that three stages of aging promote the precipitation of needle-like $[\text{Ni}_3(\text{Ti}, \text{Nb})]$ precipitates. Cold rolling increased the volume fraction of γ' and γ'' precipitates, enhancing the strengthening effect. However, at higher degrees of cold rolling, the formation of hexagonal η (Ni_3Ti) precipitates was observed. Hot tensile testing at 650 °C revealed that the η phase played a crucial role in improving hot ductility across all cold rolling conditions. These findings provide insights into optimizing the thermomechanical processing of XH43 superalloy to tailor its microstructure and mechanical performance for high-temperature applications.

Evolution of microstructure and mechanical properties as a consequence of tensile creep strain of NNS-HIPped nickel-based superalloy

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B3_4 - Nickel based superalloys II, Z1 Room (Level -3), settembre 18, 2025, 10:30 - 13:10

Nickel superalloys are being widely used in high-temperature applications such as aerospace and power generation due to their excellent mechanical properties. However, long-term exposure to high temperatures under continuous stress leads to microstructural and mechanical degradation, making it unfit for the service. Therefore, in this study, the creep behavior of Astroloy fabricated via near-net shape hot isostatic pressing (NNS-HIP) is analyzed. NNS-HIP is a powder metallurgy technique enabling precise component fabrication by densifying loose powders in a pre-designed capsule under high temperature and isostatic pressure brought by compressed inert gas. Creep tests were conducted at different temperatures (650, 760 & 820 °C) and stress conditions. Optical and scanning electron microscopy (SEM) analysis revealed that increasing temperature influences the transition of primary γ' precipitates from discontinuous to interconnected, facilitating intergranular crack initiation and propagation. Additionally, hardness testing demonstrated a direct correlation between excessive precipitates coarsening and reduced mechanical properties, with a decline in hardness at 820°C compared to 650°C. The results emphasize the necessity of optimizing operational temperature and stress parameters to mitigate detrimental precipitation and cracking, resulting in improved lifespan of the part.

Isothermal Oxidation Behavior of Mo-Ti-Si-B Multiphase Intermetallic Alloys at 1200 °C

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B3_6 - Refractory, Z1 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

The refractory intermetallic alloys are of interest for increasing the operating-temperature range beyond that of Ni-based superalloys (≈ 1100 °C) to improve the fuel efficiency of aero-engines. The Mo-Si-B based intermetallic alloys possess a strong potential for hot end aero-engine applications due to the possibility of achieving impressive oxidation resistance and fracture toughness through suitable alloying additions. The alloys of compositions Mo-14Si-10B (MSB), Mo-20Ti-14Si-10B (20Ti), Mo-30Ti-14Si-10B (30Ti) and Mo-40Ti-14Si-10B (40Ti) (at. %) have been prepared by both arc melting (AM) and spark plasma sintering (SPS). The X-ray diffraction analysis has confirmed the presence of ductile Moss and Mo₅SiB₂ (T₂) phases in both AM and SPS alloys of all the aforementioned compositions. The Mo₃Si (A₁₅) phase has been found to be absent with a small fraction of Mo₅Si₃ (T₁) phase being formed in the 40Ti alloy, as detected by electron backscattered diffraction analysis. In addition to that, formation of Ti₅Si₃ (D₈₈) phase has been observed in alloys containing 30 and 40 at.% Ti. The oxide scale has been characterized using XRD and FESEM. The X-ray diffraction and FESEM analysis have confirmed the presence of TiO₂ and SiO₂. Regardless of processing technique, the alloying with 40 at.% Ti has been found to be beneficial for improving oxidation resistance recorded on isothermal exposure at 1200 °C for 24 h. Such a trend is attributed to the presence of T₁ and D₈₈ phases, absence of A₁₅ phase with poor oxidation resistance, and the formation of a protective double-layered oxide scale comprising TiO₂ and B₂O₃-SiO₂. However, arc melted alloys have exhibited better oxidation performance than sintered alloys. The oxide scale thickness on AM alloys has decreased over time, whereas that on SPS alloys has increased with increasing Ti content, likely due to variations in TiO₂ and SiO₂ growth rates. The oxidation of the Mo-40Ti-14Si-10B alloys examined for short durations of 15 and 30 min, revealed a greater mass change in the arc-melted alloy compared to the sintered alloys, resulting in approximately 21% reduction in oxide scale thickness for AM alloys and a 3% increase for SPS alloys from 15 to 30 min. A detailed analysis of the mechanisms influencing the microstructure evolution and high-temperature oxidation resistance in the aforementioned multiphase Mo-Ti-Si-B alloys will be presented.

Keywords: Mo-Ti-Si-B alloys, Intermetallic, Oxidation

On the contribution of zirconia phase transformation on fracture properties and crack propagation at the interface of nacre-like alumina composites

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B4_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

In recent decades, researchers developed composite mimicking natural nacre “brick-and-mortar” microstructure. Nacre-Like Alumina (NLA), with a fully dense structure composed of alumina platelets in a glassy phase, garnered the most attention due to their good tradeoff between strength and toughness [1]. The main reinforcement mechanism involves crack deflection at the platelet interfaces resulting in a significant increase of the material toughness [2].

Even if NLA toughness in the specific ‘across’ direction [3] is already optimized, solutions can be envisioned to enhance their flexural strength. It may be done by modifying the interface between the platelets, e.g. incorporating tetragonal zirconia at the interface to leverage tetragonal to monoclinic phase transformation. Specifically, under tensile stress—typically at a crack tip—tetragonal to monoclinic zirconia transformation occurs, inducing compressive stresses, delaying crack propagation and thereby improving fracture toughness. This phenomenon was studied by Henry et al. [4], who incorporated yttria-stabilized zirconia into NLA composition. They revealed a notable increase in NLA flexural strength while not reducing the toughness. However, the study did not definitively establish whether this improvement was directly due to the phase transformation of tetragonal zirconia.

To sum up, zirconia-based NLA demonstrate a real potential for strength improvement. Therefore, the present study investigates several stabilization levels and amounts of zirconia to identify compositions with optimal fracture properties, with the primary aim to confirm or refute the existence of stress-induced phase transformation in these composites.

References

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Laser structuring of ceramic endoprosthesis and its influence on the strength, aging behavior and tribological properties of ATZ ceramics

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B4_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Ceramic resurfacing is emerging as a viable alternative to total hip replacement for young and active patients experiencing osteoarthritis. This approach utilizes monolithic, thin-walled implants characterized by large articulation diameters. Despite the excellent material properties, these large bearing surfaces are expected to cause increased wear. Critical factors include significantly increased friction torques during dry friction and high starting torques after long periods of inactivity. The rise in friction coefficients can result in micromovements at the bone-implant interface, potentially leading to implant loosening and the consequent need for premature revision.

One potential solution to this problem is to utilize an ultrashort pulse laser to structurally modify the articulation surface. This method creates defined microstructures (dimples), which serve to reduce the contact surface, thereby decreasing the frictional torque that occurs. The dimples also function as a microreservoir for synovia, helping to prevent the breakage of the lubricating film.

In order to identify the ideal dimple geometry for the applications mentioned above, a series of tests were conducted on dimples with varying aspect ratios and textured areas. The resulting dimple quality was evaluated by scanning electron microscopy (SEM) and tribological measurements. Furthermore, the impact of the laser structuring on the mechanical and microstructural characteristics of the Alumina-Toughened-zirconia (ATZ) ceramic is of significant importance. Therefore, the flexural strength was determined, and an analysis was conducted on the phase composition and aging behavior of the microstructured ceramic.

The results presented in this lecture were obtained within the BMBF-funded research project Self-X-For-Implants (funding programme: Biologization of Technology, FKZ: 13XP5209A).

Characterization of the deformation and damage behavior of fiber-reinforced ceramics in bending test

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B4_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Fiber-reinforced ceramics exhibit higher fracture toughness and damage tolerance than monolithic ceramics and can therefore be used as a construction material in a wide range of applications. This behavior is caused by additional microstructural mechanisms (crack-stop mechanisms) such as crack deflection, crack branching, crack bridging and fiber pull-out. For these mechanisms to be effective, the fiber and matrix properties have to be matched to each other. In particular, a sufficiently weak fiber/matrix bond is required.

The three-stage liquid silicone infiltration (LSI) process is a cost-efficient method for production of fiber-reinforced ceramics (C/C-SiC). A carbon fiber-reinforced plastic is converted into a ceramic matrix composite via pyrolysis and siliconization. By varying the starting materials and process parameters used, it is possible to develop different material qualities with a different range of properties.

The aim of this article is to describe the deformation and damage behavior of selected short-fiber and continuous-fiber-reinforced C/C-SiC ceramics. For this purpose, quasi-static bending tests were carried in-situ in a scanning electron microscope (SEM). Images were taken at defined stopping points during the test for documentation. Crack initiation, crack propagation and failure of the C/C-SiC ceramics were recorded and subsequently discussed. Conclusions were drawn for suitable material design.

Development and Integration of Novel Ultra-High Temperature Ceramics

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B4_2, Seminario 7 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

This work presents the development of high-purity single phase high entropy carbides, such as (HfZrTaNbTi)C and (MoNbTaVW)C, and high entropy diboride, such as (HfZrTaNbTi)B₂ by Spark Plasma Sintering (SPS). The main aim of this study was to develop an appropriate approach to join this novel class of Ultra-High Temperature Ceramics (UHTC). The presentation will be divided into three parts. The first part will focus on wetting and joining of (HfZrTaNbTi)C and (HfZrTaNbTi)B₂ with a commercially available AgCuTi alloy. The apparent shear strength of HEC and HEB joints was 176 ± 39 MPa and 116 ± 38 MPa, respectively. In all cases, the failure occurred in base materials, which fragmented into many small pieces, indicating that the shear strength of both joints was predetermined by the intrinsic properties of base materials. The second part will describe the joining of (MoNbTaVW)C with a NiTa eutectic alloy. The addition of 17.2 at.% Ta to Ni significantly reduced interfacial reactions and dissolution of HEC, while maintaining excellent wetting behaviour with the final wetting angle of $\leq 15^\circ$. Successful joining of HEC ceramics was achieved using a NiTa interlayer, demonstrating a high shear strength of 220 ± 17 MPa. The last part of the presentation will focus on the joining of (HfZrTaNbTi)C and (HfZrTaNbTi)B₂ with the high entropy alloy containing the same transition metals, i.e. HfZrTaNbTi. Microstructural and interfacial characterizations of the joint revealed a homogeneous, crack-free, and well-bonded interfaces. The effect of joining temperature on the mechanical strength was evaluated, revealing the strength exceeding 350 MPa for the joints made at 1800°C. High-temperature bending tests revealed no significant strength deterioration up to 1000°C.

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High Entropy Ceramics with Improved Oxidation Resistance

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B4_2, Seminario 7 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The present work reports the development of novel high entropy ceramics with improved mechanical properties, and dynamic oxidation resistance. Highly dense high entropy diboride ($\text{Ti}_{0.2}\text{Zr}_{0.2}\text{Hf}_{0.2}\text{Nb}_{0.2}\text{Ta}_{0.2}\text{B}_2$ -SiC composites with different β -SiC content (5, 10, 15, 20 and 25 vol.%) were synthesized using ball milling followed by Spark Plasma Sintering (SPS) at 1900°C. High-purity high entropy diboride (HEB) powder was synthesized using boro/carbothermal reduction of oxide precursors at 1800°C. X-ray diffraction patterns of the synthesized powders and sintered compacts of HEB showed a single solid solution with hexagonal AlB₂ structure without any residual oxide impurities. X-ray energy dispersive Spectroscopy (EDS) mapping results indicated the uniform elemental distribution of transition metals in the HEB phase. The addition of SiC improved the densification of HEB-SiC composites. The composite with 20 vol.% SiC exhibited a unique combination of mechanical properties, such as superior Vickers hardness (22.28 ± 0.25 GPa), flexural strength (750.21 ± 43.23 MPa), indentation fracture toughness (4.12 ± 0.2 MPa.m^{1/2}), Young's modulus (495.3 ± 0.3 GPa) and dynamic oxidation resistance (0.02 mg.cm⁻².s⁻¹).

Acknowledgment: This work was supported by the projects VEGA 2/0145/25 and SAS-TUBITAK/JRP/2023/807/ HiTemCom (No. 720464). The support of Slovak Research and Development Agency under the Contract no. APVV-21-0402 is also acknowledged.

Behavior of Ceramic Oxides in Durability Tests for High-Temperature Solar Receivers

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B4_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Thermochemical processes utilizing solar energy and other high-temperature solar applications require a significant concentration of solar radiation, often exceeding 100 W/cm². In this context, advanced ceramics are an ideal choice, as these materials can withstand temperatures of up to 1400 °C or higher, maintaining stability against detrimental morphological changes. Additionally, the selected materials must be capable of withstanding high flux densities and temperatures over thousands of cycles, given that these systems operate daily with start-up and shutdown procedures.

In this study, materials and operational procedures have been developed using concentrated solar energy for the characterization of materials intended for solar volumetric receivers, which can also serve as supports for solar catalysts. Various testing campaigns have been conducted in the SF40 Solar Furnace at CIEMAT-PSA for the aging of advanced ceramic specimens under concentrated solar radiation, using a specific test bench. Different ceramic materials formed by uniaxial pressing and sintered under various conditions have been evaluated. The objective is to compare their behavior under real conditions of high energy fluxes and elevated temperatures, assessing their properties in a Concentrated Solar Thermal (CST) operational environment.

The work has been carried out thanks to the project "Boost to the solar thermal H2 production via the development and validation of new materials for ceramic solar receivers with improved durability (HIDROFERR)", with project reference PID2020-118599RB-I00, funded by Ministerio de Ciencia e Innovación, Agencia Estatal de Investigación, with Digital Object Identifier 10.13039/501100011033, and FEDER Funds.

Microstructural evolution and mechanical properties of ultra-high temperature binary carbides

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B4_2, Seminario 7 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

This study investigates the microstructural evolution and basic mechanical properties of high-temperature binary carbides. Transition metal elements of group IV and V of PTP, namely Ti, Zr, Hf, V, Nb, and Ta were selected to prepare a combination of 15 binary carbides. The rationale to select these chemical compositions is due to higher thermal stability of their mono carbides, oxides or borides, known as UHTC ceramics.

Binary carbides, for example (TiZr)C, (ZrHf)C, (HfV)C, (VNb)C, (NbTa)C etc. were prepared using ball milling for 4 hours of starting powder of monocarbides. The samples were spark plasma sintered at 2100°C for 10 or 20 minutes at 70MPa in argon atmosphere, respectively. Almost fully dense single phase carbides were prepared. However, the XRD confirmed low amount of oxide phases as ZrO₂, TiO₂ or HfO₂. Longer time of sintering has not changed the grains size of binary carbides significantly. The basic mechanical and tribological properties as nano/micro hardness, Elastic modulus, fracture toughness, and coefficient of friction were measured and the influence of chemical composition of carbides on mechanical properties was studied.

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L12-type chemical short-range ordering in compositionally-complex alloys

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The formation of L12-chemical ordering is a critical phase transformation phenomenon in face-centered cubic (FCC) compositionally complex alloys (CCAs) that can significantly influence their properties. However, quantifying the early stages of chemical ordering is challenging due to the complex elemental arrangements, small domain sizes, similar atomic numbers, and subtle compositional differences from the surrounding matrix. We recently introduced a machine learning-enhanced atom probe tomography (ML-APT) approach to characterize chemical short-range ordering (CSRO) in binary and ternary alloy systems. Here, this methodology is extended to the more complex CoCrNiFeMn alloys, investigating the impact of different compositions and heat treatments on the formation of L12-type CSRO. Our findings offer solid tomographic evidence of L12-CSRO, primarily with Cr repulsion tendency, along with domain size and morphology distributions that align with reported Monte Carlo simulations. The extent of L12-CSRO is strongly dependent on both composition and heat treatment conditions. A standard workflow for applying ML-APT to CCAs is proposed, emphasizing its strengths and limitations, and setting the stage for further exploration and control of local chemical ordering to advance the design of CCAs.

Hydrogen trap characterization in 200 and 1,000 bar charged CoCrNi medium entropy alloy compared to steel AISI 316L

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B5_6 - Functionality, Andalucía I Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Multiple principal element alloys (MPEAs) represent a new class of metallic materials. MPEAs, such as the CoCrNi medium entropy alloy (MEA), have attracted considerable research attention as potential materials to replace, for example, austenitic steels in high-pressure hydrogen environments. Due to the relatively new alloy concept, studies on the specific hydrogen diffusion and trapping behavior of high-pressure hydrogen-charged CoCrNi MEAs are rare so far. For this reason, a CoCrNi-MEA was investigated and compared to an austenitic stainless steel, AISI 316L. Both materials were subjected to high pressure hydrogen loading for two different pressures: 200 bar and 1,000 bar. After charging, thermal desorption analysis (TDA) was used with three heating rates from 0.125 K/s to 0.500 K/s to clarify the specific hydrogen desorption and trapping behavior. To the best of our knowledge, this study is the first to characterize hydrogen diffusion and trapping in 1,000 bar high-pressure charged CoCrNi. For this purpose, the underlying TDA spectra were analyzed in terms of peak deconvolution into a metallurgically justifiable number of defined peaks. The individual peak temperatures and activation energies "EA" were calculated. The following conclusions can be drawn from the results obtained: (1) Exposure to 200 bar or 1,000 bar leads to an increase in hydrogen absorption, regardless of the material investigated, expressed by a significantly increased desorption rate at 1,000 bar. However, the effusion peaks typically occur only at high temperatures. The (2) TDA showed that a four-peak deconvolution scenario was sufficient to describe the trapping behavior and the "EA" indicated the dominance of irreversible traps. In addition, the average trapping energy is higher than in the 316L. The (3) charge pressure related hydrogen solubility was in the order of: CoCrNi-MEA < 316L for both pressures and (4) charging at 1000 bar results in an average concentration of 49 wt.ppm (CoCrNi-MEA) and > 75 wt.ppm (316L). In summary, the CoCrNi-MEA was characterized by a reduced solubility, but very deep entrapment compared to the 316L. For this reason, further application potentials of the MEA may arise.

Towards accurate thermodynamics from random energy sampling

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B5_1 - Thermodynamics, Andalucía I Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Special Quasi-random Structures (SQSs) are often used to model disordered alloys in small simulation cells and to compute their thermodynamic properties. Yet, SQS-based sampling yields chemical potentials (among other quantities) that do not match the equilibrium values at some finite temperature. This is due to the lack of chemical short-range order in random (or SQS) samples. In this talk, we present a probabilistic analysis of chemical potential calculations based on the distribution of substitution energies and the Widom technique.

This original approach to the thermodynamics of multi-principal element alloy is demonstrated on a model Fe-Ni alloy. Atomic-scale Monte Carlo simulations are performed systematically to check the validity and the limits of our theoretical work accross alloy compositions and temperatures.

By sampling either equilibrium configurations or SQSs, we show that they both yield different results, but that it is possible to correct the results from the random sampling in order to get a result which is much closer to the equilibrium values.

The first order correction proposed in this study is quite effective and very simple to apply. Moreover, it does not require additional energy calculations.

Using similar tools, we also show that vacancy formation free energies computed from randomly sampled local chemical environments must be corrected to ensure the consistency between various available calculations. Indeed, irrespective of the choice of the species being replaced by a vacancy, we should arrive at the same value of the vacancy formation free energy. As we did for chemical potentials, we propose a simple way to compute this correction term, and compare the outcome with equilibrium Monte Carlo results and with approximations found in the literature.

In the course of the presentation we shall also discuss the applicability of the method to other quantities of interest and to alloys beyond binary concentrated alloys.

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K. Li, T. Schuler, C.-C. Fu, M. Nastar, "Vacancy formation free energy in concentrated alloys: equilibrium vs. random sampling", *Acta Materialia* 281, 120355 (2024)

Mechanical Performance and Atomistic Modeling of polycrystal NiFeCrMn Alloy Under High-Temperature Tensile Loading

Dr. Francisco Javier Dominguez Gutierrez¹, Ms Gordana Markovic², Ms Agata Zaborowska¹, PhD. Malgorzata Frelek-Kozak¹, Dr. Ayobami Daramola³, Phd Lukasz Kurpaska¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

High-entropy alloys (HEAs) have emerged as promising materials for nuclear applications due to their exceptional mechanical properties, thermal stability, and resistance to radiation damage. Among these, FCC Ni-based high entropy alloys are particularly notable for their high strength, ductility, and structural integrity, making them ideal for extreme environments such as nuclear reactors.

This study examines the mechanical performance of a NiFeCrMn alloy under tensile loading using a combination of atomistic computational modeling and experimental validation. Analyses were conducted on both single-crystal and polycrystalline samples across room-temperature and high-temperature conditions to explore the effects of grain structure and crystallographic orientation on deformation mechanisms. A refined Embedded Atom Method (EAM) potential, optimized for NiFeCrMn alloys, was employed to ensure accurate representation of the alloy's behavior, with simulations closely replicating experimental conditions for direct comparison of stress-strain responses.

Key findings highlight the influence of temperature on ultimate stress, grain structure on twin formation, and crystal orientation on defect propagation during deformation. The study underscores the alloy's ability to maintain mechanical integrity under high-temperature conditions, advancing the understanding of HEAs for demanding applications, particularly in nuclear energy systems.

This work demonstrates the synergy between computational and experimental approaches, offering a robust methodology for evaluating advanced materials under extreme conditions.

Dislocation mechanisms in MPEAs enable simultaneously high strength and ductility

Prof. Evan Ma¹

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B5_2 - Mechanical behavior, structure and microstructure, Andalucía I Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

To expand into new territories in the strength-ductility space, we exploit additional strengthening and strain hardening mechanisms rendered possible by the widened scope of element selection and composition design in multi-principle-element alloys (MPEAs), which also help push the known plasticity mechanisms including TWIP/TRIP towards extreme. In particular, the unusual chemical inhomogeneity in these highly concentrated alloys has three prongs: i) concentration fluctuation/undulation that can be intentionally enlarged [1]; ii) local chemical orders that arise from the varying chemical affinity among the constituent species [2]; and iii) abundant interfaces due to the extraordinarily high volume fraction of nanoscale sized precipitates spaced close to one another [3]. All these help roughen the atomic and energy landscape, elevating hardening via nanoscale segment detrapping in the nano-cocktail solution. The resultant stick-slip renders the motion of dislocations sluggish/difficult, which then tend to stall, react, entangle and accumulate, sustaining the ability to work-harden on the fly with increasing tensile strain. Such defect dynamics delocalize the plastic strain to prolong tensile elongation (to as large ~50%) at >GPa flow stresses [4]. In the absence of embrittling ingredients (such as ceramic and large intermetallic precipitates with inherent dislocation starvation), as long as effective means can be found at the same time to elevate strain hardening to keep up with the strength elevation, the plastic instability such as necking that instigates damage can be suppressed/delayed. This understanding motivated us to keep developing new complex concentrated alloys for better and better strength-ductility synergy [3]. We are now at the verge of realizing yields strength up to ~1.8 GPa, not far from the best super steels, and in the meantime uniform tensile elongation ~27%, similar to that of an elemental metal such as Fe. Putting it another way via a famous/old Chinese saying, this success of having it both ways is like “having fish and bear's paw at the same time”.

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[2] X. Chen et al., Nature, 592 (2021) 712-716

[3] E. Ma and C. Liu, Prog. Mater. Sci. 143 (2024) 1012

[4] L. Wang et al., Nature Mater. 22 (2023) 950

High-temperature in-situ investigation of refractory high entropy superalloys

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B5_4 - High-temperature properties and applications, Andalucía I Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The spinodal decomposition in bcc structured refractory alloys can be used as a potential strengthening mechanism, as has been demonstrated over the last decade in research on high entropy alloys and compositionally complex alloys. Early work from the 1990s already showed the possibility of further enhancing this spinodal decomposition by adding the element Al, which in addition to spinodal decomposition also provides an ordering process in the otherwise disordered bcc phases of the alloy. Nevertheless, the knowledge of refractory high entropy (super)alloy systems, is still in its infancy and requires further research to fully exploit its potential for high temperature applications in the future. Two refractory alloys of the Al-Nb-Ta-Ti-Zr family are investigated via (high temperature in-situ) XRD, in the long run for understanding spinodal decomposition properties. Ex-situ XRD and TEM observations show the formation of at least one bcc phase and an ordered B2 phase. In addition, one or more Al-Zr rich phases are observed, which are not part of the spinodal phases and are unwanted. The high-temperature observations at 1000°C for 60 h show a remarkable increase in peak width up to 2° FWHM that does not disappear after cooling in the furnace. Ex-situ observations after 1000°C for hundreds of hours and subsequent quenching show narrow peaks (max 0,2° FWHM) at the same position. This and several other observations will be presented in this talk and possible explanations are presented.

Investigation of Thermophysical Properties and Chemical Compatibility with Alumina of High-Entropy Zirconates

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Thermal Barrier Coatings (TBCs) are used in the hot zones of airplane turbines. They protect metallic components and prevent damage caused by the high combustion temperatures and corrosive atmospheres. Since the 1980s yttria stabilized zirconia (YSZ) has been used as standard TBC material. However, its properties limit the operational temperature to around 1200 °C. It is necessary to find new materials to overcome those limitations and therefore increase the efficiency of the engine by increasing the working temperature.

In the last decade, high-entropy oxides (HEOs) are investigated as a new material class. HEOs are single-phase oxides with a configurational entropy higher than 1.5 R that can be established using five or more cations in equimolar ratio and statistical distribution in one or more sublattices. The high configurational entropy could lead into a phase stabilization over a broad temperature range and has further beneficial effects like low thermal conductivity (phonon scattering due to disorder), low sintering rate (sluggish diffusion), and adjustable properties depending on the used ions.

Single cation zirconates show promising properties as future TBC materials in gas turbine applications. Based on that, the high entropy effect can improve the usability of the zirconates as a TBC material. Therefore, zirconates with the general formula $A_2Zr_2O_7$ with five different rare-earth elements on the A sublattice were investigated in this work. Their thermophysical properties, including thermal conductivity, thermal expansion, and sintering behavior were investigated. The results show comparable behavior with YSZ or better properties.

In the application, the TBC material is in contact with alumina, which forms as a thermally grown oxide on the bond coat. Therefore, the reactions of the high-entropy zirconates with alumina were investigated in this work as well. Besides the reaction in a bulk material, the behavior at the interface of the compounds as layers needs to be investigated to explore the kinetics of the reaction in detail. Furthermore, a coating technique and the mechanical and chemical compatibility with alumina in a layer system should be investigated to estimate the lifetime of a HEO coating as a TBC.

Acknowledgements

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Strong and tough high-entropy materials with excellent multifunctionality

Prof. Zhiming Li¹

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B5_6 - Functionality, Andalucía I Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Multicomponent high-entropy materials (HEMs) composed of multiple principal elements have attracted great interest owing to their considerable potentials for achieving unprecedented properties in their practically infinite compositional space. Apart from exceptional mechanical properties such as high strength and good ductility, it has been shown that excellent magnetic, electrical and thermal properties can also be involved in HEMs via compositional and microstructural design. In this talk, we will present the unique combinations of multiple functions and even mutually exclusive properties that we have successfully achieved in recently developed multicomponent HEMs. The multiple functions include high strength, good ductility, electrical resistivity, soft magnetism, low thermal expansion (Invar), resistance to corrosion and hydrogen embrittlement. The associated design strategies will be clarified and some potential directions for further developing multifunctional HEMs will also be briefly discussed.

Martensitic islands in the AlCoNiV multicomponent alloy

Dr. Raymond Kwesi Nutor¹

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B5_7 - Architectural configuration, Andalucía I Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Multicomponent alloys including medium- and high-entropy alloys (M/HEAs) are an emerging alloy class comprising multi-principal elements with exceptional mechanical properties. Among various equiatomic single-phase face-centered cubic (FCC) MHEAs, the equiatomic CoNiV MEA has displayed impressive mechanical properties by maximizing lattice distortion. Al-addition to the CoNiV MEA further improves strength by forming Al-rich body-centered cubic (BCC) related precipitates. Like in conventional alloys, martensitic transformation is viable in these M/HEAs during rapid cooling or mechanical deformation. We observe for the first time, a martensitic transformation localized only in the BCC regions surrounded by the FCC matrix in the AlCoNiV MEA. The formation of these martensitic islands is due to the heterogeneous cooling between the FCC and BCC phases of the alloy. The martensitic islands provide significant strength enhancement due to their high hardness while the surrounding ductile FCC matrix prevents premature fracture. These findings provide valuable insights into the design of novel high-performance alloys.

Deformation mechanisms in Refractory High Entropy Alloys comprising two-phase B2/bcc microstructures

Prof. Hamish Fraser¹, Dr. Brian Welk¹, Dr. Zachary Kloenne¹, Dr. Paraic O'Kelly¹, Prof. Gopal Viswanathan¹

¹The Ohio State University, Columbus, United States

B5_5 - Refractory high-entropy alloys, Andalucía I Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The deformation mechanisms in refractory high entropy alloys has been characterized using the alloy AlMo0.5NbTa0.5TiZr as an example. Specifically, the modes of plasticity active in the B2 matrix and the precipitate bcc phase have been determined using nano-indentation. For the B2 phase, a combination of weak-beam dark-field and superlattice imaging revealed dissociation of $\langle 111 \rangle$ superdislocations into two superpartial dislocations, bounding an anti-phase boundary (APB), following the reaction: $a\langle 111 \rangle = a/2\langle 111 \rangle + \text{APB} + a/2\langle 111 \rangle$. The dislocations in the B2 phase exhibited long, relatively straight screw segments and short edge segments, such that the mobility of the edge dislocations appears to be higher than that of the screw segments. Evidence of a B2 to bcc slip transmission process has been observed through use of stereo-pair imaging and anaglyph construction. This process involves the transmission of slip from the B2 matrix, followed by the decorrelated motion of the two $a/2\langle 111 \rangle$ dislocations in the bcc precipitate, demonstrated by the increased separation of the dislocations within the bcc phase. The relative lack of ductility exhibited by this alloy has been attributed to the deformation behavior in an alloyed version of the phase Al₄Zr₅ found at grain and subgrain boundaries, which was explored also by use of nano-indentation. Regarding the deformation of the Al₄Zr₅ intermetallic phase, it was found that indentation of this phase resulted in no evidence of dislocation generation and motion, and cracking at the edges of the given indent. It has been concluded that the lack of plasticity of this phase is the cause of the room temperature brittle nature of this alloy.

Stability and properties of BCC-B2 refractory “high entropy” alloys

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B5_9 - Broad high-entropy materials, Andalucía I Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Improving energy efficiency requires the discovery of new materials for use in high-temperature environments. Refractory multicomponent alloys featuring a BCC/B2 microstructure are promising because a microstructure analogous to the famous γ/γ' in superalloys, but with refractory elements, could lead to alloys that can retain high strength at very high temperatures. Given the extensive range of possible compositions in these alloys, a key initial question is whether the B2 phase can develop within refractory metals.

In this talk, I will explain how we tackled this question via our recently developed Multi-Cell Monte Carlo (MC)² method which is suitable for predicting phase stability in multicomponent systems. We used this method to span through the extensive compositional space of these alloys, refine the trends in ordering, and identify the most promising combinations for detailed analysis. We discover that B2 phases form exclusively with the inclusion of elements from groups VII and VIII of transition metals, such as Re, Ru, and we identify these phases among a total of eleven elements. Based on these findings, we develop a machine learning interatomic potential for the most promising combination and study the dislocation structure and transfer between BCC/B2 phases using atomistic simulations.

Investigating the concept of Complex Concentrated Alloys for a sustainable alloy design of lead-free brasses

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Lead (Pb) is a commonly used alloying element in brass alloys (Cu-Zn) to enhance machinability. This improvement primarily occurs due to Pb-particles' deformation into needle-like structures, which promote discontinuous chip formation, as these structures serve as points for crack initiation. However, due to Pb's toxicity and environmental hazards, several organisations have issued regulations and guidelines, such as the DWD, REACH, ELV and RoHS, to limit the maximum Pb content in components for several industries. Different approaches have been implemented to develop novel lead-free brass solutions for various applications, such as direct Pb replacement and heat treatment. Nevertheless, none of the current solutions produce cost-effective alloys with machinability comparable to leaded brasses, therefore representing a significant drawback for the industry. To close this gap, Complex Concentrated Alloys (CCAs) could be explored as a potential solution to achieve the necessary properties and requirements without compromising brass's circularity.

The present work depicts the first phase towards the sustainable development of lead-free CCAs based on the Cu-Zn system, which covers the overall alloy design: (1) literature review; (2) definition of chemical, mechanical, and microstructural requirements; and (3) compositional alloy design based CALPHAD simulations for microstructure prediction. The current literature favours a biphasic structure with low melting point precipitates to replicate the Pb's role during machining operations. A study of the supply risk of the current elements circulating within the brass scrap circular economy versus the elements' relative cost was the first step to narrowing the window of the most attractive elements to consider for a sustainable and cost-effective alloy design. Within this window, Cu, Zn, Fe, Ni, Al, Mn, and Sn are depicted as the most promising main elements to incorporate in the lead-free alloy. Based on thermodynamic assessments, thermo-physical parameters and CALPHAD simulations show that the Cu-Zn-Al-Mn system presents a promising FCC/BCC ratio, as observed for conventional alloys. The incorporation of other elements that favour the formation of soft-phase precipitates will also be presented and discussed. This study summarises the first phase of the co-promotion project 'recyBRASS' - COMPETE2030-FEDER-00576900 - between ASBW Barbosa World Brass, S.A and the Faculty of Engineering of the University of Porto, on the development of novel lead-free brass alloys.

Fabrication and characterization of a Ni-based high-entropy alloy for the hydrogen industry

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¹Department of Mining and Metallurgical Engineering and Materials Science, Faculty of Engineering of Bilbao (UPV/EHU), Bilbao, Spain, ²Foundation Azterlan, Basque Research and Technology Alliance (BRTA), Durango, Spain

B5_4 - High-temperature properties and applications, Andalucía I Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

High-entropy alloys (HEA) are a promising class of advanced materials, whose microstructure and mechanical properties can be optimized through carefully selecting compositions and process techniques. In the present study, a nickel-based HEA with chromium, manganese, and copper additions (NiCrMnCu) was developed and characterized, being its use intended for applications requiring high strength and ductility, as well as low hydrogen permeation, and fabricated using alloy elements easily available.

The HEA was designed according to ThermoCalc simulations, to get a monophasic microstructure, and then synthesized using an induction furnace. Its microstructural characterization involves optical microscopy (OM), X-Ray diffraction (XRD), scanning electron microscopy with compositional analysis (SEM + EDX), and transmission electron microscopy (TEM) to study the crystal lattice characteristics fully. Results revealed a dendritic microstructure predominantly consisting of a face-centered cubic (FCC) phase with localized segregation of the alloy components.

Corrosion resistance was evaluated using electrochemical tests in NaCl and NaOH, including polarization curves, polarization resistance measurements, and corrosion rate calculations, aiming to obtain the right parameters to analyze its behavior towards permeation in hydrogen-rich environments. As for the mechanical characterization, Small-Punch tests (SPT) have been performed, which provide information related to its tensile and fracture properties, allowing us to estimate the ductility and tensile strength of the HEA alloy by making use of small specimens.

Superb cold-drawn deformability of NiCoCrFeMo high-entropy alloys mediated via planer defect engineering

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Metal fibers are essential key materials in the fields of textiles, aerospace, petrochemical and electronic machinery. And composite and micro refinement have become the development trend of new materials. However, the fabrication of micron-scale alloy fibers remains a challenging subject. Recently, high-entropy alloys (HEAs), also known as multi-principal-component alloys (MPCAs), have received widespread attention due to their unique characteristics such as high strength and hardness, excellent low-temperature fracture toughness, high-temperature stability, corrosion resistance, and impact resistance. Herein, we present a novel Ni-Co-Cr-Fe-Mo high-entropy alloy (HEA) fiber with a reduction rate of 99.9995% and a strain (ϵ) of 12.19 prepared by cold-drawn process without requiring intermediate annealing. The exceptional deformation strain within the fiber leads to extraordinary tensile strengths at room temperature and liquid nitrogen temperature. The in-depth investigation of the microstructure of fibers has been conducted. And the cold drawing deformation mechanisms mediated by the synergistic effects of plane defects have been studied. It has been shown that various geometrically necessary dislocation interfaces, such as dislocation walls and microbands, along with deformation twins and long-period 9R structures, was formed in response to external stress when $\epsilon \leq 2.7$. As the strain increases, the saturated layered structure emerges and progressively evolves into a 3D equiaxed crystal. Moreover, the formation and evolution of the 9R structure (i.e., the migration of incoherent twin boundaries), coupled with the interaction of partial dislocations and the role of deformation twins, are crucial factors determining the fiber's plastic response. This work is supposed to provide an alternative approach for the process of high-strength metallic fibers with excellent deformability through plane defects engineering.

Empowering high-entropy alloys with unique nanostructure for exceptional oxygen evolution performance through self-replenishment

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¹University Of Science And Technology Beijing, Beijing, China

B5_6 - Functionality, Andalucía I Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Oxygen evolution reaction (OER) catalysts suffer from degradation under harsh oxygen evolution conditions, especially at large current densities, which is a longstanding challenge when developing OER catalysts for industrial applications. In this talk, we will report ultra-stable high-entropy catalysts with outstanding OER performance, created by forming two-layered nanostructures in noble metal-free high-entropy superlattice alloys, which boost activity and stability simultaneously through a counterintuitive parallel-mechanism strategy. The outer high-entropy amorphous oxide layer endows compelling OER activity (235 mV at 10 mA cm⁻²), while the underneath layer affords dynamic self-healing capability for sustainable performance (working stably for 1600 h at 500 mA cm⁻²) in alkaline electrolytes. More appealing is that the catalyst can be easily revitalized, significantly extending its service durability and reducing its cost. This finding can be applied to developing other cost-efficient catalysts with considerable potential for industrial applications, but also offers a design paradigm to break the activity-stability trade-off of electrocatalysts.

Mechanical properties of the quaternary high-entropy alloy Zr₄₅Ti_{31.5}Nb_{13.5}Al₁₀ after plasma nitriding or nitrogen ion implantation followed by heat treatment

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B5_3 - Structure, defect and mechanical behavior, Andalucía I Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

High-entropy alloys (HEAs) are materials of great interest due to their unique composition, consisting of multiple principal elements. This contrasts with traditional alloys, which typically contain only one or, at most, two base elements. The number of possible HEA compositions is significantly larger than that of conventional alloys [1]. HEAs exhibit a range of exceptional properties, including high corrosion resistance, excellent mechanical strength, and remarkable fracture toughness.

In this study, the mechanical properties of the quaternary high-entropy alloy Zr₄₅Ti_{31.5}Nb_{13.5}Al₁₀ were investigated. The alloy underwent plasma nitriding or nitrogen ion implantation and subsequent heat treatment. The primary objective of this research was to examine and compare the effects of these two modifications on the alloy's mechanical performance and microstructure.

Plasma nitriding leads to the formation of a high-entropy nitride phase within the material. In contrast, nitrogen ion implantation introduces a supersaturated solid solution but disrupts the crystal structure, primarily incorporating interstitial nitrogen atoms. To restore the crystalline structure and promote the formation of high-entropy nitrides, heat treatment was applied to homogenize the material.

Mechanical testing was performed using nanoindentation and micropillar compression to evaluate hardness, elastic modulus, and yield strength. The surface of the samples was primarily characterized using atomic force microscopy (AFM), which was employed to measure adhesion, surface roughness and friction. To analyze the microstructural changes induced by the different treatments, thin lamellae were prepared for transmission electron microscopy (TEM) observations. X-ray diffraction (XRD) analysis was conducted to confirm the presence of high-entropy nitride phases. Additionally, energy-dispersive X-ray spectroscopy (EDS) was used to determine elemental distribution both on the surface and in cross-sections of the lamellae.

Samples with nitrogen incorporated into their lattice exhibited increased hardness compared to the untreated alloy. Furthermore, the deformation mechanisms were altered following the introduction of nitrogen.

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Notable local lattice distortions in BCC refractory high-entropy alloys probed by total scattering

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B5_3 - Structure, defect and mechanical behavior, Andalucía I Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

The remarkable flexibility in tuneable chemistry and promising application prospects have driven the development of high-entropy alloys (HEAs). One particular category of HEAs, body-centred cubic (BCC)-structured refractory high-entropy alloys (RHEAs), have attracted great interest due to their exceptional mechanical properties at high temperatures. Despite the fast development in the field of HEAs, one of their key features, local lattice distortion (LLD), remains rarely explored and a comprehensive understanding of it is lacking. Considering that there has been plausible evidence suggesting that LLDs contribute to solid solution strengthening, a deeper understanding of LLDs through systematic studies might provide a promising route for decoding the structure-properties relationship and tailoring mechanical properties of RHEAs.

Total scattering and pair distribution function (PDF) analysis have been presented as potent techniques in quantitatively investigating LLDs. The effect of LLDs on the PDF peak broadening provides a way to quantify them by fitting the PDF data. However, since LLDs as static displacements are coupled with thermal displacements resulting from thermal oscillations of atoms, it is essential to separate the thermal component. One approach is to conduct measurements at cryogenic temperatures, which allows the fitting of Debye curves and the quantification of the thermal component as a function of temperature.

In this work, LLDs in BCC-structured RHEAs were quantified through variable temperature neutron total scattering measurements under cryogenic conditions. Notable LLDs were quantified in the studied BCC-structured RHEAs, compared to their face-centred cubic (FCC)-structured counterparts. Results from both a homogeneous bulk sample and inhomogeneous powder were compared to evaluate the combined effects of chemical segregation and vacancy on PDFs. Additionally, Debye temperatures of the investigated RHEAs were experimentally determined, which is one step forward in understanding their thermodynamic properties.

High temperature oxidation behavior of high entropy alloys elaborated by Spark Plasma Sintering and Hot Isostatic Pressing

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B5_4 - High-temperature properties and applications, Andalucía I Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Interest in high entropy alloys (HEAs) has increased in recent years, as they exhibit promising mechanical properties and phase stability at elevated temperatures, making them promising candidates to replace superalloys [1]. The high temperature oxidation behavior of HEAs elaborated by arc-melting, a classical metallurgical process, is widely reported in the literature [2-6]. In the present study, HEAs were elaborated by pressure assisted-sintering techniques (Spark Plasma Sintering (SPS) and Hot Isostatic Pressing (HIP)) from atomized and atomized-milled powders. The alloy under study is Al_{0.3}CoCrFeNi, formed by an FCC single-phase solid solution. Isothermal oxidation tests were performed at 900 °C for several durations up to 3000 h. SEM-EDS characterizations combined with XRD analyses revealed that the oxide scale formed on HIPed samples elaborated from atomized powder is composed of an outer Cr₂O₃ layer and α -Al₂O₃ at the metal /oxide scale interface. A spinel-type oxide containing Cr, Co, Ni, and Fe grew on top of the Cr₂O₃ scale. SEM cross-section analyses showed the formation of Al₂O₃ inside the alloy, at powder particle grain boundaries. Al₂O₃ internal oxidation tends to increase with the oxidation time. Additionally, AlN precipitates were observed inside and below the internal Al₂O₃ oxidation layer. Samples elaborated by SPS from atomized-milled powder showed a completely different oxidation behavior. The oxide scale was only formed by an α -Al₂O₃ layer, presenting two different grain morphologies. No internal oxidation (Al₂O₃) phenomenon was observed. For both HIP and SPS samples, deeper in the bulk, the high temperature ageing promotes the precipitation of B2 AlNi enriched phase inside the grains (in the form of rods) and at the grain boundaries (with equiaxed shape). Finally, the influence of the elaboration process and the initial mechanical state of the powder particles (atomized or atomized-milled) was also investigated.

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Chemically architected high-entropy alloys: exploring composition space to generalize the concept

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B5_2 - Mechanical behavior, structure and microstructure, Andalucía I Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

In addition to the various strategies already widely known and exploited, a new strengthening mechanism for metallic alloys has recently been proposed [1]. Thanks in particular to the specific features of the Spark Plasma Sintering process, an area with a pronounced chemical gradient, called interphase, was generated between the grains of two jointly sintered powders, one of pure nickel and the other corresponding to the equimolar high-entropy alloy CrMnFeCoNi. Having shown that the characteristics of the interphase were controllable [2] and that an increase in mechanical resistance, attributed to this chemical gradient, was obtained [3], the study is now being extended to other combinations of metals and/or alloys. The main objectives are to generalize the description of the phenomena already observed, while maximizing the effect of the chemical gradient on strengthening. More specifically, the aim is to find alloys with the same crystalline structure (face-centered cubic, fcc) and a significant difference in lattice parameter, which is assumed to be the main driver of hardening.

The exploration of new alloy systems was assisted by the CALPHAD method (CALculation of PHase Diagrams). Firstly, the accuracy of this tool for lattice parameter predictions, which is not a common use case, was investigated. Next, equilibrium calculations were carried out at a fixed temperature (1373 K) and in such a way as to broadly screen the compositional space within 16 alloy systems: 14 quinary and 2 quaternary, from the 13 elements considered (Al, Ti, Cr, Mn, Fe, Co, Ni, Cu, Zn, Nb, Mo, Sn and W), were explored numerically with a predefined meshing for each. From around 350,000 compositions, we selected those that were fcc single-phase and then calculated their lattice parameter. The aim is to maximize the difference in lattice parameter between the selected alloy and pure nickel. Taking into account other criteria, such as chemical complexity and manufacturability, a limited number of compositions were selected. These were then processed by melting, casting and homogenization treatment, and their microstructure was characterized. Finally, the experimental results were compared with predictions.

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Phase stability and mechanical behaviour of oxygen-doped refractory high-entropy alloys.

Ph.D. Mariano Casas-Luna¹, Ph.D. Michal Knappek¹, Ph.D. Milos Janecek¹, Ph.D. Josef Strasky¹

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B5_8 - Alloying effect, Andalucía I Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

In recent years, there has been a growing interest in exploring the central regions of multi-element phase diagrams, leading to the development of a new class of alloys known as complex concentrated alloys (CCAs). Among these, high-entropy alloys (HEAs) are characterized by a high configurational entropy that can stabilize a single-phase microstructure. These alloys exhibit a wide range of attractive physical properties, making them promising candidates for advanced applications even at high-temperature conditions.

One approach to further enhancing HEA properties is the introduction of interstitial elements, such as oxygen, which can significantly influence phase stability and mechanical behaviour. Although the impact of interstitial oxygen has been observed in specific traditional alloy systems, such as TiZrNb, its role in HEAs remains largely unexplored.

This study focuses on four refractory HEAs composed of quinary systems based on the AlTiNb system, incorporating Cr, Fe, Mo, and/or Zr, specifically designed to achieve low-density single-phase alloys. The alloy compositions were carefully tailored by CALPHAD method to ensure a single-phase body-centred cubic structure. To investigate the effects of oxygen doping, interstitial oxygen was introduced at concentrations of 0.5 and 1.0 atomic percent. The study systematically examines its influence on phase stability and mechanical properties, particularly microhardness and compressive strength. The experimental results shed light on the role of oxygen in enhancing phase stability, as demonstrated by microstructural observations and X-ray diffraction analyses. Additionally, interstitial oxygen improved the hardness and mechanical performance of most of the studied alloys, which has significant implications for the development of next-generation CCAs with controlled oxygen content.

Interstitial solid solution high-entropy thin films

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B5_7 - Architectural configuration, Andalucía I Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Face-centered-cubic (fcc) high-entropy alloys (HEAs) have attracted significant research interest over the past two decades mostly due to their exceptional mechanical properties, which are attributed to their low stacking fault energy and the resulting activation of deformation twinning and/or martensite formation [1,2]. However, their respective room temperature yield strength is low. Common methods to enhance yield strength, such as partial recrystallization or grain refinement, often lead to a significant reduction in ductility at least when a significant increase in yield strength is targeted [3].

Interstitial elements, like carbon and nitrogen, are the most effective solid-solution strengtheners. Nevertheless, the interstitial content in HEAs is typically kept low to prevent the formation of carbides and/or nitrides, which are known to degrade mechanical properties, particularly ductility, and corrosion resistance. This limitation restricts the degree of solid-solution strengthening achievable through interstitial elements. To incorporate significant interstitial content into HEAs, nitrogen must be introduced at high temperatures where nitride formation is thermodynamically unstable, followed by rapid quenching to suppress precipitation during cooling. Reactive DC magnetron sputtering provides a viable pathway to produce interstitial-rich thin films due to its ability to achieve very high cooling rates. However, research on nitrogen-containing HEA thin films often focuses on the formation of high-entropy nitrides, with relatively few studies investigating high-interstitial solid solutions.

This study explores the effect of nitrogen flow rate on the microstructure and mechanical properties of Co-free Cr_{0.5}FeMnNi(100-x)N_x HEA thin films using a combination of nanoindentation, transmission electron microscopy (TEM), and X-ray photoelectron spectroscopy (XPS). The findings demonstrate that HEA thin films significantly supersaturated with nitrogen with a significant increase in mechanical properties can be successfully synthesized via reactive DC magnetron sputtering.

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Active learning prediction of the enthalpy of mixing of BCC, FCC and HCP solid solutions

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B5_1 - Thermodynamics, Andalucía I Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Predicting the formation of solid solution is essential in a large field of research, particularly for high-entropy alloys, for which the properties can be modulated by adjusting the composition and nature of elements. To design these alloys, it is important to know the enthalpy of mixing in the face-centered cubic (FCC), body-centered cubic (BCC), and hexagonal compact (HCP) phases, because this property is key to predict their formation using machine learning [1] or thermodynamic [2] approaches. At present, these approaches rely on enthalpy of mixing data that are either approximations from Miedema's model [3], which is valid only for the liquid phase, or obtained by Density Functional Theory (DFT) methods, which are time-consuming, and make it challenging to explore all possible configurations and combinations for all phases. In both cases, the enthalpy of mixing of multicomponent solutions is obtained by summing the pairwise interactions of all binary subsystems.

In this study, we develop a machine learning model to predict the enthalpy of mixing in the FCC, BCC, and HCP phases generated by binary combination of dozens of elements. The training dataset is built from literature data, and is completed using active learning to identify where new data is most needed, and the Special Quasi-random Structures methods combined with the DFT method are used to simulate news data. The agreement between experimental and theoretical data, as well as between enthalpies of mixing calculated for complex concentrated solutions and those extrapolated from binary systems, is discussed. Our results can be used to improve and extend to other elements predictions of FCC, BCC and HCP phase formation that are necessary for the design of high entropy alloys.

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Experimental and computational analysis of nanoindentation-induced plasticity in arc-melted equiatomic Mo-Ta-W refractory bcc single-phase alloy

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B5_3 - Structure, defect and mechanical behavior, Andalucía I Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Medium and high entropy alloys (MEAs and HEAs) have been studied for the last twenty years. Many compositions are still unknown due to the vast field of possible systems. Alloys based on refractory elements are very promising for high-temperature applications due to their very high strength. However, their brittleness at room temperature, relatively poor oxidation resistance, and difficulty in preparation due to very high melting points of constituent elements limit the application of refractory multicomponent alloys. Moreover, the deformation mechanisms of refractory alloys are poorly understood, which slows down advancements in the field.

The aim of this study was to investigate nanoindentation-induced plasticity in a single-phase equiatomic Mo-Ta-W alloy. The experimental results were compared with molecular dynamics (MD) simulations. Mo-Ta-W alloy was prepared using the arc melting technique. The alloy was characterized by various methods such as XRD, SEM-EDS, EBSD, TEM, and nanoindentation. After casting, the microstructure of the Mo-Ta-W alloy reveals a segregation of molybdenum, which has a significantly lower melting point than tantalum and tungsten. The annealing at 1550°C for 24 h was performed to homogenize the microstructure. The XRD confirms a single bcc phase structure and large grains of a few hundred micrometers. The nanoindentation was carried out in the grains with different orientations, i.e., [001], [111], and [101], to study plastic response. The effect of grain boundaries was diminished in this study. The pile-up formation and slip traces were analyzed by SEM and TEM and, subsequently, compared with the MD simulations. It was found that experimental and computational results are in good agreement. The dislocations in Mo-Ta-W alloy are distorted compared to pure W. The studies that were conducted deliver new knowledge about the understanding of nanoindentation-induced plasticity of refractory multicomponent alloys.

Microstructure evolution and excellent mechanical properties of TiVNbHf refractory High Entropy Alloy fabricated by powder metallurgy

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B5_5 - Refractory high-entropy alloys, Andalucía I Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

This study introduces a powder metallurgy (PM) approach combining mechanical alloying (MA) and hot press sintering (HPS) to fabricate high-performance TiVNbHf refractory high entropy alloys (RHEAs), which consist of BCC and V-Hf-rich phases. The ball milling process and HPS sintering temperatures were optimized to enhance the alloy's properties. Notably, the average grain size of the TiVNbHf RHEAs was only 1 μm , two orders of magnitude smaller than that of as-cast TiVNbHf alloys. This fine microstructure resulted in a low density (8.12 g/cm³) and significantly improved mechanical properties, with yield strength, fracture strength, and fracture strain reaching 1880 MPa, 2227 MPa, and 24.4%, respectively, at room temperature—approximately 500 MPa higher than those of as-cast TiVNbHf alloys. Furthermore, reducing the V and Hf content led to the complete elimination of the V-Hf-rich phases, contributing to further improvements in density (7.49 g/cm³). In addition, the yield strength, fracture strength, and fracture strain reached 1630 MPa, 2198 MPa, and 34.4%, respectively, at room temperature—approximately 41% higher in strain than that of the TiVNbHf alloys. Notably, at 800 °C, the yield strength was 859 MPa. Consequently, the specific strengths of these TiVNbHf RHEAs significantly surpass those of publicly reported Ni-based superalloys, especially above 800 °C, indicating potential for partial substitution of conventional Ni-based superalloys in aerospace applications, where both weight reduction and performance improvement are critical. Finally, the microstructural evolution and the underlying strengthening-toughening mechanisms of the PM TiVNbHf RHEAs are discussed.

Phase transformation and texture evolution in a metastable medium entropy alloy

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B5_2 - Mechanical behavior, structure and microstructure, Andalucía I Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The metastable Fe₄₅Co₃₅Cr₁₀V₁₀ medium-entropy alloy (MEA) exhibits a single-phase face-centred cubic (fcc, γ) structure after casting and homogenisation at 1100 °C for 6 h. During cold rolling (CR), the MEA undergoes deformation-induced martensitic transformations via $\gamma \rightarrow \epsilon \rightarrow \alpha'$ and $\gamma \rightarrow \alpha'$ pathways with variant selection. Beyond 40% CR thickness reduction, the γ phase develops a Brass-type texture due to the preferential transformation of $\text{Cu}\gamma$ and $\text{S}\gamma$ orientations to ϵ and α' -martensite, accompanied by shear banding. The ϵ -martensite texture features $\sim(01\bar{1}5)$ $[[3742]]$ ϵ and $\sim(1126)$ $[[[1]\bar{1}21]]$ ϵ orientations along the $\{hkil\}$ -fibre, arising from $\text{Cu}\gamma$ and $\text{S}\gamma$ orientations via the Shoji-Nishiyama orientation relationship (OR) and variant selection. Similarly, the α' -martensite texture, typical of bcc materials, aligns along the alpha and gamma fibres after 80% CR, with the former originating from $\text{G}\gamma$, Br_γ Cu_γ and S_γ orientations, and the latter mainly from Br_γ and S_γ via the Kurdjumov-Sachs OR and variant selection.

Isochronal annealing of the metastable MEA at 625–900 °C for 300 seconds after 80% cold rolling (CR) results in the formation of the Cr- and V-rich sigma (σ) phase between 625–725 °C. Beyond 725 °C, the microstructure consists solely of the γ phase due to $\alpha' \rightarrow \gamma$ reverse transformation, which begins at 675 °C and completes above 725 °C, driven primarily by shear martensitic transformation. Recrystallisation of the reverted γ phase completes at ≥ 850 °C, with nucleation occurring preferentially within shear bands. The reverted γ phase retains a rolling texture with high intensities at $\text{G}\gamma$, Br_γ , and GT_γ orientations after annealing between 625–750 °C. Above 750 °C, annealing twinning weakens $\text{G}\gamma$ and Br_γ orientations while strengthening GT_γ and (120) $[[2\bar{1}0]]$ γ orientations, driven by first-order twinning of $\text{G}\gamma$ and GBr_γ orientations. Twinning within $\text{G}\gamma$ and Br_γ also produces new (214) $[[2\bar{1}1]]$ γ and RBr_γ orientations, characteristic of low stacking fault energy alloys.

Isothermal annealing at 625 °C reveals that the MEA develops B2-like chemical short-range ordering (CSRO) domains within 300 seconds. These CSRO domains gradually transform into a long-range ordered B2 phase after more than 6 hours of annealing at the same temperature. A combination of scanning transmission electron microscopy and thermodynamic calculations indicates that this disorder-to-order transformation is driven by the formation of the σ phase, which depletes the disordered α' -martensite (bcc) matrix of Cr and V elements. The ordered B2 phase is predominantly FeCo-rich, resembling the chemical composition of Fe-Co binary or Fe-Co-V magnetic alloys that undergo disorder-to-order transformations at low annealing temperatures.

Optimizing oxide dispersoid content towards enhancing mechanical properties of ODS Ni-based high entropy alloy

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The oxide dispersion strengthened high entropy alloys (ODS HEAs) represent an advanced material that integrates the distinctive properties of high entropy alloys with the strengthening effect of oxide nanoparticles. The excellent high-temperature stability, strength, hardness, and corrosion resistance of the ODS HEAs thus offer new avenues for developing structural materials to meet high-temperature applications like aerospace, nuclear power plants, etc. The current research work provides a comprehensive approach for optimizing oxide dispersoids in oxide dispersion strengthened high entropy alloy (ODS HEA) to enhance the strength-ductility alliance, thereby widening its applicability. The study focuses on fabrication of ODS HEA featuring a composition of Ni₄₇Al₆Co₁₈Cr₈Fe₁₂Ti₈W₁ at. % via mechanical alloying (MA) and spark plasma sintering (SPS). The investigation encompasses variations in Y₂O₃ content, including 1 vol. %, 3 vol. % and 5 vol. %. The effect of Y₂O₃ addition on the microstructural evolution and mechanical properties of the sintered alloys was evaluated. Phase analysis reveals that presence of Y₂O₃ promotes the formation of Y₂Ti₂O₇ complex oxide precipitation in ODS HEAs. A significant enhancement in both hardness and strength is evident in the pristine HEA upon Y₂O₃ addition. However, a reduction in these properties is observed in the 5 vol.% Y₂O₃ ODS HEA due to agglomeration of Y₂O₃ nanoparticles. Notably, the ODS HEA containing 3 vol.% Y₂O₃ exhibits exceptional mechanical characteristics, achieving a compressive yield strength of 1517 MPa and a compressive strain of 27%, demonstrating a synergistic combination of strength and ductility. Enhancement of the mechanical properties in the ODS HEA is ascribed to both oxide dispersion strengthening resulting from addition of Y₂O₃ as well as presence of in-situ formed Y₂Ti₂O₇ complex oxide coupled with solid solution strengthening effect of the HEA matrix.

Keywords: High Entropy Alloy, Oxide dispersion strengthening, Mechanical alloying, Spark plasma sintering, Solid solution strengthening

Development of High Specific Modulus Multicomponent Alloys with An FCC Structure

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B5_2 - Mechanical behavior, structure and microstructure, Andalucía I Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

This project aims to design a new single-phase FCC High Entropy Alloy (HEA) with a high specific modulus, employing a combined computational and experimental approach. The goal is to develop a lightweight engineering material that achieves ductility through an FCC structure, and a high stiffness and low density, using the compositional freedom of HEAs. Firstly, computational modelling methods are used to efficiently explore the vast compositional space and identify promising candidates. After promising compositions are found through modelling studies, these alloys are manufactured experimentally, and the modelling results are verified by characterization studies. In this direction, CASTEP, an atomistic modelling method based on density functional theory, is used in assessing lowest energy phases and their elastic properties. In addition to this method, phase estimation is supported using Thermo-Calc (CALPHAD method software). In the experimental side, Vacuum Arc Melting is used in sample manufacturing. SEM, EDX and XRD are used to characterise the structure, with mechanical properties assessed by nanoindentation.

Despite the power of computation, employing particular search strategies is useful in narrowing the compositional space to explore. To do this, two different approaches are being followed. The first approach designs a new alloy from scratch, while the second manipulates a previously known single-phase FCC HEA to retain the FCC structure while increasing the specific stiffness. Within the scope of the first approach, modelling and experimental studies were initially conducted with aluminium and nickel, with the subsequent introduction of cobalt. The second approach explored the individual effects of copper, molybdenum, vanadium, and aluminium additions to an CoFeMnNi base. The results of modelling and experimental studies on these alloys will be presented.

TiVCr-based High Entropy Alloys for solid-state hydrogen storage

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B5_6 - Functionality, Andalucía I Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

High-entropy alloys (HEAs) emerged as promising materials having a significant potential for solid-state hydrogen storage due to their very good sorption properties. The high mixing entropy, resulting from their multi-elemental composition, favors the formation of solid solution phases with simple crystallographic structures (bcc, fcc or hcp). The wide range of relevant chemical elements and adjustable compositions offers a favorable playground for optimizing HEAs with excellent hydrogen sorption properties and equilibrium pressures above 1 bar at 25°C in order to target industrial applications.

Our work focused on TiVCr-based HEAs with a small percentage (4 to 8 at. %) of Mn, Fe or Mn and Fe, synthesized by induction melting. Structural analysis was performed by X-ray and neutron diffraction. The as-cast alloys contain a predominant bcc phase and a minority hexagonal C14 Laves phase, of which amount seems to depend on the Mn-Fe proportion. The co-existence of these two phases is supported by CALPHAD thermodynamic calculations. Upon hydrogenation, two distinct hydride phases are observed: a β -bcc monohydride which forms at the lowest hydrogen pressures and a γ -fcc dihydride at higher pressures. Microstructural and chemical analyses were carried out using scanning electron microscopy, coupled with energy-dispersive X-ray spectroscopy. They revealed some degree of elemental segregation at grain boundaries, correlated to the wide range of melting points and an uncontrolled cooling process. These local spatial inhomogeneities, together with the variable bcc/C14 proportion, play a crucial role in the overall hydrogen sorption properties. These latter were assessed by pressure-composition isotherms, using the Sievert's volumetric method. The alloys demonstrated fair hydrogen storage capacities (1.5 to 3.6 wt. %) with fast kinetics (< 3 min) and equilibrium pressures exceeding 1.5 bar at 25°C, making them potential candidates for industrial hydrogen storage applications.

The complementarity of the experimental techniques we used sheds light on the subtle structural and chemical variations existing at the micrometric scale and promotes a better understanding of the parameters that could influence the hydrogen sorption properties. These promising results motivate in situ diffraction studies during hydrogen absorption and desorption to better understand the structural transitions occurring during hydrogenation.

Nitrogen Ion Implantation in Refractory High Entropy Metallic Glass HfMoNbTaTiVWZr: Structural and Mechanical Effects

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

High entropy metallic glasses (HEMGs) combine the superior mechanical and chemical properties of metallic glasses with the compositional complexity of high entropy alloys. Among them, refractory high entropy metallic glasses (RHEMGs) stand out for their high thermal stability, oxidation resistance, and superior mechanical properties at elevated temperatures. Despite extensive studies on their thermal behavior, mechanical performance, and glass-forming ability, ion implantation remains an underexplored method for optimizing their surface properties.

This study investigates the effects of nitrogen ion implantation on a thin film of HfMoNbTaTiVWZr, a RHEMG with exceptional stability and hardness. While ion implantation has been successfully employed to enhance hardness and wear resistance in both conventional metallic glasses and high entropy alloys, its influence on RHEMGs is not well understood. Previous studies have shown that argon ion implantation has minimal impact on the hardness of this material, suggesting high radiation resistance. However, nitrogen implantation may lead to significant changes, including nitride formation, densification, and modifications in atomic bonding.

Our research explores the impact of nitrogen incorporation on hardness, elastic modulus, tribological performance, and fracture resistance. Special attention is given to nitrogen diffusion mechanisms, penetration depth, and potential nitride formation. Preliminary findings indicate that nitrogen implantation can significantly alter the material's surface characteristics without compromising its bulk properties. These results provide critical insights for tailoring RHEMGs for high-performance applications in extreme environments, where enhanced surface properties are required without sacrificing structural integrity. Samples with nitrogen incorporated into their lattice exhibited increased hardness compared to the untreated alloy. Furthermore, the deformation mechanisms were altered following the introduction of nitrogen.

Size effects and strain rate sensitivity in nanocrystalline High-Entropy CuMoTaWV

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B5_3 - Structure, defect and mechanical behavior, Andalucia I Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

High-entropy alloys (HEAs) are materials known for their exceptional mechanical properties, resistance to thermal effects, radiation, and even corrosion, properties, which are often unattainable with conventional materials [1]. From a nanomechanics point of view nanocrystalline structure is particularly interesting [2] and because of that, this work investigated size effects and strain rate sensitivity in nanocrystalline CuMoTaWV prepared using single target DC-magnetron sputtering.

To achieve objective comparison of the behaviour of novel HEA under various loads and different loading rates were investigated with nanoindentation and compression of micropillars in situ Scanning Electron Microscopy with an Alemnis nano-indenter. Therefore data from experiments were correlated with taken images and videos, which extended the analysis. To analyze the microstructural changes induced by compressive stresses due to nanoindentation and micropillar compression tests thin lamellae under indents and in cross-sections of pillars with the use of Focused Ion Beam were conducted. Prepared lamellae were investigated using Transmission Electron Microscopy in order to enhance knowledge of the behaviour of the nanocrystalline HEA after loading.

Experimental work will help with the evaluation of the influence of the different effects on the mechanics of HEAs. The overall project objective is to bring a wider understanding of mechanical properties and underlying rules affecting the behaviour of nanocrystalline HEA.

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Influence of Carbon Content on the Microstructure and Mechanical Properties of High-Entropy (Mo Nb Ti V W)C Carbides

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B5_8 - Alloying effect, Andalucía I Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

High-entropy carbides (HEC) have attracted much interest because they combine several, at least five, elements in a unique way, giving these ceramics excellent mechanical properties and heat resistance. In this study, we investigate how varying carbon content affects the microstructure and mechanical properties of (Mo Nb Ti V W)C high-entropy ceramics. (Mo Nb Ti V W)C system was prepared by carbothermal reduction route using metal oxides and carbon as starting materials. Powder compositions were tailored based on thermodynamic predictions. The synthesized powders were then subjected to spark plasma sintering at high temperatures.

The microstructural analysis focused on the changes induced by the carbon content, such as grain structure, distribution of elements, and secondary phase formation. Mechanical properties were investigated by nanoindentation to obtain information on hardness and elastic modulus. The results revealing the causalities between design, processing and properties of HECs are presented in this study, focussing on the influence of carbon content. Understanding the role of carbon content in these ceramics is essential to tailor their properties for advanced structural applications.

Processing of Biphasic High-Entropy Alloys by Laser Powder Bed Fusion and Optimization of Heat Treatments: Enhancing Strength at High Temperatures via Precipitates Strengthening.

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B5_7 - Architectural configuration, Andalucía I Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

High-entropy alloys (HEAs) have attracted significant attention in recent years due to their unique microstructures and exceptional mechanical properties. Among these, biphasic HEAs (FCC+BCC phases) offer a promising balance of strength and ductility, especially when their phases are precisely tailored. In this study, Laser Powder Bed Fusion (LPBF) is employed to fabricate two novel Al-containing biphasic HEAs based on the Cantor alloy from commodity powders. Using these powders, rather than elemental ones, helps to reduce the overall cost of developing HEAs. These commodity powders contain the essential alloying elements required for fabricating the alloys, offering a more affordable and sustainable option by allowing the recycling of metal scraps from these commodity alloys. Besides, the alloys will receive post-processing based on heat treatments involving solution treatment and aging. These treatments are designed to finely disperse the BCC phase as precipitates within the FCC matrix, thereby enhancing mechanical strength and hardness at room and high working temperatures (600-750 °C). Microstructural characterization was performed by SEM, EDS, EBSD, and TEM explorations, while the mechanical performance was assessed by hardness measurements, profilometry-based indentation plastometry (PIP), and micro-compression tests at room and high temperatures. Correlating the microstructural features with the final mechanical performance will be a key step in demonstrating the effectiveness of the dispersed BCC precipitates in the FCC matrix. This research represents a novel integration of advanced additive manufacturing and precise thermal processing to optimize biphasic HEAs. By optimizing the post-printing heat treatments, it is possible to obtain tailored strength-to-ductility ratios for specific applications by dispersing differently the BCC precipitates in the FCC matrix. Furthermore, their development through LPBF offers the consecution of complex geometries, increasing their overall added value. Finally, evaluating their mechanical properties at room and high temperatures showcases the alloys' potential for high-performance applications in critical engineering sectors.

Oxygen-induced decomposition of the BCC HfNbTaTiZr high-entropy alloy

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B5_8 - Alloying effect, Andalucía I Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The HfNbTaTiZr alloy is one of the most thoroughly investigated body-centered cubic (BCC) high-entropy alloys, due to its ductility and malleability at room temperature. However, experimental studies on the phase stability of this alloy have produced conflicting results. While some studies report a single-phase solid solution above 900 °C, others mention the presence of secondary phases or short-range clustering up to 1450 °C.

The aim of this work is to investigate the factors affecting the stability of an initially single-phase BCC HfNbTaTiZr alloy by heat treatments at 900 °C up to 1000 hours in different atmospheres. The BCC solid solution remains stable at this temperature but O contamination originating from the aging atmosphere leads to the co-precipitation of an O-enriched hexagonal close-packed (HCP) Hf-Zr-rich phase and a second Nb-Ta-rich BCC phase. Diffusion of O in the atmosphere from the surface to the core of the sample is faster along grain boundaries than through the grain interior. This results in an inhomogeneous distribution of precipitates, formed at grain boundaries by a monotectoid reaction. Similar phases were observed in a HfNbTaTiZr enriched with 3 at.% O, thus confirming the role of O in phase stability.

During this presentation, the influence of O on the BCC phase stability will be demonstrated and the crystallographic aspects of the oxygen-contaminated microstructure will be discussed and compared to the BCC-HCP microstructure found in other type of alloys. These aspects will include the orientation relationship between the different phases, the location of the precipitation, and the growth orientation of the precipitates.

Development of layered Cu-Mo composites with tailored thermal properties

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B5_7 - Architectural configuration, Andalucía I Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Keywords: Cu-Mo-Cu composites, thermal management, ARB, diffusion bonding, interfacial bonding.

Nowadays, the demand for materials with tailored thermal and mechanical properties is growing rapidly, particularly in the electronics and aerospace industries, where thermal expansion mismatches pose significant challenges. Copper-molybdenum (Cu-Mo) composites are promising candidates due to their exceptional thermal stability, high thermal conductivity, and adjustable coefficients of thermal expansion (CTE).

In this work, attempts have been made to produce and characterize Cu-Mo composites with layered structures and optimized properties for advanced thermal management applications. Two distinct manufacturing approaches were applied to achieve unique microstructures and performance characteristics, i.e. accumulative roll bonding (ARB) supported with diffusion bonding and electroplating for submicron laminates.

The ARB process, combined with diffusion bonding, was employed to produce Cu-Mo laminates with submicron layers thickness. This method ensures strong interfacial bonding between the Cu and Mo layers, which is crucial for thermal and mechanical properties. Electroplating was integrated into the process to enhance the active surface and refine layer uniformity at submicron scales prior to the diffusion bonding step. This approach provided a cost-effective pathway for scaling up production while maintaining precise control over composite properties.

Comprehensive characterization of the composites was conducted, including microstructural analysis using SEM and TEM, thermal conductivity and mechanical strength measurements, along with CTE evaluation. The investigated method allowed us to obtain promising materials and outline guidelines for the design and fabrication of novel layered composites with tailorable thermal and mechanical properties.

Acknowledgment

The research was conducted as a part of the NCN OPUS-22 (LAP) project: “Development of submicro- and nanostructured Cu-Mo composites with tailored properties for thermal management” (grant agreement UMO-2021/43/I/ST5/01701)

High-throughput screening of Al-Co-Cr-Fe-Ni-Ti compositionally complex alloys: from CALPHAD simulation to AM-generated component

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B5_1 - Thermodynamics, Andalucía I Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

The accelerated design of high entropy alloys (HEAs) and compositionally complex alloys (CCAs) aims to expedite the discovery and optimization of these materials through computational techniques and high-throughput experimental methods. By leveraging thermodynamic simulations techniques such as CALPHAD, it is possible to predict phase stability of various alloy compositions, significantly reducing the time and resources required for traditional trial-and-error approaches.

In the research project NovMat-AM a high-throughput screening approach has been utilized and further improved, enabling characterization of more than 60 novel alloys in the Al-Co-Cr-Fe-Ni-Ti system. The aim was to develop a dual-phase alloy comprising FCC matrix and L12 precipitations after age hardening heat treatment for application in harsh environment. From the screened compositions one selected alloy Al₇Ti₆Cr₁₆Fe₁₄Co₁₄Ni₄₃ (in at.%) has been cast and then processed to 20 kg powder for additive manufacturing. This powder was successfully used to produce a turbine stator as a demonstrator part by means of laser powder bed fusion (LPBF). Furthermore, the mechanical properties of the synthesized alloy at elevated temperature of $T = 600\text{ }^{\circ}\text{C}$ were determined by means of tensile test.

The alloy Al₇Ti₆Cr₁₆Fe₁₄Co₁₄Ni₄₃ exhibited a phase structure consisting of FCC matrix, L12 precipitations and small amounts of BCC B2, Ni₃Ti and sigma phase in the as cast state. In the as-built state the LPBF-produced samples had a much finer dendritic solidification structure than the as cast samples. However a precipitation of the L12 phase could not be detected in the as-built state of the LPBF samples. After homogenisation heat treatment at $T = 1,150\text{ }^{\circ}\text{C}$ for $t = 24\text{ h}$ and subsequent age hardening at $T = 850\text{ }^{\circ}\text{C}$ phase composition comprises FCC matrix, L12 precipitations and small particles of BCC B2 and sigma phase at the grain boundaries. This is true for both. i.e. cast and LPBF processed material, although the LPBF samples exhibit finer grain structures. With a tensile strength of $R_m = 1,056 \pm 37\text{ MPa}$ at $T = 600\text{ }^{\circ}\text{C}$ the heat treated LPBF samples show promising results for future use in high-temperature application. However, the low ductility of the alloy with elongation at break of $A = 0.5\%$ still needs to be improved. A slight reduce of Al and Ti content could be a possible solution for avoidance of the formation of BCC B2 and sigma phases, which are presumed to be the main reason for the decreased ductility of the material.

Laser metal deposition of NbTaTiV Refractory High Entropy Alloy

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B5_5 - Refractory high-entropy alloys, Andalucía I Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Mechanical resistance at high temperature is a critical challenge for the aerospace and aeronautical industry. A new category of alloys, refractory high entropy alloys (RHEA), made of refractory elements in close to equimolar proportions, shows very promising high temperature resistance. However, they encounter multiple manufacturability issues, and are still held back by cost and density issues, and by the number of possible alloy composition.

In parallel, additive manufacturing is an ever-growing technology, allowing the production of highly complex parts. This could lead to simpler and lighter structures, and to more efficient material usage. Moreover, the Laser Metal Deposition (LMD) technique can be used as a high throughput scanning tool to identify new RHEA compositions. However, this process comes with its own set of problems.

This study therefore offers to analyze the manufacturability of NbTaTiV by LMD process.

Procedure

The samples are manufactured on commercial BeAM Mobile and Modulo400 LMD machines.

A mixture of pure elemental powders was used to manufacture single-beads, 5-layer walls and bulk samples, using various deposition parameter. A second laser exposure without powder addition was tested to homogenize the deposited microstructure. All samples were produced under argon atmosphere. The samples were observed with an optical and a scanning electron beam microscope. The composition of the samples was analyzed by EDS. The microhardnesses of the deposits were also measured, and tensile samples were extracted from the bulk samples and tested.

Combined CFD+DEM simulations were conducted to help with the composition control of the powders. Upon analyzing the samples, it appears that their composition strongly deviates from the expected equimolar one. The ratio between the obtained concentrations and expected ones was 0.78, 0.57, 0.94 and 2.01 for Ti, V, Nb and Ta, respectively. Ta powders therefore have a better deposition efficiency. DEM+CFD simulations showed that this discrepancy was mostly due to variations in term of powder impact velocity.

Upon performing an EDS mapping of the samples' cross-section, large quantities of Ta and Nb powder (elements with the highest melting point) can be observed. The 2nd laser exposure allowed to homogenize the microstructure and reduce the number of Ta and Nb particle.

The tensile tests returned an average yield strength of 832MPa and an average maximal elongation of 5.55%

The next step in the study is the high-scale, high-temperature testing of the alloy, and the application of a thermal treatment to further homogenize them.

Structural and mechanical properties of refractory alloy thin films: TiZrHfTa system

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Complex concentrated alloys (CCAs), including medium- and high-entropy alloys, offer attractive thermomechanical properties which make them promising candidates for various technologies such as corrosion resistant or radiation tolerant structural materials. Among the various CCAs, alloys with multi-principal refractory elements (RCCA) have drawn significant attention for hydrogen (H) storage applications [1-3] due to their ability to reversibly absorb H in the form of metal hydrides. However, up to now, studies on RCCA for H storage have only focused on bulk materials, with limited attention to thin film counterparts, which could be considered as model materials enabling an easy tailor of composition, phase and microstructural features (grain size, porosity or texture), providing valuable insights on the mechanisms of hydride formation and

dissolution in RCCAs. In this work, (TiZrHf)_{100-x}Ta_x thin films, with thickness up to 700 nm and Ta content ranging from 0 to 60 at.%, were synthesized by co-sputtering deposition. The phase composition, crystal structure, morphology and elemental composition was determined using a combination of analytical techniques (XRD, SEM/TEM, EDS), while the intrinsic stress was measured in situ during deposition by wafer curvature method. The mechanical properties of the films were assessed by nanoindentation and opto-acoustics (Brillouin light scattering and picosecond laser ultrasonics) methods. By tuning the Ta content, different phases were stabilized in these quaternary alloys, from hcp to bcc and amorphous. These structural changes are accompanied by variation in growth morphology (evolving from nanocolumns to vein-like patterns), stress reduction and a progressive softening of hardness, shear and elastic modulus with increasing Ta content. The experimental findings are discussed and compared with results obtained from atomistic models of random alloys and amorphous phases, using ab initio molecular dynamics simulations combined with machine-learned interatomic potentials, as well as relevant data from the existing literature [4]. Preliminary hydrogenation tests will be also reported.

References:

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Spinodal Decomposition in FeMnNiCoCu High-Entropy Alloys: A Combined Theoretical and Experimental Study

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B5_8 - Alloying effect, Andalucía I Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Spinodal decomposition in complex multi-component alloys is less explored and not yet fully understood. While chemical thermodynamics provides robust predictions of a spinodal character, the inclusion of elastic energy contributions can shift the boundaries of phase stability. In this study, we explore the interplay between chemical and elastic contributions in the spinodal decomposition of FeMnNiCoCu High-Entropy Alloys (HEAs) with a focus on Fe₂₀Mn₁₀Ni₂₀Co₃₀Cu₂₀. Notably, this alloy lies outside the chemical spinodal for 873 K but within the elastic spinodal, which showcases the potential significance of elastic contributions. To test our predictions, we performed annealing experiments at 873 K over durations ranging from 0 to 240 h. X-ray diffraction (XRD) measurements are employed to track phase evolution. Selected samples are further analysed using transmission electron microscopy (TEM) to provide insights into the resulting microstructural changes. The results of the thermodynamic and kinetic models suggest that elastic energy may play a decisive role in phase decomposition processes. The experimental data will also serve to critically assess the validity of the elastic spinodal and their potential overestimation. This combined theoretical and experimental approach provides a deeper understanding of the mechanisms driving phase evolution in multi-component alloys.

High temperature corrosion resistance of HEA for application in hydrogen energy

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B5_4 - High-temperature properties and applications, Andaluc a I Room (Level +1), septiembre 15, 2025,
17:00 - 19:00

The constant need to reduce greenhouse gas emissions and the desire to improve the efficiency of gas turbines lead to a continuing trend in increasing the operation temperature of gas turbines. Higher operating temperatures reduce fuel consumption and higher combustion temperatures reduce emissions of pollutants. In addition, hydrogen is increasingly being used as a cleaner alternative fuel. However, the use of hydrogen or hydrogen-rich fuels increases combustion temperatures and increases water vapour content in exhaust gases. Typically used Ni-based alloys reached their operation temperature limit. In addition, the presence of water vapor exacerbates the oxidation behaviour of Ni-based alloys at high temperatures. It is therefore necessary to use a new brand of materials in gas turbines running on hydrogen-rich fuels. High-entropy alloys (HEAs) are a very promising material to replace commonly used Ni-based alloys. HEA is a group of materials composed of at least five major atomic elements. These alloys can be doped with other elements in quantities below 5 at. % in total. Thus, in this study, NiCoCrAlFe-X alloys are studied for oxidation behavior when exposed to dry and humid atmospheres for 1000 h. NiCoCrAlFe-X alloys are doped with alloy elements of 1–5 at. %. The effects of chemical composition on oxidation resistance in dry and wet atmospheres will be explained and discussed.

Chromium effect on the behavior of NbTiZr refractory medium entropy alloys

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B5_5 - Refractory high-entropy alloys, Andalucía I Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The objective of this study is to examine the effect of chromium addition on the microstructure, mechanical behavior and environmental properties of a refractory medium entropy alloy (RMEA).

The alloy that has been selected for this study is an equimolar NbTiZr alloy, which has been comprehensively researched in the literature and features a microstructure composed of a single-centered cubic solid solution. The addition of chromium to this system results in the emergence of brittle Laves phases in relatively limited quantities. Utilizing thermodynamic calculations employing the Calphad method (Thermocalc), a series of alloys with chromium contents of up to 8% at. were developed and subsequently exposed to temperatures at the dissolution temperature of the Laves phases, with the objective of establishing the solubility limit of chromium in the solid solution. The microstructure was then prepared to a size close to 100 μm by a cold rolling step and heat treatment at 1100°C.

Structural analyses were conducted by X-ray diffraction, while microstructural analyses were performed using scanning electron microscopy (SEM), including EBSD orientation mapping. The alloy composition was verified by ICP-OES, and the mechanical behavior was measured by micro-indentation tests, tensile tests and relaxation tests. The environmental resistance of the alloys was studied by thermogravimetric analysis (TGA).

Observations demonstrate that Laves phases emerge at grain boundaries as soon as 4.5% at. chromium is incorporated, despite thermodynamic calculations indicating the presence of a single solid solution for contents of up to 6% at.

Vickers microhardness and tensile yield strength increase with chromium content, reaching a plateau at 4.5% at. These results therefore suggest that the solubility limit of chromium is approximately this level. However, Rietveld refinement of the diffractograms demonstrates that the cell parameter of the solid solution continues to evolve above 4.5% at.

It is shown that chromium, even when added in small quantities, exerts a significant effect on the behavior of the NbTiZr alloy. The results of this study indicate that up to 3% at. chromium can cause significant solid solution hardening, although this content is insufficient to form a protective oxide layer and protect the alloy against oxidation.

Microstructural Evolution and Deformation Mechanism Analysis of AlTiVCr High-Entropy Alloy with Varying Al-Ti Ratios

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

High-entropy alloys (HEAs) are multi-component metallic systems composed of four to five or more principal elements, each within a composition range of 5–35 at.%. Due to their high configurational entropy, HEAs reduce free energy, promoting the formation of a stable single-phase solid solution while suppressing intermetallic compound formation. Among various HEAs, body-centered cubic (BCC) structured HEAs exhibit superior strength, making them promising candidates for high-performance structural applications such as aerospace components and lightweight automotive parts. However, their inherently low ductility poses challenges in processing, necessitating further research to enhance their mechanical properties.

In this study, a novel lightweight BCC-based HEA was designed to achieve an optimal balance between strength and deformation characteristics. Alloy compositions were systematically adjusted based on experimental evaluations of microstructural evolution to ensure homogeneity and improve mechanical performance. Specifically, Ti, V, and Cr—elements with minimal atomic size differences—were selected as primary alloying components, while Al, a widely used lightweight element, was incorporated to mitigate brittleness. The study aimed to develop an AlTiVCr HEA with enhanced mechanical properties. Furthermore, the influence of Al and Ti ratio variations on the formation of intermetallic compounds was experimentally analyzed, and their impact on mechanical performance was assessed.

The alloys were fabricated using arc melting and suction casting to produce rod-shaped specimens with a diameter of 3 mm and a length of 50 mm, with compositions of Al_xTi_{80-x}V₁₅Cr₅ (x = 35, 40, 45 at.%). Microstructural characterization and phase analysis were conducted using scanning electron microscopy (SEM, JEOL JSM-6390) and X-ray diffraction (XRD, Panalytical). Additionally, chemical composition analysis was performed via transmission electron microscopy (TEM, JEM-ARM200F, Jeol) and energy-dispersive spectroscopy (EDS). Mechanical properties were evaluated through room-temperature compression tests using a universal testing machine (UTM), and the experimental data were analyzed using SEM to establish correlations between microstructure and mechanical properties.

Chemical short-range order and local lattice distortions in High-Entropy Alloys: state of the art

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B5_5 - Refractory high-entropy alloys, Andalucía I Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Understanding the complex atomic-scale structures of High-Entropy Alloys (HEAs) is crucial for tailoring their properties to diverse applications. The present contribution aims to provide an overview of the state-of-the-art experimental techniques employed in probing local lattice distortions and chemical short-range order in HEA solid solutions: from synchrotron/neutron-based techniques such as X-ray absorption spectroscopy and X-ray / neutron total scattering to novel and less known techniques such as single-crystal diffuse scattering and atomic-resolution holography. A key challenge in analyzing multi-component alloys lie in the inherent low scattering contrast among the five or more alloying elements, which are often neighbors in the periodic table. Additionally, HEAs generally exhibit simple crystal structures with few or even one single Wyckoff site further complicating the extraction of local structural information. These characteristics pose significant challenges for data interpretation, including in transmission electron microscopy.

At the laboratory level, the more accessible thermo-physical methods such as differential scanning calorimetry and electrical resistivity have proven valuable in the corroboration and quantitative estimation of ordering within HEAs.

It becomes evident that rather than relying solely on individual techniques, it is the combination of several experimental approaches, ideally complemented by simulations, that can effectively assign the contribution of each element to the alloy structure and, ideally, to the overall alloy performance. However, it is important to recognize that each experimental method has its own strengths and weaknesses, which will also be shortly addressed within this contribution.

Hydrogen-assisted spinodal decomposition in a TiNbZrHfTa complex concentrated alloy

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B5_8 - Alloying effect, Andalucía I Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Understanding hydrogen-metal interactions is critical for developing refractory complex concentrated alloys (CCAs), applicable to the hydrogen economy. In this study, we revealed a hydrogen-assisted spinodal decomposition phenomenon at the nanoscale in an equiatomic TiNbZrHfTa CCA upon its exposure to H₂ at 500 °C. Such a decomposition pathway was characterized by a periodic compositional modulation with an up-hill diffusion behavior of the principal metallic elements, particularly Zr, over an extended treatment period (from 0.5 h to 2 h) in an H₂ atmosphere, probed by three-dimensional atom probe tomography. Consequently, the decomposed alloy consisted of a needle-shaped phase enriched in Zr and Ti and a phase enriched in Nb and Ta. Crystallographically, the spinodal features aligned preferentially along $\langle 001 \rangle$ directions of the matrix phase to minimize elastic strain energy. To better understand the role of hydrogen in spinodal decomposition, a statistical thermodynamic model was further developed by incorporating hydrogen to predict the phase stability of the TiNbZrHfTa-H system. This analysis suggested that hydrogen destabilizes the single solid-solution phase by expanding the spinodal region. Such nanoscale spinodal decomposition enhanced the hardness and anti-abrasive properties of the investigated alloy. Thus, this study not only provides fundamental insights into the effect of hydrogen on phase stability, but also demonstrates a novel alloy design strategy by introducing hydrogen as an interstitial alloying element to tailor the microstructure.

Investigation of phase content of TiZrAlNbMo high entropy alloys with compositional gradient

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B5_5 - Refractory high-entropy alloys, Andalucía I Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Elemental powder mixtures were sintered by SPS to produce samples with intentional chemical variations to study the effect of chemical composition on the phase content of the TiZrAlNbMo based high entropy alloys (HEA). Annealing and quenching from 1200°C produce material with phase content associated with the thermodynamic equilibrium at 1200 °C. The microstructural characterization was conducted by means of scanning electron microscopy, including EDS and by x-ray diffraction. It was revealed that major phase is the bcc-matrix, depending on composition, AlZr based intermetallic particles were also present. The threshold of Nb and Mo content for stabilization of single-phase bcc matrix was revealed. The experimental results were complemented by Thermocalc calculations using TCHEA4 database. It was revealed that qualitative predictions and trends are correct, while explicit quantitative determination is not fully consistent with experimental data. We consider high-throughput experimental determination of phase content and microstructure irreplaceable for HEA development and tailoring. Manufacturing and characterization of gradient samples allows efficient analysis of the effect of individual elements on microstructure and phase content in HEA.

Micromechanical characterization of multimetal carbides

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B5_9 - Broad high-entropy materials, Andalucía I Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

High entropy carbides (HEC) are multi-metal carbides containing at least four metal atoms at near-equiatomic concentrations. They exhibit unconventional mechanical and physical properties due to the disorder in terms of metal cation packing, but the inherent brittleness of these carbides limits their applicability. Recent micromechanical studies have revealed that certain grain orientation promotes the activation of slip in these multimetal carbides with enhanced yield and failure strength compared to their monocarbides¹. Up till now, the high entropy carbide compositions presented in literature have been rich in critical raw materials (CRM), such as hafnium, tantalum, zirconium.

In this study, we explore the feasibility of fabricating certain sustainable multimetal carbide compositions which are free from at least one CRM and analyze their micromechanical behavior. Based on the entropy forming ability, certain compositions were synthesised – HfNbTaTiZrC and MoNbTaVWC. X-ray diffraction and electron microscopy techniques confirm the crystal structure and formation of single-phase multi-metal carbides with chemical homogeneity. The hardness and elastic modulus dependance on the grain orientation were studied with high throughput nanoindentation mapping studies. The elastic modulus and hardness of the multimetal carbide phases were found superior to HfC and TaC monocarbides. Moreover, the experimental interpretations of the operative deformation mechanisms based on the strain rate sensitivity and activation parameters for deformation will also be detailed.

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The phase transition of multi-component (TiZrVNb)C ceramics: The phase decomposition induced by carbon content

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B5_9 - Broad high-entropy materials, Andalucía I Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The phase decomposition can enhance the mechanical properties of carbide ceramics effectively, which can overcome the difficulty of enhancement of mechanical properties for single-phase multi-component carbide ceramics. In this work, a series of non-stoichiometric (TiZrVNb)C_x ceramics were prepared by spark plasma sintering (SPS) at different temperatures. The effects of carbon content on phase compositions, microstructure evolution, and mechanical properties were investigated in detail. The phase decomposition took place with the reduction of carbon content. Two different solid solutions of (Ti, V)-rich and Zr-rich phases formed originating from the decomposition of equimolar single-phase solid solution, namely the Zr-poor phase and Zr-rich phase, respectively. The distribution of Nb element is relatively uniform. The semi-coherent interfaces between the Zr-poor phase and the Zr-rich phase can harden and strengthen effectively under the synergistic effect of grain refinement. The ceramics with phase decomposition structures have apparent advantages compared to single-phase high-entropy carbides. This work provides an important train of thought for the microstructure tailoring and properties optimization of multi-component carbide ceramics.

From binary to high-entropy : tailoring microstructure and mechanical properties of diboride-carbide composites through reactive sintering

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B5_9 - Broad high-entropy materials, Andalucía I Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Ultrahigh-temperature ceramics, such as diborides (MB_2s) and carbides (MCs) of transition metals (Ti, Zr, Hf, Nb, Ta), possess outstanding physical and chemical properties, including high hardness, modulus, thermal conductivity, and excellent resistance to thermal shock and ablation. These materials are therefore well-suited for extreme environmental applications. Notably, certain MCs can react with MB_2s at specific temperatures, leading to the formation of multi-component solid solutions. Compared to the self-diffusion mass transfer in single-phase MB_2s , the reaction-driven interdiffusion between MB_2s and MCs enhances mass transfer and facilitates densification. This in-situ reaction and solid solution coupling process not only improves densification but also suppresses excessive grain growth and may introduce additional solid solution phases. The formation of these multi-phase solid solutions, along with the microstructure refinement induced by reactive sintering, typically results in improved mechanical properties. Since diborides and carbides exhibit similar exchange reactions and solid solution behaviors, a binary system (boride + carbide) can serve as a starting point for designing more complex multi-component systems. When diborides and carbides of different metal atoms are employed for reactive sintering, the resulting materials tend to form high-entropy ceramics (HECs), which exhibit intricate phase formation, microstructure evolution, and tunable mechanical properties dependent on phase fractions. This work offers new insights into the design of diboride-carbide dual-phase composites from a binary to high-entropy systems.

Influence of Si on structure, mechanical properties, and thermal stability of reactively and non-reactively sputtered high-entropy (Hf,Ta,Ti,V,Zr) carbides

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B5_8 - Alloying effect, Andalucía I Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

High-entropy metal-sublattice carbide thin films, (Hf,Ta,Ti,V,Zr)C, with and without Si addition, are synthesized via reactive and non-reactive magnetron sputtering. Structural analysis confirms a stable single-phase face-centered cubic (fcc) structure across all coatings, even at Si contents up to 21 at% and after annealing at 900 °C and 1400 °C. Unlike for binary nitrides, the increasing Si content promotes grain-growth rather than refinement, as evidenced by detailed X-ray diffraction and transmission electron microscopy studies. Mechanical testing shows hardness and elastic modulus values of 31–36 GPa and 397–427 GPa, respectively, with no strong dependence on Si content. Si addition increases deposition rate and grain size while preserving a dense, fine-fibrous growth-morphology. Dynamic simultaneous thermal analysis up to 1400 °C reveals minor carbon loss in Si-free reactively and non-reactively prepared samples above 850 °C and 1000 °C, respectively. Despite this, all coatings retain their single-phase fcc structure and the Si-free (Hf_{0.19}Ta_{0.24}Ti_{0.25}V_{0.21}Zr_{0.11})C film only softened from 33.12±3.2 GPa to 29.08±2.57 GPa upon annealing at 900 °C. These findings highlight the exceptional thermal stability and mechanical resilience of high-entropy carbide thin films, positioning them as promising candidates for high-temperature applications.

Elucidating the Equilibrium Vacancy Concentration and Diffusion Behaviour in Refractory High-Entropy Alloys from First-Principles

Mr. Damien Lee¹, Mr. Yann Müller¹, Prof. Anirudh Natarajan¹

¹EPFL, Lausanne, Switzerland

B5_3 - Structure, defect and mechanical behavior, Andalucía I Room (Level +1), septiembre 15, 2025,
14:30 - 16:30

Refractory high-entropy alloys (HEAs) have emerged as promising candidates for high-temperature applications due to their exceptional mechanical properties and thermal stability. Atomic diffusion plays a crucial role in microstructural evolution and long-term stability. In most metallic systems, diffusion primarily proceeds through substitutional diffusion, where diffusion constants are directly proportional to vacancy concentrations. However, accurately determining vacancy concentrations from ab initio methods is computationally demanding due to the vast compositional space of HEAs and extremely low vacancy concentrations. In this work, we investigate HEAs composed of Group 4, 5, and 6 elements and introduce an efficient statistical-mechanical approach for calculating equilibrium vacancy concentrations. By leveraging first-principles calculations and Monte Carlo simulations, we systematically assess how composition and local atomic interactions influence vacancy formation. We then employ kinetic Monte Carlo (kMC) simulations to compute diffusion constants, providing a quantitative understanding of atomic mobility in HEAs. Our results reveal key insights into diffusion mechanisms, emphasizing the role of short-range order and chemical environment. Our work demonstrates how first-principles methods can effectively model diffusion behavior in complex composition space of HEAs.

High-entropy MAX phase with high strength and large plasticity mediated by local chemical fluctuations

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B5_9 - Broad high-entropy materials, Andalucía I Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

MAX phases are an emerging kind of material with a unique combination of metallic and ceramic properties, and they have great potential to be utilized as high-temperature components. However, their lack of plastic deformation capability and low strength (particularly at high temperatures) result in unsatisfactory mechanical properties, which restricts their potential applications. In this study, we introduced local chemical fluctuations (LCFs) into atomic packing layers of MAX phases by applying the high-entropy concept learned from the metal community. We substituted Ti in the model Ti₂AlC MAX phase with Zr, Nb, and Ta and successfully developed a high-entropy MAX phase (TiZr_{0.6}NbTa)₂AlC while preserving its lattice structure. The enhanced LCFs in this new MAX phase created strong lattice strains, increasing the resistance to dislocation slip and then leading to a high compressive yield strength of over 500 MPa even at 1473 K. Also, the LCFs stimulated cross-slips and stacking faults during deformation, effectively alleviating strain localization, promoting uniform deformation, and eventually enhancing plasticity at room temperature and the elevated temperature. Our work not only sheds light on understanding the deformation mechanisms of MAX phases in general, but also offers a valuable route for improving their mechanical properties, making them competitive as the next-generation lightweight high-temperature materials.

Radiofrequency plasma spheroidization of mechanically alloyed complex concentrated alloy NbTiVZr

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The recent progress in additive manufacturing increased the demand for high quality metal powders with tailored composition. The refractory complex concentrated alloys are peculiar for conventional metallurgy due to their high melting point and reactivity. Therefore, the cold spray additive manufacturing method is ideal for utilization of this type of material. Radiofrequency plasma spheroidization provides powders with suitable collection of properties for further processing. In addition, the combination of our cold spray additive manufacturing and refractory complex concentrated alloys is suitable for cladding of heat sensitive parts. This work focuses on production of spherical powder of a selected refractory complex concentrated alloy NbTiVZr from a powder produced by high energy milling from elemental commercial powders. Various processing parameters will be discussed in order to optimize the quality, homogeneity and powder size distribution. Each additive manufacturing method requires different size distribution of powder particles. However, powder sieving significantly decreases efficiency of production. Therefore, provided optimization of milling and spheroidization processes are crucial. Main focus of this study is to investigate microstructure and quantitative phase composition of spheroidized powder particles from initially mechanically alloyed powders with the atomic-level homogeneity. High-enthalpy plasma reaction in protective atmosphere liquifies intermixed powder particles and thus interesting microstructures and phase composition are formed during fast cooling in the collector and on the walls of the spheroidization chamber. Such powder does not require complicated heat treatment nor surface reduction annealing and is ready for further additive manufacturing. The first samples of cold spray additive manufacturing method of high entropy alloy NbTiVZr will be presented after thorough analyses of microstructure, quantitative phase composition and mechanical properties.

Fatigue properties of nitrogen-strengthened high Cr-Ni austenitic stainless steels at 77 K

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B6_3 - Fatigue and Fatigue corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The low fatigue resistance of nitrogen-strengthened austenitic steels in the high-cycle fatigue range at cryogenic temperatures is related to the subsurface crack generation. This failure mode was favored by the coarse microstructure. The high-cycle fatigue properties of 24Cr-15Ni-4Mn-0.3N and 22Cr-12Ni-4Mn-0.3N-(Nb,V), in mass%, austenitic stainless steels were examined at 77 K. Nb and V show the advantages of high strength and excellent weldability owing to grain refinement by their precipitates. The present study is concerned with obtaining a systematic understanding of the microstructure of the fatigue strength and examining its subsurface crack generation. The solution-treated and cold-groove-rolled steel bars were annealed at temperatures that controlled the partially recrystallized (PR), fine recrystallized (FR), solution-treated (ST), and grain-grown (GG) microstructures. Their average grain diameters were in the range of a few μm to hundreds μm . Uniaxial load-controlled fatigue tests were performed at 77 K with a stress ratio of $R=0.01$, using liquid nitrogen immersion. The high-cycle fatigue strength of the heat-treated materials was not directly proportional to their tensile strength, and the ratio of the fatigue strength at 10^7 cycles to the tensile strength decreased approximately from 0.8 to 0.3 in the order of PR, FR, ST, and GG. Subsurface crack initiation was detected in the lower peak stress and/or in the longer life range for all materials. In particular, ST and GG exhibited a sharp drop in fatigue strength over 10^6 cycles owing to subsurface crack initiation. Grain refinement in the microstructure predominantly resulted in a higher fatigue resistance to this mode of failure. Movable dislocations on various types of slip systems may provide less strain incompatibility at grain boundaries owing to a rather homogeneous deformation; however, improving the fatigue strength between the PR and FR was not remarkable because of the maintenance of the planar slip mode. In contrast, coarsened grains provide larger subsurface crack sizes to initiate crack propagation, resulting in a lower fatigue strength.

Effect of the residual stress induced by surface treatment processes on the mechanical behavior

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Residual stress is the stress that remains inside the material during the manufacturing process of the material and parts. Depending on the magnitude and direction of the stress, the mechanical properties of the material can be improved, and sometimes it can cause fracture. Processes that artificially apply compressive residual stress to surfaces to improve the mechanical properties of materials include those such as shot peening, laser peening, and ultrasonic peening. This surface treatment process establishes plastic deformation on the surface, improves the surface hardness, and induces compression residual stress, which delays the fatigue failure occurring on the surface. In addition, for shot peening, nano-grain grains are formed on the surface to improve yield strength and tensile strength. However, the magnitude of the residual stress decreases after plastic deformation or fatigue. In the case of fatigue crack growth, a low fatigue load is imposed, but existing residual stress changes around the tip of the crack due to the presence of plastic regions at the tip of the crack. In this study, various methods such as XRD and contour methods were used to measure the change in the residual stress distribution after tensile, fatigue, and fatigue crack propagation tests using materials with compression residual stress on the surface to which shot peening and laser shock peening were applied. In addition, the tensile and fatigue crack propagation behavior of materials with residual stress were studied after the shot peening and the laser shock peening processes.

Effect of Pitting Corrosion on Fatigue Behaviour of a Cast, Anodized Aluminium-Silicon alloy

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B6_3 - Fatigue and Fatigue corrosion, Seminario 6 Room (Level +1), settembre 17, 2025, 17:00 - 19:00

Aluminium-Silicon (AlSi) alloys are excellent materials for the metal casting of complex-shaped automotive components, thanks to their optimal castability and strength-to-weight ratio.

During the service life, automotive components can be exposed to corrosive environments. For this reason, cast AlSi alloys are typically anodized to grow a protective, micrometric Aluminium oxide layer on their surface with an associated improvement of the corrosion resistance. However, the presence of chlorides (e.g., on-road de-icing salts and coastal air) can trigger pitting corrosion in anodized AlSi components, despite the presence of the anodic layer.

Since corrosion pits are known to play a crucial role in fatigue performance, it becomes fundamental to study the effect of pitting corrosion on the mechanical performance of cast, anodized AlSi alloys.

At this regard, the work aims at correlating the increasing exposure time to a chloride-rich environment (i.e., neutral salt spray chamber) to the fatigue life of a cast, anodized AlSi_xMg_y-T6 (where x=7%wt and y=0.5%wt) alloy. Three batches of cast, anodized AlSi specimens are produced and placed in a neutral salt spray (NSS) chamber for 0, 480 and 1000h. The evolution of corrosion pits is monitored by means of X-ray microtomography. Then, tensile and high-cycle fatigue tests, metallography and fracture surface analyses are performed to understand the effect of pitting corrosion on the fatigue behaviour. It is demonstrated that corrosion pits nucleate within the first 480h of exposure to NSS and, as the time increases to 1000h, they increase in dimensions. Consequently, as the dimension of corrosion pits increases, the fatigue life of the cast, anodized AlSi alloy decreases. Moreover, surface fracture analysis reveals that after 1000h of NSS exposure corrosion pits become the predominant and sole nucleation site for the fatigue crack, despite the presence of casting defects (i.e., shrinkage pores and entrapped oxides) and defects in the anodic layer.

In conclusion, this work not only unveils the mechanism of corrosion pit formation in cast, anodized AlSi alloys, but also demonstrates the detrimental effect of corrosion pitting on the fatigue performance of these materials.

Fatigue Corrosion Performance of Cast- and Chip-Based Produced AA6060 under Varied Heat Treatments

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B6_3 - Fatigue and Fatigue corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Over the last few decades considerable efforts have been made to cope with the energy waste in material production methods. This is aimed at the increasing sustainability level to be aligned with modern environmental, social, and economic requirements.

A promising approach to overthrow this problem is the utilization of solid-state recycling route in converting aluminum machining chips directly into semi products to save time, reducing the CO₂ footprint and cost-consuming experimental try-outs. This model may make the process an intriguing alternative solution due to its clear environmental benefits in the production of complex profiles.

In the present work, chips of aluminum alloy (AA6060) were subjected to compaction and then hot extrusion conducted at 500°C through porthole die, followed by various heat treatment profiles to study the resultant material fatigue corrosion behavior. The same tests were also conducted on Cast based hot extruded specimens for comparison reasons.

This alloy was submitted to fatigue corrosion tests under the conditions of $R = 0$, $f = 25\text{Hz}$ and simulated sea water 3.5% NaCl corrosion solution.

Optical and scanning electron microscopy (SEM) were used to conduct detailed fractographic analysis of the micro-morphological fatigue failure features.

Comparisons were also directly made connected to materials deriving from various production routes to highlight the role of the homogenization heat treatment on the fatigue corrosion resistance. The influence of corrosion on the fatigue crack propagation was also investigated.

The findings revealed that the corrosion fatigue life of chip-based specimens was comparable to that of the cast-based specimens (conventionally produced) and that the ensuing heat treatment (homogenization) enhanced the performance of the chip-based materials and corrosion resistance.

The study concluded that (heat treatment determination control) contamination control is essential to prevent galvanic corrosion during solid-state recycling of machining chips. This work suggested that solid-state hot extruded recycling of aluminum machining chips can improve fatigue and corrosion behavior in aluminum alloys.

Fretting wear of a B₄C-SiC composite spark-plasma-sintered at 1400°C from B₄C+Si

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B6_5 - Wear, Seminario 6 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The fretting wear of a B₄C-SiC composite fabricated by spark-plasma-sintering of B₄C+20vol.%Si at 1400°C is investigated in various friction pairs with other ceramics. To this end, fretting tests of 50 mm stroke were performed against diamond, Al₂O₃, and borosilicate glass, at 1 and 5 N loads for up to 100000 cycles. The resulting fretting tracks were characterized in detail by optical microscopy, scanning electron microscopy, energy-dispersive X-ray spectroscopy, and optical profilometry, which was used together with the fretted volumes and the friction coefficients to identify the corresponding fretting modes and mechanisms. Finally, implications arising from the study are presented.

Assessment of early-stage degradation of coil coated steel

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B6_4 - Fatigue II, Seminario 6 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Continuous coil coating lines have been producing materials for domestic appliances and building industry for over a century. The synergistic combination of metal sheets with organic coatings (polyvinyl chloride (PVC) in the 1960's, followed by polyester in the 1970's and epoxy, polyvinylidene fluoride (PVDF) and polyurethane from the 1980's onwards has spawned a multitude of end applications with tailored properties for aesthetics, corrosion resistance and durability. Currently, the European coil coating industry produces about 1600 million m² of coated metal per year. The industry faces pressure to cut costs in the curing section, pushing for novel radiation curable coating formulations and sustainable practices, such as reducing fossil-based constituents and incorporating recycled and biobased binders and additives.

Some of the bottlenecks related to introducing these novel coating formulations to the market are related to relatively long testing and verification procedures. Currently, quality control during development of coil coatings for steel is carried out with extensive accelerated exposures, UV-weathering, constant salt/humidity resistance and cyclic corrosion tests, followed by gloss and color measurements, and finally assessment of blister density, delamination and paint adhesion. One of the reasons behind the slow pace of approval is that the testing relies heavily on changes in macroscopic coating properties. For a long time, paint deterioration can remain invisible to the naked eye and undetectable by commonly used evaluation techniques. Formation of any visual signs of the degradation may take many several years even at highly corrosive sites. A significant improvement would be to be able to observe and understand the degradation mechanisms at an earlier stage.

This paper explores weathering-induced chemical degradation in coil-coated steel using modern techniques like high-throughput ion beam milling, high-resolution SEM-EDS imaging, and depth-resolved FTIR. Using examples from exposed coil coated materials, it is illustrated how hidden interfaces and molecular-level changes appear before macroscopic signs of corrosion. Being able to observe and understand these mechanisms enables tailoring of more corrosion-resistant coatings and speeding up the lab-to-market cycle.

Influence of the mesostructure on the cyclic fracture-mechanical behavior of Al/Cu-Laminates

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B6_4 - Fatigue II, Seminario 6 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Damage tolerance is a critical aspect designing components subjected to cyclic loading for various commercial applications such as the aviation industry. Especially in safety-relevant areas, increasing the service life of components without compromising on safety is of fundamental importance. For this reason, laminated metallic composites (LMC) are of particular interest due to their numerous advantages including an improved strength-to-weight ratio and tailored mechanical properties compared to monolithic materials [1,2]. Among others enhancing the resistance against fatigue crack propagation due to toughening mechanisms is very promising. This feature is based on the so-called material inhomogeneity effect at interfaces. By introducing a gradient in hardness or elastic properties at the interfaces, the resistance against crack propagation is increased due to the formation of a complex 3D-crack network with toughening mechanisms such as crack deflection, bifurcation or bridging [3].

In this work, monolithic materials and Al/Cu-LMCs with a hardness and Young's modulus gradient were fabricated via the accumulative roll bonding (ARB)-process. The LMC samples were heat-treated after the fabrication in order to create a continuous intermetallic layer along the interface. The mesostructure formed was characterized in more detail in terms of hardness, Young's modulus and chemical composition using nanoindentation and EDS. In addition, fatigue tests were carried out using a 3-point bending setup on samples that show no or, respectively, different thicknesses of the intermetallic layer. The fatigue crack growth rates are effectively reduced compared to those of the monolithic materials in crack arrester orientation. Monitoring of selected experiments using a far-field microscope setup and post-mortem light microscopy investigations revealed the formation of various fatigue crack paths. Toughening mechanisms like crack deflection, crack bifurcation and crack bridging are strongly pronounced when defined intermetallic layers in the LMC exist.

[1] D. R. Lesuer, et al. , "Mechanical behaviour of laminated metal composites," *Int. Mater. Rev.*, vol. 41, no. 5, pp. 169–197, 1996.

[2] F. Kümmel, et al. , "Ultrafine-Grained Laminated Metal Composites: A New Material Class for Tailoring Cyclically Stressed Components," *Adv. Eng. Mater.*, vol. 23, no. 7, p. 2100070, 2021

[3] P.M. Pohl, et al. , "About the Role of Interfaces on the Fatigue Crack Propagation in Laminated Metallic Composites," *Mater.*, vol. 14, 2021

In-situ investigation of the influence of corrosion protection systems on microbially influenced corrosion inside offshore monopiles

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B6_4 - Fatigue II, Seminario 6 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Offshore wind parks are crucial to a successful energy transition towards renewable energy. With a financial break-even point close to the service lifetime, offshore wind energy is expensive. In addition, microbially influenced corrosion further shortens the service time. While the issue of electrochemical corrosion is already addressed by the corrosion protection system, microbially influenced corrosion and its inhibition are little studied for offshore wind farms, resulting in a substantial need for further investigations.

Monopiles, tube-like structures anchored in the seabed, are common foundations for offshore wind turbines. The water column within these structures exhibits only a limited mixing with ambient seawater, which can lead to decreasing oxygen levels in greater water depth and therefore offers a unique environment for microbially influenced corrosion. Currently, deployed corrosion protection systems are designed for electrochemical corrosion and do not take microbially influenced corrosion into account. However, previous studies show a dependence of the incubation depth on the overall corrosion patterns and associated microbial corrosion. In the present in-situ study, two test series were incubated for several months to determine the effect of corrosion protection systems on microbially influenced corrosion. Both test series contain commonly used structural steel incubated at three water depths. The first water depth at -6 m shows fully oxic environmental conditions. Seasonally, the water parameters start to transition at -15 m (second water depth) until they reach anoxic conditions close to the seabed at -21 m (third water depth). Test series 1 was incubated without any corrosion protection system, while test series 2 was electrically connected to the mass potential of the monopile, thus being connected to the corrosion protection system.

To determine the influence of the corrosion protection system, corrosion rates regarding incubation depths were measured gravimetrically. The obtained corrosion products were then analysed further using 3D and scanning electron microscopy as well as X-ray diffraction. In addition, the environmental water conditions and the microbial communities associated with the incubated steel specimens were investigated. First results demonstrate the dynamic and depth-dependent corrosive situations inside offshore monopiles with and without corrosion protection system. In a later stage, these findings will also be used to calculate the lifetime of offshore monopiles, taking microbially influenced corrosion into account, as well as to find suitable coating strategies. This investigation is carried out as part of the joint project “MiCorFe” funded by the German Federal Ministry for Economic affairs and Climate Action.

Effect of Surface treatment on Residual Stress distribution and mechanical properties of Butt-Welded S45C Joints

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B6_1 - Fatigue I, Seminario 6 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Residual stress generated during the welding of automotive components significantly affects their fatigue life and fatigue crack growth. Welding defects and residual stress can lead to crack initiation in the welded joint, ultimately resulting in failure. To address this issue, this study aims to control residual stress in welded joints and evaluate its impact on mechanical performance.

In this research, laser peening was selected as a surface treatment method to introduce compressive residual stress and improve the fatigue life of butt-welded S45C medium-carbon steel. The residual stress distribution before and after surface treatment was measured and analyzed using the Contour method and X-ray diffraction (XRD) method.

To evaluate the effect of compressive residual stress on mechanical performance, tensile and fatigue tests were conducted before and after the surface treatment. Additionally, the microstructural changes induced by the surface treatment were analyzed to understand their influence on material properties. The results provide insights into the effectiveness of laser peening in enhancing the fatigue resistance of welded joints.

The enrichment behavior of Ni in austenitic stainless steel during the corrosion in liquid lead-bismuth eutectic at 550 °C

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B6_4 - Fatigue II, Seminario 6 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Currently austenitic stainless steels (AuSS) are viewed as promising candidate structural materials for key components of lead-based fast reactors (LFRs), owing to their exceptional high-temperature mechanical properties, processability, and resistance to liquid metal embrittlement. However, as a crucial major element for the structural stability of AuSS, Ni has a very high solubility in the coolant of LFR, namely liquid lead-bismuth eutectic (LBE). Moreover, Ni typically exhibits a significant segregation tendency in the oxidation zone, and numerous researchers have observed Ni-rich structures within the inner oxidation layer (IOL) of AuSS. This may pose risks of solution corrosion and LBE penetration to AuSS. At present, the enriching behavior of Ni and the effects of Ni-rich structures on the oxidation and solution processes of AuSS in LBE remain unclear. In this study, the internal oxidation behavior of 15-15Ti alloy in oxygen-saturated static LBE at 550°C (up to 6000 h) was systematically investigated, focusing on the initial corrosion behavior and evolution process of Ni in the matrix in front of the oxide/metal (O/M) interface. A new Ni-rich structure was found at grain boundaries in the unoxidized matrix using the method of small-angle inclination polishing. This structure is coherent with the grain on one side and grows into the incoherent grain on the opposite side driving grain boundary migration. A sharp compositional difference is present at the coherent interface. The Ni-rich structure stores Ni, facilitates the participation of Cr in oxidation processes, and alters the composition of oxides as well as distorts their growing path. In this study, with an intact oxide film and no LBE penetration, Ni-rich particles augment the intergranular oxidation resistance of 15-15Ti. However, their impact is constrained by their limited size and number. By increasing the quantity and enhancing the size of Ni-rich particles, further suppression of the preferential oxide thickening along grain boundaries could be achieved. Furthermore, investigations on the interactions between Ni-rich structures and the infiltrated LBE along grain boundaries are currently ongoing.

Surface inspection to detect early fatigue crack initiation in low cycle fatigue regime of high carbon steel using a scattered light sensor

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B6_1 - Fatigue I, Seminario 6 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Fatigue damage is the major factor in the failure of components. During the fatigue loading, the local plastic strain deformation is formed as persistent slip bands (PSBs) and emerges on the surface as persistent slip markings (PSMs). The PSM can develop roughness and be observed on the surface as extrusions and intrusions. The intrusions are possible sites of crack initiation. Thus, surface roughness development is a reasonable way to inspect fatigue damage. Many techniques were utilized to inspect and monitor the cracks and fatigue damage to protect the components and predict the remaining lifetime. Most of these techniques consume a lot of measuring time. In this study, a scattered light sensor from Optosurf will be performed to measure and determine the roughness evolution during cyclic loading of a high-strength steel 115CrV3. As a result, the profile measurement, areal measurement, and the derived Aq values are suitable to illustrate severe surface changes before failure. Moreover, the Aq values using a scattered light sensor are comparable with the results using a confocal microscope (Nanofocus).

Study of the tribological behavior of SnO₂ coatings under low atmospheric ethanol contamination

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 17, 2025, 13:10 - 14:30

Friction and wear at the interface between solids have a major impact on the service life of all kinds of mechanical systems. The development of high-performance dry lubricants to deal with this problem must take into account the surrounding atmosphere, including the presence of contaminants. Different physico-chemical mechanisms involving the materials in contact and their internal and external (ambient) contaminants can compete and give rise to the formation of lubricating interfaces through mechanically activated chemical reactions involving particles generated at the contact [1-2]. Traces of contaminants (in the ppm or ppb range) are enough to initiate the creation and maintenance of this lubricating and anti-wear interface [3,4].

The aim of the present work is to investigate the influence of very low concentration of volatile compounds, at ppm level, on the tribological behavior of surface coatings. To this end, tin oxide, known for its sensitivity to the adsorption of ethanol molecules, was chosen as the material to study. Indeed, SnO₂ is used as a sensitive material for ethanol gas sensors.

PVD-deposited SnO₂ thin films on silicon substrates were subjected to friction in three different atmospheres: laboratory air, dry N₂ and dry N₂ contaminated with 1000 ppm ethanol vapor. Contact conditions: sliding speed 8 mm/s, average contact pressure 330 MPa, room temperature, 100Cr6 sliding counterpart and 500 reciprocating friction cycles.

The results showed a strong impact of the gaseous environment on the coefficient of friction, as well as on damage and wear. This effect, expected for N₂ compared with laboratory air, was also observed in the case of N₂ contamination with traces of ethanol, with a reduction in average friction by a factor of 2.5 to 3, and much lower friction damage.

The study of friction tracks on SnO₂ films and steel counterparts using surface analysis techniques is essential to advance our understanding of the tribochemical mechanisms involved. Here, SEM observation of friction scars and elemental EDX analysis have been complemented by XPS, SIMS and micro-Raman spectroscopy. Surface analysis shows that material composition at the interfaces varies, particularly in terms of the proportion of iron oxides. The formation of a mixed Fe-Sn-O compound has also been investigated.

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Investigating the correlation between wear and fatigue properties of cryogenically treated high-alloyed tool steels using cyclic indentation testing

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B6_3 - Fatigue and Fatigue corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The service life of tools made from high-alloyed tool steels is determined by their wear and fatigue properties, which are influenced by the microstructure formed during thermal treatments. Conventional heat treatments, including quenching and tempering, aim to achieve a balance between strength and toughness for various applications. However, in high carbon steels, this process often results in significant amounts of retained austenite, compromising dimensional stability. To address this, cryogenic treatments at temperatures between -80 °C and -196 °C can be applied to reduce the retained austenite content. In addition, when combined with subsequent tempering, these treatments refine the carbide and martensite structure, improving both hardness and toughness.

As tools are often subjected to cyclic loading during their service life, it is essential to consider the cyclic deformation behaviour in addition to the commonly investigated properties such as hardness and toughness. However, the analysis of cyclic deformation behaviour requires extensive experimental effort, making the optimisation of cryogenic treatment parameters time consuming. As described by Kramer et al. [1], the PhyBaLCHT method, which is based on instrumented cyclic indentation testing (CIT), allows an efficient assessment of the cyclic deformation behaviour and thus offers great potential for characterising the effects of cryogenic treatments. Accordingly, previous studies [2] have shown a strong correlation between the mechanical properties obtained in CIT and the wear resistance of cryogenically treated blanking tools made of Vanadis 4E.

Consequently, the aim of this study is to develop an evaluation procedure for cryogenic treatments based on CIT. This requires a thorough understanding of the relationship between cryogenic treatment parameters, the measures obtained in CIT, and the corresponding wear and fatigue behaviour. Therefore, Vanadis 4E specimens were subjected to various cryogenic treatments and compared with conventionally heat treated specimens. Subsequently, more than 40 different heat treatment conditions were analysed using CIT. Based on these results, sufficiently different conditions were selected for broad analyses of the fatigue behaviour, the microstructure and the wear performance in blanking tests. In accordance with [2], the results confirmed a strong correlation between the fatigue strength and the wear resistance with the mechanical properties determined in CIT. Moreover, these correlations could be attributed to microstructural phenomena, in particular the differences in carbide and martensite structure. In conclusion the work presented confirms the applicability of CIT for the characterisation of cryogenically treated tools.

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Fatigue strength enhancement of welded steel through residual stress tailoring by electrodeposition of a Cu/Ni multilayer thin film

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B6_1 - Fatigue I, Seminario 6 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The integrity and longevity of industrial structures heavily depend on the performance of their connections. This is especially relevant for welded joints in civil engineering, where, despite their widespread use and importance, they present significant implications related to permanence. The geometry of welds and the inherent metallurgical changes occurring within the heat-affected zone predispose these areas to premature failure under cyclic loading, leading to a reduced lifespan compared to the surrounding base material. Moderating the effects of fatigue results in increase of material usage, which raises weight, handling difficulties and sustainability concerns. Methods of post-weld treatments increase the usable lifetime of welded structures by changing its geometry or the residual stress states in the surface to postpone crack initiation and propagation.

Here, a novel post-weld treatment is investigated, which enables the tailoring of the residual stress states in the surface proximity by deposition of a Cu/Ni nano-structured multilayer onto the weld and its surroundings. Energy dispersive X-ray diffraction experiments across the depth on a variety of electrodeposition process conditions are conducted, thereby gaining insights into the change of residual stresses in the heat affected zone and base material. Across all process parameter sets, the superficial residual stresses are transformed to be compressive in nature, resulting from strain equilibration between the tensile residual stresses in the 10 μ m thin film and the steel substrate. Subsequent fatigue testing is conducted to correlate the tailored residual stress data to the lifetime enhancement of the welded specimen. The results indicate, that a dramatic increase in cycle numbers with a decrease in the slope of the S/N curve is achieved, yielding to a multifold increase in the usable lifetime of welded components. For the design process of welded structures, FAT classes above 200 are proposed, far exceeding the fatigue strength of the base material.

Effect of Grain Size on Corrosion Behaviour of Rolled Pure Magnesium

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B6_2 - Corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Grain refinement is one of the most widely used processing techniques for enhancing the strength and ductility of metals and alloys. This grain size variation impacts the electrochemical characteristics of the system. Systematic research on the impact of grain size on corrosion is lacking in the existing literature. Prior studies address the impact of grain size of pure Magnesium on corrosion behaviour without separating the effect of texture and localized stresses. The impact of grain size on corrosion has been investigated using pure magnesium that has been rolled and annealed while maintaining a consistent texture. A wide range of grain sizes was considered while keeping localized stresses and texture consistent. The corrosion rate was calculated and the corrosion behaviour was studied using potentiodynamic polarisation testing, electrochemical impedance spectroscopy, and corroded surface characterization to get a broader insight into the corrosion mechanisms. It has been noted that as grain size increases, the corrosion rate increases. This study contributes to the systematic and thorough understanding of the impact of grain size on the corrosion behaviour of pure Mg.

Type I-Pitting of Copper Tubes in Drinking Water Supply Networks - Recent Insights into Damage Patterns and Corrosion Mechanism

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B6_4 - Fatigue II, Seminario 6 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Pitting corrosion is a kind of corrosion that again and again is observed on copper tubes in water supplying networks. It appears when there are no stable protective layers developed on the copper tubes' contact surfaces exposed to water.

DIN EN 12502 distinguishes between different types of pitting, especially cold water pitting (type I), warm-mild water pitting (type II) and microbial-influenced pitting (MIC). That classification corresponds on the water temperature, the water composition and some conditions of operation.

According to DIN EN 12502 type I-pitting is generally "characterised by hemispherical cavities at and of green pustules above the corroded area, that consist of basic copper carbonate. Below these spots, the cavities are always covered by a continuous copper(I)oxide film at the previous surface level. Beneath this copper(I)oxide-film ruby-red copper(I)oxide-macrocrystallites and sometimes finely white copper chloride crystals are observed."

Type I-pitting occurs in cold water systems or hot water circuits having cold water characteristics due to long-term stagnations. The Type I-pitting rate is particularly high. For usually tube wall thicknesses of 1 to 2 mm, first damages are soon observed after 3 to 5 years after commissioning.

There are various reasons that trigger pitting corrosion only by interaction. In the case of type I-pitting, the chemical composition of water is essential. Water having a $\text{pH} \leq 7.5$ containing high concentrations of sulphate and nitrate is considered to be corrosive. However, the pitting likelihood decreases if chlorides and hydrogen carbonates are increasing. Due to water quality dependence type I-pitting frequently occurs in certain water supply areas.

This publication presents a case of damage caused by copper pitting in the service line of a single-family house located in Cologne on the left bank of the river Rhine. There, the sulphate content of tap water is $\approx 70 \text{ mg/L}$. As expected, the regional damage incidence is very high. The damage pattern, the appearance of the corrosion phenomena and the morphology of corrosion products are visualised by high-resolution light-optical and electron-optical procedures. The chemical compositions are analysed using EDX analysis and Raman microscopy. This enabled to identify specific compounds and their associated morphologies at the respective sites, to explain how and why they develop and, last but not least, to describe the entire mechanism of type I-pitting from the bare copper metal via the hollowed surfaces to the perforated pipe. It could be explained, too, why sulphates in tap water are so harmful to copper and increase its pitting likelihood.

Microcrack initiation of a second-generation nickel-based single crystal superalloy during thermal fatigue

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B6_1 - Fatigue I, Seminario 6 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Ni-based single crystal superalloys consisting of γ/γ' microstructure are widely used in the turbine blades of aero-engines due to their extraordinary high-temperature mechanical properties. Compressive and tensile stresses induced by the thermal cycle are inevitable and may lead to crack formation during the service of the turbine blade. However, how these cracks nucleated is still unclear. In this work, the nucleation process was simulated and investigated by performing a thermal fatigue test (ranging from room temperature to 1100 °C) on a second-generation Ni-based single crystal superalloy. The results show that the γ/γ' microstructure in both dendritic and interdendritic regions almost remains unchanged during thermal fatigue. In contrast, the micropores were mainly observed in the interdendritic region. Their volume fraction and equivalent diameter increase with the increase of thermal fatigue cycles, while the sphericity shows an opposite trend and transforms from the spherical shape to the irregular morphology. Meanwhile, the kernel average misorientation (KAM) map analysis indicates a stress concentration around the micropores. A high density of dislocations was observed at the γ/γ' interface, and some of them even sheared into the γ' precipitates to form low-angle grain boundaries around the micropores. These low-angle grain boundaries were subsequently transformed into high-angle grain boundaries due to crystal rotation along with the local intense plastic deformation during thermal fatigue. Thus leading to the local recrystallization near the micropores. The area of the recrystallized region increases as thermal fatigue proceeds, contributing to the microcracks nucleation at the grain boundaries near the interdendritic micropores. The local recrystallization and microcracks nucleation were closely related to the equivalent diameter and shape of micropores. The quantitative analysis indicates that the recrystallization-associated micropores were larger than 20 μm in equivalent diameter and less than 0.4 in sphericity, while the microcrack-associated micropores exhibited a larger equivalent diameter and lower sphericity. This study will be helpful in understanding the microcracks initiation of Ni-based single crystal superalloys during thermal fatigue and improvement of process control of turbine blade production.

Corrosion behavior and mechanical properties of ER70S-6 Wire Arc Additively Manufactured Steel

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

One of the most widely utilized Additive Manufacturing processes for construction steel is Wire Arc Additive Manufacturing (WAAM), exploiting its agile deposition rates and large-scale printing, as it is performed in ambient environments. WAAM manufactured steel is also suitable for the construction industry due to higher tolerance indicated for mechanical properties. The Cold Metal Transfer (CMT) printing technique was employed in the current study, which results in better distribution of the drops transfer rate, because of the reverse movement of the electrode and the zero current supporting the transfer process. In the present research work, the corrosion behavior and mechanical properties of WAAMed ER70S-6 wire steel are investigated via potentiodynamic polarization and tensile tests. Cooling methods of the printed samples used for these experiments include Natural Cooling (NC) and compressed Air Cooling (AC) with and without water admixture. Potentiodynamic Polarization tests were performed using a 3.5 wt.% NaCl solution at three different values of pH, namely 4, 7 and 9, and the corresponding results were plotted on Tafel diagrams. Post-corrosion observations were made employing Light Optical Microscopy (LOM), Scanning Electron Microscopy (SEM) and Energy-Dispersive X-ray Spectroscopy (EDS). The mechanical properties were assessed via stress - strain diagrams and the results were correlated to the different cooling methods implemented.

Keywords: ER70S-6 wire; WAAM; Low Carbon Steel; Tensile Strength; Corrosion; Microstructure

Low Cycle Fatigue of High Manganese Steel with Variable Microstructure Processed by Laser Powder Bed Fusion

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B6_1 - Fatigue I, Seminario 6 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

In this study, the low cycle fatigue behaviour of a high manganese steel X30Mn22 was investigated in several microstructural variants featuring different predominant crystallographic orientations. Metastable austenitic solidification structure of studied material underwent strain-induced martensitic transformation which is crystallographic orientation-dependent. Therefore, the studied types of structures, {011}- and {111}-textured, and without predominant texture, showed different cyclic behaviour characterized by various magnitude of cyclic hardening. Notable variations in fatigue lifetime were found also with respect to the type of microstructure. To explain underlying deformation mechanisms a detailed SEM characterization was carried out on initial microstructures, surface relief after cyclic loading, and internal deformation structures. Localization of cyclic plastic deformation resulted in martensitic transformation via γ (FCC) $\rightarrow$ ϵ (HCP) $\rightarrow$ α' (BCC) sequence, which was identified in all microstructural variants. These processes created a distinct surface relief which induced fatigue crack initiation and promoted fatigue crack propagation.

Premature Failure of a Coated Gas Turbine Compressor Rotor at SP Subang: A Synergistic Effect of Corrosion, Erosion, and Coating Degradation

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B6_2 - Corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

This study investigates the premature failure of a coated gas turbine compressor (GTC) rotor at SP Subang, Indonesia, focusing on the mechanisms contributing to deposit formation, coating degradation, and subsequent rotor damage. The compressor in question utilizes a three-stage rotor-stator configuration. A key observation is the significantly shorter operational lifespan of the coated rotor (292 days) compared to its uncoated predecessor (606 days), suggesting that the coating, intended to enhance durability, may have inadvertently contributed to the accelerated failure.

Analysis of deposits collected from the rotor blade leading edges revealed the presence of iron carbonate (FeCO_3) and iron hydroxide ($\text{FeO}(\text{OH})$), indicating a corrosion process driven by the presence of water and CO_2 . Laboratory analysis of the inlet gas stream confirmed exceptionally high levels of both water (167 lb/mmscf) and CO_2 (23.16-33.30 % mol), significantly exceeding the NORSOK P-001 standard of 13.3 L/mmscf (~ 29.3 lb/mmscf) for water content. These elevated levels promote the formation of carbonate ions, which are highly corrosive to steel components.

Furthermore, the presence of silica (sand) particles in the deposits and the observation of flow-induced scratches on the stator stage suggest erosive wear as a contributing factor. The combined action of corrosion and erosion likely exacerbated the damage to the Sermalon coating, which was found to be damaged, particularly at the rotor blade tips where the deposits were concentrated. Analysis of the soaking solutions used for turbine cleaning (Petroce and Army) revealed the presence of corrosive elements, potentially hydrochloric acid (HCl), which could have further compromised the coating integrity. The presence of iron, carbon, and oxygen in the residual particles from both the soaking solution and the suction scrubber water reinforces the formation of FeCO_3 .

The study underscores the critical influence of gas composition, particularly high water and CO_2 content, on GTC rotor lifespan. It highlights the complex interplay between corrosion, erosion, and coating degradation in accelerating component failure. The findings emphasize the need for improved material selection, more effective coating strategies, and optimized cleaning procedures to mitigate these detrimental effects in gas turbine compressors operating in challenging environments like SP Subang. Further investigation into the specific mechanisms of coating failure and the synergistic effects of corrosion and erosion is recommended.

A Case Study of Gas Turbine Failure: Unraveling the Impact of Soot Ingestion on NGV, Heat Shield, and Turbine Impeller Damage

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This study investigates the failure of an OPRA OP16-3A gas turbine engine that occurred at PT Pertamina EP's Xray-Jatibarang Platform in September 2021. The investigation focuses on identifying the root cause of the failure through detailed examination of the damaged components and laboratory analysis. The primary components of the OPRA OP16-3A gas turbine include the compressor, combustion chamber, and turbine. The failure affected several key components: the nozzle guide vanes (NGVs), turbine impeller, heat shield, and heat shield hanger ring. Damage was observed in the form of erosion, deposit formation, and material loss. The damaged components were analyzed using various techniques to determine material composition and assess the damage mechanisms. The NGVs, made of Alloy 754 (an oxide-dispersion-strengthened superalloy), exhibited erosion of the thermal barrier coating (TBC) and substrate material. The heat shield, composed of Udimet 500, showed evidence of deposit buildup and subsequent material loss. The turbine impeller, constructed from Alloy 718 and Udimet 720, displayed wear and damage, particularly in the clearance region. Based on the laboratory findings, the failure sequence was reconstructed. Soot particles ingested into the compressor were carried through the gas path, leading to erosion of the NGV's TBC. The eroded TBC particles, along with other debris, deposited on the heat shield. These deposits, combined with the high-temperature and high-pressure operating conditions, caused cracking and detachment of the heat shield material. The detached particles acted as abrasive agents, leading to wear and damage of the turbine impeller and heat shield. The root cause of the failure was determined to be the ingestion of soot particles into the compressor, which initiated the erosion process and triggered the subsequent damage to downstream components. The analysis concluded that the failure was not due to overheating but rather a sequence of events initiated by soot-induced erosion. The study highlights the detrimental effects of environmental contaminants on gas turbine performance and emphasizes the importance of effective filtration systems to prevent such failures. Further investigation into the specific mechanisms of soot erosion and the development of mitigation strategies are recommended.

Ground WC-Co hard metal grades evaluated under service-like working conditions: mechanical and microstructural evolution

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B6_5 - Wear, Seminario 6 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The unique combination of hardness, toughness and wear resistance exhibited by heterogeneous hard materials (e.g. PcBN systems, cemented carbides, among others) has made them preeminent material choices for extremely demanding applications, such as metal cutting/forming tools or mining bits among others, where improved performance together are required. This presentation is focused on WC-Co cemented carbide material surface integrity evolution at high/intermediate temperature. A systematic micro and nanomechanical study of several WC-Co (in terms of metallic binder content and WC particle size) ground materials is presented. In general, three different aspects are investigated to accomplish the main goal of this research: (1) assessment of the intrinsic hardness of the deformed layer from room temperature up to 600 °C, (2) correlation of the compressive residual stresses with the hardness and elastic modulus maps by high indentation speed tests at the different temperature tested and (3) evaluation of the damage and plastic deformation mechanisms induced in the deformed layer. It was found that for different WC-Co composites, the intrinsic hardness of the deformed layer starts to slightly decrease at temperatures ranging between 400 and 500 °C, depending on the amount of metallic binder. This effect is attributed to different effects which take place simultaneously when the testing temperature increases: dislocation motion, reduction of compressive residual stresses and layer oxide generation mainly constituted by CoWO₄, WO₃ and Co₃O₄.

Effect of dynamically reconstructed microstructure on the precipitation of secondary phases and their impact on corrosion properties in a cast UNS 32760 super duplex stainless steel

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B6_2 - Corrosion, Seminario 6 Room (Level +1), settembre 17, 2025, 14:30 - 16:30

This study investigates the impact of hot plastic deformation on the precipitation of secondary phases during cooling in cast UNS S32760 super duplex stainless steel (SDSS). Due to their dual-phase microstructure and chemical composition, SDSS optimally balance mechanical strength and corrosion resistance. However, thermomechanical treatments can induce the formation of intermetallic phases such as sigma (σ), chi (χ), and chromium nitrides, which may negatively affect the alloy's overall performance.

To explore these effects, experimental tests were conducted to assess how the degree of deformation and strain rate influence dynamic softening mechanisms and secondary phase precipitation during cooling. The deformation was simulated using open-die forging at 1100 °C, followed by two different cooling conditions: a slow cooling rate (0.25 °C/s) and water quenching. This setup enabled the examination of ferrite decomposition under two distinct scenarios: precipitation of thermodynamically stable secondary phases at equilibrium, and the formation of nitrides due to nitrogen supersaturation of ferrite during rapid cooling. A thorough microstructural characterization, combined with phase quantification and corrosion testing, was carried out to assess the impact of these phases on mechanical integrity and corrosion resistance. The results show that hot plastic deformation significantly promotes sensitization, with a clear relationship between deformation parameters and the extent of secondary phase precipitation. Moreover, variations in strain conditions influence the dynamic reconstruction mechanisms, leading to significant changes in the kinetics of both stable and metastable intermetallic phase precipitation. This study offers new insights into the complex interactions between hot deformation, dynamic softening, and secondary phase precipitation kinetics, enhancing our understanding of their role in corrosion performance. The findings can be applied to optimize thermomechanical processing strategies, reduce the formation of detrimental phases, and improve the durability of SDSS in aggressive environments.

Effect of isothermal annealing on phase transformation and corrosion properties of UNS S32760 cast SDSS

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Because of their exceptional strength and corrosion resistance, with a PREN above 40, super duplex stainless steels (SDSS) are widely used to manufacture large valves and pipelines in off shore and desalination installations. In such applications, long-lasting and low maintenance cast metallic components are considered a viable option. However, in the temperature range where the precipitation of harmful phases is critical, cast components are particularly susceptible to slow cooling rates. This study investigates the mechanisms and kinetics of secondary phase formation in UNS S32760 super duplex stainless steel, subjected to isothermal ageing at temperatures ranging between 850 °C and 950 °C for 3 to 210 minutes. Among the possible secondary phases, the sigma (σ) and chi (χ) phases were identified as the main contributors to the instability of the duplex microstructure. Increasing the ageing time led to a higher percentage of secondary phase precipitation. It was observed that the kinetics and morphology of secondary phases are strongly influenced by variations in isothermal annealing temperatures. Since these aspects have a significant impact on corrosion properties, it was found that the finer the structure of intermetallic phases, the larger the sensitized surface area. Consequently, at the same volume fraction of secondary phases, a different degree of sensitization can be observed. This behavior was confirmed through DLEPR (Double Loop Electrochemical Potentiodynamic Reactivation) and CPT (Critical Pitting Temperature) corrosion tests. All isothermally aged samples were characterized using SEM-BSD combined with EDX analysis and quantitatively assessed using ImageJ software.

Design and realization of a tribometer for journal bearing applications in non-lubricating fluids

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B6_5 - Wear, Seminario 6 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Friction and wear phenomena are now viewed as a key area of research in support of the European Union's sustainability objectives. Recent studies suggest that tribological advancements could lead to a potential reduction of up to 24% in primary energy consumption [1]. In the extensive domain of tribology concerning shaft-journal bearing systems, the mechanics of non-lubricating fluid environments remains a largely uncharted scientific territory. Numerous industrial sectors grapple with the challenge of transporting and storing non-lubricating fluids, often employing mechanical technologies that prove to be insufficient for this task. Poor material selection and unbalanced operating conditions not only shorten the lifespan of numerous mechanical components but also force users to adopt inefficient technologies to address industrial challenges. This situation becomes even more problematic when non-lubricating fluids contain solid particles, which can act as abrasive agents against materials.

The present study is based on an industrial problem to analyze this engineering issue. A novel, custom-designed tribometer is proposed to simulate the performance of various materials, treatments, and coatings for shaft and journal bearings in non-lubricating environments. The instrument is designed to operate under high rotational speeds, heavy radial loads, and fixed operative temperature. A statistical approach is proposed to correlate torque and heat outputs with operating parameters, according to models proposed in previous literature [2]

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Effect of air, vacuum, and liquid metal environment on fatigue crack growth in 316L stainless steel at 450 °C

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B6_4 - Fatigue II, Seminario 6 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Despite numerous demonstrations that the mechanical properties of austenite steels remain largely unaffected in liquid lead-bismuth eutectic (LBE) environment, the effect of LBE on the propagation of fatigue cracks in 316L stainless steel is not yet fully understood. The main reason is that the immunity of 316L stainless steel has been established from relatively short time exposure testing campaigns at temperatures below 400 °C, therefore limiting corrosion effects. Additionally, low cycle fatigue tests in LBE often suffer from experimental inconsistencies, causing the large data scatter. In this study, the fatigue crack growth rates (FCGRs) in 316L stainless steel, measured in air, vacuum and LBE at 450 °C, are contrasted with the microstructural properties at the crack tips investigated by transmission electron microscopy (TEM). FCG tests were performed on the compact tension (CT) specimens following the ASTM standard. The specimens were pre-cracked under the same environment as those used for the FCGR tests. TEM lamellas with the crack tips were extracted from the fracture surface. For all the samples, the strong deformation field in the form of multiple low angle grain and twin boundaries are observed along the cracks and at the crack tips. Morphological characteristics of crack branching are in agreement with the slip plane activation mechanism, with irregular crack paths that closely follow the striation pattern observed at the fracture surface. Interestingly, the chemical mapping of the region in front of the crack tip revealed the enrichment of deformation induced low angle grain and twin boundaries by oxygen, and lead/bismuth in the samples that are measured under air and LBE, respectively. These changes, governed by the stress enhanced diffusion, affect chemical bonds, and could potentially lower the material strength locally, causing early fracture. At the macroscopic scale, this results in higher FCGRs in 316L exposed to air and LBE with respect of FCGRs in vacuum. Even though we observed almost two orders of magnitude higher FCGRs in 316L stainless steel exposed to LBE in comparison to those measured in vacuum, the fracture surface investigation clearly indicates that the fracture mode of 316L remains ductile in the whole ΔK range explored in this work.

THE MULTISCALE NATURE OF MATERIALS DEGRADATION: USE OF ION SELECTIVE SENSORS FOR HIGH RESOLUTION IMAGING AND CHEMICAL CHARACTERIZATION

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B6_2 - Corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The performance of metallic components is often limited by the loss of their properties due to environmentally induced degradation. Advanced research in corrosion science mainly aims for a better understanding of the surface chemical processes involved in the microscale, thus promoting the efficient and durable application of metallic materials to new societal expectations. To better control corrosion and its effects, researchers must integrate emerging advances in many areas of science and technology to understand mechanistic effects and relate them to underlying structures, compositions, and dynamics.

It has long been known that corrosion processes start at micrometre or nanometre scales, although until recently no suitable techniques were available to study reactions at such scales. Additionally, surface chemical heterogeneity is frequently observed for many metallic materials, particularly when dealing with alloys or joined (galvanically coupled) metals, but this can also occur with individual metallic materials that were once mistakenly considered stable and uniform in their passive state, examples of which are stainless steels and prosthetic-quality titanium. The issue of surface inhomogeneity is even more relevant when corrosion protection methods involve the chemical modification of surfaces. Progress in corrosion research will therefore depend on the availability of experimental techniques capable of probing materials with high spatial and chemical resolution in operation. In this context, the use of scanning electrochemical microscopy (SECM) in corrosion science has been shown to be a powerful technique.

However, the application of SECM to the study of corrosion reactions has been significantly slower than that for other electrochemical applications, partly because in its early stages SECM was mainly an amperometric and potentiostatic technique. Although attractive advantages were recognised in regard to performing local quantitative electrochemical experiments, the possibility of using all the electrochemical techniques on both the probe and the substrate, and the possibility of coupling in situ electrochemical measurements with other techniques, their application to corrosion systems was limited by the requirement of a redox process at the tip for imaging (feedback mode). In fact, the addition of a redox mediator to the solution for its faradaic conversion at the tip would inevitably generate a Nernst potential at the metal surface under investigation, which may significantly alter the spontaneous mixed potential state of the corrosive system, and thus produce changes in the mechanism of the process under investigation. Advances have resulted from the application of potentiometric operating modes, involving ion-selective microelectrodes as tips, as described in this contribution.

Role of Chemical and Physical Conditions on Nitrogen Insertion During High-Temperature Oxidation of titanium in Air

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 17, 2025, 13:10 - 14:30

Metals and alloys are used in many technological applications requiring extreme temperature conditions. Their resistance to high-temperature oxidation becomes a major challenge, enabling them to be used for longer or shorter periods of time, depending on the type of application. In the aeronautics sector, an additional selection criterion for reducing operating costs is material density. Titanium combines low density with good specific strength and wear resistance, as well as good corrosion and oxidation resistance up to 550°C. Many ways were explored to increased High Temperature resistance of alloys, specially titanium ones.

Then, we will present various studies focusing on the role of physical conditions which govern formation of the oxide layer and also in the case of oxidation of titanium in air the insertion of nitrogen into metal substrates. And so, various reactive surface treatments using a laser source and classical oxidation in a furnace are displayed for at high temperature oxidation in air in the case of different metallic bases (iron, titanium and aluminum).

We will discuss the role of the coalescence rate on nanoparticle formation in the case of a laser plasma plume for laser ablation (Ti, Al and Fe) [9,10], but also the role of the solidification temperature of the different phases during cooling of the liquid bath formed by laser marking treatment of titanium [6,7, 10]. In the case of high-temperature oxidation in air of titanium alloys, we will also discuss presence of additional elements, or the surface state on the role of additional elements in the formation of the nitride layer at the metal-oxide interface [2].

In these studies, the choice of analytical techniques to determine the location of nitrogen and quantify its insertion was of great importance. Specific and complementary analyses were carried out under synchrotron radiation (ID22-ESRF and SWING-Soleil), or by techniques using ion beams (Saclay) such as Rutherford backscattering spectrometry (RBS) or Nuclear Reaction Analysis (NRA). Other characterization techniques such as electron microscopy, electron microprobe (EDX, WDS), X-ray diffraction and Raman spectroscopy have also been used to complete the studies.

The challenge of understanding the conditions of formation of such nitride phases results in the different properties for those kind of oxynitride layers, in terms of adhesion, protection against oxidation and also accommodation of various mechanical stresses such as friction or wear.

Slurry and cavitation erosion behavior of HVOF sprayed Metallic and Cermet Coatings

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B6_2 - Corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

HVOF thermal spraying is a deposition process that aims to increase the service life of engineering products in various types of media, such as corrosion, abrasion, and erosion. The intended study seeks to understand the effect of the residual stresses on the cavitation and slurry wear resistance of different metallic (316L and Hastelloy C276) and composite coatings, (WC17Co, Cr3C2 25NiCr). This study aims to observe how different coating materials are affected by the stresses generated during and after deposition, which is a result of the impact of the particles and their cooling and thermal contraction process. The coatings were characterized by metallographic techniques optical and electronic microscopy, and microhardness. After surface preparation (grinding and polishing), cavitation and slurry tests were performed. It was observed that the WC and Cr3C2 coatings are more clearly influenced by stresses generated during the deposition, where a minor peening effect and formation of a tensile residual stress reduce the cavitation resistance. Two different Cr3C2 25NiCr powders were performed; agglomerate and sintered showed more sensitivity for these deposition parameters. In contrast, the metallic coatings, 316L and C276, are more affected by different deposition aspects which affect the oxidation and porosity process. 316L and C276 coatings presented lower cavitation resistance for the samples with higher oxide phase content, probably reducing the adhesion between splats. The slurry resistance of the coatings are not so sensible to the processes parameters and stresses, and are only affected by metallurgical aspects, like presence, quantity and type of the hard phase. WC17Co show better slurry resistance than other coatings.

Design and implementation of an in-situ electrochemical setup for fatigue testing under the influence of hydrogen charging

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B6_3 - Fatigue and Fatigue corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

In view of the increasing use of hydrogen in the energy industry, a comprehensive understanding of hydrogen embrittlement is essential to ensure the safety of materials under real operating conditions. The complex interplay between cyclic loading and hydrogen-induced degradation requires advanced experimental methodologies for reliable assessment.

For this purpose, an electrochemical in-situ hydrogen charging cell was integrated into a fatigue test rig to systematically investigate the influence of hydrogen on fatigue performance of metallic materials. The setup consists of a two-electrode configuration with a platinum counter electrode in a double-walled laboratory glass cell, enabling precise temperature control of the electrolyte. The soft martensitic steel 1.4313 (X3CrNiMo13-4) was selected as a model material to validate the experimental approach. Fatigue tests were carried out at a stress ratio of $R=0.1$ and a frequency of 10 Hz with varying hydrogen charging durations in a 22% NaCl solution containing 1 g/l Thiourea at 50°C. Experiments were conducted using both pre-charged samples and in-situ hydrogen charging to distinguish between general fatigue effects and those driven by hydrogen diffusion. Samples that were pre-charged failed immediately during the first cycle, indicating a purely hydrogen-induced failure. In contrast, in-situ charging reduced the number of cycles to failure compared to tests conducted in air. Hence, the fracture surfaces still exhibited significant regions of fatigue crack growth, indicating the interplay between fatigue and hydrogen-induced failure. Beyond evaluating the number of cycles to failure, the study focused on analysing fracture surfaces through scanning electron microscopy. Beside the typical fatigue characteristics (e.g. striations), the fracture surfaces showed typical features of hydrogen embrittlement, including intergranular brittle fracture with gaping grain boundaries, ductile deformed hairlines on the grain surfaces and transcrystalline 'feathered' sections, as well as quasi-cleavage fracture.

These findings confirm the reliability of the developed setup, which is therefore suitable for further investigations into hydrogen-related degradation of various metals and alloys. To further elucidate the role of hydrogen in fatigue crack initiation, correlative studies employ high-resolution SEM and atom probe tomography to analyse the fracture initiation sites at the atomic scale.

Advances in Cermets for harsh environments: Unlocking Wear and Corrosion Resistance Through Microstructure and Binder Optimization

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B6_2 - Corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The performance of cermets (ceramic-metal composites) in harsh environments depends significantly on their microstructure, binder phase, and the interplay between material properties under varying conditions. This presentation explores our recent advances in the design of high-performance cermets, particularly focusing on the optimization of wear resistance and corrosion behavior. Key innovations include the development of TiC-based and WC-based cermets incorporating multi-principal element alloy binders (e.g., CoCrNi, CoFeAl) and rare-earth dopants, which enhance the toughness, wear resistance, and corrosion resistance of these materials. The research employs advanced experimental techniques, including high-temperature tribological testing and electrochemical corrosion studies, to characterize the degradation behavior of these materials under harsh conditions. Coupled with these experimental investigations, data-driven modeling and simulation approaches, including thermodynamic phase stability analysis and microstructural modeling, offer deeper insights into the mechanisms controlling wear and corrosion. The formation of oxide tribolayers, along with the role of binder composition and phase stability, is identified as key to mitigating degradation, especially in high-temperature and corrosive environments. Furthermore, a deeper understanding of the complex tribocorrosion mechanisms will be discussed, shedding light on how these insights can guide the future development of cermets for demanding industrial applications such as mining, drilling, and high-temperature machinery. The findings offer a robust framework for enhancing the durability of materials in extreme service conditions, which could pave the way for new high-performance composites.

Influence of Hybrid Silica-Based Sol-Gel Coatings on the Fatigue and Corrosion Behaviour of 16Mo3 Steel

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembere 17, 2025, 13:10 - 14:30

Surface morphology significantly influences the fatigue life of metallic materials. Therefore, improving surface performance is crucial for both economic and safety-related applications. Coatings can be beneficial in two ways: (i) mechanically suppressing slip bands and (ii) acting as a chemical barrier to mitigate corrosion. Sol-gel coatings have gained interest due to their tunable properties, which can be optimised by adjusting the synthesis parameters, such as synthesis steps, precursors, solvents, and catalysts. This has led to the development of silica-based hybrid coatings at Wroclaw University of Science and Technology, Poland, where the addition of organic moieties enhances flexibility while reducing porosity compared to pure inorganic coatings. These improvements can be beneficial for mechanical performance under cyclic loading and corrosion resistance. Our previous studies have shown that such coatings increase fatigue life in the very high cycle fatigue regime when tested using an ultrasonic fatigue system at a working frequency of 20 kHz. However, in this study, coated and uncoated specimens were tested in the high cycle fatigue regime under significantly higher stress levels. The tests were carried out at a stress amplitude of 295 MPa, a frequency of 5 Hz, room temperature, and zero mean stress using a servo-hydraulic fatigue testing system. The results indicated that the coating had no noticeable effect on fatigue life in the high cycle fatigue regime. Interestingly, analysis of the stress-strain hysteresis from the fatigue tests showed that, while both coated and uncoated specimens exhibited cyclic softening, this phenomenon began later in the coated specimens but developed more pronounced. To investigate the cause of this behaviour, the development of slip bands was studied in interrupted fatigue tests at specific load cycles using a scanning electron microscope. Additionally, the corrosion resistance of the coatings was evaluated by immersing both coated and uncoated specimens in a 3.5% NaCl solution for 72 hours prior to fatigue testing. The uncoated specimens exhibited early failure, whereas the coated specimens maintained the same fatigue life as those not exposed to immersion. To assess the impact of prior corrosion on fatigue behaviour, the fracture surfaces of failed specimens were closely analysed and investigated.

“Hybrid” multi-component alloys: chemical composition optimization to enhance an abrasive wear resistance

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The presentation is devoted to the “Three-body abrasion” wear behavior of “hybrid” multi-component alloys which are Fe-B-C alloys containing 5 wt.%W; 5 wt.%Mo; 5 wt.%V; 10 wt.%Cr and 2.5 wt.%Ti. The contents of carbon (0.3 wt.%, 0.7 wt.%, 1.1 wt.%) and boron (1.5 wt.%, 2.5 wt.%, 3.5 wt%) were varied according to a full factorial design 32 method. The alloys were fabricated by sand-casting. In the as-cast state, the alloys performed near-eutectic (at 1.5 wt.% B) or hypereutectic (at 2.5-3.5 wt.% B) structure. The structural micro-constituents were (in different combinations): (a) (W,Mo,V)-rich borocarbide $M_2(B,C)_5$ as the coarse primary prismatoids or the fibers of “Chinese-Script” eutectic, (b) Ti-rich carboboride $M(C,B)$ of equiaxed shape, (c) Cr-rich carboboride $M_7(C,B)_3$ as the plates of “Rosette”-like eutectic, (d) Fe-rich borocementite $M_3(C,B)$ as the plates of “Coarse-net” and Ledeburite eutectics. The metallic matrix was ferrite (at 0.3-1.1 wt.%C and 1.5 wt.%B) and “ferrite+pearlite” or martensite (at 0.7-1.1 wt.%C and 2.5-3.5 wt.%B). Bulk hardness varied from 29 HRC (0.3 wt.% C-1.5 wt.% B) to 53.5 HRC (1.1 wt.%C-3.5 wt.%B). The wear test results were mathematically processed and the regression equation of the wear rate as a function of carbon and boron contents was derived and analyzed. At any carbon content, the lowest wear rate was attributed to the alloy with 1.5 wt.% B. Adding 2.5 wt.% B led to an increase in wear rate because of the appearance of coarse primary borocarbitides $M_2(B,C)_5$ which were prone to chipping under abrasion. At higher boron content (3.5 wt.%) wear rate decreased due to increasing the amount of the eutectic carboborides. The optimal chemical composition was found as 1.1 wt.%C-1.5 wt.% B with a near-eutectic structure having total 35 vol.% of carboborides ($M_2(B,C)_5$, $M(C,B)$, $M_3(C,B)$ and $M_7(C,B)_3$). The heat treatment (quenching and low-temperature tempering) resulted in a substantial increase in hardness and wear resistance. As the quenching temperature increased to 1150-1200 °C, hardness gradually increased to 66-67 HRC while the wear rate decreased by 3-6 times as compared to the as-cast state. The highest abrasive resistance was attributed to the alloys with 1.1 wt.% C which had a 2.36-3.20 times lower wear rate as compared with reference alloy (13 wt.% Cr cast iron, 66 HRC). The effects of carbon and boron on hardness and wear behaviour are analyzed using the regression models developed according to the factorial design procedure.

Investigation of High-Temperature Fatigue and Microstructural Influences on Crack Propagation in Nickel-Based Superalloy IN718

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B6_3 - Fatigue and Fatigue corrosion, Seminario 6 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Nickel-based superalloys such as IN718 are essential for high-temperature applications in aerospace, power generation, and oil and gas industries. These alloys are characterized by their excellent mechanical properties and corrosion resistance, primarily optimized by precipitation hardening using secondary phases such as γ' and γ'' precipitates.

The fatigue life of IN718 at elevated temperatures is significantly influenced by environmental effects and mechanisms such as dynamic embrittlement (DE) and stress assisted grain boundary oxidation (SAGBO). Experiments with varying dwell times under peak load conditions have shown that longer dwell times weaken grain boundaries and lead to a transition to time-dependent crack growth. Interrupted tests and microstructural analysis after specific load cycles provided insights into crack propagation behavior and the damage mechanisms.

The influence of grain boundary properties and precipitates on crack propagation has been investigated to better understand transgranular and intergranular cracking behavior. The role of special grain boundaries (CSL boundaries) and the positioning of precipitates in influencing crack deflection were of particular interest. A combination of imaging techniques such as light optical microscopy (LOM) and scanning electron microscopy (SEM), together with 2D and 3D electron backscatter diffraction (EBSD) were used to correlate crack path evolution with microstructural features.

This study aims to provide insights into the complex interplay between time of mechanical loading, microstructure, and fatigue mechanisms. The ultimate goal is to achieve a deeper understanding of crack behavior in IN718 under high-temperature fatigue loading, which can be used to design future optimization strategies for advanced applications.

Very high cycle fatigue behavior and failure mechanism of Fe-24Mn-10Al-1C lightweight steels

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Numerous studies have demonstrated the viability of lightweight Fe-Mn-Al-C steels for exhibiting an improved balance of high strength and high ductility in industry applications. However, there are few reports on the very high cycle fatigue (VHCF) performance and fracture mechanism of lightweight steels, which undoubtedly greatly limits its further application. Currently, we have achieved a good mechanical properties (tensile strength 750MPa, elongation 42%) in the investigated duplex lightweight steels. In addition, the investigated steels also exhibited a good fatigue strength (310 MPa) and high ratio of fatigue strength to ultimate tensile strength (σ_f / σ_{UTS} , 0.42). According to our previous research, the investigated steels are composed of austenite. During the quasi-static tensile test, movement of dislocations are dominated planar slip in austenite. However, the cyclic loading may change the dislocation configuration and dislocation structures, which may influence the VHCF performance of the investigated steels. Therefore, in order to further clarify the relationship between microstructure and fatigue performance in Fe-Mn-Al-C lightweight steels, the dislocation structures evolution has been characterized by TEM. In addition, the fracture surfaces will be analyzed by SEM. The three stages of fatigue failure (crack initiation, stable crack propagation and sample failure) could be identified. Through analysis the results of Electron Backscatter Diffraction (EBSD), the effect of ferrite and austenite on VHCF performance and fracture mechanism could be also discussed. Based on above results, we systematically discussed VHCF behavior and fracture mechanism of the investigated steels.

Damage nature in metallic material during very high cycle fatigue

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B6_1 - Fatigue I, Seminario 6 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The primary cause for material damage under cyclic loading has been considered to be intimately related to plastic deformation irreversibility. Intrusion and extrusion of persistent slip bands (PSB) formed at the surface cause fatigue crack initiation (stage I) and then crack propagation follows (long crack propagation, stage II). For fatigue in a very high cycle regime ($>10^7$ cycles), surface damage becomes negligibly small due to low stress amplitude. Crack initiation may shift from surface to subsurface with increasing fatigue life or decreasing applied stress. Fatigue crack initiation starts at subsurface defects such as inclusions, pores, and microstructure inhomogeneities by stress localization or concentration. Based on the recent results, this work will provide a review or discussion on fatigue damage and crack initiation in polycrystalline metallic materials without any defect as mentioned. They include the following four processes: formation of stress/strain localization; formation of dislocation sub-cells and grain fragmentation; fully grain fragmentation; fatigue crack initiation. During cyclic loading, the soft grains with larger Schmid factors can undergo higher plastic strain amplitude in the crystal plane. This results in strain localization and formation of dislocation sub-cells and grain fragmentation in the grains. Very high cycle fatigue will also result in exhaustion of local plasticity and consequently lead to crack initiation in the matrix. They start mainly at grain boundaries or triple junction points. Once a critical size (crack origin or FGA) has formed or the crack length has reached a threshold value (or stress intensity factor threshold), the stage II crack propagation will occur. This work can increase our understanding on the material nature for fatigue damage and crack initiation during very high cycle fatigue.

New Thermal Barrier Coatings with Polymer Derived Ceramic Bond Coats for TiAl alloys

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Current state-of-the-art materials for blades in jet turbine engines are monocrystalline nickel-based superalloys. For application in the hot section, they are coated with thermal barrier coatings (TBCs) made of an outer layer of zirconium oxide stabilised with yttrium oxide (YSZ) with a thickness of 100-300 µm. An inner layer (bond coat) based on a diffusion aluminide layer or a metallic interlayer of MCrAlY (M=metal) with a thickness of approx. 80 µm is applied below the TBC and additionally protects the turbine blade from oxidation. TiAl alloys represent a very interesting alternative for the lower temperature section of the jet engine with a much lower density than Ni (3.7-3.9 vs. 8.0-8.7 g/cm³) and are already used in the cold section of some jet engine turbines. Application of a TBC could allow the use of TiAl turbine blades at higher temperatures. However, when combining TBCs and TiAl alloys, a compatibility problem with the bonding layer (MCrAlY) arises due to the formation of brittle phases at the interface.

To address this the application of TBCs on the Ti48Al2Cr2Nb (4822) alloy with a bond coat based on polymer-derived ceramic coatings from the SiAlOC system are being explored for higher temperature applications. SiAlOC coatings were already shown to improve the corrosion resistance of 4822 [1]. TBCs of YSZ were obtained at several different temperatures using an EB-PVD process. SEM and EDS microstructural studies along with advanced structural studies using Raman confocal imaging showed that using a hollow cathode (HC) plasma in the EB-PVD process formed columnar ceramic coatings successfully at temperatures up to 200°C lower than typical, while still meeting the requirements for TBC applications. The TiAl specimens with a SiAlOC bond coat and EB-PVD TBC were oxidized in lab air for up to 800 h. Metallographic cross-sections were prepared to study the impact of oxidation and the overall adhesion of the coatings.

Keywords: Thermal Barrier Coatings; High temperature corrosion; Polymer Derived Ceramics

Acknowledgment

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Type of presentation: poster

Impact of the initial HAZ microstructure of low alloy steels on intergranular embrittlement due to thermal ageing

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B7_9, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 14:30 - 16:30

The reactor vessel, the pressurizer and the steam generators used in nuclear power plants are fabricated from low alloy steels. Due to their large size, each component is made of smaller parts, that are welded together. The area where two steel pieces are welded together is composed of the weld metal, the Heat Affected Zone (HAZ) and the base metal.

These components are exposed to temperatures up to 345°C, during long period of time, leading to thermal ageing. Current norms define HAZs to be the most susceptible regions to thermal ageing. Indeed, it is commonly assumed that the shift of their ductile-to-brittle transition temperature (DBTT) upon ageing is three times larger than that of the base metal.

Under these conditions, thermal ageing is due to Reversible Temper Embrittlement (RTE) or intergranular embrittlement, which is a non-hardening thermal ageing mechanism. This mechanism is characterized by impurities segregating to grain boundaries (mainly phosphorus). The phosphorus segregation at prior austenite grain boundaries reduces grain boundaries cohesion, which lowers the critical intergranular fracture stress, resulting in an increase in DBTT. Consequently, a ductile fracture at a given temperature before thermal ageing can switch to a brittle fracture at the same temperature after thermal ageing.

This study aims to understand how the initial HAZ microstructure influences the embrittlement due to thermal ageing. While the base metal microstructure of low alloy steels is mainly bainitic, HAZ gather many different microstructures, each with their own susceptibility to thermal ageing. In this study, a variety of simulated HAZ microstructures was generated using a Gleeble thermomechanical simulator. After performing a post-welding heat treatment, half of the specimens created were aged using an accelerated ageing heat treatment. Instrumented Charpy V-notch impact tests were conducted on the different microstructures, both in the initial and aged conditions, to build DBTT curves. The 'load diagram' method was applied to analyze the force-displacement curves measured during the Charpy tests, to estimate the critical cleavage fracture stress for each microstructure before and after thermal ageing. The intergranular segregation was measured by Auger Electron Spectroscopy (AES). According to the first AES results, it seems that the HAZ microstructure has little influence on the phosphorus concentration at grain boundaries after thermal ageing, although it significantly affects the shift in DBTT.

Evaluation of Damage Models for Predicting Bending Failure in Advanced High-Strength Steels (AHSS)

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B7_3, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 14:30 - 16:30

The prediction of bending failure in conventional constitutive models and numerical analysis remains underexplored, particularly for advanced high-strength steels (AHSS). These materials present unique challenges in bending fracture, as surface cracks initiate without necking, raising doubts about the applicability of traditional ductile damage models. This study evaluates two advanced damage models across three AHSS grades with tensile strengths ranging from 980 MPa to 1500 MPa to predict the macroscopic onset of failure. The micromechanical-based Gurson-Tvergaard-Needleman-Shear (GTNS) model was modified to better calibrate and distinguish between pure shear and plane-strain tension fractures. Additionally, the Hosford-Coulomb model, integrated with the Generalized Incremental Stress-State Dependent Damage Model (GISSMO), was employed—a framework frequently used in industrial shell analysis for sheet metal forming. A finite element analysis (FEA)-free calibration method was developed to rapidly and systematically identify the coefficients for each model. Calibration was conducted for shear, plane-strain bending, and biaxial tension paths. Both models showed good agreement with experimental load-displacement results for AHSS with low bendability in shear, bending, and tension modes. However, significant errors were observed for AHSS with high bendability due to their unique fracture behavior. The result shows that even with small three-dimensional elements, current ductile fracture models fail to accurately predict the onset of failure in high-bendability AHSS, as these materials exhibit very slow propagation of microcracks at the bending tip. These findings highlight the need to account for slowly propagating bending cracks when developing finite element-based failure models for AHSS.

The effect of Mo segregation on the grain boundary precipitation behavior in Fe-Ni-Mo-X alloys

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Maraging steel shows superior strength and toughness through the significant precipitation of intermetallic compounds. Its development started from high amounts of Ni- and Co-containing alloys, but nowadays, the entire or partial substitution of high-cost elements (Ni, Co) to cheap ones is being studied to reduce its cost. Fe-Ni-X (X=Mn, Ti) alloys show excellent hardening responses during aging treatment. However, these alloys suffer grain boundary embrittlement and show no tensile ductility even after very short aging treatment. Precipitation of intermetallic phases, θ -MnNi in Fe-Mn-Ni alloys and η -Ni₃Ti in Fe-Ni-Ti alloys, at grain boundaries was suggested as the reason for the weakening of grain boundary strength. After extended aging, grain boundary strength is recovered when these precipitates transform to austenite. Dislocation glide or dislocation climb was critical in converting these grain boundary precipitates to austenite. To overcome the grain boundary embrittlement at the early stage of aging treatment, adding Mo is considered to strengthen the grain boundary. Although the Mo effect improving strength and ductility was reported, the effect of Mo segregation on the change of the grain boundary precipitation behavior has not been elucidated yet. This study clarifies the roles of Mo segregation on the grain boundary precipitation behavior and its related recovery of grain boundary strength in Fe-Ni-Mo-X alloys.

Microstructural and mechanical evolution of IN718 alloy produced by additive manufacturing after heat treatment optimization

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B7_6, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 14:30 - 16:30

This research investigated the effects of different heat treatments on microstructure and mechanical properties of additively manufactured Inconel 718 (IN718) superalloy, produced using laser powder bed fusion technique. Samples included bulk materials and lattice structures, with three different geometries. In order to investigate the above-mentioned properties of the specimens, many experimental techniques have been used, such as optical microscopy, scanning electron microscopy, electron backscattered diffraction, differential scanning calorimetry, X-ray diffraction and Vickers hardness measurements.

After a full characterization of the as-built samples, they were heat treated, starting from the standard industrial treatment employed for IN718 alloy. It includes a solution annealing at 980 °C for 1h then air cooling, followed by a first ageing at 720 °C for 8h and a second ageing at 620 °C for 8h. The resulting microstructure shows some fine γ'/γ'' precipitates, dispersed inside the grains of the γ matrix. Along grain boundaries, coarser precipitates were continuously distributed, attributable to both δ and Laves brittle phases.

The standard heat treatment is often optimized for traditionally manufactured products, such as samples produced via casting. In this case, the involved production technique is additive manufacturing, so an optimization of the heat treatment should be considered. In fact, the embrittlement observed on annealed samples suggested an optimization of the standard heat treatment, being the lattice structures employed for structural applications. The study has been then focused on the tunability of the heat treatment by varying both the annealing and the aging temperatures, to understand which step is the most critical for defining the final microstructure and mechanical properties. In order to reach this goal, some modifications have been successfully applied to the standard heat treatment, by firstly modifying the solution annealing temperature, which has been increased up to 1150 °C. The obtained samples showed different microstructural features, in terms of secondary phases, with a low amount of brittle phases. Then, being the ageing responsible of the hardness increment, the two steps of ageing have been investigated, in order to evaluate the impact of these steps on both microstructure and mechanical properties. Finally, all samples, both bulk and lattice structures, were heat treated with the optimized treatment, and better microstructural features have been observed, in terms of fraction of secondary brittle phases. Furthermore, mechanical properties have been also improved, being suitable for application purposes of selected structures.

High-temperature deformation behaviour of nickel-based superalloys

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In this study, the high-temperature deformation behaviour of INCOLOY alloy 925 was investigated through deformability and microstructure evolution in the (1050 - 1200) °C temperature range. The microstructure evolution of INCOLOY alloy 925 was investigated by X-ray diffraction (XRD) and Scanning Electron Microscopy - Electron Backscatter Diffraction (SEM-EBSD) techniques. The deformability of INCOLOY alloy 925 was investigated by the up-setting method, using a gravity-drop hammer, with the following deformation energy/impact energy (E): 545.2 J, 1,021.5 J, 1,480.6 J, and 1,905.3 J. Data referring to deformation resistance (σ) and mechanical work (A) as a function of deformation temperature (T) and deformation energy/impact energy (E) was obtained and analysed. It was shown that increasing the deformation temperature leads to an increase in the obtained deformation degree (degree of reduction in height). By analysing the rate of increase in the deformation degree as a function of the applied impact energy, it was shown that the rate of increase in the deformation degree rises with the increase in the applied impact energy. Also, it was observed that the evolution of the deformation resistance (σ) as a function of temperature (T) shows a decreasing tendency while increasing the deformation temperature, for all impact energies, and that, the evolution of the mechanical work (A) as a function of temperature (T) shows a decreasing tendency while increasing the deformation temperature, for all impact energies.

Keywords: nickel-based superalloys; INCOLOY alloy 925; plasticity.

Acknowledgements: This work was supported by a grant from the Ministry of Research, Innovation and Digitization (Romania), CCCDI—UEFISCDI, project number PN-IV-P7-7.1-PTE-2024-0364, within PNCDI IV.

Overcoming the Strength-Ductility Trade-Off in FCC Metals: TWIP Effects in Cu-Al and Cu-Si Alloys

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The strength and ductility of metals are traditionally constrained by a trade-off relationship, governed by the dislocation mechanism that dominates plastic deformation in crystalline metals. Achieving high strength often necessitates suppressing the generation and movement of dislocations that contribute to ductility. This trade-off, however, can be mitigated by employing deformation twinning as a complementary strengthening and deformation mechanism. This concept is exemplified by TWIP steels, where deformation twinning in single-phase austenitic steels results in exceptional strength and ductility. Since the TWIP effect arises from deformation twinning behavior rather than intrinsic chemical composition, other FCC metals capable of deformation twinning hold potential for similar enhancements.

Building on recent insights into Cu-Al alloys [1], where deformation twinning supports plastic deformation, this study explores the potential of Cu-Si alloys. Silicon, a known reducer of copper's stacking fault energy (SFE), was incorporated to enhance twinning activity. Cu-Al and Cu-Si binary alloys were fabricated, including pure copper, Cu-8at% Al, Cu-16at% Al, Cu-2.2at% Si, Cu-4.4at% Si, and Cu-6.6at% Si, using vacuum arc melting. Following homogenization heat treatment, cold rolling, and annealing at 600°C for 30 minutes, the mechanical properties were assessed via tensile tests and microstructural analysis. Deformation behavior at low temperatures (−80°C) was also evaluated.

Experimental results demonstrated that increasing alloying element content in both Cu-Al and Cu-Si alloys enhanced strength and elongation, confirming the TWIP effect. Notably, Cu-Si alloys exhibited greater improvements in strength and elongation compared to Cu-Al alloys under similar conditions. This is attributed to Si's superior ability to reduce copper's stacking fault energy, enabling more effective twinning. Additionally, work-hardening rates increased with strain in both alloys. Microstructural analysis revealed active deformation twin formation during plastic deformation, with the TWIP effect persisting at low temperatures.

These findings underscore the potential of Cu-Si alloys as high-performance TWIP materials, demonstrating their ability to achieve superior mechanical properties through optimized deformation mechanisms. This research contributes to advancing FCC metal applications by addressing the strength-ductility trade-off and enhancing understanding of microstructural evolution.

[1] Liu, R., Zhang, Z., Li, L. et al. Microscopic mechanisms contributing to the synchronous improvement of strength and plasticity (SISP) for TWIP copper alloys. *Sci Rep* 5, 9550 (2015).

Analyses of UNSM treatment on mechanical properties and microstructures of Inconel 718 alloy

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The ultrasonic nanocrystalline surface modification process(UNSM) is a physical surface treatment method in which ultrasonic vibrations are applied directly to the surface. Nanocrystalline grains and compressive residual stress at the surface formed through the ultrasonic nanocrystalline surface modification process improve yield and tensile strength and are particularly effective in suppressing fatigue failure.

In this study, the ultrasonic nanocrystalline surface modification process was applied to Inconel 718 alloy and confirmed the mechanical properties at room temperature, and the microstructure was examined using a scanning electron microscope and electron backscattered diffraction analysis. The ultrasonic nanocrystalline surface modification process was treated on the surface of the Inconel 718 tensile specimen. For the mechanical properties analyses, tensile tests at room temperature were conducted, and nanoindentation was conducted to analyze hardness up to 200 μm from the surface.

The effect of the nano-surface layer and the compressive residual stress formed during the ultrasonic nanocrystalline surface modification process on the mechanical properties were obtained from this study.

Dynamic Strain Aging in CP-Titanium: Insights from Tensile and Cyclic Loading Tests

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

Dynamic strain aging (DSA) is a critical phenomenon influencing the mechanical behavior of materials, driven by the interaction between dislocations and diffusing solute atoms. This study investigates the occurrence of DSA in commercially pure titanium (CP-titanium) under quasi-static tensile and cyclic tension-compression loading. Tensile and low-cycle fatigue (LCF) tests were carried out in a wide temperature range from 25 – 600 °C at strain rates of 10^{-5} – 10^{-1} /s. A systematic comparison is conducted to identify and analyze the temperature, strain rate/frequency, and incubation strain conditions where DSA manifests in these loading modes. Microstructural and mechanical properties, such as microhardness, are also evaluated to elucidate the impact of DSA under each loading regime. During tensile deformation, DSA manifests through several distinct features, including a plateau in the strength-temperature relationship, serrated yielding in stress–strain curves, and negative strain rate sensitivity (SRS). In the case of cyclic deformation, DSA can be observed as a plateau or peak in the cyclic peak stress-temperature relationship and a negative temperature dependence of the plastic strain amplitude or hardening trend. These findings provide new insights into the mechanisms of DSA in CP-titanium and lay the foundation for optimizing CP-titanium for applications where tensile and cyclic loading are critical.

During tensile deformation, DSA manifests through several distinct features, including a plateau in the strength-temperature relationship, serrated yielding in stress–strain curves, and negative strain rate sensitivity (SRS). In the case of low-cycle fatigue deformation, DSA can be observed as a plateau or peak in the cyclic peak stress-temperature relationship and a negative temperature dependence of the plastic strain amplitude or hardening trend. These findings provide new insights into the mechanisms of DSA in CP-titanium and lay the foundation for optimizing CP-titanium for applications where tensile and cyclic loading are critical.

X-ray diffraction for characterization of materials in nuclear industry

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B7_2, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 10:50 - 13:10

X-ray diffraction (XRD) is an effective technique for studying different kinds of materials, providing valuable information about their crystal structure and phase composition. One of the main benefits of XRD is its ability to detect even small amounts of secondary phases that can affect the mechanical and chemical properties of materials. This method also allows for monitoring changes in the crystal structure over time or under non-standard conditions (e.g. high temperature, high pressure, or gamma/neutron irradiation), for example concrete aging or changes due to irradiation. Knowing how the phase composition changes on/in a material is important because from that we can conclude about their physical properties, which is especially important in the nuclear industry ensuring the safe operation of the components.

In this work we would like to present examples of how XRD help us to “see” the expansion of unit cell on granite after neutron irradiation, changes of the phase composition on the surface of cement-matrices, and corrosion of steel surface after years embedded in cement-matrices under water in anaerobic conditions.

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Sample shape effects on the experimental characterization of compressive and shear moduli

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B7_3, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 14:30 - 16:30

Accurate determination of the elastic properties, such as the compressive and shear moduli, is essential for understanding the mechanical behavior of materials. While the influence of specimen geometry on compressive modulus measurements is well-documented, its effect on shear modulus measurements in torsion tests has not been studied in-depth, and no correction models are currently available. The present work investigates the geometric dependencies of these moduli and introduces a novel correction model for torsion tests. The elastic properties of cylindrical samples of silicone rubber were evaluated using compressive and torsion experiments. Compressive modulus measurements were conducted with a Dynamic Mechanical Analyzer (DMA), and shear modulus measurements were performed via torsion tests using a rheometer. The results confirmed that both moduli are influenced by the shape factor of the cylindrical samples. To address these effects, a correction model was developed for torsion tests, while an existing model was applied to compressive tests. Application of the proposed correction model led to physically consistent values for both the compressive and shear moduli, demonstrating the reliability of this approach for accurate characterization

Dynamic Response and Challenges in High-Frequency Testing of Elastomeric Specimens

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B7_3, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 14:30 - 16:30

The accurate characterization of elastomeric materials under high-frequency dynamic excitation is fundamental for applications requiring vibration isolation, energy dissipation, and structural damping. However, the behavior of these materials at frequencies above 1 kHz shows singular challenges, as the interaction of viscoelastic properties, resonance phenomena, and wave dispersion effects becomes increasingly significant. This study focuses on the dynamic response of elastomeric specimens subjected to excitation frequencies up to 3 kHz, highlighting the mechanical impedance behavior, the strain field distribution, and the limitations of conventional testing methodologies.

Using a custom-built test bench designed for high-frequency applications, the dynamic response of elastomeric specimens was evaluated through an indirect measurement approach compliant with ISO 10846-3. This setup incorporates a seismic mass to decouple external interference, ensuring accurate measurements of force and displacement. Piezoelectric accelerometers and force transducers were employed to capture dynamic data across a wide frequency range, revealing critical phenomena such as resonance-induced strain concentrations and transitions from stiffness-dominated to inertia-dominated behavior. At resonance frequencies, significant deviations in mechanical impedance were observed, attributed to non-uniform deformation patterns and internal energy dissipation mechanisms.

Finite element modeling (FEM) was used to validate experimental results and analyze the strain field under high-frequency excitation. The simulations confirmed the resonance-induced strain localization observed experimentally and provided further insights into the deformation modes of elastomeric specimens. The analysis demonstrated how standard elastic models fail to capture the material's dynamic behavior at high frequencies, requiring more advanced viscoelastic or fractional-order modeling approaches.

This research identifies several challenges in high-frequency testing, including the influence of resonance on measurement accuracy, the role of boundary conditions, and the limitations of current testing standards. The findings underline the importance of integrating experimental and numerical approaches to fully understand the high-frequency dynamics of elastomeric materials.

The outcomes of this study have implications for multiple industries, including automotive, aerospace, and civil engineering, where elastomeric components are crucial for mitigating high-frequency vibrations and ensuring structural reliability. By addressing the challenges of high-frequency testing, this work provides a foundation for optimizing the design and performance of elastomeric systems in demanding dynamic environments.

Effect of humidity on the wear behaviour of a medium carbon high silicon nanostructured bainitic steel

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B7_8, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 10:30 - 13:10

Nanostructured bainitic steels (NBSs) have attracted significant attention due to their exceptional combination of strength, ductility and wear resistance. These materials exhibit ultimate tensile strengths exceeding 1.5 GPa alongside fracture elongations of approximately 20%. Additionally, their chemical composition requires limited amounts or even the complete absence of expensive alloying elements such as Cr, V, Mo, and Nb, making them highly attractive for various industrial applications, particularly in the transportation sector.

The mechanical performances and wear resistance of NBSs under dry sliding conditions align with the transportation industry's current demands for reduced CO₂ emissions and improved passenger safety. The high strength of these materials enables the production of thinner, lighter components, leading to lower fuel consumption without compromising intrusion resistance. Moreover, their remarkable durability reduces maintenance costs and enhances vehicle safety. As a result, significant research efforts have been dedicated to comprehensively understanding the in-service properties of NBSs.

While numerous studies have explored the wear behaviour of NBSs under dry sliding conditions, focusing on the influence of heat treatment parameters, applied forces, sliding speed and lubrication, the impact of environmental humidity remains poorly understood. Investigating the role of humidity is crucial to accurately describing material degradation under real-world operating conditions, considering that a large part of the technological applications operate in the open air. Indeed, a potential shift in the wear mechanisms at different humidity levels due to the lubrication effect of moisture and the modification of the oxide layer that covers the steel can occur. This study examines a 0.45C-2.8Si-2.7Mn-0.56Al nanostructured bainitic steel under three humidity levels: low (<25 %), medium (~50%), and high (~90%). The microstructural characterization was carried out by SEM, XRD, Vickers microhardness before and after wear tests. The tribological tests comprised ball-on-disc configuration (ASTM G99-17 standard) using nanostructured bainitic steel discs 45 mm in diameter and 5 mm in thickness and a 100Cr6 steel ball 6 mm in diameter as counter-body material. The obtained wear tracks were analyzed by optical profilometer to evaluate the wear rates and by SEM to analyze the wear mechanisms. The results showed that relative humidity has a noticeable effect on wear damage and oxide layer formation with significant modification of the wear rate with the humidity level. These outcomes enable to describe the effects of environmental conditions and oxide layers on the wear performance of NBSs and so to predict the behavior in different practical applications.

Microstructural Changes in Zr-4Nb-2Al Alloy During Hot Rotary Swaging

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Zirconium and its alloys are widely utilised in various industries, from nuclear reactors to biomedical implants, owing to their excellent corrosion resistance, low neutron absorption cross-section, and superior mechanical properties. The low neutron absorption cross-section, in particular, makes zirconium an ideal structural material for nuclear reactor components. To enhance the material's mechanical strength and achieve a favourable microstructure comprising hexagonal close-packed (hcp) α -phase and body-centred cubic (bcc) β -phase, new zirconium alloys have been developed. The studied alloy, Zr-4Nb-2Al, contains a high concentration of α -phase-stabilising aluminium and β -phase-stabilising niobium, resulting in a favourable $\alpha+\beta$ microstructure.

This study examines the microstructural changes in the Zr-4Nb-2Al alloy during thermomechanical processing using hot rotary swaging. A key focus of the research was analysing the phase transformations occurring in the alloy, which were studied using differential scanning calorimetry and resistometry. These methods provided insight into the α -to- β phase transformation, which was later used to establish the temperature parameters for hot rotary swaging. The swaging process began in the β -phase region to refine the typically large β grains. This was followed by processing in the $\alpha + \beta$ coexistence region to achieve the desired final microstructure.

The microstructural changes after each processing step were analysed using scanning electron microscopy, which revealed a transition from a lamellar to a globular microstructure. Mechanical properties were then evaluated through compression and microhardness tests, demonstrating the material's performance enhancement.

This research provides insight into the steps involved in the hot rotary swaging of zirconium alloys. It also offers a detailed summary of the microstructural and mechanical property changes that occurred during the thermomechanical processing of the Zr-4Nb-2Al alloy.

Characterisation of a cast iron alloy produced with the addition of TiC nanoparticles

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B7_4, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 17:00 - 19:00

The simultaneous improvement of strength, ductility, and toughness in cast iron alloys is a key goal in the metallurgical industry. A promising strategy to achieve that is to modify the alloys by adding nanoparticles (NPs) with high hardness and thermal resistance. An example of valuable NP is titanium carbide (TiC), which has been reported to originate microstructural changes in the Fe-base alloys and to enhance their mechanical properties. A base cast iron with a high Mg content and a low Si content was first produced and then remelted with different additives in a centrifugal casting furnace to cast two medals in a metallic mould. One of them was produced with no addition of NPs and the other one with 3.8% of TiC NPs (about 20 nm in diameter). These NPs were previously introduced in Ni crucibles to promote good wettability (homogeneous dispersion of the particles) and to prevent agglomeration effects. The microstructure and the particles present in each medal were characterized using optical microscopy and Scanning Electron Microscopy (SEM). Both cast medals show a matrix composed of a high fraction of carbides, areas with martensite and low amounts of graphite particles with some having degenerated shape. The casting produced with an addition of TiC NPs comparatively show a microstructure with slightly lower amounts of graphite particles than that in the casting without any NPs addition. These graphite particles are mainly located in the central areas of both castings due to the low solidification rate at that location. For the case of non-graphitic particles, they were analysed using EDS-SEM microanalyses and then classified into six composition classes, very often containing Mg or Ti as main elements. Although the average density of non-graphitic particles are in the range 20000-25000 mm⁻² for both castings, the most frequent composition strongly depends on the addition of the NPs. Thus, the highest density of particles corresponds to compounds (Mg, Si, O, P, RE) for the casting produced without NPs addition, while class (Ti, C) is predominant in the case of the casting with the addition of TiC NPs. Further, it is observed that the size of the (Ti, C) particles present in the matrix ranges between 140 and 430 nm, i.e. about 7-20 times bigger than the size of the added TiC particles.

Impact of different types of fillers into the UV-ageing behavior of rotomolded PE composites

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Composite samples were produced by rotational molding, using a polyethylene (PE) matrix and different proportions of mineral dust (ignimbrite) and lignocellulose fibers (*Arundo donax* L.). Ignimbrite is based on silica, with high proportions of alumina and iron oxides (60-65%, 18-20%, and 3-5 %, respectively) [1]. The interfacial interactions between the fillers and the polymers are critical for achieving optimal performance, including the lifetime of the composite when exposed to various environmental factors, including UV light [2]. A good interfacial adhesion contributes to distribute stress more evenly throughout the material, thereby reducing the likelihood of crack propagation and degradation.

While the integration of different types of fillers into PE-based composites is expected to yield improvements in mechanical, and thermal properties (for silica), the evidence specifically supporting significant enhancements in UV-aging behavior is limited, finding even less studies for rotomolded items. For this purpose, composites with 5 and 10 wt% filler were prepared and characterized (tensile properties, FTIR spectroscopy and thermal behavior by DSC) before and after accelerated weathering in a UV-chamber for up to 500 h, analyzing the test samples properties every 100 h of exposure. Similarly, 5 and 10 wt% composites were prepared with a combination of both fillers (2.5 and 5 % of each filler). The tensile properties (tensile strength, elastic modulus and elongation at break) were determined for all formulations in the 6 analyzed times, also calculating their carbonyl and vinyl index to determine the extent of the degradation. As expected, modulus increases for the composites, keeping this behavior for the entire analyzed period of time, except for lignocellulose. Elongation at break has been found to decrease with exposure time, in general, although some distinct behavior occurs for the different composites, as also happening for maximum strength and elastic modulus. The neat matrix increases rigidity with UV-exposure, for a later decrease, thus evidencing that the incorporation of the fillers has a significant influence in the photodegradation of the PE. Hybrid composites at 5 % loading shows in general the highest properties, while 5 % composites (with single filler) exhibits the lowest variations along the exposure.

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In-situ neutron microstructural and mechanical characterization of WL –DED 316L stainless steel

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B7_6, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 14:30 - 16:30

Additive manufacturing (AM) of metals is generally more environmentally friendly than conventional casting-based manufacturing (CM), as it reduces material waste and produces complex, lightweight and repairable components. Among AM techniques, wire laser directed energy deposition (WL-DED) is increasingly utilized to fabricate large parts, especially with AISI 316L stainless steel, given its corrosion, creep, and oxidation resistance. However, the broader industrial uptake of AM faces challenges. Rapid thermal cycles during the process result in complex microstructures with coarse grains and epitaxial growth, which can compromise the predictability and safety of AM components in structural applications.

Characterizing these intricate microstructures requires analysis over representative sample volumes, which neutrons facilitate due to their ability to penetrate up to 6 cm into steel. The Institut Laue-Langevin (ILL) aims to support the implementation of AM in industry through neutron diffraction characterization, in this particular case of WL-DED 316L samples manufactured by the Technical University of Catalonia (UPC). These samples exhibit a two-phase, γ -austenite matrix and δ -ferrite, microstructure. The δ -ferrite is undesirable due to its chromium reaction, promoting the formation of brittle intermetallic FeCr (σ -phase) and reducing both corrosion resistance and mechanical properties. 3D Residual stress distribution was determined at SALSA, a strain analyzer for engineering applications. Three strain components (longitudinal, transverse, and normal) were measured in as-printed 15x150x15 mm³ prisms still attached to the baseplate. Initial results of the as-printed condition indicated areas with significant differences in stress concentration that could lead to material failure. A stress relief treatment at 700 °C for 2 hours was applied to study stress evolution and relaxation. High-temperature tensile tests conducted at SALSA and Engin-X provided diffraction elastic constants (Ehkl, v_{hkl}) to understand their influence on the mechanical properties of the material by analyzing the load partitioning under mechanical stress and its temperature dependence.

To understand phase evolution with temperature, in-situ neutron diffraction using the XTREMED instrument was performed on 4x4x5 mm³ coupons. These were subjected to cycles at room temperature (RT), 300, 400, 600, 700, and 900 °C and RT again, producing full high-resolution diffraction patterns. Rietveld refinement revealed a thermal expansion coefficient of $1.89 \times 10^{-5} \text{ } ^\circ\text{C}^{-1}$, as lattice parameters increased from 3.599 Å (RT) to 3.658 Å (900 °C). At RT, 4.36 vol.% δ -ferrite transitioned to 7.21 vol.% σ -phase after 7 hours at 800 °C and continued increasing at 900 °C.

Copper-Free, Eco-Friendly, Composite Brake Linings: Optimization of Manufacturing Parameters

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B7_8, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 10:30 - 13:10

Brake pads are critical for the safety of vehicles, ensuring reliable performance on speed control. The frictional behavior of automotive brakes is defined by the active surfaces of the disc, pad, and particles between them, making this a complex tribological system. There are several criteria that have to be met. First of all, the coefficient of friction should remain as stable as possible with time, temperature, erosion, etc. In addition, the optimization of wear performance is crucial to maintain a long service life of the pad while not damaging the opposite surface, the disc. Moreover, the particles generated as a result of wear should not harm the environment. It was found that the copper particles, which is one of the primary constituents of the brake pads, had toxic effects on aquatic life. As a result, in 2010, U.S. Environmental Protection Agency initiated a phase-out of copper in brake pads. Accordingly, this study focuses on the production of an eco-friendly, copper-free brake pad. A phenolic resin is used as the binder of the lubricants, friction modifiers, abrasives, fillers and the copper-replacement material. Hot-pressing technique is employed in the production of brake pad samples. The effects of processing parameters (pressure, temperature and time) on the friction and wear performance were analyzed within the scope of this study. The thermal transitions of the resin were characterized with thermogravimetric analysis (TGA) while pin-on-disc wear tests according to ASTM G99 were employed for measuring the coefficient of friction (COF) and wear rates at a temperature range of 100°C-350°C. The wear surfaces were examined with both stereo and scanning electron microscopes.

Aging-Induced Embrittlement in Short-Fiber Reinforced Thermoplastics: A Micromechanical Approach Using Numerical Homogenization

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B7_12, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 14:30 - 16:30

Aging studies are critical for ensuring that engineering plastic components can endure physico-chemical degradation under operating conditions. The degradation kinetics can be assessed by exposing parts to aging environments and testing them afterwards. However, this empirical approach is time-consuming and costly. An advantageous approach would be to simulate those aging tests. The aim of this research program is to develop a simulation method for virtualizing the aging tests of injection-molded thermoplastic parts, specifically addressing aging of the mechanical behavior at the component level. To achieve this in the framework of finite element (FE)-based mechanical simulations, it is crucial to establish failure criteria based on local aging descriptors. This work is focused on the hydrolytic degradation of polyamide 6.6, reinforced with 30 wt.% short glass fibers. Hydrolytic aging of 4 mm thickness PA66-GF30 part results in non-limited diffusion hydrolysis leading to an uniform reduction in molecular weight of the polymer matrix, causing progressive embrittlement, which manifests as a reduction in strain at break during uniaxial tensile tests. To achieve accurate simulations, the research aims to develop a failure criterion based on local aging descriptors. Using micro-mechanical analysis of a 3D representative volume element (RVE), the study links local degradation effects (such as molecular weight reduction) with the overall mechanical response of the composite. This approach allows finite element (FE) simulations to predict aged component failure. The study also discusses the construction of the RVE, which accounts for fiber microstructure, and the identification of the elastoplastic constitutive law for the PA66 matrix. The focus is on proposing a physics-based failure criterion that correlates with damage initiation under various levels of hydrolytic degradation.

Optimization of aluminum content in the zinc bath to improve wettability and galvanizing performance of AHSS

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Advanced high-strength steels (AHSS) contain Si and Mn, which form surface oxides during annealing, hindering zinc coating. To address this, aluminum is added to the zinc bath to promote oxide reduction. This study investigates the effect of aluminum content by measuring wetting force and Fe-Al coverage across different steel grades. A comparative study was conducted on interstitial-free (IF), high-silicon (P2, Si/Mn = 1.0), and low-silicon (P4, Si/Mn = 0.3) steels. The wetting force and $\text{Fe}_2\text{Al}_{5-x}\text{Zn}_x$ inhibition layer coverage were evaluated.

IF steel exhibited optimal wettability at 0.25 wt.% Al, while higher Al concentrations reduced the wetting force due to the formation of coarse $\text{Fe}_2\text{Al}_{5-x}\text{Zn}_x$ particles. In contrast, both P2 and P4 steels showed a monotonic increase in wetting force with increasing Al content. In both P2 and P4 steels, the aluminothermic reaction facilitated oxide reduction and aluminum consumption, suppressing abnormal $\text{Fe}_2\text{Al}_{5-x}\text{Zn}_x$ growth and improving wettability.

FactSage calculations revealed that the aluminothermic reaction significantly reduced the residual MnSiO_3 coverage, while SiO_2 showed minimal reduction, indicating greater resistance. Even at 0.50 wt.% Al, complete oxide reduction was not achieved, leading to the retention of residual oxides. The penetration of $\text{Fe}_2\text{Al}_{5-x}\text{Zn}_x$ beneath these residual oxides was observed, further enhancing wettability.

Influence of microstructural features on Charpy impact toughness properties of low alloy steels.

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

Keywords: Fracture mechanics, ductile-brittle transition, Low alloy steels, Microstructure.

Summary :

One of the primary challenges in the nuclear industry is ensuring the safety and security of the installations. Critical structures such as large forged components in low-alloy steel require an in-depth understanding of their mechanical properties to guarantee long-term reliability and performance under normal, incidental, or accidental operational conditions.

The exceptional scale of these components, obtained through ingot forging, inherently leads to localized chemical heterogeneities and variations in thermal history. Consequently, these variations result in a wide range of microstructures, inducing a substantial variability of mechanical properties within a single component. Despite extensive research, a satisfactory predictive tool for fracture properties remains elusive.

This research systematically investigates the key microstructural features influencing fracture properties of low alloy steel, with a focus on explaining and quantifying the statistical aspects of brittle cleavage failure in the ductile-brittle transition.

Our methodology employed mechanical tests on four precisely controlled microstructures. Starting from a reference tempered bainitic microstructure, we methodically varied three metallurgical parameters suspected influent on fracture properties: precipitate size (controlled by tempering conditions), prior austenite grain size (controlled by austenitizing temperature), local chemical composition (controlled by sampling area). Advanced scanning electron microscopy (SEM) and fractographic analyses provided comprehensive insights into mechanical property variations.

The result of this research will be instrumental in developing an advanced numerical model using a micromechanical approach [1] to simulate brittle failure at the microscopic scale.

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Investigation of recrystallization in high strength Ti-10-2-3 forged alloys: impact of the stored mechanical energy on active mechanisms

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B7_7, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 17:00 - 19:00

Due to its high strength Ti-10-2-3 titanium alloy is commonly used in the design of aircraft landing gear. It is well known that the final properties of the structural parts are closely linked to key microstructural parameters such as the size and orientation (texture) of the beta phase, as well as the volume fraction of the different phases present in the final bimodal microstructure. As far as the beta phase is concerned, it is an important factor on the control of the recrystallization stages during the forging route. However, the underlying recrystallization mechanisms during the final thermomechanical treatment of the Ti-10-2-3 alloy remain poorly understood due to the simultaneous occurrence of multiple phenomena during the annealing above the beta transus temperature step. At this temperature, the dissolution of the alpha phase occurs. Concurrently, several mechanisms related to the release of stored energy take place, including strain-induced boundary migration, continuous and discontinuous recrystallization, grain coarsening, substructure misorientation evolution, and heteroepitaxial recrystallization. The forging paths are highly complex, and among the important parameters influencing the beta phase are the temperature and deformation rate, as well as the amount of local deformation, which is directly responsible for the amount of stored mechanical energy. The latter is a key value as it constitutes the essential driving force behind the recrystallization phenomena. The use of forged double truncated cones is particularly advantageous for investigating local deformation and the activation of stored energy release mechanisms. This geometry provides access to a wide range of deformation levels due to its shape, while eliminating the influence of deformation temperature, strain-rate and chemical variation parameters—all of which impact as well the selection of mechanisms. Sampling specific areas on the forged double truncated cones allowed for precise determination of the deformation levels in the sampled materials. EBSD mapping was performed to observe the morphological evolution as a function of local deformation levels and post-processing temperatures. Finally, the competition between the different recrystallization mechanisms is discussed as a function of the quantity of mechanical energy stored in the microstructure during the processing path.

Characterization of microstructure in bent Al-Mg-Si-Cu alloys and their correlation to crack development at high and low quench rate

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

Al-Mg-Si-Cu alloys are widely utilized in automotive applications due to their excellent formability and mechanical properties. However, during bending processes, material failure can occur in the form of cracks, the development of which is strongly influenced by the microstructural features and the quench rate. This study investigates the microstructural characteristics and grain boundary precipitates that contribute to crack development. To explore these phenomena, laboratory samples were produced and subjected to high and low quench rates after solution heat treatment, with subsequent bending until failure and ex situ analysis in the scanning electron microscope (SEM). This enabled a systematic evaluation of the correlation between microstructure, bending angle, and quench rate.

Using advanced electron backscatter diffraction (EBSD) combined with conventional SEM, a geometrical transformation method was applied to precisely correlate EBSD data with SEM secondary electron (SE) and backscattered electron (BSE) images. This integrated approach facilitated a detailed microstructural analysis and allowed a clear allocation of features, such as precipitates, in relation to grains or grain boundaries. Additionally, it provided a robust means to distinguish between transgranular and intergranular fracture, an aspect of studying crack development that is often challenging with conventional BSE imaging due to insufficient grain contrast, especially in highly strained materials.

In the bend tests, the high quench rate material successfully achieved the full bending angle before failure, whereas the low quench rate material failed at a significantly lower bending angle. Experimental observations revealed intergranular fracture as the dominant failure mechanism in the low quench rate material, indicating weakened grain boundaries. Further analysis using energy dispersive X-ray spectroscopy (EDX) identified the presence of needle-shaped Q-phase grain boundary precipitates in the low quench rate material, which appeared to play a critical role in crack development. These precipitates exhibited mechanical degradation, forming pores under strain during bending. This pore formation, coupled with mechanical stress, explains the grain boundary weakening leading to intergranular crack propagation. In contrast, the high quench rate material exhibited no Q-phase precipitates at the grain boundaries, correlating to improved resistance to crack formation during bending and thus explaining the difference in bend angle.

This study highlights how microstructural features might be correlated with mechanical performance in aluminium alloys. By employing the geometrical transformation technique for EBSD-SEM data alignment, critical insights into the interplay between grain boundary precipitates and crack development were obtained.

The use of High Temperature Profilometry-based Indentation Plastometry (HT-PIP) for the Rapid Characterisation of High Temperature Alloys

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B7_9, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 14:30 - 16:30

Profilometry-based indentation plastometry (PIP) is a technique that enables the rapid characterisation of the stress-strain curve of a material. It combines experimental readings of the residual profile from indentation testing and an iterative inverse FE model to extract plasticity characteristics, such as yield stress and work hardening rates, more rapidly than tensile testing.

A recently developed hot stage now allows PIP to be performed at temperatures up to 800°C. The low thermal inertia of this stage and small material volume requirements offers advantages in terms of minimising heating times and time at temperature. The effects of oxidation and oxygen uptake are monitored for several alloys. The short time at high temperatures has prevented the formation of oxides thick enough to change the indent profile significantly.

A wide range of materials - including steels, nickel superalloys, aluminium, tungsten, niobium and copper – have been tested. Results across the materials spectrum are aligned with high temperature tensile testing in cases where the mechanical behaviour is not significantly affected by creep.

This advancement should enable high-throughput, high temperature mechanical testing, offering a faster and more efficient alternative to conventional methods.

Experimental and numerical study of the interaction of a Zinc based alloy with Stainless Steel 430

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B7_13, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 17:00 - 19:00

The ATRUIM reactor design, a loop-type Sodium-cooled Fast Reactor (SFR), stems for the necessity of enhanced safety for the next generation of nuclear reactors. One of the key feature of this concept, introduced to meet the required safety standards, is the design of a compact and passive Decay Heat Removal System (DHRS). This component is tasked with storing the excess heat from the nuclear core during an emergency shut down, operating without external intervention and electricity for multiple days. To ensure the system's compactness, the design choice fell onto a modular storage, where the metallic Phase Change Material (PCM) selected to store the excess thermal heat, Zamak (Zn-4%Al), is encapsulated in multiple SS430 boxes.

In working condition, the encapsulated Zamak will first interact mechanically with the walls of the box, then it will undergo phase change (i.e. melting), that will lead to thermochemical reactions. This study requires the characterization of the intrinsic properties of the individual materials and their interaction behaviour as it may modify the thermal response of the system. Thermal properties are acquired by Differential Scanning Calorimetry (DSC, Netzsch Jupiter F3). For the thermochemical interactions between Zamak and SS430, an experimental setup is developed to study their wetting behaviour. Small samples of Zamak set on SS430 plates are placed inside a tubular furnace (Nabertherm RHTH 120/600/17). The temperature inside the furnace is brought over melting temperature at 450°C in a N₂ atmosphere. A different behaviour is observed when the surface of Zamak is left untreated compared to when it is cleaned with 37% HCl; the untreated Zamak does not adhere to the SS430, a phenomenon that is observed when the surface oxide is chemically removed. We simultaneously develop a numerical model (STAR-CCM+, Siemens) representative of the melting behavior experimentally observed. The experimental and numerical data are utilized to accurately represent the materials and the effects of their interactions.

To further explore the thermal behavior of the modular storage system, an experimental setup for the elementary unit box (15x15x25 cm) is developed. The box is filled with an ingot of Zamak and heated on one side. A reciprocal CFD numerical model is defined to include the heat transfer mechanisms and the phase change behavior. Experimentally, IR thermography is used to measure the temperature distribution on the external surface. The dynamic of this temperature field coupled with numerical simulations will be used to identify the thermal evolution of the system.

In-situ synchrotron X-ray diffraction study on the deformation mechanisms of advanced steels under various load paths from cryogenic to high temperatures

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B7_2, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 10:50 - 13:10

In-situ synchrotron x-ray diffraction was applied to investigate the mechanical and microstructural responses of advanced steels such as TWinning Induced Plasticity (TWIP) steel and Quenching and Partitioning (Q&P980) steel under monotonic uniaxial tensile and cyclic loading-unloading from 173 K to 523 K. It is well known that in fcc materials the temperature-dependent stacking fault energy (SFE) dictates the prevailing deformation mode such as dislocation sliding (i.e., $SFE > 45 \text{ mJm}^{-2}$), twinning (i.e., $SFE \approx 18\text{-}45 \text{ mJm}^{-2}$) and fcc-austenite to hcp/bct-martensite transformation (i.e., $SFE < 18 \text{ mJm}^{-2}$) [1-3]. Despite the well documented studies on deformation under uniaxial tension, this work aims to address the deformation behaviour in these materials under complex thermomechanical conditions, which is critical in predicting and controlling microstructure for engineering alloys.

The diffraction peak profile convolutes microstructural parameters such as stacking faults, twinning, and dislocations [4]. The deviation of lattice strains of successive grain families in fcc phase indicates stacking fault. Diffraction peak profile analysis was carried out to calculate the SFE based on stacking fault probability and mean-square strain. The dislocation density and character (edge/screw) was determined based on the modified Williamson-Hall method, taking into account the effect of stacking faults and twinning. The twin fault probability was drawn from peak asymmetry parameters (Lorentzian and Gaussian peak width of left and right side). Transformation was tracked by evaluating the phase specific integrated intensity. Coupled with in-situ texture analysis via Rietveld refinement of the 2D diffraction images and post-mortem EBSD, the temperature and load paths dependent deformation behaviour is interpreted in terms of phase specific planar faults, dislocation glide and reversal, twinning and detwinning, transformation and their synergistic activities.

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Evaluation of Springback Prediction of the 980MPa High Strength Steel Sheet Using a Yield Function with a Hardening Model

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The ongoing need for vehicle weight reduction and safety improvement results in many challenges in selecting and replacing automotive materials. Advanced high strength steel(AHSS) remain one of most common materials in automotive applications due to its continuous property improvement. In spite of their major advantage, large springback is one of major drawbacks of AHSS sheets. As a way to overcome such a drawback, the computational method is utilized in the design stage for the proper analysis of spring-back in the forming process.

In the current study, springback of 980MPa high strength steel sheet was numerically evaluated for U-bending and S-rail component using a yield function with a hardening model. For springback prediction, two types of yield functions - Hill'48 and Yld2000-2d - were considered. Additionally, isotropic hardening and the Yoshida-Uemori model were used to investigate the springback behavior. The parameters for each model were obtained from uniaxial tension, uniaxial tension-compression, uniaxial tension-unloading and hydraulic bulging tests. The numerical simulations were performed using the commercial software, AUTOFORM. The results were compared with experimental data from a U-bending and S-rail component stamping process.

Secondary Grain Boundary Dislocations Modulate Segregation Energy Spectra in Fe-W Alloys

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B7_8, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 10:30 - 13:10

Grain boundaries (GBs) are key sites for structure-specific chemical segregation of solute atoms. While traditionally defined as planar defects, GBs inherently exhibit curvature due to the three-dimensional (3D) topology of grains, necessitating the formation of secondary grain boundary dislocations (sGBDs). In this study, we demonstrate that these topologically necessary sGBDs have a significant impact on segregation energy spectra, often surpassing the effects of defect-free GBs. Using advanced nanoscale correlative tomography, which integrates crystallographic and chemical analysis, we establish a direct quantitative relationship between sGBDs and segregation energy in a model Fe-W alloy. Our findings introduce an additional degree of freedom for tailoring segregation behavior, presenting new opportunities for microstructural engineering and the development of next-generation materials.

Characterization of the fracture toughness of material interfaces

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B7_10, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 17:00 - 19:00

The study of fracture modes is essential for the characterization of fracture toughness of material interfaces, whether adhesive or chemical. This work presents a methodology for the experimental measurement of fracture modes. The experimental setup includes standardized mechanical testing procedures, such as double cantilever beam (DCB) and end-notched flexure (ENF) tests, to quantify mode I and mode II fracture toughness, respectively. Additionally, specimens have been designed whose constitutive laws facilitate the characterization of the mechanical properties of the interface. Furthermore, the study incorporates a numerical correlation that enables the validation of experimental results through finite element analysis (FEA). The numerical simulations employ cohesive zone models (CZM) based on the traction-separation law.

Kinetic degradation determination of the Ion Exchange Resins used as a solid-active media for dry-electropolishing applications

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B7_4, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 17:00 - 19:00

The increasing use of ion exchange resins in the industry presents the need to determine the main mechanism of loss of efficacy for dry-electropolishing applications. Ion exchange resins for the polishing process of titanium alloys are used to study the effectivity reduction in terms of surface quality and therefore reduce the polishing cycles. Two different resins will be employed, one new (considered as a reference) and the other after reaching the end-life (around 100 hours of dry-electropolishing). Along the process, the electrochemical activity of the solid particles decreases, due to several factors; as: moisture retention, saturation of the ionic exchange points, closure of the porosity due to Joule's effect, among others.

The main goal behind this study, is to evaluate the degradation process of cationic-based ion exchange resins to highlight the chemical, physical and thermal properties along the life-time of the electrolyte. Furthermore, the functional groups evolution as well as the mean decomposition temperature of the solid/liquid part of the ion exchange resins investigated will be characterized by using Fourier Transformed Infrared (FT-IR), thermogravimetric analysis, and Time-of-Flight Secondary Ion Mass Spectrometry respectively. Finally, the microstructure of the ionic exchange porosity will be evaluated by means of scanning electron microscopy.

To conclude, after the dry-electropolishing process is possible to appreciate, a reduction of the acid and water content filled in the internal porosity due to the Joule's effect induced during the dry-electropolishing process. The dehydration process presents two different rates: (1) high-dehydration rate induced during the initial dry-electropolishing process mainly attributed to the local temperature change near the surface of the resin and (2) at lower dehydration rates, mainly attribution to a diffusion process of the liquid media, from the central to external part of the resin. These hypotheses agree with the O-H groups present in the FT-IR spectra.

DURABILITY TESTING OF NEXT-GENERATION MATERIALS FOR SOLAR REFLECTORS

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B7_4, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 17:00 - 19:00

The global transition toward more sustainable energy solutions has driven exciting innovations in solar reflector production. Manufacturers are moving away from traditional materials like copper and lead, opting instead for more environmentally friendly alternatives. At the same time, there is growing interest in using glass with higher impurity levels to reduce production costs and enhance the competitiveness of concentrating solar thermal (CST) technology compared to photovoltaics. These new materials haven't been studied yet, especially when it comes to how well they perform optically or how durable they are in real-outdoor exposure conditions. The long-term performance of solar reflectors for CST systems is closely related to the interplay between their material structure (comprising the chemical composition and layer stack) and the environmental factors they are exposed to.

In this study, several different silvered-glass solar reflectors were evaluated, including state-of-the-art samples and several advanced materials combining copper-free samples with varying silver layer thicknesses, enhanced lead-free back protective paints and innovative front glass layers (with different impurity levels). These specimens underwent accelerated aging tests, in addition to outdoor exposure at several global locations, to assess the degradation of their optical properties over time. The accelerated aging test selected in this experimental campaign was the UV radiation exposure in a controlled UV chamber, since it is the most representative for analyzing the potential degradation of this type of novel materials.

The results showed that the initial optical properties of all the materials studied are equivalent, with the maximum difference in solar hemispherical reflectance being less than 0.1 percentage points. This suggests that the use of an innovative silver layer allows the removal of the copper layer without affecting significantly the initial optical performance of the reflector material. However, the composition of the glass layer directly influences the initial reflectance, with a maximum decrease of 0.5 percentage points observed in samples containing higher impurity levels. Additionally, materials with thinner silver layers showed a decrease in solar hemispherical reflectance over time, primarily due to tarnishing (a surface deterioration of the silver layer that impacts reflectance across the visible and near-infrared spectra).

These results emphasize the need for a comprehensive approach to the design of the new generation of solar reflectors, balancing optical efficiency, durability, sustainability, and cost, highlighting the critical role of both material composition and environmental factors in ensuring long-term performance.

Influence of the Pt addition on the primary microstructure of heat-resistant Ni-based superalloy for aerospace applications

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B7_9, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 14:30 - 16:30

Single crystal (SX) Ni-based superalloys are currently utilized in civil and military aeroengines at temperatures up to 1100–1150°C. This is due to their excellent combination of environmental resistance to corrosion and oxidation, along with superior mechanical properties, particularly under creep conditions. A distinguishing characteristic of Ni-based superalloys is the high volume fraction of γ' precipitates, which remains stable up to 1000 °C. However, their strength diminishes rapidly beyond 1000 °C, primarily due to a reduction in precipitate volume fraction, accelerated diffusion rates, and directional coarsening. To develop Ni-based superalloys capable of maintaining microstructural stability at operating temperatures of approximately 1150–1200 °C, it is essential to explore new compositional domains. The intermetallic γ' phase is key in strengthening the γ matrix and its chemical composition, distribution, morphology, size and volume fraction determine the stability of turbine blades during service.

In this work, the SX Ni-based superalloy René N5 (Ni-7.0Cr-8.0Co-2.0Mo-3.0Re-5.0W-6.2Al-7.0Ta-0.2Hf) has been subjected to chemical composition modifications with platinum (Pt). Observations and analyses of five variants were carried out using thermodynamic simulations, differential scanning calorimetry (DSC), X-ray diffraction (XRD), light microscopy (LM), scanning electron microscopy (SEM), and X-ray spectroscopy (EDX). Thermodynamical simulations showed that the Pt addition effectively influences the stability of γ' and increases its volume fraction. Pt is partitioning mainly in the γ' not γ matrix. Microstructure of produced castings characterized by a typical dendritic structure with a dominant amount of cubic-like intermetallic γ' phase.

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Effects of specimen geometry and tensile testing system on the ductility and stability of ausferrite

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B7_3, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 14:30 - 16:30

Ausferrite is a metallic matrix consisting of Widmānstatten acicular microstructure of bainitic ferrite and metastable austenite rich in C. In ductile irons, where graphite nodules are imbedded, it results from the two-step industrial heat treatment of austempering, coming into a first step of austenitization at high temperatures for high carbon austenite, followed by quenching in salt bath for an isothermal austempering transformation to produce proper ausferrite, and a final slow cooling to room temperature. The resulting Austempered Ductile Irons (ADIs) have outstanding physical and mechanical properties, with excellent strength-to-density ratio, and so ADIs are valid substitutes to steel castings and forgings in many weight-saving transportation applications with considerable cost and CO₂ production benefits, like in heavy trucks, military, railroad and agricultural applications. However, the main concern in the use of ADIs, is the stability of ausferrite, as during loading the metastable austenite may transform into martensite causing rupture. So, the assessment of the stability of ausferrite in industrial thin-walled ADI components is paramount, but, first of all, it is needed to assess the eventual sensitivity of ausferrite ductility and stability to the tensile specimen geometry and the tensile testing system. So, different tensile specimen geometries (round and 2 mm flat with different gauge geometries) have been tested with different gripping systems to investigate the ductility and stability of ADIs. A procedure based on the tensile strain hardening analysis has been implemented to assess the stability of ausferrite, and microstructure investigations have been carried out through Scanning Electron Microscopy and XRD measurements, while Digital Image Correlation (DIC) technique and Finite Element Modeling (FEM) have been used to investigate the local plastic behavior of ADI with different specimen geometries and gripping systems.

Residual Stress Analysis for Aluminum Cast Alloys

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B7_8, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 10:30 - 13:10

The measurement of residual stresses in aluminum castings is a challenging task due to the coarse grain microstructure. The small number of large grains that can be analyzed is a limiting factor for X-ray based analysis methods such as the $\sin^2(\psi)$ method. In addition, if the microstructure is too coarse, it can be difficult to interpret the results from the drilling method.

To address this challenge, in the present work we use a wrought alloy with comparatively small grains and produce parts with similar geometry to the cast part. The heat treatment process of the wrought alloy is analogous to that of the cast alloy, involving solution annealing followed by water quenching and subsequent artificial aging. During the quenching process, residual stresses are induced which are subsequently relieved during aging. Accurate knowledge of the material behavior during all stages of heat treatment is critical to predicting the residual stress state. The microstructural state of the alloy is analyzed metallographically, and the mechanical behavior of the material is characterized using a dilatometer.

In addition to the experimental characterization, a state parameter based material subroutine called Simple-MSE is employed in a finite element simulation, which takes into account the temperature and strain rate dependent mechanical properties of the material. The subroutine is implemented in ANSYS-Mechanical. To verify the simulated results, the residual stresses of the wrought alloy parts are measured using the hole-drilling method and the $\sin^2(\psi)$ method. The results of both methods are compared with the simulation and the advantages and challenges are discussed.

Microstructure evolution of alloy 625 subjected to concentrated solar radiation at 600°C

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B7_7, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 17:00 - 19:00

Solar thermal systems concentrate sunlight by directing it with adjustable mirrors towards a solar receiver. This receiver absorbs the intense solar radiation, transforms it in thermal energy and transfer it to the heat-transfer fluid (such as water/steam, molten salts, liquid sodium, or air) that flows through it, causing the fluid's temperature to rise. In central tower setups, the solar receivers, predominantly made of nickel-based superalloys with tubular shape, experience challenging working conditions due to solar radiation intensities exceeding 1MW/m² and operational temperatures nearing 1000°C. The receivers are not exposed to steady temperatures; rather, they face daily cycles of heating and cooling because of the inherent variability of solar radiation. These cycles become more frequent on cloudy days, as cloud cover can intermittently block the sunlight.

This study presents the initial results of a comparison of the aging processes in one of the most commonly used alloys for manufacturing tube-type high concentration solar receivers, i.e. alloy 625. A set of flat specimens, 20mm square and 0.8mm thick each, made of alloy 625, was aged at 600°C constant temperature in a muffle furnace during different times to study the effect of thermal radiation in the alloy microstructure evolution. Simultaneously, a second set of samples with an identical design was exposed to concentrated solar radiation in a solar furnace to compare the aging when this material is selected for solar thermal applications. The microstructure evolution was characterised by optical and electron microscopies after preparing the metallographic sections of the specimens. Vickers micro-hardness tests were also used to follow the possible evolution of the mechanical properties.

The results indicate that concentrated solar radiation (CSR) significantly impacts both the rate and nature of alloy 625 aging at 600°C. On the one hand, with only 13h of CSR treatment, an increase in hardness equivalent to 30 hours of isothermal treatment has been observed, which is equivalent to an aging rate of more than double when using this alloy with CSR. On the other hand, the shape and grain size of the phase producing this hardening is different, suggesting an onset of δ phase formation with RSC rather than the γ'' phase that forms in isotherm treatment. The abundance of intermetallic precipitates at the interface between grains and in the grains themselves suggests that RSC accelerates the aging of about 8 times with respect to the isothermal case.

Damage and delamination behaviour of oxide scale layers

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B7_10, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 17:00 - 19:00

In hot bulk forming processes of steel, oxide scale layers are formed in dependence of the occurring process conditions. As remaining oxide scale can weaken the formed workpiece, it has to be removed at the end of the process. Through this, the oxide scale formation can lead to a mass loss of up to 3 % in addition to influencing the forming process for example by affecting the friction conditions or increasing the die wear [1]. However, oxide scale layers can protect against further oxidation and limit the mass loss as long as they are not damaged, for example through cracks [2]. For the precise numerical description of a forming process using a finite element simulation, it is therefore necessary to model the formation and damage behaviour of the oxide layer. This paper presents a characterisation and modelling approach to describe the damage behaviour depending on the process conditions as well as the alloy composition.

Procedure

The properties and layer structure of the oxide scale was characterised through nanoindentation. The damage behaviour was investigated by means of compression and tensile tests with oxidated specimens. The tests were carried out at varying oxidation and testing conditions such as the forming temperature or strain rate. In addition, the occurring oxide layers and their properties for multiple steel alloys, with different contents of carbon and chromium, were compared.

The experimental data was used to develop a numerical modelling approach for finite element simulations. A mesh splitting algorithm was applied to describe the damage behaviour of the oxide scale layers in forming processes through the occurring stresses.

Key findings

- The damage behaviour of oxide scale layers is dependent of the oxidation parameters, the occurring stresses and the particular alloy contents of chromium and carbon.
- Oxide scale failure can be modelled in dependence of the process parameters and stress state using a mesh splitting algorithm.

Keywords: Oxide scale layers, Nanoindentation, FEM, Tensile test

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Design and assessment of Si enriched innovative alloys resistant to liquid lead corrosion

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 17, 2025, 13:10 - 14:30

The growing need for decarbonized and sovereign energy has renewed interest in nuclear energy, and particularly in advanced reactors designs. Among them, Lead-cooled Fast Reactors (LFRs) offer many advantages. However, their implementation requires the development of high-performance materials combining ductility, mechanical strength, creep and corrosion resistance in high-temperature liquid lead. These requirements can be contradictory. For instance, Ni-rich alloys exhibit excellent mechanical properties, but Ni has a high solubility in liquid lead. To address these challenges, research efforts have focused on protective coatings development and innovative material solutions. Among them, Alumina-Forming Austenitic Steels (AFA) have been proposed for their ability to form protective alumina layers in high-temperature oxidizing environments. Despite these progresses, alternative strategies are still underexplored.

Literature suggests that addition of silicon to stainless steels improve their resistance to liquid lead corrosion. Silicon promotes the formation of silica, a very stable oxide in liquid lead. From a long-term perspective, Silica Forming Austenitic steels (SiFa), which are not widely explored yet, represent a promising solution for structural elements in LFRs. This study aims to evaluate the potential of silicon-enriched austenitic steels for structural applications in LFRs. Two reference alloys, the Russian EP302M-sh and a high-Ni alloy, were selected as a base for comparison. Using these references, new compositions have been designed through thermodynamic calculations with Thermo-Calc. The design strategy is to stabilize a silica layer on the surface while maintaining a microstructure and mechanical properties close to those of the reference alloys.

Several alloys have been cast by cold crucible melting and their microstructures have been optimized (grain size, presence of secondary phases). The coherence between thermodynamic predictions and experimental results have been systematically verified to ensure the reliability of the alloy design. The mechanical behavior has been evaluated through hardness and compressions tests. In addition, oxidation tests revealed the presence of Si-rich oxides for some alloys.

Microstructural and mechanical characterization of PBF-LB 316L by neutron and synchrotron diffraction

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B7_6, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 14:30 - 16:30

Additive manufacturing (AM) technologies offer a great opportunity for spaceflight by saving materials, and lowering transport weight. In particular, Laser-based Powder Bed Fusion (PBF-LB) is one of the most versatile AM technologies due to its ability to produce complex geometries and its adaptability to a wide range of materials. In this work, a microgravity-compatible system using PBF-LB was designed to meet environmental requirements in space, such as resisting the dynamic loads and vibrations during rocket launch and stabilizing the powder in microgravity. This study focuses on the microstructural and mechanical properties of 316L parts produced in the printer-designed device. The printing strategy considered a single-pass cylindrical wall with an external diameter of 30 mm and a thickness of 1 mm. The region of interest lies in the initial layers, from the base plate to the printed material, due to the high RS expected there. Samples were printed with heights 3 and 10 mm to analyze the impact of RS distribution with time and build height. The microstructure was analyzed by x-ray diffraction during printing in the DiffAbs beamline at SOLEIL (Paris, France). The set-up considered a lateral resolution of 250 μm and an exposure time of 5 s/acquisition. Results disclosed the dynamic evolution of the lattice parameter of the γ matrix and precipitating phases such as ferrite (α). Regarding stress analyses, neutron diffraction was carried out on SALSA strain diffractometer at ILL (Grenoble, France). In this case, the lateral resolution is higher than 0.01 mm and acquisition required 3 c/s, proving enough to disclose RS gradients and enhance a full tensor analysis. Note that for the first time worldwide, the printer and SALSA set-ups allow in-situ monitoring in the BD direction of samples thanks to the tailored baseplate powder suction system. The evolution of γ matrix and in particular the Fe(311). Initial ex-situ tests were conducted for preparation of in-situ monitoring experiments: the first involved rotation of the baseplate to simulate the movement during printing meaning averaging one build height condition, and the second was static meaning just one single point acquisition in build height and radial positions. The results disclosed similar RS values between static and dynamic conditions (compare statistics/count times for both conditions). For the three strain components, the longitudinal and radial directions displayed a similar trend (-1000 $\mu\epsilon$), while the hoop direction exhibited different behavior, from 1000 $\mu\epsilon$ on the surface to -1000 $\mu\epsilon$ in the cylinder.

Tensile deformation behavior of CoNi-based single crystal superalloys at different temperatures

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B7_9, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 14:30 - 16:30

γ' -strengthened Co-based superalloys have been considered as the candidate for high-temperature applications due to their analogous $\gamma+\gamma'$ configuration and higher melting temperature compared to the widely used Ni-based superalloys. Moreover, the compositions have been optimized into CoNi-based superalloys to obtain good comprehensive properties, such as microstructural stability and environmental resistance. To further enhance the mechanical property of CoNi-based superalloys, a high-Cr CoNi-based single crystal was developed, and its tensile deformation performance at different temperatures was investigated by analyzing the featured deformation substructures and their elemental segregation. The 0.2 % yield strength initially decreases up to 650 °C. Subsequently, the yield strength anomalously increases at 760 °C before abruptly dropping off at higher temperatures. At 760 °C, the deformation behavior is characterized by continuous strain hardening with increased plastic strain. The plastic deformation is initially dominated by forming anti-phase boundary (APB)-coupled dislocation pair shearing γ' precipitates. With the increase of strain, the leading partial dislocations of stacking faults (SFs) shear γ' precipitates. Subsequently, the interactions of SFs further enhance the deformation resistance due to the formation of sessile stair-rod dislocation and coherent SF interfaces preventing further expansion of other SFs. Different from 760 °C, with the increase of temperature, the flow stress decreases first and increases with the increasing strain during the yield process. The initial decrease of flow stress is mainly ascribed to the formation of SFs inside the γ' precipitates. A similar strengthening mechanism of SF interactions was observed for the increase of flow stress. Interestingly, APB-related complex deformation substructures, such as APB-SF, were also observed up to a strain of 2%, and its interaction with SFs is responsible for the further strain hardening process. The Co and Cr segregation at SF was investigated to be associated with the formation of APB-related complex deformation substructures. In addition, a comparison of the deformation mechanism was made among the Co-Al-W, CoNi and Ni-based single crystal superalloys to further understand the strengthening mechanism of γ' -strengthened superalloys, which is also meaningful for enhancing the mechanical properties of CoNi-based superalloys.

Influence of heat-treatment-induced microstructural evolution on the low-cycle fatigue behavior of 316L stainless steel fabricated by laser powder bed fusion

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B7_2, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 10:50 - 13:10

Additive manufacturing, particularly the laser powder bed fusion (PBF-LB/M) process, has gained significant attention in recent years due to its ability to produce complex geometries with enhanced mechanical properties. Among the various materials used, 316L stainless steel (SS) is highly favored for cyclically loaded components due to its exceptional mechanical strength, high-temperature performance, and corrosion resistance, making it widely applicable across various industries. 316L SS fabricated by PBF-LB/M (PBF-LB/M/316L) exhibits a unique hierarchical microstructure, with high density of low-angle grain boundaries (LAGBs), nano-dispersed silicates, chemical micro-segregations, and solidification-induced cellular structures. Particularly, the submicron-sized cellular walls that enriched with chromium (Cr) and molybdenum (Mo), along with high dislocation densities, contribute to a superior strength-ductility balance compared to conventionally manufactured 316L SS. The dispersed silicate particles act also as a strengthening phase, impeding dislocation movement and enhancing plastic deformation resistance.

This study explores the effect of heat treatments on the low-cycle fatigue (LCF) behavior of PBF-LB/M/316L at room temperature (RT) and 600 °C. First, three heat treatments were applied to the as-built material: 450 °C for 4 hours (HT450/4), 800 °C for 3 hours (HT800/3), and 900 °C for 1 hour (HT900/1) to investigate their influence on microstructural evolution. Microstructural analysis revealed that the HT450/4 condition preserved the cellular structure with high dislocation density, while the HT800/3 condition showed partial dissolution of cells together with reduction in both segregated elements along the cell walls and dislocation density. The HT900/1 condition resulted in complete segregation and cellular structure dissolution with comparable dislocation density to HT800/3 while maintaining the crystallographic texture and grain morphology. Intermetallic χ phase was mostly observed at the grain boundaries in HT800/3, but not in HT900/1. Fully reversed LCF tests were conducted under strain-controlled conditions with a strain amplitude of 0.8 %. Tests were interrupted at specific intervals to analyze the interaction between hierarchical microstructural features and deformation mechanisms in the three heat-treated conditions. Due to the pronounced dislocation cell structures and elemental segregation, the microstructure of the HT450/4 condition significantly impacts deformation and damage mechanisms during cyclic loading, which in turn, differ from the conventionally produced counterparts. The results provide insights into the relationship between microstructural features and fatigue performance, highlighting key deformation and failure mechanisms under cyclic loading. A comparative analysis with conventionally manufactured 316L SS is also made. These findings help optimize post-processing strategies to enhance the structural integrity of additively manufactured components.

Effect of the tempering on microstructure development and mechanical properties of bainite in a 42CrMo4 steel

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B7_5, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 10:30 - 13:10

Medium- and large-sized forged steel components are usually subjected to additional Q&T (Quenching and Tempering) heat treatments to achieve the required final mechanical properties (MP). The tempering conditions are of special interest as MP can be accomplished by its fine control. Additionally, depending on the dimensions of the component, its chemical composition and quenching conditions, different microstructures are developed from the surface to the core, that behave differently with the tempering conditions. Traditionally, the tempering treatment aim to improve the outer martensitic layer mechanical performance in terms of toughness and to produce additional stress relief due to quenching. However, due to the volumetric character of the heat treatment, not only the hardened martensitic layer is affected, but also deeper regions in the forged parts. In the case of 42CrMo4 (4140) steel, widely used as a forging steel grade, the region just below hardened layer is chiefly made up of bainite. The effect of tempering on its microstructure evolution and MP has drawn less attention than in martensite.

In the present work, two heat treatment strategies have been undertaken in a dilatometer to create bainitic microstructures: bainitic quenching (BQ) and anisothermal cooling paths, which simulates the thermal profile at several positions in a large-sized cylindrical specimen quenched in water. The BQ temperatures have been chosen in the region of bainite and some prior martensite formation, whereas tempering temperatures have been set at 480 °C and 640 °C for 1h. A thorough microstructure (optical, FEG-SEM and X-ray) and hardness characterizations have been performed.

The experimental results have shown that bainite may lead to a wide range of mechanical properties and microstructures, which are controlled by the specific complete thermal cycle (Q&T). Specifically, tempering conditions have been proven to affect the microstructure development and hardness in different manner depending on the nature of the bainite formed on the previous quenching step.

In-situ time resolved synchrotron X-ray imaging and tomography at Diamond I12-JEEP

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B7_1, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 9:20 - 10:20

The high energy (50-150keV) synchrotron beamline I12-JEEP has the capability to install a variety of large and complex user-supplied equipment in support of the study of materials processing and testing in-situ. Experiments under high pressure, elevated temperature or in full mechanical testing machines use radiography, tomography and diffraction to observe the behaviour of materials during processing and testing at the micron-to-millimeter scale and subsecond to multi-seconds time scales.

Radiography at millisecond timescale is used to observe the behaviour of the active zone during additive manufacturing ; the development of porosity and the flow of fluid in the liquid pool under various conditions as well as ejection of material and other defect forming behaviours.

Tomography on the scale of seconds or several seconds reveals the growth behaviour of crystals from liquid of complex mixtures, alloys or natural geological materials under the pressure found in magma chambers.

Large tomography of samples held in a 100kn mechanical testing machine allows the internal observation of damage accumulation in metals or civil engineering materials.

Combined synchrotron diffraction and imaging studies elucidate the processes occurring in the multiple phases present in such materials

Correlated Analysis with a Nanomechanical Microscope

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B7_5, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 10:30 - 13:10

Correlated Analysis with a Nanomechanical Microscope

When nano-indentation and AFM experiments are done at separate instruments, the spatial correlation of the data from the two methods is an inherent problem. We solved this problem by integrating a standard Alemnis nanoindenter, a new very compact dedicated AFM-scanner employing cantilever with integrated strain sensors [1] and an optical USB-microscope into the measurement head (200x200x200mm³). The distance between nanoindenter and AFM cantilever tip is 20mm. Their position relative to the sample is secured by a patented reference procedure.

This means that this new table-top instrument allows to switch between the 2 methods back and forth to investigate the area of interest by either of the two methods – real-time: The operator can decide on the sequence of indentation, scratch or imaging experiments at different point(s) of interest (PoI) on one sample: real interactive correlated analysis.

WE will report the data from the following experiments:

- Indents on thin Cu-, Al and Ni-films with Berkovich nanoindenters:
 - o Subsequent to higher force (<100mN) indents, indents with much lower forces (5mN) were made precisely into the contour ridge of the previous bigger indent. This was possible by the sub-micron positioning accuracy of various indents relative to each other combined with nm-resolution AFM topography. By comparing the force-distance curves from such small indents with indents of equal force in the surrounding film we determined the difference in hardness very accurately and concresolved strain hardening effects. .
- Investigation of hardness-effects on multilayer organic solar cells :
 - o A series of indents through the sandwich structure at certain positions and depths were performed - with subsequent AFM imaging @ nm resolution –
- Analysis of nano-crystals embedded in electro-chemically plated 300nm-thick Cu-films:
 - o Nanometer sized Copper-nuclei were located via AFM and subsequently directly probed by indents with different forces. Hence, direct probing of nanoparticles has been achieved by the 100nm-positioning accuracy and the nm-resolution of the AFM-topography image.

The extension of the AFM functionality with KPFM and c-AFM modes is in progress.

References

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High-Throughput Mapping of Dislocation Recovery in Low-Carbon Graded Alloys via In Situ HEXRD

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B7_1, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 9:20 - 10:20

Alloy design requires exploring a wide parameter space where both composition and processing routes dictate the resulting microstructure and material properties. To streamline this process, a high-throughput methodology, termed COMPASS, has been developed by the SIMaP laboratory of Grenoble INP. This approach integrates space- and time-resolved High-Energy X-ray Diffraction (HEXRD) with in situ thermal processing in a continuously translating sample environment, creating graded samples that facilitate space-resolved diffraction and enabling rapid mapping of microstructure evolution kinetics over various heat treatment conditions.

The aim of the present work is to determine the influence of substitutional solutes on dislocation recovery in low carbon steels. For this purpose, we investigate low-carbon steels with graded molybdenum, manganese and silicon compositions to understand their recovery behavior under thermal treatments following a cold rolling step. A dedicated furnace, designed by researchers at the Institut Jean Lamour (IJL) and operated at ID31, enables real-time tracking of dislocation density through modified Williamson–Hall and modified Warren–Averbach methods. By synchronizing continuous sample translation with fast data acquisition (10 Hz), the methodology provides an efficient route to quantify the dislocation density evolution as a function of local composition and temperature.

Preliminary results confirm that the in situ measurements successfully capture how solute additions slow down the recovery kinetics across compositional gradients. The ability to monitor dislocation structures in real time reveals how subtle variations in molybdenum content influence recovery kinetics. This integrated approach offers a significant advance over traditional ex situ techniques, reducing experimental timescales and preserving critical transient states that often go undetected in post-mortem analyses.

Overall, this new methodology opens the door to a more comprehensive understanding of alloy behavior by linking compositional variations to microstructural evolution in real time. The insights gained will serve as valuable input for refining computational models of material behavior and guiding the design of next-generation alloys with optimized properties.

Advanced Correlative Characterization of a Gas-Nitrided 42CrMo4 Steel: Insights into Gradient Microstructure and Mechanical Properties

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B7_7, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 17:00 - 19:00

Gas nitriding is a widely used thermo-chemical surface modification process to enhance the hardness, wear resistance and fatigue strength of steels. In this process, a gradual modification of the base material is created by nitrogen diffusion. Additionally, a ceramic compound layer can form at its surface, which consists of iron nitrides. While the formation and process parameter correlation of this layer had been intensively studied by research groups worldwide, there is still a lack of knowledge of its mechanical properties and residual stress distribution with high spatial resolution. These results are critical for increased simulation accuracy and industrial design efficiency.

In this study, a gas-nitrided 42CrMo4 steel was comprehensively analyzed using correlative techniques to elucidate gradients in phase composition, microstructure, mechanical properties, and residual stresses at micro- and nanoscales. Cross-sectional X-ray micro- and nanodiffraction (CSmicroXRD, CSnanoXRD) experiments were performed in transmission diffraction geometry at the High-Energy Materials Science beamline HEMS at PETRAIII in Hamburg and at the ESRF in Grenoble, respectively, the latter achieving spatial resolutions below 500 nm. The synchrotron results were correlated with optical and scanning electron microscopy, microhardness profiling, nanoindentation and micromechanical cantilever bending tests.

CSmicroXRD revealed a compressive residual stress profile with a peak of -192 MPa at 100 μm depth, which could be correlated with the depth of nitrogen diffusion in the martensitic base material. The diffusion induced broadening of the XRD peaks extending to 169 μm . This is consistent with results from energy dispersive X-ray spectroscopy and microhardness data. CSnanoXRD showed that tensile stresses within the porous ϵ -nitride Fe_{2-3}N layer (approximately 3 μm thick) relax at the γ' -nitride (Fe_4N) interface. In the γ' -nitride, comprising an additional 3 μm , maximal tensile stresses of 500 MPa were determined, which further relaxed into the martensitic base material.

Micro-cantilever bending tests of the γ' -nitride revealed a Young's modulus of 158 ± 18 GPa and a fracture toughness of 1.8 ± 0.2 MPa·m^{0.5}. In addition, mechanical properties were also determined by nanoindentation. This method yielded Young's moduli of 201 ± 8 and 142 ± 6 GPa for the γ' -nitride and ϵ -nitride, respectively. The higher Young's moduli determined by nanoindentation experiments compared to micro-cantilever tests can be attributed to the different scales, measurement regions, and specific test conditions of each technique.

This study demonstrates the power of advanced correlative characterization to deepen the understanding of gradient materials and provides deeper insights for optimizing material performance in industrial applications.

Advancements and Challenges in Automated Non-Destructive Testing: AI-Driven Techniques, Emerging Trends and Future Directions

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B7_12, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 14:30 - 16:30

Non-Destructive Testing (NDT) is essential for ensuring the structural integrity and reliability of critical components in industries such as aerospace, automotive, electronics, and energy. The growing need for precision, repeatability, and efficiency has driven the adoption of automated NDT techniques, which leverage advanced imaging, sensors, and AI-driven analysis to improve defect detection and characterization. This paper provides a comprehensive review of key automated NDT methods, including Automated X-ray Inspection (AXI), Automated Ultrasonic Testing (AUT), Automated Optical Inspection (AOI), Acoustic Emission Testing (AET), Eddy Current Testing (ECT), and Infrared Thermography (IRT). While these methods offer significant advantages in terms of speed, accuracy, and scalability, challenges remain in standardization, reliability assessment, and the mitigation of false positives and negatives.

A critical evaluation of these techniques is presented, highlighting their strengths, limitations, and areas where AI and machine learning can further enhance defect detection and classification. The paper also examines the integration of real-time monitoring, digital twin technology, and hybrid NDT approaches as emerging trends that could address current gaps in reliability and uncertainty quantification. Additionally, industry adoption challenges, regulatory compliance, and the need for improved Probability of Detection (POD) metrics are discussed. The findings emphasize that while automation has revolutionized NDT, further advancements in AI-driven analytics, sensor fusion, and adaptive algorithms are necessary to achieve higher accuracy and broader applicability across industries.

The potential of Scanning Microelectrochemical Techniques to monitor chemical activity across surface layers and coatings on metals

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B7_10, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 17:00 - 19:00

Advanced methodologies for protection against material degradation aim at the design, development and synthesis of new materials and characterization procedures operating at the micro and submicrometer scale of complex microstructures. Environmentally induced degradation of a material involves chemical reactions initiated at the micrometer and submicrometer scales. On the other hand, the choice of protection strategies for a specific surface depends on a judicious choice of surface layers and coatings as well as active molecules (such as corrosion inhibitors). Unfortunately, very often the limiting step for the development of effective functionalized anticorrosion coating systems is the lack of information on the local dissolution rate as a function of physicochemical characteristics, such as pH, aggressive ion concentrations and dissolved oxygen for a given metal/coating system, as to properly design the triggering condition for the smart release of active protective agents from the functionalized material. Therefore, to properly design and fabricate a functionalized surface layer or coating suitable for a certain metal-environment combination, it will be necessary to address information on the chemical changes occurring in the corroding substrate, and the actual surface protection mechanism at the micrometer scale in situ, that is, at finer levels of spatial resolution and time scales that can facilitate advances in lifetime prediction compared to conventional macroscale corrosion monitoring strategies.

The recent application of new characterization techniques based on electrochemically sensitive scanning probe methodologies, which are an extension of local probe techniques originating from the use of microelectrodes as probes in near-field microscopic techniques to operate inside a small electrochemical cell, has found potentially-broad applicability in Corrosion Science. Among them, scanning electrochemical microscopy (SECM) takes advantage of the successful combination of chemical and/or electrochemical selectivities provided by microelectrode probes with the fine spatial resolution of the scanning microscopies to probe reaction dynamics in the complex environments and microstructures of alloys and composite materials, creating new opportunities to explore the design of materials and tailored corrosion protection methods (including inhibitors, coatings and smart materials) and to achieve a link between micrometer- and submicrometer-level processes and macroscopic behaviors.

In this work we report our new advances in the monitoring of the chemical reactivities of surface layers and coatings applied on metal substrates exposed to humid environments by using scanning microelectrochemical techniques in situ with spatial resolution.

A case study of polymeric capsule failure in cold thermal energy storage applications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Cold thermal energy storage (CTES) technologies are used in applications that need to keep the temperature below ambient temperature, even near or below 0 °C, such as refrigeration and freezing systems. These are especially important in cooling using solar energy, in order to maintain the thermal energy needs during cloudy conditions and the night. For that reason, they are considered a key point for the necessary transition to renewable energies in the near future [1]. One of the most studied CTES systems is based on encapsulated phase change materials (EPCMs) inside a tank through which the heat transfer fluid circulates. Capsules are usually made of a polymeric material, and must withstand the pressure of the fluid, and possible volume changes of the phase change material during the phase transition.

Within the European COOLSPACES4LIFE project we are developing a solar-powered air conditioning system, to be installed in the CIESOL building at the University of Almeria, which includes a new prototype of CTES system with EPCMs [2]. Commercial EPCMs with the appropriate properties for this installation have been purchased and they have been tested in a pilot tank. Some of these capsules have not withstood the operating conditions and have broken, causing the PCM to mix with the heat transfer fluid. This failure can seriously affect the operation of the whole facility if it occurs in the CIESOL installation.

In this work we studied the mechanical resistance of this commercial EPCM by subjecting it to the working conditions of the pilot tank, with thermal cycles between 25 and -10 °C, external pressures in the order of 1 bar and heat transfer fluid flow rates of about 4 L/min. Both, thermomechanical fatigue experiments and simulations using the computer-aided design software SolidWorks and its finite element analysis module (SolidWorks Simulation), were carried out to identify the causes of the failure and be able to propose solutions to improve the design and manufacture of new capsules. Cracks will be studied with advanced material characterisation techniques. Preliminary results in the pilot tank show all broken capsules developed a crack between 2 and 8 cm long, which always started in the same point and propagated in the same direction, which indicate that the failure will be due to a manufacturing defect detected in that area.

[1] L. Yang, et al. Applied Energy 288 (2021) 116555

[2] <https://www.coolspaces4life.com/en/>

Advanced Characterization of Coating Microstructure for CERN Future Circular Collider

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B7_2, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 10:50 - 13:10

The Future Circular Collider (FCC) study aims to advance next-generation, high-performance particle colliders and accelerating structures, with a focus on optimizing the performance of Superconducting Radio Frequency (SRF) cavities. These cavities, typically made of niobium (Nb), operate at superconducting temperatures (below 2 K), enabling highly efficient energy transfer with minimal RF losses.

At CERN, research on Nb-coated, copper-based cavities with thin-film deposition techniques such as diode sputtering and DC-Magnetron Sputtering (DC-MS) were successfully developed and implemented in projects like LEP-II, LHC, and HIE-ISOLDE. These methods demonstrated enhanced RF performance by reducing residual surface resistance while also lowering costs. However, for future accelerators, further understanding of the effects of deposition parameters on the microstructural and mechanical properties of these coatings remains essential to optimize their RF performance.

The study utilizes state-of-the-art preparation and characterization techniques to thoroughly evaluate the microstructural features and stress states of Nb films deposited on Cu via bipolar High Power Impulse Magnetron Sputtering (HiPIMS). Large cross-sectional views were prepared using laser-focused ion beam (FIB) technology, while characterization was carried out through Scanning Electron Microscopy (SEM) and Scanning Transmission Electron Microscopy (STEM). Additionally, advanced diffraction techniques such as Electron Backscatter Diffraction (EBSD) and Grazing Incidence X-Ray Diffraction (GI-XRD) were employed for dislocation density evaluation, texture analysis, and residual stress assessment.

This comprehensive approach facilitates the selection of optimal deposition parameters, enabling the development of high-quality coatings with controlled microstructural and mechanical properties. Consequently, it enhances the efficiency and performance of Nb-coated, copper-based SRF cavities. The findings of this study will contribute to cost-effective designs, which are essential for large-scale accelerators like those envisioned at CERN, while also advancing thin-film coating applications in related fields.

Role of precipitates on deformation processes in Al alloys

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B7_1, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 9:20 - 10:20

Advanced high-strength Aluminum alloys owe their mechanical properties to microstructure, typically consisting of aluminum matrix and strengthening secondary particles. The size distribution, volume fraction and number density as well as the type of secondary particles determine the nature of the particle-dislocation interactions and, thus, resulting properties of the alloys. The present study aims to describe the role of different precipitate types upon uniaxial plastic deformation in wrought Al alloys. Modern Al-Cu-Li alloy was subjected to various heat treatment regimes, resulting in different microstructures with various types of strengthening particles. The five series of specimens strengthened with GP zones, θ' , T1 were prepared and subjected to the incremental uniaxial tensile loading while employing digital image correlation (DIC) and various electron microscopy techniques to follow precipitating particles – dislocations interactions and overall dislocation slip character. The results help to understand the role of different precipitate types on dislocation slip character and allow to establish a more accurate prediction of contribution to mechanical properties from certain type of particles.

Adhesion properties of carbide-rich nano-coatings produced by ion irradiation

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B7_10, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 17:00 - 19:00

The good adhesion of coatings to the substrate is essentially important in various applications e.g.: catalysis, protective coatings etc. By applying ion irradiation, it is possible to improve the adhesion of coatings due to the ion mixing of coating to the substrate. Herein, carbide-rich nano-layers are formed by means of noble gas irradiation. Various multilayer structures (C/Mo and C/W with individual layer thicknesses of 10-20 nm) on a silicon substrate were irradiated by argon and xenon ions with energy in the range of 40-120 keV and fluences between $0.25-1 \times 10^{16}$ ions/cm². At the interfaces molybdenum-carbide and tungsten-carbide were formed. The carbide in-depth distributions have been detected by XPS depth profiling [1]. The adhesion of the coating has been tested by ramped load scratch test in a nanoindenter with a spheroconical diamond tip. The critical loads for the coating delamination were obtained from the optical microscopic images of the individual scratches. Depending on the irradiation conditions the adhesion of the coatings has been increased. The structural changes along the scratches were investigated extensively by cross-sectional transmission electron microscope. Serious changes were observed (amorphization, crystallization) in the coating and the silicon substrate due to scratching.

[1] A.S. Racz, M. Menyhard XPS depth profiling of nano-layers by a novel trial-and-error evaluation procedure Sci. Rep. 14, 18497, 2024

Effect of selective laser remelting on microstructure and tensile properties of 304L stainless steel processed by laser powder bed fusion

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B7_6, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 14:30 - 16:30

Laser powder bed fusion presents a processing technology for fabricating slender and complex components of variable sizes. Although the technology has great potential, multiple challenges and uncertainties lie in the consistency of the process. For instance, optimized processing parameters, usually verified on small test cubes, may be unsuitable for the fabrication of significantly larger bodies. Such process discrepancies can lead to lower overall build quality, for instance, extensive porosity. In this study, we investigated the effect of an additional laser scanning sequence, remelting, on microstructure character and tensile properties at ambient and decreased temperatures. The study demonstrates that remelting has a distinctively beneficial effect on inherited porosity without dramatic changes in other microstructural characteristics. Moreover, remelted microstructure exhibits more reliable mechanical properties. The results suggest a possible application of remelting during the LPBF process of complex-shaped components to maintain a nearly defect-free microstructure.

Study on microscale strain localization and slip activity in ferrite-carbides steel: An integrated study of SEM-DIC and crystal plasticity modeling

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B7_12, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 14:30 - 16:30

This work investigates microscale strain localization and slip activity in ferritic AISI 420 stainless steel using an integrated approach of scanning electron microscopy-based digital image correlation (SEM-DIC), electron backscatter diffraction (EBSD) and crystal plasticity (CP) modeling. The microstructure, consisting of ferritic grains with finely dispersed carbides, exhibits early strain localization that intensifies under increasing global strain, ultimately forming interconnected shear bands. Statistical analyses indicate that localized deformation does not arise from any single microstructural parameter—such as grain size, grain boundary misorientation, maximum Schmid factor, or carbides' effect—but rather from an interplay of constraints. Specifically, poor geometrical alignment of slip transfer at misaligned grain boundaries, constrained slip paths between ferrite grain boundaries and carbides, and limited accommodation in smaller grains collectively promote strain localization. The CP model, enhanced by a realistic representative volume element (RVE) that incorporates nanoscale carbides, reveals local stress heterogeneities and clarifies slip transfer/blocking behavior. To enhance the identification of active slip systems, a new accumulated shear methodology integrates loading history, overcoming the transient limitations of velocity-gradient-based methods. Collectively, these findings underscore the role of microstructural incompatibilities in driving strain localization and point to strategies—such as optimizing grain boundary alignment, refining annealing processes to minimize the formation of small grains, and promoting a more dispersed distribution of carbides—to improve formability in ferritic steels.

Precipitation evolution in FeNbVC microalloyed steels during welding

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B7_13, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 17:00 - 19:00

This study explores the precipitation of (Nb,V)C carbides in microalloyed steels during welding and stress relief heat treatment (SRHT) of nuclear power plant secondary circuit pipes. A focus is made on how the heat history influences the mechanical properties of the material through particle size distribution evolution. This research investigates the effect of thermal cycles and alloying elements (Nb and V) on the nucleation and growth of precipitates within the Heat-Affected Zone (HAZ). Four model steel alloys (without Nb and V, with Nb, with V, with both) are studied and a thermomechanical simulator is used to reproduce welding cycles and SRHT. The chemistry and the distribution of precipitates are characterised using electron microscopy. Hardness and Charpy impact tests are performed to assess the link between precipitation and mechanical properties. Simultaneously, a KWN model [1] is developed to simulate the evolution of the precipitation distribution at each point of the HAZ, during welding and SRHT, incorporating classic nucleation and growth theories (CNGTs). This study provides valuable insights that emphasise the link between thermal cycles, precipitation and mechanical properties. In particular, far from the weld, precipitates do not evolve; in the opposite, near the weld, they are completely dissolved. However, in the sub-critical HAZ (just below Ac1), precipitates can grow up and be one of the causes of the ductility drop observed at these distances.

[1] Wagner R, Kampmann R, Voorhees PW. Homogeneous Second-Phase Precipitation. In: Kostorz G, editor. Phase Transform. Mater., John Wiley & Sons, Ltd; 2001, p. 309–407.

Simulation of Steel Plate Response undergoing Differential Cooling with Air and Water Impinging Jets

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B7_5, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 10:30 - 13:10

Differential cooling is widely used in the automotive industry to tailor the microstructure and the mechanical properties in thin-walled beams through tool or spray quenching. However, thicker steel plates, such as those used in soil-working agricultural tools, typically require high hardness and are conventionally quenched by immersion in water. While this ensures strength, it does not account for the spatial variation of mechanical loads that these tools experience in service. By implementing differential cooling, it is possible to engineer hardness gradients that optimize both wear resistance and structural integrity.

This study explores the use of Impinging Jet Quenching Technique (IJQT) to achieve differential cooling of 15 mm-thick carbon steel plates by employing different water and air jet flow rates. The cooling process was monitored using embedded thermocouples, generating spatial and temporal temperature evolution data, which was then utilized in finite element simulations to predict phase transformations and final hardness gradients. The simulation framework enables extrapolation to other steel grades, using their chemical composition as an input parameter to a machine learning tool for phase transformation data generation, making the methodology adaptable for various industrial applications. The experimental trials produced a wide range of cooling rates (0–43 °C/s) along the steel plate, depending on the quenching strategy and cooling medium. The simulated phase transformations revealed distinct hardness distributions across three steel grades with different hardenability levels (0.26, 0.27, and 0.38 mass-% C). The results showed that higher-hardenability steels retained a greater proportion of martensite, whereas lower-hardenability steels exhibited increased bainite, ferrite, and pearlite fractions, particularly in the slower cooling regions. The results clearly show how different steels react on different cooling medium and flow rates in terms of hardness profile variations along a potential component. Furthermore, it was found that differential air cooling could, in some cases, replicate the effects of slower water quenching, providing an alternative method for controlled microstructure tailoring.

These findings highlight the potential of IJQT as a flexible and scalable approach for achieving site-specific material properties in thick steel components. The demonstrated simulative and experimental approach opens new possibilities for enhancing the durability of steel components exposed to variable mechanical loads, offering an efficient means to optimize hardness distributions through controlled cooling strategies.

In situ DSC of homogenization in 6xxx aluminium alloys

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B7_5, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 10:30 - 13:10

6xxx-series aluminum alloys are widely used in automotive and construction industries due to their low weight, recyclability, and excellent mechanical properties. The homogenization heat treatment plays a critical role in optimizing these alloys for subsequent hot forming (e.g., rolling or extrusion) by influencing dispersoid precipitation and the dissolution and re-precipitation of Mg-Si phases. However, common experimental methods for studying these phenomena are time- and labor-intensive. In this study, we employ in situ differential scanning calorimetry (DSC) to analyze the homogenization behaviour of three 6xxx aluminum alloys under varying soak temperatures and cooling rates. The resulting heating and cooling curves provide insights into phase transformations, dispersoid number density, and Mg-Si-phase evolution, supported by microstructural investigations using scanning electron microscopy (SEM) and transmission electron microscopy (TEM). Our findings show that soak temperature has the most significant impact on microstructural changes, while cooling rate variations within an industrially relevant range have a lesser effect. This study demonstrates that in situ DSC is a rapid, cost-effective tool for optimizing homogenization parameters, reducing the need for extensive furnace trials, and enhancing alloy performance in industrial applications.

Wire-arc directed deposition of Ti-6Al-2Sn-4Zr-2Mo: insights on mechanical behavior and high temperature creep dynamics

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B7_9, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 14:30 - 16:30

Ti-6Al-2Sn-4Zr-2Mo (wt.%) was developed in the late 1960s as a high-temperature alloy, known for its excellent tensile and creep strength, with long-term service capability at temperatures up to 425°C. It is widely used in aerospace applications, including compressor blades, impellers, and engine exhaust nozzle structures. Despite its established role in industry, its application in wire-arc directed energy deposition (waDED) has remained largely unexplored. To date, only one study has examined Ti-6242 in this context, focusing on microstructural details and dissimilar alloy bonding. The present study investigates the feasibility of processing Ti-6242 using cold metal transfer-based waDED. Deposited samples were heat-treated following industry recommendations and mechanically tested. Room-temperature mechanical properties were evaluated through hardness measurements and tensile testing, while high-temperature behaviour was assessed using full-scale tensile creep tests under varying temperatures and constant loads. After a two-stage heat-treatment, a solution heat treatment at 955°C for one hour and aging at 650°C for eight hours (both cooled to room temperature using air cooling), the deposited material, achieved a yield strength of 922.01 ± 22.4 MPa, 1023.1 ± 16.8 MPa ultimate strength and an elongation to fracture of 7.3 ± 1.8 %. The microstructures of the deformed and crept samples were further characterized using scanning electron microscopy and electron backscatter diffraction to evaluate the deformation mechanisms under different loading modes and temperatures. The results demonstrate that, despite its limited prior exploration, this process is capable to produce Ti-6242 samples with mechanical properties that meet industry standards. These findings provide a basis for expanding the use of the wire-arc DED process for high-temperature alloy applications.

Development of curve smoothing systems for a more accurate and automated Ball-on-Disc test analysis

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B7_5, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 10:30 - 13:10

The Ball-on-disc (BoD) test is the most employed for the study of wear. Various factors influence the signal obtained during friction tests. In addition to material-related factors, sample alignment, equipment accuracy, sampling frequency, and transitions between wear mechanisms can introduce noise and fluctuations in the recorded coefficient of friction (CoF), complicating precise value determination, particularly during the steady-state phase but also in the early stages. In some cases, the average coefficient of friction during equilibrium may not be accurately defined, which is particularly relevant when comparing samples with very similar friction values. These variations can impact the interpretation of wear rates and other tribological phenomena and the evaluation of materials for final uses.

This study presents a smoothing method designed to improve result accuracy in the study of CoF curves. The selected method applies Nyquist's criterion for setting the correct sampling frequency to prevent aliasing, ensuring proper signal capture and processing. This technique is compared against ten other filtering techniques, including Gaussian, Butterworth, Savitzky-Golay, to evaluate the best balance between reducing noise and preserving essential signal features.

The results show that applying the moving average filter improves the precision of the friction coefficient values and reveals delicate but significant phenomena that may otherwise remain undetected. Also, some transient events such as delamination, adhesion, or microstructural changes during the wear become more apparent after applying appropriate smoothing. These phenomena are crucial for understanding wear mechanisms, especially in materials with complex microstructures or new alloy formulations.

Additionally, the comparative analysis demonstrates that different methods may be more suitable depending on the characteristics of the signal depending on tested materials. While the moving average method is effective in reducing high-frequency noise and providing clear trends, methods like Butterworth or Gaussian filtering may be optimal for preserving signal fidelity when necessary.

In conclusion, implementing a suitable smoothing method, enhances the reliability of friction test data, allowing for a more accurate interpretation of tribological behaviour. This approach not only improves the precision of coefficient of friction measurements but also enables a better understanding of key wear mechanisms that might otherwise remain undetected.

The study has been performed in a new patented multi-phase aluminium alloy and the AlSi9Cu3 cast alloy.

Small-specimen methods for extreme temperature and plastic strain rate material characterisation

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B7_3, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 14:30 - 16:30

Material processes like fusion and friction welding expose materials to extreme conditions, requiring detailed characterisation of properties such as high-temperature conductivity and plastic flow behaviour for accurate finite element modelling [1,2]. The integration of novel small-specimen testing, co-simulation FE methodologies, and high-temperature DIC has demonstrated an effective approach for determining high-temperature material properties with reduced uncertainty. The research presented here introduces small-specimen testing methodologies and co-simulation techniques designed to optimise experimental setups for high-temperature material characterisation. Building upon prior research conducted to establish temperature fields through material emissivity and optimised speckle patterns using high-speed digital thermography [3,4], this research integrates these methodologies with small-specimen tests to characterise material properties under extreme conditions. A coupled electromagnetic-thermomechanical simulation is developed to optimise both the specimen geometry and experimental setup, ensuring accurate strain field capture while minimising uncertainties such as electromagnetic noise and thermal gradient variations. The simulation results are validated against experimental digital image correlation data to ensure accuracy. The experimental and simulation results reveal that the proposed setup reliably captures complex plastic strain fields and thermal gradients under extreme conditions. These findings contribute to more accurate constitutive models for high-temperature materials, which are critical for simulating processes such as friction welding in finite element models. The methodology provides a robust framework for advancing material characterisation techniques at high temperatures, with potential applications in manufacturing processes requiring precise plastic flow and residual stress predictions.

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Uncertainty quantification of composite failure

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

The failure of composite materials is a complex phenomenon, but one which must be understood by engineers during the design process in order to generate an optimised design solution. A major challenge when designing large scale composite structures, notably those utilised in the aerospace sector, is the uncertainty associated with mechanical simulation models (finite element models, for example) which are used to drive the design process. Model solutions are typically generated using low fidelity representations due to the scale of the assemblies. Such practices yield expedient results however key quantities of interest, particularly at failure “hot spots”, may be subject to relatively large levels of uncertainty. This paper considers the challenge of interpreting uncertainty within low fidelity finite element models of composite materials. A goal orientated error estimator is implemented in a finite element model of a reference carbon fibre reinforced plastic component. This allows for a quantifiable error field in the stress field to be developed. These stress value distributions are then used to compute a range of composite failure potentials, with confidence bounds of the failure metrics quantified and the most likely failure mode suggested. The combination of the discretisation error estimated from the goal orientated error estimator alongside the error in the composite failure metrics are then compared with empirical data from fibre reinforced composite tests, demonstrating the failure of the falls within the range computed by the error estimator scheme. This work is conducted with the intention of expanding this methodology onto large composite aerospace structures, allowing for the design engineer to iterate during the design concept phase at low computational expense.

Low temperature Peltier-based nanoindentation setup for in-situ measurements in SEM

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The mechanical properties of materials at subzero temperatures are critical for various applications in aerospace, electronics, and polar engineering. However, conventional cryogenic nanoindentation systems face limitations in achieving precise thermal control and integration with in situ measurement setups. We present a novel Peltier-based nanoindentation system, designed for in situ testing within a scanning electron microscope (SEM), offering a compact, vibration-free, and energy-efficient alternative to the traditional liquid nitrogen cooling method at low temperatures, which often requires bulky liquid-based cooling systems and introduce mechanical instabilities through bubbling in the system.

Using a multistage Peltier cooler integrated into an in situ micro/nanomechanical testing platform (Alemnis AG), for the first time, the system achieves stable subzero temperatures down to -30 °C. Key innovations besides using the Peltier cooler include detachable sample and indenter holders, efficient thermal management via copper braids, a PTFE clamping mechanism, and an optimized heat sink design to maximize cooling efficiency while ensuring mechanical stability. A glycol-water circulating system is used to dissipate heat effectively while a graphite pad is applied on the interface between the heat sink and Peltier cooler, preventing overheating of the Peltier element and maintaining long-term stability. To ensure precise temperature monitoring, Type K thermocouples are strategically placed near the indenter tip and sample, providing real-time temperature readings and enabling fine control during experiments. The integration of precision heating elements behind the sample and indenter tip allows fine temperature control via a PID controller, minimizing thermal drift to fluctuations within ± 0.05 K. Unlike nitrogen cooling systems, this setup eliminates the need for specialized tubing inside the SEM, reducing system complexity and potential thermal instabilities. Additionally, avoiding liquid nitrogen lowers operational costs, as Peltier cooling does not require continuous refilling and offers more controlled and localized cooling compared to cryogenic fluids.

Initial characterization and thermal performance assessments demonstrate rapid cooling times (10–15 minutes) and effective stabilization (over hours) of temperature down to -30 °C for long-duration nanoindentation experiments. Next steps will include performing indentation tests on reference samples, like fused silica or single-crystalline copper. Future work aims to expand the system's applications by investigating water ice micro-mechanics, a key challenge in glaciology, planetary science and cryo-engineering, as well as other materials where traditional cryogenic systems that reach -150°C or lower are unnecessary but precise low-temperature control is already sufficient.

Uncertainty quantification and validation for centre hole-drilling residual stress measurement: A combined finite element and experimental framework for enhanced reliability in advanced materials

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

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Residual stress assessment is critical for ensuring structural integrity in aerospace, automotive, and energy applications. The hole-drilling method, standardized in ASTM E837 [1], is widely used in industry but its accuracy is limited by uncertainties in calibration coefficients linked to geometric parameters, material properties, and drilling conditions. While ASTM E837 provides a foundational framework, it does not address error propagation from material properties or tooling variability, which this study quantifies. Our work employs finite element analysis in ABAQUS to investigate these uncertainties, focusing on isotropic materials such as steel. A 3D model simulates incremental drilling using the model change function, removing material in discrete steps. A parameterized python script automates variations in hole diameter, material properties (such as Young's modulus and Poisson's ratio), and drilling increments, enabling strain computation based on these parameters.

This computational strategy bridges experimental and numerical approaches, offering a scalable platform for isotropic/anisotropic materials and complex geometries. Automated parametric scripting enhances calibration reliability, addressing manual system limitations. By isolating hole size, step increments, and material isotropy effects, the methodology in our study provides actionable guidelines to reduce measurement bias. These findings improve the confidence in residual stress evaluation for safety-critical applications like welded aerospace components, where precise stress quantification reduces premature failure risks.

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Micromechanical study of the influence of ion irradiation on the mechanical properties of anodized Al6061-T6 alloy

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B7_12, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 14:30 - 16:30

In the nuclear industry, materials are subjected to extreme environments, including high radiation flux, elevated temperatures, and corrosive conditions. Ensuring the durability and mechanical integrity of protective coatings is essential for the long-term performance of critical components. Anodized alumina coatings are widely used for their corrosion resistance and mechanical properties, but their behavior under irradiation remains insufficiently understood. Ion irradiation can induce structural modifications, affect mechanical strength, and alter residual stress distribution. Understanding these effects is crucial for optimizing materials intended for nuclear applications. This study investigates the micromechanical response of an alumina-based anodized layer subjected to silicon ion irradiation, providing insights into its potential durability in radiation-intensive environments.

A hard anodized layer with an average thickness of $49.1 \pm 1.9 \mu\text{m}$ was developed on an Al6061-T6 alloy through anodization in oxalic acid, followed by sealing in boiling water. SEM and TEM analyses revealed a U-shaped columnar structure in the longitudinal cross-section, while the top surface exhibited a flaky and/or gel-like morphology. X-ray diffraction and TEM confirmed the anodized layer was amorphous.

Silicon ion irradiation, performed at energies from 3.5 MeV to 0.5 MeV, resulted in a damage dose estimated between 6 and 7 dpa up to $\sim 2 \mu\text{m}$ depth. This irradiation also led to Si implantation within the anodized layer at $\sim 0.6 \text{ at.}\%$. Post-irradiation microscopic examination revealed curled or rolled surface features on the exposed top layer, while the irradiated zone exhibited a smoother texture. Despite irradiation, the affected region remained amorphous.

To assess irradiation effects on mechanical properties, in situ micropillar compression and splitting tests were conducted using SEM. These tests enabled direct comparison of plasticity and fracture toughness between non-irradiated and irradiated layers. Micropillar compression experiments demonstrated irradiation-induced hardening of $\sim 30\%$, with a plastic flow stress of $\sim 3 \text{ GPa}$. Fracture toughness (K_{IC}) measurements from micropillar splitting indicated this property remained unchanged after irradiation, with $K_{\text{IC}} \approx 2.2 \text{ MPa}\sqrt{\text{m}}$.

By testing over a dozen micropillars with different geometric shape factors, unrelaxed compressive residual stresses of $\sim 1 \text{ GPa}$ were measured in the irradiated layer. Finally, in situ observation of deformation and cracking mechanisms provides insights into the mechanical properties in relation to the previously characterized microstructure, contributing to a broader discussion on the impact of ion irradiation on anodized layers.

The Microstructure Evolution and Mechanical Response of Cold-Worked and Heat-Treated Heterostructured Materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Titanium alloys are widely used in aerospace due to their high strength and excellent corrosion resistance. One efficient way to improve the performance of titanium alloys is to increase the strength/specific strength further. Through traditional solid solution strengthening, precipitation strengthening, and fine-grained strengthening, material strength can be increased while sacrificing a certain degree of ductility. Heterostructured (HS) materials can alter their microstructure through heat treatment, forming heterogeneous regions composed of hard and soft zones. When HS materials undergo plastic deformation due to stress, geometrically necessary dislocations (GNDs) accumulate at the boundaries of heterogeneous regions, exhibiting a unique deformation mechanism that achieves both high strength and high ductility.

Based on these reasons, this research will adjust the heat treatment parameters of titanium alloys, which introduced GNDs by cyclic loading, to obtain a heterogeneous microstructure composed of different proportions of fine α phase (hard region) and coarse β phase (soft region). And investigate the impact of GNDs density accumulated in various microstructures on their mechanical properties.

Mechanical Testing at Elevated and Cryogenic Temperatures with Concurrent Acoustic Emission and Electrical Resistivity Monitoring

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B7_3, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 14:30 - 16:30

Understanding the deformation mechanisms of materials under extreme temperature conditions is crucial for their reliable application. This study presents an advanced mechanical testing methodology that integrates acoustic emission (AE) and electrical resistivity measurements during tensile loading at both elevated and cryogenic temperatures. The combination of AE and resistivity monitoring provides real-time insights into microstructural changes, and phase transformations. The results highlight the correlation between mechanical behavior, and defect evolution, offering a comprehensive approach to material characterization under non-ambient conditions.

Texture Evolution in Transforming and Twinning Materials: A Comparison of Neutron Diffraction and MTEX-Based Simulations

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The evolution of crystallographic texture during deformation plays a crucial role in defining the mechanical properties of materials, particularly those undergoing phase transformations or twinning. This study compares neutron diffraction experiments with MTEX simulations to analyze texture development under mechanical loading. By correlating experimental and simulated texture evolution, we assess the accuracy of modeling approaches in capturing grain reorientation, variant selection, and twinning behavior. The results provide insights into the microstructural mechanisms governing deformation in complex materials and highlight the predictive capabilities of computational methods.

Defect detection in composite materials with lab-based X-ray scattering

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B7_5, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 10:30 - 13:10

Glass fabric reinforced thermoplastics (GFRT) represent a promising class of composite materials ideal for automotive and similar applications due to their lightweight, ease of production, and favorable mechanical properties. Despite these advantages, defects can arise during the manufacturing process - particularly during the forming of prefabricated laminates - which can jeopardize the safety and longevity of the final components. Therefore, it is crucial to detect these defects and understand their formation for production monitoring and recycling. The latter is especially crucial as the safety of the to-be-recycled component necessitates information about fiber integrity and local distribution on the micrometer scale.

Various NDT techniques, such as ultrasonic imaging, X-ray computed tomography, and infrared thermography, have been investigated for the purpose of defect detection in GRFTs. Among these, laboratory-based X-ray scattering using the edge-illumination (EI) principle has shown promise for defect detection. The EI technique utilizes two line masks in the beam, one close to the sample and another close to the detector, in order to sense sub-pixel structural changes in the order of micrometers. The corresponding contrast is called scattering or dark-field contrast.

We have demonstrated the detection of local fiber shifts in GRFT samples with scattering EI in radiographic imaging, i.e. without the need for time consuming high resolution x-ray tomography [1]. Further, data analysis with EI is straight forward compared to potentially work intensive fiber segmentation in tomography. In addition, we will demonstrate the quantitative determination of projected fiber densities with EI. Both of these milestones have obvious applications in current composite materials research as well as in future production monitoring and recycling efforts. Finally, we demonstrate the high sensitivity of this approach by the ability to distinguish the protein networks in raw versus cooked egg yolk – for a bit of fun.

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3D strain heterogeneity and fracture studied by absorption and diffraction contrast X-ray tomography and crystal plasticity in an aluminium alloy

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B7_7, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 17:00 - 19:00

Strong correlations between measured strain fields and 3D crystal plasticity finite element (CPFE) predictions based on the real microstructure are found for a plane strain tensile specimen made of 6016 T4 aluminium alloy. This is achieved using multimodal X-ray lab tomography giving access to both the initial grain structure and the strain evolution. The real microstructure of the central region of interest (ROI) of the undeformed specimen is obtained non destructively using lab-based diffraction contrast tomography (DCT) and meshing. An in situ tensile test, using absorption contrast tomography (ACT) is then performed for twelve loading increments up to fracture. Taking advantage of the plane strain condition, the evolution of the internal strain field is measured by two-dimensional digital image correlation (DIC) in the material bulk using the natural speckle provided by intermetallic particles. Early strain heterogeneities in the form of slanted bands, that are spatially stable over time, are revealed and the fracture path – determined from the post mortem scan – is found to coincide with the bands exhibiting maximum strain. CP-FE simulations are performed on the meshed microstructure of the specimen acquired by DCT and are compared with image correlation measurements. The measured strain fields are well described by 3D CP-FE predictions, whilst it is shown that neither a macroscopic anisotropic plasticity model nor a CP-FE simulation with random grain orientations could reproduce the measurements.

Effect of Surface Defects and Oxide Layers from Different Stages during Hot Rolling on the Bendability of Martensitic Wear-resistant Steel

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B7_8, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 10:30 - 13:10

During hot rolling of steel, various defects are introduced on and below the surface of the steel strip. These defects will propagate and evolve through the different stages of the hot rolling process and may finally affect the material performance during subsequent manufacturing processes when components are produced. In forming operations, the bending behaviour of high-performance steel is critical to ensure an efficient and robust production process. Understanding the connection between surface defects and oxide layers and the bendability of high-performance steels is critical for forming process optimisation. The aim of this study is to investigate the surface/near surface defects and oxide layers for a high-performance martensitic wear-resistant steel at different stages of the hot rolling process (roughing mill, finishing mill, and after the final processing stage) and correlate these to the bendability. Pre- and post-bend test analysis was performed using scanning electron microscopy with energy dispersive spectroscopy, 3D white light interferometry, X-ray diffraction, and microhardness measurements. Friction free standard bend tests VDA 230 were conducted at a 90° bend angle with the bend axes parallel and perpendicular to the rolling direction. In general, the bendability of samples in levelled condition after finishing process is less compared to as-rolled condition. The results show that the formation of red scale between the steel substrate and primary oxides significantly affects the bendability of the martensitic wear-resistant steel in both as-rolled and levelled conditions. Red scale is a type of oxide rich in silicon called fayalite, which is formed during the hot rolling process and was found to be embedded non-homogeneously across the surface. Detailed characterisation indicated that crack initiation during bending was primarily concentrated at the red scale region. The presence of sub surface cracks parallel to the bend axis in this area further shows that presence of red scale negatively affect the formability. Abrasive wear grooves that are formed during the finishing process have also been found to affect the bendability.

Temperature and Grain-Size Dependence of Deformation Behavior in Commercial-Purity Titanium

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Thermo-mechanical treatments, including multi-directional forging and cold rolling, were employed to produce ultrafine-grained (UFGed) Grade 2 commercial-purity titanium sheets. A subset of these UFGed sheets underwent annealing under various conditions to prepare specimens with three distinct average grain sizes (0.07, 0.8 and 12 μm). These specimens were subjected to tensile tests both at room temperature (RT) and cryogenic temperature of 77 K. The deformation behaviors changed complicatedly depending on temperature and grain size. Regardless of grain size, all specimens exhibited significantly higher 0.2% proof stress, ultimate tensile stress and elongation to failure at 77 K compared to those at RT. Microstructural observations revealed that prismatic $\langle a \rangle$ slip was the primary deformation mechanism in all specimens, also with pyramidal $\langle c + a \rangle$ slip in the ones with grain sizes of 0.07 and 0.8 μm . Mechanical twinning in these specimens at RT was few. However, twinning, particularly $\{11\bar{2}2\} \langle 11\bar{2}3 \rangle$ compression twins, was considerably stimulated at 77 K. While twinning frequently occurred even at RT in the coarse-grained (12 μm) specimen, it was much more promoted at 77 K. It can be concluded, therefore, that uniform deformation caused by twinning-induced-plasticity effect largely contributed to the larger ductility at 77 K, improving the strength-ductility balance. These findings suggest that mechanical twinning, rather than slip activity, is the main factor influencing the temperature dependence of the mechanical properties in the CP-Ti specimens composed of different grain sizes.

Influence of the crystallographic orientation on the crystal rotation under tribological load

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B7_4, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 17:00 - 19:00

Tribological loading leads to a change in the microstructure of metallic materials, resulting in nucleation points for defects, ultimately resulting in wear particle formation and component failure. The sequentially first microstructural change is crystal rotation, followed by sub-grain formation. A fundamental understanding of these microstructural changes, which form the basis of the friction properties, is required to increase component life time and to design more efficient metallic materials employed in tribological contacts. It is known that the microstructure develops differently for different-orientated normal directions. In order to investigate this orientation dependence in more detail and to understand the influence of the crystallographic orientation parallel to the sliding direction, single trace tribological experiments were carried out on a copper single crystal with [110] normal direction. The sliding directions were systematically varied according to the following criteria: crystal symmetry and the reduction of activatable slip systems. For analyses, the topography of the wear track was measured, SEM images of the wear tracks and cross-sectional STEM images were taken. The crystal rotation was measured using EBSD and TKD. We found that sliding directions that create a mirror plane together with the normal direction result in symmetric material pile-ups on both sides of the wear track, whereas off-symmetry sliding directions result in asymmetric pile-ups. Slip steps form inside the wear track which can be assigned to the same crystallographic orientation in each experiment. The crystal rotation occurs in all cases around an axis perpendicular to the sliding and to the normal direction of the single crystal. The rotational misorientation increases towards the surface and is most pronounced directly underneath the sliding interface. In the microstructure, different features such as a grain boundary-like structure parallel to the surface or a more continuous transition to a higher misorientation are formed depending on the sliding direction. Our results are a first step towards a strategic texture engineering for tribologically loaded materials.

As-built microstructure characterization of thin walled laser wire directed energy deposited (LW-DED) AISI 316L with different process parameters

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B7_6, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 14:30 - 16:30

Laser wire directed energy deposition (LW-DED) is a versatile manufacturing method for relatively large structures. The relation between process, microstructure and mechanical properties has been described in detail in recent publications. However, these studies are typically limited to rather thick specimens where the surfaces have been machined prior to testing, in some cases after post annealing. Hence, there is a gap in understanding the mechanical properties of as-deposited thin walled structures without further machining and/or heat treatment. In this work, stainless steel AISI 316L wire was deposited with two different process parameter sets on a carbon steel substrate with a nominal wall thickness of 2 mm using a co-axial laser. The parameter sets were chosen to maintain approximately constant energy densities while simulating slow and fast production scenarios. The layer height in the fast scenario was twice that of the slow scenario. Specimens near the substrate and at mid-height of the deposited walls were characterized using metallographic methods such as LOM, SEM/EDS, EBSD and microhardness. The parameter sets resulted in surprisingly different microstructures despite the same energy density. The low layer height sample had, comparably, larger fraction of large grains in the centre but finer recrystallized grains at the surfaces. We explore the reasons for this difference through comparison of the solidification rate and the residual stresses during cooling and its influence on recrystallization. Furthermore, the carbon steel/stainless interface microstructure showed very little mixing for both parameter sets with some pores originating from the infill design. Surface waviness of the low layer height sample was also lower and had smoother valleys, indicating more flow during solidification. These differences in microstructure and surface topography are expected to have significant impact on fatigue properties due to possible notch effects.

Influence of the annealing parameters on the development of microstructure and porosity due to the Kirkendall effect in diffusion couples of Ni/Ni-based Superalloy CMSX-4

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B7_7, Federico García Lorca Auditorium (Level 0), septiembre 16, 2025, 17:00 - 19:00

Turbine blades are critical components in aircraft engines and landbased gas turbines because they operate at high temperature and load. These turbine blades therefore consist of thermo-mechanically highly resistant nickel-based superalloys. If they are exposed to high temperatures over a longer period of time and are connected to a material of a different composition, interdiffusion occurs. The diffusion couple technique is applied for the experimental investigation of interdiffusion. A diffusion couple of high-purity Nickel and the Nickel-based superalloy CMSX-4 was used here, which was joined by diffusion welding. CMSX-4 is a two-phase material with a γ/γ' microstructure directionally solidified with a uniform orientation. At high temperatures elements fluxes accompanied with vacancies flux across the Ni/ CMSX-4 diffusion welding interface take place. While the alloying elements of the CMSX-4 diffuse to the pure-Ni side, a reverse flux of Ni and vacancies to the CMSX-4 side occurs. From this follows a nucleation and evolution of porosity induced by Kirkendall effect in the CMSX-4 part near the joints interface. The issues of diffusion mobility of alloying element atoms and pore formation are of practical importance. So, it is relevant for welded and brazed joints of gas turbine blades, as well as the interface "blade material - protective coating". In the worst case this leads to failure of the material joint by separating of the both materials or by cyclic mechanical loading. Forming and evolution of the Kirkendall porosity depends strongly on the composition of the joined materials, crystallographic structure, annealing temperature, and annealing duration. The microstructure of three different diffusion couples, Ni/ CMSX-4 [001], Ni/ CMSX-4 [001]-HIPed and Ni/ CMSX-4 [111], exposed to three different temperatures (1200 °C, 1250 °C, 1300 °C) and three different time durations each, was investigated by synchrotron X-Ray radiation 3D μ -tomography (3D-XCT), optical and electron microscopy and energy dispersive spectroscopy (EDS). This provides a more information regarding the underlying complicated mechanisms of the void formation and evolution and a deeper insight into the kinetics of Kirkendall porosity, microstructural changes due to forming of topologically close pack (TCP) phase and dissolution of the γ' -phase. The obtained experimental 3D-XCT and EDS data are accompanied by phase-field and continuum simulations.

Microstructural and Mechanical Characterization of Ultra-Pure Aluminum for Low-Vibration Cryogenic Applications

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B7_4, Federico García Lorca Auditorium (Level 0), settembre 15, 2025, 17:00 - 19:00

Sensors operating below liquid helium temperatures are highly sensitive to vibrations, which can affect the sensitivity of high-performance particle detectors. Pulse Tube cryocoolers [1], while generating vibrations lower than those of conventional refrigerators, may still introduce disturbances in delicate applications [2]. Flexible thermal connections are commonly used to mitigate these effects [3].

In the present study, a comprehensive investigation was undertaken to characterize the mechanical and microstructural properties of three ultra-pure aluminium alloys intended for the fabrication of thermal links with low stiffness, specifically designed to reduce vibration transmission in cryogenic environments. Static mechanical behaviour was evaluated through detailed tensile tests, providing insights into yield strength, ultimate tensile strength, and ductility. Complementarily, dynamic elastic moduli were determined by measuring the natural resonance frequency, thereby assessing the alloys' response to vibrational loads [4]. Moreover, dynamic modulus measurements were extended to temperatures approaching those of liquid nitrogen, offering a deeper understanding of the temperature dependence of the elastic properties under conditions that closely simulate practical cryogenic applications. Concurrently, an extensive microstructural analysis was conducted using Electron Backscatter Diffraction (EBSD) and X-ray Diffraction (XRD). These techniques facilitated the development of detailed crystallographic texture maps and enabled the identification of specific preferential orientations within the material. The correlation between the observed microstructural features and the elastic properties was systematically examined [5]. The findings of this study underscore the pivotal role of microstructural characteristics in dictating the elastic behaviour of ultra-pure aluminium alloys. The integrated analysis advances the understanding of the fundamental relationships between microstructure and mechanical performance and provides valuable guidelines for optimizing materials employed in cryogenic systems, where stringent vibration control is critical for maintaining high operational performance.

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Advanced quenching of steels for controlled and improved properties

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B7_9, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 14:30 - 16:30

Proper and precisely controlled heat treatment of steel components can significantly enhance their mechanical properties. Processes like hardening of carbon steels or quench annealing of duplex stainless steels involve specific phase transformations that must be accurately controlled during quenching. The cooling rate directly influences the final microstructure of the steel, which in turn determines its mechanical properties. Improper cooling can lead to insufficient hardening, undesired residual stresses, or even cracks, resulting in premature failure of the component.

As the complexity of steel component geometries increases and the demand for tailored mechanical properties grows, traditional quenching methods often fall short. There is a need for advanced quenching techniques that can provide tailored or uniform and precise control over cooling rates and subsequently microstructures. These techniques must be adaptable to various component sizes and shapes, ensuring desired properties throughout the material.

One promising approach is the use of impinging jet quenching. This technique provides high quenching rates and the ability to create tailored microstructures within a single component. By varying parameters such as jet location, number, spacing, and flow rate, impinging jet quenching can be customized to meet the specific needs of different steel components.

This study investigates carbon steels and super duplex stainless steels (SDSS), focusing on creating microstructure gradients and optimizing mechanical properties using the Impinging Jet Quenching Technique (IJQT).

For steel with varied hardenability, the quenching process resulted in a transition from a fully martensitic state to a softer ferritic/bainitic condition. This gradient was confirmed through microscopy, tensile tests and hardness measurements. The steel with higher hardenability predominantly remained in a fully hardened martensitic state with slight ferritic and bainitic features. Temperature evolution during quenching was recorded and used to predict phase transformations, final hardness, and residual stresses, showing good correlation with experimental results.

For the SDSS results showed a consistent decrease in impact toughness with decreasing cooling capacity, although intermetallic precipitation was observed only in some locations. Bars cooled with higher air flow rates met toughness and precipitation quality criteria, making air cooling with IJQT applicable for 80 mm and smaller diameters.

These results highlight IJQT's potential to precisely control the quenching process, optimizing mechanical properties in both boron-containing carbon steels and SDSS, enhancing their durability and performance in various industrial applications.

Exploring three dimensional orientation and residual stresses in railway steels

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

Railway wheel steels, comprising a fine lamellar pearlitic microstructure interspersed with pro-eutectoid ferrite, experience combined thermal and mechanical loads that may induce material failure due to increased local residual stress.

In this study, we use an advanced synchrotron technique, dark-field X-ray microscopy, in which the X-ray diffracted beam is magnified by an objective lens, forming a 2D projection of a grain. By using a line beam, this technique enables the 3D mapping of lattice variations, including both crystallographic orientation and lattice strain. This non-destructive method allows for the characterisation of grains embedded in bulk with a resolution down to 100 nm and is applied here to pro-eutectoid ferrite grains.

In addition to an as-manufactured sample, we studied samples that underwent low-cycle fatigue tests followed by isothermal heat treatments at 300–600°C. The as-manufactured sample shows an orientation variation up to 0.5° and compressive elastic strain up to 1.8×10^{-3} but no direct correlation between the measured compressive strain and lattice orientation. The low-cycle fatigue tested samples exhibit an increase in orientation spread up to 3–4°. These grain-level observations were correlated with bulk X-ray diffraction results, which revealed a non-monotonic evolution of residual stress levels with annealing temperature, as well as with macroscopic mechanical tests.

Such an analysis of the evolution and distribution of residual stress, as proposed here, is essential to inform finite element models that can predict the mechanical behaviour of these materials.

Fatigue performance of steels for next generation electric heavy-duty vehicles leaf springs

MSc Yuan Tian¹, Prof. Mattias Calmunger¹, Dr Jinghao Xu¹, Prof. Ru Lin Peng¹, Prof. Johan Moverare¹

¹Linköping University, Linköping, Sweden

B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

The automotive suspension system is the link between the structure of the vehicle and its wheels. Thus, its crucial for the absorption of road induced vibrations and for improving vehicle maneuverability and user comfort. For heavy-duty vehicles, the leaf springs are an important part of the suspension system, responsible for supporting the vehicle weight and absorbing the vertical vibrations and impacts due to the road conditions. Thus, the springs are exposed to dynamic forces and need to withstand many cycles without failure during their service life. It should also be noticed that failure of a main leaf spring may significantly affect the steering behavior of the vehicle and must be regarded as a critical safety component. To fulfill the safety requirements and the increasing demand for lightweight structures it is typically required to have an optimized design and accurate manufacturing processes, especially from the point of view of fatigue.

This study aims to investigate the possibility to enhance the durability of leaf springs for electric heavy-duty vehicles by introducing advanced high-strength steels and optimizing surface treatments. The study will investigate the impact of surface treatments such as shot-peening on different high-strength steels and their fatigue life. The findings are expected to be applicable to various automotive components, promoting broader adoption of advanced materials and manufacturing techniques in the industry.

The results showed that the fatigue life can be enhanced by selecting the appropriate high-strength steel and by optimizing the surface treatments. Fatigue performance of the different advanced high-strength steels as well as residual stress evolution of different surface treatments will be discussed.

The formation of solid-state zinc thermal diffusion coatings on steel surfaces and their wear performance

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This study investigates the formation of solid-state zinc thermal diffusion coatings on high-strength steel surfaces and evaluates their wear performance. Traditionally, hard chromium electroplating coatings are applied to improve bicycle steel gears' wear and corrosion resistance, raising environmental and health problems. The gears are typically made from steel and are applied after carburising or through hardening to endure high and cyclic stresses in service. Bicycle gears are components of rear hubs that connect the rim to the spokes, maintaining the wheel's integrity and containing bearings and springs that enable the wheels to rotate around the axle. Solid-state zinc thermal diffusion coatings offer an alternative, as they do not carry the environmental risks and the hydrogen embrittlement associated with hard chromium electroplating. In this study, quenched and tempered 40 CrMnNiMo 8-6-4 steel rings were embedded in zinc powder within a sealed alumina container. This assembly was then placed in a furnace for diffusion heat treatment with varying temperatures. Optical and scanning electron microscopy, energy-dispersive X-ray spectroscopy and X-ray diffraction were used to analyse zinc thermal diffusion coatings. Vickers microhardness profiles were also determined on uncoated and coated steel rings. Pin-on-disk wear tests were conducted on the solid-state zinc thermal diffusion-coated steel rings, using a DIN 100Cr6 steel ball as the counter body to study wear performance. Zinc diffused into the steel surface during the solid-state diffusion heat treatment, forming the Γ and δ phases with increasing zinc content. This study's temperatures and holding times for the zinc thermal diffusion treatments did not significantly change the hardness profiles for the quenched and tempered 40 CrMnNiMo 8-6-4 steel substrates. This investigation contributes to a better understanding of solid-state zinc diffusion coating formation on steel substrates as a viable alternative to hard chromium electroplating for bicycle rear hub gears.

Electrochemical diagnostics for molten salt corrosion

Ph.D. Maria Elena Gennaro¹, Mr Fabio Todesco¹, Ms Silvia Vicini¹, Mr Enrico Tognella¹, Mr Alberto Pontarollo¹

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Recently, molten salts have been proposed for numerous applications: as coolants for advanced nuclear fission and fusion reactors, and as thermal vectors for thermal energy transfer. The characterization and understanding of the chemical behavior and mass transport of corrosion products and other solutes in the molten salt is critical for the design, licensing and operation of the various plants. Electrochemical techniques provide a powerful set of tools to investigate these phenomena. In addition, electrochemical techniques provide a direct approach to continuously monitor salt quality during operation, avoiding the need for sampling and subsequent analysis. The present study aims to investigate high temperature electrochemical techniques for the study and monitoring of corrosion in molten salt environments. A further objective is to assess the applicability in field cases of interest and to explore challenges in key areas of the energy transition (e.g. fusion, TES, CCUS). In order to carry out these analyses, an experimental cell for molten salts electrochemistry is proposed that can operate up to 800°C, in controlled environment, with the possibility of gas sweep, gas sampling and analysis. The cell can support a variety of materials and electrode configurations and potentiodynamic sweep, linear polarization resistance and other DC techniques have been applied.

Detection using computer vision and analysis of the mechanical effect of fiber orientation degree in composite materials.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

A precise understanding of mechanical properties of materials enables a more efficient use, reducing resource consumption during manufacturing and optimizing the final weight of components. In long-fiber-reinforced composites, predicting and correcting fiber alignment deviations during production is especially beneficial in Industry 4.0.

This study presents advances in fiber orientation monitoring in thermoplastic and thermosetting composites. A methodology is described to analyze fiber orientation distribution over large material areas. Computer vision and image processing algorithms help control fiber alignment throughout manufacturing. Before production, improper fiber orientations can be detected and adjusted. After manufacturing, the method helps estimate the final mechanical properties of the laminate based on fiber distribution.

Results show high detection accuracy across various composite materials, allowing for reliable mechanical property predictions. This approach can also be applied to more complex composites using advanced vision techniques.

Mechanical properties of 304L stainless steel at 4K

Dr. Young-Kyun Kim¹, Dr. Young-Sang Na¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In this study, the mechanical properties of 304L stainless steel (SS) fabricated via the laser powder bed fusion (LPBF) process were investigated at room temperature and cryogenic conditions ($\sim -269^{\circ}\text{C}$) under controlled oxygen concentration (0.2%). Compared to conventionally wrought SS304L, LPBF-fabricated SS304L exhibited a significantly increased yield strength, reaching approximately 336 MPa at room temperature and up to 398 MPa at -269°C . Additionally, it demonstrated an additional yield strength increase of approximately 64 MPa at room temperature compared to previously reported LPBF SS304L. This enhancement in strength is primarily attributed to the oxide dispersion strengthening effect induced by controlled oxygen concentration, as well as grain boundary and dislocation strengthening, without a significant reduction in ductility. Furthermore, strain-induced martensitic transformation (SIMT) did not occur at room temperature and showed a decreasing trend at cryogenic temperatures compared to wrought SS304L. This behavior is interpreted as a result of the high dislocation density and nitrogen-stabilized austenite. Additionally, the "discontinuous plastic flow (DPF)" observed at -269°C was associated with the adiabatic heating effect induced by plastic deformation, consistent with the material's low thermal conductivity. Based on these findings, the correlation between the unique hierarchical microstructure of LPBF SS304L and its cryogenic mechanical properties at -269°C was thoroughly examined.

Ultra-Low Temperature Tensile properties and Fracture Toughness of L1₂ Precipitation-Strengthened Medium-Entropy Alloy

Mr. Seong-June Youn¹, Ph.D. Young-Sang Na¹, Ph.D. Young-Kyun Kim¹

¹Korea Institute of Materials Science, Extreme Materials Research Institute, Changwon, South Korea
B7_4, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 17:00 - 19:00

With growing concerns about global warming, the demand for eco-friendly energy sources, such as liquid hydrogen (LH₂), has been increasing. Consequently, ensuring the reliability of structural materials in cryogenic temperature ranges has become crucial. Medium-entropy alloys (MEAs) with a face-centered cubic (FCC) structure are promising candidates for cryogenic applications because they have excellent mechanical properties and fracture resistance at low temperatures. However, MEAs have low yield strength, and at temperatures below about 20K, they experience discontinuous plastic flow, causing sudden stress changes. This makes it difficult to predict the material's reliability. In this study, Aluminum and titanium were added to a CoCrNi-based MEA to form L1₂ precipitates. The newly developed alloy was tested under 77K and 4.2K to evaluate its tensile properties and fracture toughness. Compared to the equiatomic CoCrNi alloy, the modified MEA showed a significant increase in yield strength and a lower serration amplitude. Additionally, the K_{Ic} fracture toughness value at 4.2K was measured to be over 300 MPa·m^{1/2}, which is higher than that of austenitic stainless steel commonly used in cryogenic applications. The deformation and fracture behavior of L1₂ strengthened MEA was also identified based on the deformed microstructure and fractography observation results.

Hidden insights of Friction Welding Processes - Linking material behaviour to process performance

Prof. Chris Bennett¹

¹University of Nottingham, Nottingham, United Kingdom

B7_8, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 10:30 - 13:10

Friction welding is a group of high-integrity, solid-state joining processes that are widely used in the joining of advanced materials employed in the aerospace industry. These processes use mechanical friction to generate heat at the interface between two workpieces, followed by the application of pressure to forge them together. These processes are highly dynamic in nature, with materials experiencing both high heating and deformation rates, leading to complex material evolution. While these techniques offer numerous advantages over traditional fusion welding processes, they also present several material-specific challenges that engineers must address to achieve successful welds, for example, material flow behaviour represents a significant challenge as during friction welding, materials must undergo plastic deformation to create intimate contact at the interface. Materials with high flow stress or low ductility at elevated temperatures can be difficult to process.

Throughout his career, Prof. Chris Bennett has been dedicated to understanding the detail of these processes and his talk will cover a range of experimental and modelling techniques that have been employed to develop a deeper understanding of the processes, revealing their effects on the material both during the process and the characteristics of the joints and properties of the resulting material. The talk will include both experimental and modelling characterisation approaches, residual stress prediction and measurement, and the characterisation of mechanical material properties of the resultant material. Through this work, new insights and a holistic understanding of the processes have been gained, and suggestions for further work to further enhance the understanding and optimisation of processes for existing and new materials will be presented.

Damage tolerance of nanostructured thin films during multiaxial deformation using polymer supported tensile tests

Dr. Barbara Putz¹

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B7_10, Federico García Lorca Auditorium (Level 0), septiembre 17, 2025, 17:00 - 19:00

Brittle layers are often dominating the fracture behavior of flexible thin film nanolaminate structures through stress concentration, whereby the modulation period ($t_{\text{brittle}} + t_{\text{ductile}}$, film thickness t) and the modulation ratio ($t_{\text{brittle}}/t_{\text{ductile}}$) influence the extent of embrittlement. Atomic layer deposition (ALD) holds enormous potential to design nanolaminates with tailored mechanical properties, due to the unique way in which materials are built in an atomic layer-by-layer fashion. When combined with other thin film techniques, such as magnetron sputtering (PVD), without breaking vacuum, the layer-by-layer nature of ALD can be harvested to design (sub)nanoscale interface and nanolaminate architectures with extremely good control over the layer thicknesses. For metal-oxide interfaces (Al/Al₂O₃), the minimum ALD layer thickness of one monolayer (nominal thickness 0.14 nm) far exceeds the thickness restrictions of natural oxidation of Al (2-10 nm¹). The mechanical behavior of resulting nanolaminates consisting of Al (10-150 nm, PVD) and Al₂O₃ (0.1-10 nm, ALD) is studied in-situ under uni- and biaxial tensile loading using polymer substrates. Ultrathin oxide layers confine the grain growth of the metallic thin films, creating sub-layer architectures with unique properties. In-situ film stress and electrical resistance measurements as a function of varying oxide and metal layer thickness show that brittle failure of the nanolaminates can be avoided for oxide thicknesses ≤ 2 nm and the maximum strength is obtained with 25 nm Al layers.

In the second part of the talk, the potential of modifying the deformation behavior of metallic thin films via incorporated nanoparticles will be discussed, produced via combined magnetron sputtering and a nanoparticle source. The thin films contain nanoparticles with a tailored size, shape, distribution and volume density without precipitation-related restrictions concerning phase diagrams and solubility. Their microstructures and nanoparticle concentrations were confirmed and characterized by TEM. For inherently brittle films (200 nm Mo), suffering from through-thickness crack formation at low applied strains, incorporating various amounts of Al nanoparticles (20 nm diameter) can significantly improve the electro-mechanical behavior. The observed changes in the developing crack pattern, through crack deflection at nanoparticles, correlates well with a lower electrical resistance at equivalent strains and changes in the stress-strain curve. For ductile films (50 - 200 nm Cu and Au) the observed influence of nanoparticles (W, 4 nm diameter and Co, 10 nm diameter) strongly depends on the grain size and film thickness, whereby both softening and strengthening mechanisms have been observed.

Exploring Texture and Residual Stress in Additively Manufactured Steels Using Advanced Diffraction Techniques

Dr. Steven Van Petegem¹

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B7_2, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 10:50 - 13:10

The crystallographic texture of a material plays a crucial role in determining mechanical properties, deformation behavior, and residual stress development. In additively manufactured (AM) metals, rapid solidification, complex thermal histories, and repeated heating-cooling cycles strongly affect texture, often leading to highly heterogeneous and anisotropic microstructures. Importantly, AM techniques allow not only for shaping components but also for manipulating local texture, offering opportunities to tailor mechanical performance in specific regions. However, the resulting microstructures are often complex and three-dimensional, making it critical to develop methods that can capture both the texture evolution and the coupled residual stress development under processing and loading. This contribution presents two complementary case studies that apply advanced diffraction techniques to tackle these challenges. The first investigates residual stress formation and its link to texture during AM processing, while the second focuses on grain-resolved texture evolution under mechanical deformation.

The first case study examines the evolution of residual stresses and crystallographic texture in 2205 duplex stainless steel during laser powder bed fusion (LPBF) additive manufacturing. Operando neutron diffraction experiments were performed using a neutron-optimized LPBF machine to monitor real-time strain evolution during the layer-by-layer build process. Complementary Bragg-edge imaging mapped texture variations shaped by local thermal history and solid-phase transformations. Results show that stress redistribution occurs predominantly in the earliest printed layers and that crystallographic texture has a direct and significant influence on the magnitude and direction of residual stresses. Ignoring orientation-dependent elastic constants can lead to residual stress calculation errors of up to 96 MPa, emphasizing the importance of integrating texture into stress analysis models.

The second case study focuses on the use of texture tomography to study deformation behavior in additively manufactured TWIP (twinning-induced plasticity) steels. This non-destructive x-ray-based approach was motivated by the need to probe three-dimensional, grain-resolved texture evolution in microstructures with high local complexity and large intergranular misorientations, where conventional 3D diffraction methods struggle. By scanning a micro-focused x-ray beam and reconstructing orientation distribution functions (ODFs) across the sample, texture tomography enables tracking of reorientation mechanisms such as slip and twinning during interrupted tensile loading. The method provides critical insight into how texture evolves under mechanical strain, complementing stress-focused measurements by revealing the grain-scale deformation pathways that contribute to macroscopic material behavior

Laser-Driven Surface Design of Ti-Alloys: A Path Towards Biofunctionality and Beyond

Dr. Oktawian Bialas¹

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B7_2, Federico García Lorca Auditorium (Level 0), septiembre 15, 2025, 10:50 - 13:10

Titanium and its alloys are among the most prominent materials in biomedical engineering, especially for load-bearing implants, due to their favorable mechanical properties and biocompatibility. However, achieving optimal biofunctionality—encompassing osteointegration, antibacterial resistance, and long-term stability—requires precise control over surface characteristics. In this context, laser-based surface engineering has emerged as a promising strategy for tailoring surface topography, chemistry, and phase composition at micro- and nanoscale levels.

In this work, we investigate the effects of laser machining of the near-surface modification of titanium-gold (Ti-Au) alloy system. Using a laser treatment under ambient conditions, surface remelting, oxidation, and alloy redistribution phenomena were systematically examined. The resulting laser-affected zones exhibited significant morphological and microstructural transformations, including the formation of surface ripples, grain refinement, and the emergence of metastable Ti oxides and intermetallic phases such as Ti_3Au . These features are known to influence biological interactions, including improved cellular interaction and antibacterial properties.

Advanced characterization techniques such as SEM/EDS, EBSD, and XRD were employed to elucidate the phase transformations and crystallographic orientations induced by laser treatment. Moreover, the complex interplay between thermal gradients, convection, and rapid solidification was analyzed to understand the driving forces behind the observed surface architectures.

The results underscore the versatility of laser-based approaches in designing functional surfaces on biomedical alloys. By fine-tuning process parameters such as power, scan speed, and repetition rate, it is possible to engineer surface zones with tailored morphology and chemistry aimed at specific biological outcomes.

This study lays the groundwork for developing next-generation implant surfaces that go beyond passive biocompatibility toward active biofunctionality, highlighting the role of laser-material interaction in the emerging field of surface bioengineering.

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Effect of Ti and Nb on hydrogen trapping in welded S690 HSLA steel and effect on delayed cold cracking

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Fine-grain, high-strength, low-alloy (HSLA) structural steels with yield strengths > 600 MPa are now the state of the art in construction applications such as mobile cranes and civil engineering. HSLA grades derive their strength from a combination of specific heat treatment and the underlying chemical composition. In this context, Ti or Nb are essential to obtain a fine-grained microstructure as well as the necessary carbides or nitrides for precipitation strengthening. In this context, the specific effect of Ti or Nb-rich compounds on hydrogen trapping and diffusion is well known for special laboratory cast alloys, but unknown for realistic steel compositions. For this reason, a series of S690Q-based alloys were synthesized, close to a real steel composition, but with well controlled Ti or Nb additions in different amounts. Specimens were obtained from these alloys by electrochemical discharge machining (EDM). The specimens were tested using the well-established electrochemical permeation technique. From the experimental results, the hydrogen diffusion coefficients and the analytical subsurface hydrogen concentration were calculated. In addition, the hydrogen trapping behavior at elevated temperatures was interpreted by thermal desorption analysis (TDA) using different heating rates of hydrogen charged samples. The results showed that in contrast to metallurgically "pure" laboratory cast alloys, realistic chemical compositions were similar in their hydrogen trapping behavior, despite some small differences. All investigated steel grades exhibited shallow and reversible hydrogen trapping, regardless of their chemical composition. Of course, the experiments only allowed the calculation of effective diffusion coefficients and trapping energies, which represent an average of the entire microstructure. Nevertheless, HSLA steels are typically joined by arc welding, which includes the risk of delayed hydrogen assisted cracking. From the point of view of welding practice, however, a more or less identical hydrogen diffusion behavior means that no special "metallurgically specific", justifiable measures need to be considered, despite the well-established processes such as "soaking" or dehydrogenation heat treatment. Of course, a closer look at the heat-affected zone (HAZ) or the weld metal of the specific welds is necessary. However, especially in the case of thick-walled welds, it is assumed that the weld metal and HAZ are similar to the base material due to the multi-layer welding, which results in multiple annealing cycles of the weld metal and HAZ.

Influence of hydrogen on the γ -matrix lattice parameters of a polycrystalline Ni-based superalloy – a synchrotron diffraction study

Dr. Massimo Fritton-Fantini¹, Dr. Alexander Mutschke¹, MSc. Oliver Nagel², Dr. Andreas Stark³, Dr. Masood Hafez-Haghighat⁴, Dr. Bodo Gehrman⁴, Dr. Steffen Neumeier², Dr. Ralph Gilles¹

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B8_2, Seminario 8 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

To reduce reliance on fossil fuels and combat climate change, hydrogen has emerged as a versatile and sustainable alternative, offering a pathway to carbon neutrality. Its dual role as an energy carrier and industrial feedstock makes it an essential component in transitioning to cleaner energy systems while enabling decarbonization across sectors like transportation, power generation, and chemical production. However, hydrogen dissolved in alloys can drastically alter their deformation behavior, transitioning from ductile to brittle, a phenomenon known as hydrogen embrittlement (HE). Understanding this effect is critical, particularly, as hydrogen becomes increasingly important as a possible candidate for future mobility applications.

The objective of this study was to investigate the hydrogen uptake of Ni-based superalloy VDM® Alloy 780 through electrochemical charging via high-energy X-ray diffraction (HEXRD). The results demonstrate that hydrogen incorporation at interstitial sites of the fcc lattice causes a slight increase in lattice parameters compared to hydrogen-free samples. In-situ HEXRD measurements reveal that at elevated temperatures the lattice parameters of uncharged and charged specimens gradually converge. This suggests the reversibility of hydrogenation through diffusion and subsequent effusion of hydrogen. Hot gas extraction (HGE) measurements were conducted to quantify the hydrogen content, showing that prolonged electrochemical charging increases hydrogen uptake. Temperature-dependent quantification confirmed that hydrogen diffusion rates increase with temperature, as evidenced by higher measured hydrogen content at elevated temperatures.

To evaluate the mechanical impact of hydrogen, tensile tests were performed, supported by fractographic analysis via scanning electron microscopy (SEM). The hydrogen-charged specimens exhibited cleavage fractures near the surface, contrasting with the ductile fracture patterns observed throughout the entire reference sample. These findings provide valuable insights into the effects of hydrogen on superalloys, offering a foundation for further research on their performance in hydrogen-rich environments.

Comparison of hydrogen embrittlement fractures of tempered martensitic steel obtained by various test methods

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Conventionally, slow strain rate test (SSRT) and constant load test (CLT) have been widely used to evaluate the hydrogen embrittlement susceptibility of high-strength steels. High-strength bolts are typically subjected to a constant displacement tensile load under actual service conditions. However, there are few reports on evaluating hydrogen embrittlement susceptibility using constant displacement tensile test (CDT). Furthermore, differences in hydrogen embrittlement susceptibility obtained by SSRT, CLT, and CDT have not been clarified. In the present study, we compared the fracture strength and fracture morphology of hydrogen-charged tempered martensitic steel using SSRT, CLT, and CDT. Tempered martensitic steel specimens with a tensile strength of 1530 MPa were prepared as smooth round bars with a gauge length of 30 mm and a diameter of 6 mm. Specimens were charged with hydrogen in a 0.1N NaOH aqueous solution containing 1.0 to 3.0 g·L⁻¹ NH₄SCN at a temperature of 30 °C for 96 h using the constant current cathodic electrolysis at a current density of 20 to 50 A·m⁻². Following hydrogen precharging, three types of tensile tests were conducted. For SSRT, tensile tests were performed at strain rates of 5.56×10^{-6} to 5.56×10^{-7} s⁻¹. For CLT, the load was applied at a rate of 3.33 MPa·s⁻¹ until reaching a predetermined stress value in the range from 400 to 1200 MPa, after which the constant stresses were applied for up to 48 h. For CDT, the load was applied at the same rate as CLT, but displacement was fixed upon reaching the predetermined stress value in the range of 500 to 1200 MPa, and held constant for up to 10 h. The critical fracture strengths were determined for each test method, and fracture surfaces were observed using a scanning electron microscope. Under low amount of hydrogen, the critical fracture strengths for SSRT, CDT, and CLT were 1420 MPa, 1400 MPa, and 1350 MPa, respectively, which were no significant differences among the three testing methods. Fracture surfaces obtained by three testing methods commonly exhibited quasi-cleavage facets initiating from the base material at the edge on the circumference of the specimens. Under high amount of hydrogen, the critical fracture strengths for SSRT, CDT, and CLT were 900 MPa, 500 MPa, and 400 MPa, respectively, indicating significant differences between SSRT and the other two testing methods. Fracture surfaces for all three methods showed a mixture of quasi-cleavage and intergranular fractures, where the crack initiation occurred around the internal precipitates.

Evaluation of the activation energy of hydrogen desorbed from the vicinity of dislocation cores in α -iron

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Hydrogen embrittlement, which deteriorates mechanical properties such as strength and ductility of metallic materials due to absorbed hydrogen, is a significant issue. It has been well known that hydrogen diffusing into metallic materials is preferentially trapped at sites with high binding energy according to Fermi-Dirac statistics. Therefore, clarifying the activation energy for hydrogen desorption (E_a) from various lattice defects acting as trap sites for diffusible hydrogen is crucial to understanding the states of hydrogen present in metallic materials. However, previous studies on the E_a for hydrogen desorbed from dislocations in α -iron have only been able to determine values considered as average for hydrogen trapped at edge dislocation cores, screw dislocation cores, and the strain fields around dislocation cores. In the present study, we attempted to evaluate the E_a for edge dislocation cores and their vicinity, which have the highest binding energy among dislocations, by reducing the amount of tracer hydrogen as much as possible. Cold-rolled iron containing 6 ppm C (Fe > 99.98 mass%) was prepared. The iron was processed into flat plate tensile specimens with a parallel part of 30 mm and annealed at 900 °C for 30 min. The tensile specimens were subjected to plastic strain of 25 % at a strain rate of $8.3 \times 10^{-6} \text{ s}^{-1}$ at R. T. to induce sufficient lattice defects into the specimens. A 10-mm square specimen was cut out from the parallel part of the tensile specimen and polished to reduce the specimen thickness to 0.3 mm. To detect lattice defects in these specimens, tracer hydrogen was charged by constant current cathodic electrolysis at a current density of $10 \text{ A}\cdot\text{m}^{-2}$ in a 0.1 N NaOH solution containing $0.05 \text{ g}\cdot\text{L}^{-1} \text{ NH}_4\text{SCN}$ at 30 °C for 1 h. Tracer hydrogen spectra were then obtained by thermal desorption spectroscopy at heating rates of 1, 2, and $2.5 \text{ }^\circ\text{C}\cdot\text{min}^{-1}$ and in a temperature range of -200 to $200 \text{ }^\circ\text{C}$. The peak of hydrogen desorption corresponding to dislocations was extracted from the tracer hydrogen spectra, and then the E_a values were calculated from the heating rate and the peak temperature of hydrogen desorption using the Choo and Lee's equation. The E_a for dislocations with approximately 1/40 of the tracer hydrogen amount compared to the previous study was found to be $53.1 \text{ kJ}\cdot\text{mol}^{-1}$, which is higher than $30.4 \text{ kJ}\cdot\text{mol}^{-1}$ reported previously and is considered to be the E_a for the edge dislocation cores and vicinity in α -iron.

States of hydrogen and hydrogen embrittlement susceptibility of flake and spheroidal graphite cast irons

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B8_3, Seminario 8 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

It is essential to investigate the safety of cast iron used in hydrogen environments to apply cast iron to hydrogen-fueled internal combustion engines. However, there has been little research on hydrogen embrittlement of cast iron. The present study attempts to clarify factors causing hydrogen embrittlement based on the relationship between states of hydrogen present in cast iron and hydrogen embrittlement susceptibility. Flake graphite cast iron (FC) and spheroidal graphite cast iron (FCD) were employed. Specimens were electrochemically charged with hydrogen in a 0.1 N NaOH solution at a temperature of 30 °C at a current density of 30 A·m⁻². Charging times were 96 h and 192 h for FC and FCD, respectively. States of hydrogen were analyzed using thermal desorption analysis (TDA). The activation energy for hydrogen desorption (E_a) was calculated from the dependence of peak temperatures of hydrogen desorption on heating rates for TDA. Specimens with the parallel part were used in tensile testing. A crosshead speed of 0.01 mm·min⁻¹ with/without hydrogen charging was employed. TDA results showed that FC and FCD specimens had two and three peak temperatures of hydrogen desorption, respectively, which are labeled as Peak 1H, 2H, and 3H in order from the lower temperature. The E_a value of Peak 1H was calculated to be 28 kJ·mol⁻¹ for both FC and FCD specimens. The E_a value of Peak 2H was calculated to be 76 kJ·mol⁻¹ for both specimens. The E_a value of Peak 3H was calculated to be 103 kJ·mol⁻¹ only for FCD specimen. Based on the E_a values, Peak 1H presumably desorbs from dislocations, whereas Peak 2H presumably desorbs from interfaces and/or voids between graphite and matrix in addition to casting defects for FC and FCD specimens. Peak 3H only for FCD specimens probably desorbs from graphite. The results of tensile testing showed elongations of hydrogen-charged FC and FCD specimens decreased compared with those of non-charged specimens. However, the elongations of FC specimen only with Peak 2H and FCD specimen only with Peak 2H and 3H were the same as those of non-charged specimens. These findings indicated that Peak 1H, i.e. hydrogen present at dislocations directly causes embrittlement, while Peak 2H and 3H, i.e. hydrogen present on the interfaces between graphite and matrix, in casting defects, and in graphite are not related to hydrogen embrittlement at a room temperature.

Comparison of hydrogen embrittlement susceptibility of tempered martensitic steels adding Mo and Mo-V

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B8_4, Seminario 8 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Recent studies have reported that the precipitation of fine carbides with co-addition of molybdenum (Mo) and vanadium (V) in a matrix improved the resistance to hydrogen embrittlement of tempered martensitic steel due to the interfaces with high binding energy with hydrogen atoms under low hydrogen content. However, the effect of fine precipitation of co-added Mo and V carbides on reducing the susceptibility to hydrogen embrittlement of tempered martensitic steel under high hydrogen content has not been clarified. This study investigates the effect of finely precipitated Mo and V carbides on the susceptibility of hydrogen embrittlement of tempered martensitic steels with different Mo and V amounts evaluated by both slow strain rate testing (SSRT) and constant load testing (CLT) under low to high hydrogen charging conditions. Three kinds of steel (Base steel, 1%Mo steel, and 1%Mo-0.1%V steel) were compared. The specimens with a diameter of 5 mm and a gauge length of 30 mm were pre-charged with hydrogen in a 0.1 N NaOH solution with the addition of NH₄SCH of 5 g·L⁻¹ at current densities ranging from 1 to 50 A·m⁻² for SSRT and at a current density of 50 A·m⁻² for CLT at 30 °C for 192 h, respectively. SSRT was conducted at a crosshead speed of 0.02 mm·min⁻¹ while maintaining hydrogen charging under the same conditions. In CLT, hydrogen-charged specimens were loaded to an initial stress of 0.8 σ_B (tensile strength: σ_B) under the same conditions of hydrogen pre-charging. When no fracture occurred after 48 h, the applied stress was incrementally increased by 0.05 σ_B every 48 h. The critical stresses for delayed fracture were determined. Stress relaxation tests were also performed with an initial stress of 0.7 σ_B to evaluate the degree of dislocation mobility. SSRT results show that the difference in fracture strength among the three kinds of steel was smaller at lower current densities, whereas that at higher current densities was larger. The order of fracture strength was Base steel < 1%Mo steel < 1%Mo-0.1%V steel. In CLT, the order of the critical stress for delayed fracture was the same as the fracture strength obtained by SSRT. Stress relaxation increases in the order of 1%Mo-0.1%V steel < 1%Mo steel < Base steel. These results indicate that the co-addition of Mo and V not only enhances hydrogen trapping but also reduces dislocation mobility, thereby reducing the susceptibility of hydrogen embrittlement even under higher hydrogen content.

Effects of Pressure and Frequency on Hydrogen-induced Fatigue in X65 Pipeline Steel

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B8_4, Seminario 8 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Repurposing natural gas pipelines for hydrogen transport is crucial for sustainable energy transition, necessitating an understanding of hydrogen degradation mechanisms. While much research exists on hydrogen-induced failure, fatigue loading remains underexplored due to its complexity. This study examines the effects of hydrogen gas pressure and loading frequency on the fatigue crack growth behaviour of X65 pipeline steel. Constant force amplitude tests were conducted at hydrogen gas pressures of 0.2, 2, 5 and 10 MPa and loading frequencies of 0.01, 0.1 and 10 Hz. Paris regimes of base and weld metals were obtained in both nitrogen and hydrogen environments. The hydrogen-assisted crack growth rate increased with higher pressure and lower frequency. Moreover, the crack growth rate ratio in hydrogen to nitrogen was higher at lower ΔK . Constant ΔK experiments were performed at various pressures and frequencies, followed by electron backscattered diffraction to analyse deformation near the crack flanks. Postmortem fractographic analysis identified degradation mechanisms and weak links in the microstructure.

Hydrogen-induced effects on plasticity in austenitic steels: Role on deformation behavior and hydrogen embrittlement resistance

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B8_1, Seminario 8 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

The influence of hydrogen on the deformation behavior of structural materials is still a controversial topic largely due to the limited understanding of the role of hydrogen-induced effects on the collective behavior of plasticity. In austenitic steels, the influence of hydrogen on plasticity has been mainly associated with slip localization. This effect has been ascribed to the locking of dislocations by hydrogen atmospheres and the hydrogen-induced reduction of dislocation cross-slip. According to these processes, hydrogen tends to localize the emitted dislocations into a narrow slip band formed by unrelaxed pileups that, at interacting with GBS, result in the initiation of a microcrack via void nucleation at GBs (hydrogen embrittlement, HE). However, these hydrogen-related phenomena do not explain the small influence of hydrogen on the fracture behavior of austenitic steels (316L and 310S) and austenitic FeMnAlC low-density steels. In this presentation, we present unrevealed hydrogen-induced effects on plasticity that evidence the complex influence of hydrogen on the collective behavior of dislocation plasticity and their impact on strain-hardening in austenitic steels. The quantitative analysis of the hydrogen-related deformation structure by several electron microscopy techniques, such as electron channeling contrast imaging (ECCI), electron backscatter diffraction (EBSD), and scanning transmission electron microscopy (STEM), reveals novel dislocation-based processes associated with hydrogen-induced strain localization phenomena. These processes have a significant influence on the deformation and strain-hardening behaviors of the steels. Two cases will be presented. On the one hand, we will show experimental evidence of the hydrogen-induced promotion of dislocation structures associated with inhomogeneous plasticity (deformation bands) and strain localization (microbands) in an austenitic Fe₃₀Mn_{6.5}Al_{0.3}C low-density steel with a solute hydrogen content of 101 mass ppm [1]. These hydrogen-induced mechanisms contribute to plastic accommodation by accommodating local lattice rotation gradients and relaxing the elastic field associated with dislocations, favoring the excellent HE resistance exhibited by the steel. On the other hand, we will show experimental evidence of hydrogen-induced effects on the GB-assisted nucleation of dislocations in an austenitic 310S stainless steel with a solute hydrogen content of 131 mass ppm. These processes modify the dislocation structure of slip bands, favoring slip localization. Upon straining, the propagation of hydrogen-induced coarse slip bands results in the localized shear of the primary dislocation structure. The grain orientation dependence of this process is evaluated, and its contribution to the deformation behavior is discussed.

References:

[1] I. Gutierrez-Urrutia et al., *Acta Materialia* 280 (2024) 120335.

Tritium-based micro-fracture experiments for mechanistic understanding of hydrogen embrittlement

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B8_3, Seminario 8 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Abstract – FEMS EUROMAT 2025

Tritium-based micro-fracture experiments for mechanistic understanding of hydrogen embrittlement

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Presentation in the symposium “B8 – Hydrogen embrittlement of structural materials”

Green hydrogen is considered a potential game changer in the transition to cleaner energy systems with lower CO₂ emissions. However, for safe storage and transportation of hydrogen, hydrogen embrittlement (HE) has remained a major concern. The ERC-funded project, TRITium based microMEchanics (TRITIME), aims to isolate, observe, and quantify the debated mechanisms responsible for HE, leveraging the unique properties of tritium.

In this talk, we will present the concept of using tritium (³H) charged single-crystal Fe-3wt-%Si samples for micro-fracture tests to elaborate the fracture behavior under the influence of hydrogen (tritium). The notched microcantilevers are prepared using a combination of a femto-second ablation laser and a focused ion beam, prior to the charging with a hydrogen-tritium gas mixture. The microcantilever fracture experiments are conducted inside an SEM using an in situ nanoindentation system. Post-deformation imaging of the hydrogen isotopes ¹H and ³H (tritium) across the relevant length scales is done applying various methods, including atom probe tomography (APT). This combination enables the quantitative correlation of the (fracture)-mechanical properties with the locally resolved hydrogen content. The results will be discussed in the framework of the Hydrogen Enhanced Decohesion (HEDE), Hydrogen Enhanced Localized Plasticity (HELP), and their interplay.

Ab initio study of hydrogen trapping at coherent and semicoherent interfaces

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B8_4, Seminario 8 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Small and dense carbide precipitates in steels increase the resistance to hydrogen embrittlement by providing deep trapping sites which reduce the concentration of mobile hydrogen content. The critical factors affect hydrogen trapping capacity of carbide precipitates remain unclear. The present study uses ab initio calculations to study the complicated interactions between hydrogen and metal carbides (e.g., VC, NbC, TiC) in steels aiming at revealing and quantifying the effects of interfacial properties, e.g., chemistry, coherency, local strain, and interfacial dislocations etc. on hydrogen trapping and distribution. We compare the calculated atomic site-specific trapping energies (energy spectrum) with the experimentally determined hydrogen de-trapping activation energies for interfaces from thermal desorption spectroscopy measurements.

Fracture Toughness of Hybrid Laser-MAG and MAG Welded API 5L X65 Steel in air and hydrogen: Influence of Nano-Chemistry Change

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B8_1, Seminario 8 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

This study examines the microstructural and mechanical properties of ferritic steel specimens welded using the metal active gas (MAG) and hybrid laser-MAG welding (HLAW) processes, focusing on their behavior in both air and hydrogen environments. Using atom probe tomography, we conduct a detailed atomic-scale analysis to investigate element distribution and oxide inclusion composition. The results show distinct nano chemistry differences, with HLAW specimens exhibiting layered oxide structures and Mn depletion zones around the inclusions that lead to the formation of the higher densities of acicular ferrite and high-angle grain boundaries (HAGBs). These microstructural features are linked to mechanical properties assessed using single edge notch tension testing. The results show that the higher density of HAGBs in HLAW enhances fracture toughness in air and resistance to hydrogen embrittlement. In contrast, the MAG specimens which show more uniform elemental distribution in oxide inclusions and lower HAGB density adopt a lower fracture toughness in air and high hydrogen embrittlement sensitivity. This study concludes that the HLAW process is better suited for applications like pipeline welding, where high strength, resistance to hydrogen-induced damage, higher speed, and lower cost are essential.

Tensile Properties of X70 Pipeline Steel Under In-Situ Electrochemical Hydrogen Charging

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B8_3, Seminario 8 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

This study investigates the influence of hydrogen embrittlement susceptibility of X70 pipeline steel through uniaxial tensile testing under electrochemical hydrogen charging. Specimens were strained at $1.25 \times 10^{-5} \text{ s}^{-1}$ and electrochemically charged with hydrogen in 0.1 mol/L NaCl containing 1 g/L Thiourea. Hydrogen absorption induced severe loss in ductility. Effects of stress concentrations as well as pre-strain are also investigated. Fractographic analysis revealed a transition from ductile dimple rupture in hydrogen-free specimens to a mixed-mode fracture of quasi-cleavage and intergranular fracture in hydrogen-charged samples, confirming the embrittling effect of hydrogen.

Hydrogen compatibility of internal combustion engine components

Prof. Paolo Matteis¹, Prof. Giorgia Ghiara¹, Dr. Sujith Surendran Vijayamma¹, Prof. Emilio Bassini¹, Prof. Daniele Ugues¹, Dr. Alberto Vassallo², Dr. Massimo Ferrera², Graziano Ubertalli¹

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

In the broader context of the transition from fossil fuels to cleaner and renewable energies, the introduction of hydrogen in the transport field necessitates the testing of metallic components that are compatible with hydrogen-powered vehicles. Numerous studies have been conducted to address the question of whether hydrogen embrittlement affects hydrogen-powered vehicles. The results of these studies have indicated that the answer to this question is in the affirmative. This conclusion is based on the composition, manufacturing procedure and mechanical properties of the component in question, as well as the hydrogen partial pressure and operating conditions.

Several prominent private enterprises (for instance, Toyota, Hyundai, Honda, BMW, GM) have directed their research and development departments to explore the potential compatibility of internal combustion engines (ICEs) with hydrogen-based fuels. The selection of materials is therefore a pivotal consideration, with particular attention to the operational conditions to which they are exposed.

In accordance with this trend, the present study constitutes a component of a project promoted by the Italian company Dumarey Automotive Italia S.p.A., the objective of which is to ensure full compatibility of internal combustion engine (ICE) components in the context of a transition from hydrocarbon to hydrogen engines. A primary objective of the project is the identification of hydrogen embrittlement-(HE)-resistant alloys, with a focus on the selection of components, including but not limited to pistons, engine heads, and engine blocks, deemed suitable for these applications.

A series of experiments were conducted on a set of alloys (comprising various aluminium alloys and cast irons) in order to evaluate their mechanical performance and susceptibility to hydrogen degradation. Slow strain rate testing (SSRT) of hydrogen-charged samples was performed on selected alloys. In addition, fractographic analyses were carried out to identify characteristic fracture features connected to hydrogen embrittlement (HE).

Metallographic analysis of end-of-test metal components of hydrogen-fueled internal combustion engines

Graziano Ubertalli¹, Prof. Giorgia Ghiara¹, Dr. Sujith Surendran Vijayamma¹, Dr. Alberto Vassallo², Dr. Massimo Ferrera², Prof. Paolo Matteis¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The ability to detect hydrogen embrittlement in internal combustion engines is of pivotal importance to ensure the reliability, safety, and durability of engines, particularly those that utilise hydrogen as a fuel source. Metallography can reveal microstructural changes, crack propagation and fracture characteristics in hydrogen-exposed metals. Therefore, it facilitates a comprehensive understanding of the mechanisms underlying hydrogen embrittlement (HE) and the evaluation of material susceptibility.

This study constitutes a part of a collaborative initiative with the company Dumarey Automotive Italia S.p.A., which received financial support from the Italian government in ensuring the full compatibility of internal combustion engine components in the context of transitioning from hydrocarbon-based fuels to hydrogen-powered engines. The objective of the present study is to determine, through metallographic techniques, the susceptibility of metallic components of internal combustion engines (pistons, engine heads and blocks, valves and valve seats, and gas inlet and outlet manifolds) to degradation caused by hydrogen. To this end, equivalent components from diesel and hydrogen-powered engines were examined and compared after engine bench tests lasting approximately one thousand hours. Optical microscopy and scanning electron microscopy were performed to verify the presence of microstructural changes and crack propagation. In addition, microhardness measurements were employed to assess changes in the hardness of the material.

Simulation of hydrogen behavior at crystal defects in Fe-based alloys

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B8_2, Seminario 8 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

With atomistic simulations we consider hydrogen behavior in iron and its alloys (Fe-Cr, Fe-Ni). Simulations are based on a new interatomic potential developed by the authors [1]. Namely, we concentrate at cases of lattice distortions, such as crystal defects, alloying elements or deformation due to applied stresses. We characterize hydrogen segregation at typical defects: from vacancy to grain boundaries (GBs). Equilibrium distribution of H in the presence of crystal defects is discussed. A role of hydrogen in alternating vacancy diffusion is illustrated by results of finite-temperature diffusion simulations. We also report hydrogen diffusion coefficients at GBs, for fcc and bcc phases. The interplay of H with GBs depends on the phase structure. For fcc-Fe, GBs provide an accelerating path for hydrogen diffusion. As opposite, GBs in bcc-Fe may retard hydrogen mobility compared to bulk case. Calculated hydrogen concentration and diffusivity at GBs were used to interpret experiments on H permeation [2]. For bcc Fe we show that GBs of the considered type do not act as diffusion accelerating channels. Hence, we may assume that a picture of H permeation observed in situ came from a combination of fast H diffusion in bulk and strong segregation at GBs.

[1] Smirnova, D., Starikov, S. (2023). Atomistic study of hydrogen diffusion in presence of defects in bcc and fcc iron. *Comp. Mater. Sci.*, 230, 112433.

[2] Koyama, M., Yamasaki, D., Nagashima, T., Tasan, C. C., Tsuzaki, K. (2017). In situ observations of silver-decoration evolution under hydrogen permeation: Effects of grain boundary misorientation on hydrogen flux in pure iron. *Scripta Materialia*, 129, 48-51.

Integrating in-situ performance tests, advanced materials characterization, and computational modelling to understand hydrogen-material interactions

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B8_4, Seminario 8 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

To realise the promise of the hydrogen economy, the structural integrity and operational reliability of components, assets and infrastructures needs to be ensured all through the hydrogen value chain: production, storage and transfer, and utilization. Particularly in the storage and transport phase, materials are retained long times in interaction with gaseous hydrogen (H₂), that has the capacity to dissociate in the atomic form. Hydrogen as the smallest of atoms diffuses readily into and within materials, with diffusion characteristics relying strongly on the material microstructure and chemical composition. On the macroscale, hydrogen may contribute to the dramatic loss of plastic deformation capability and/or load bearing capacity of structural materials, a phenomenon called hydrogen embrittlement (HE). This may occur already at ppm levels of hydrogen in the material.

For components, assets and infrastructures to perform as planned, interactions between materials and hydrogen need to be understood well. This work gives an overview, how the combination of advanced tools in materials research: in-situ performance tests, advanced materials characterization methods, and multi-scale multi-physics computational modelling can deepen the understanding of material-hydrogen interactions. Selected example cases are demonstrated.

A comparative study of hydrogen trapping kinetics and embrittlement susceptibility of additively manufactured and wrought 316L austenitic stainless steel: influence of post-processing

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B8_3, Seminario 8 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Selective laser melting (SLM) is one of the common methods of additive manufacturing technology. SLM can be employed to customize mechanical components with complex geometry such as elbows and valves, which are expected to work in hydrogen atmospheres under high-pressure hydrogen gas. However, more studies are still needed to characterize the behavior of the printed mechanical components intended to work in contact with gaseous hydrogen. It is known that additively manufactured 316L boasts superior mechanical properties than those of conventional state. However, greater absorption of hydrogen can be induced in the SLMed 316L because of its higher density of dislocations, induced due to the rapid cooling rates during solidification. Accordingly, new production techniques, especially additive manufacturing, require re-evaluation of hydrogen susceptibility of austenitic stainless steels.

In this work, microstructural and mechanical behavior, in the presence of internal hydrogen, of the 316L wrought series and the as-built and post-heat-treated additively manufactured 316L samples, is studied.

Experimentally, thermal desorption analysis (TDA) and electrochemical hydrogen permeation (EP) experiments are both used to analyze hydrogen trapping and diffusion kinetics, in the different series. In this regard, the hydrogen concentration, the apparent hydrogen diffusion coefficient (D_{app}), the density of traps (NT) and hydrogen activation energies (E_a) attributed to the desorption of hydrogen from various microstructural singularities, are compared among the analyzed series. TDA analysis was carried out on hydrogen precharged samples at high temperature.

Besides, mechanical behavior is analyzed at room temperature by Slow Strain Rate Tests (SSRTs) on smooth tensile samples, precharged in a high-pressure hydrogen reactor at 195 and 300°C for 24h. Fracture mechanisms (HELP -Hydrogen Enhanced Localized Plasticity- and HEDE -Hydrogen Enhanced Decohesion-) and micromechanisms are deeply analyzed.

Hydrogen damage was especially noted in the 316L wrought series (i.e. hot-rolled and annealed grade), where fracture micromechanism changed from ductile in the absence of hydrogen to quasi-brittle in the presence of internal hydrogen. In this case, the presence of HELP (Hydrogen Enhanced Localized Plasticity) mechanism was also confirmed. On the other hand, HE resistance enhanced in the printed samples, especially in the post-heat-treated SLM 316L series, where the fracture micromechanism was ductile.

To explain the impact of the internal hydrogen on the mechanical properties of the studied series, the role of the strain-induced martensite, dislocation glide, deformation twinning, and cellular structures is discussed.

Evaluation of the hydrogen embrittlement index for a martensitic advanced high strength steel using ex-situ tensile tests

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Car body-in-white lightweighting is a pathway to improved sustainability of the automotive industry due to the following increased fuel efficiency. For this reason, ever higher-strength steels with moderate ductility are being actively developed in the field.

Hydrogen does interact with steels in multiple ways, in a series of phenomena collectively known as hydrogen embrittlement. Even low amounts of hydrogen can significantly impact ductility of automotive high strength steels, which is required both for sufficient formability and crashworthiness.

A commonly used technique for better performing such risk assessment is the identification of an hydrogen embrittlement index, which correlates loss of mechanical or technological properties of the steel to hydrogen content. In this work an advanced characterization of the hydrogen embrittlement index for a martensitic advanced high strength steel is performed. To that aim, ex situ electrochemically charged tensile specimen are tested in the slow strain rate regime and the effects of hydrogen on the tensile curve are evaluated. The interpretation of the tests is aided by their FEM simulations which allow for a better understanding of the stress and strain conditions in the specimen at fracture nucleation conditions. Further, a simulation of hydrogen diffusion and trapping considering its outgassing kinetics at room temperature allows for a better understanding of the hydrogen concentration present in the specimen. Correlation of both the concentration data and the stress-strain state at fracture nucleation may provide a better formulation of the hydrogen embrittlement index.

Hydrogen-Enhanced Entropy (HEENT) Mechanism For Hydrogen Embrittlement in Metals: An Umbrella Over HELP, HEDE and HESIV Mechanisms

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

One of the most serious challenges in materials science is hydrogen embrittlement (HE). It mainly concerns structural elements that are cyclically loaded in an environment rich in hydrogen, such as in a pressure vessel. Though Paris' law and Coffin-Manson laws are fundamental models for estimating the propagation of fatigue cracks and the lifetimes in low-cycle fatigue, their conventional forms are not able to capture the rather complex hydrogen/material interactions. This study attempts to bridge this fundamental gap by addressing the hydrogen effects on the fatigue performance, proposing new versions of the Paris' and Coffin-Manson laws, and validating these modifications via numerical simulations and experimental data.

The law of Paris was used to analyse the rates of crack growth (da/dN) under variable hydrogen concentrations, pressures, and cyclic loading conditions. A new modified model was developed to include hydrogen-specific parameters associated with the crack tip such as the hydrogen concentration, activation energy for embrittlement, and those environmental factors such as temperature and pressure. The Coffin-Manson law, on the other hand, was modified to incorporate a direct account of reduced ductility and accelerated initiation associated with hydrogen embrittlement effects. Important parameters such as fatigue ductility coefficient (ϵ_f) and exponent (c) were determined experimentally for high-strength steels and aluminium alloys in hydrogen environments. Further, the work focuses on the impacts of hydrogen on threshold stress intensity factors (ΔK_{th}) and fatigue limit, providing more insight about the environmental sensitivities of these parameters.

Finite Element Simulations with the Aid of Abaqus for verification of revised laws. The model considered hydrogen diffusion, a localized plasticity, and crack development for analysing crack propagation under simultaneously applied mechanical and environmental stress. The comparative exercise indicated the extent to which the revised laws significantly improve prediction accuracy for materials undergoing hydrogen embrittlement. This shows that hydrogen increases the rates of crack growth and shortens the fatigue lifetimes, thereby underlining the need for incorporating hydrogen-sensitive factors in models.

This research addresses a significant gap in the literature by presenting a cohesive framework for predicting fatigue life in environments rich in hydrogen, integrating experimental findings with computational modelling. It presents practical consequences for sectors like aerospace, automotive, and energy, where hydrogen embrittlement threatens the integrity of components. Upcoming research will concentrate on broadening the material database and investigating multiscale modelling techniques to enhance the predictive abilities of these adjusted laws.

Hydrogen Distribution in FCC and BCC Alloys: Impact of Electrochemical Charging Conditions

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B8_2, Seminario 8 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Hydrogen charging into a material is typically achieved through either gaseous or electrochemical methods. Gaseous charging involves exposing the material to a high-pressure hydrogen gas environment at elevated temperatures, whereas electrochemical charging takes place in an electrolytic solution under either galvanostatic or potentiostatic conditions, usually at or near room temperature. Due to safety concerns associated with the use of pressurized hydrogen gas, electrochemical charging is sometimes employed as an alternative for hydrogen gas exposure when investigating hydrogen embrittlement susceptibility of a material. The severity of hydrogen embrittlement effects is highly dependent on the hydrogen charging conditions. Therefore, the optimization of the charging conditions is crucial for accurately assessing material behaviour. Thermal desorption spectroscopy (TDS) is a prevalent analytical method used in the study of hydrogen absorption behaviour and distribution in metals, which can lead to hydrogen embrittlement (HE). In our study, cathodic charging at different temperatures was conducted in sulfuric acid and neutral NaCl solutions using various steel samples with both face-centered cubic (FCC) and body-centered cubic (BCC) structures. The effect of the charging conditions on hydrogen uptake and distribution was studied via TDS, aiming to improve the accuracy and effectiveness of hydrogen charging, which is essential for assessing hydrogen embrittlement susceptibility in metallic materials.

Influence of environment and crystallographic factors and on hydrogen embrittlement in Al-Zn-Mg alloy

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Al-Zn-Mg alloys possess high strength but also exhibit high sensitivity to hydrogen embrittlement. Hydrogen embrittlement occurs not only by hydrogen present within the material but also by external hydrogen from the environment (e.g., through corrosion). To develop materials with high resistance to hydrogen embrittlement, it is crucial to identify the microstructural features that are most susceptible and most resistant to hydrogen embrittlement. In a previous study, we proposed a method for identifying the strongest and weakest grain boundaries with respect to internal-hydrogen-induced intergranular cracking using three-dimensional (3D) image-based statistical analysis. However, the effect of external hydrogen is known to be higher in promoting hydrogen embrittlement than that of internal hydrogen. Therefore, this study investigated the dominant factors influencing external-hydrogen-induced fracture behavior in an Al-Zn-Mg alloy by analyzing hydrogen embrittlement under controlled environmental conditions using multi-modal 3D image-based analysis.

Al-9.6%Zn-1.8%Mg ternary alloy was prepared. Specimens for in-situ tensile testing were prepared using electrical discharge machining in water, which resulted in hydrogen charging during the cutting process. The in-situ tensile tests were conducted in both water and a pure argon atmosphere. X-ray computed tomography (CT) and diffraction contrast tomography (DCT) experiments were performed at BL20XU in SPring-8 to visualize the 3D microstructure and hydrogen embrittlement behavior.

On the fracture surface, ductile fracture was dominant in the argon atmosphere. On the other hand, intergranular and quasi-cleavage fracture surfaces were observed in the water environment. This result clearly demonstrates that the external environment promotes hydrogen embrittlement. Crack initiation sites were identified by superimposing 3D crack and grain images. Design parameters representing the shape and size of grains and grain boundaries were determined for all grains and grain boundaries. Principal component analysis (PCA) and global sensitivity analysis (GSA) were employed to select the design parameters that had the greatest influence on hydrogen embrittlement.

Using the selected design parameters, metamodeling analysis was used to predict the weakest microstructures, i.e., those with the highest probability of cracking, for both transgranular and intergranular cracks. Intergranular cracks initiated at grain boundaries where three constituent grains at a triple junction exhibited different shapes and high Schmid factors. These grains are likely to undergo plastic deformation more readily, which facilitates the reaction between external water and aluminum, leading to localized hydrogen enrichment and promoting early initiation of intergranular cracking. Eliminating grains and grain boundaries exhibiting these weakest microstructural characteristics represents an effective approach to designing materials resistant to external-hydrogen-induced fracture.

Hydrogen embrittlement of 316L stainless steel studied by synchrotron tomography.

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B8_2, Seminario 8 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Europe's decarbonization program aims to replace gas, petrol and coal with green energies such as green hydrogen, which is produced by renewable energy such as windmills. Green hydrogen needs to be transported and stored in pipelines or tanks. Hydrogen storage structures are often made from austenitic stainless steel, like 316L.

However, the materials used in this application may experience hydrogen embrittlement (HE). In storage or transport applications, gaseous hydrogen will diffuse into the bulk. Following the time exposure, different conditions can be observed: gaseous hydrogen is present as a gradient or is uniformly present inside the bulk.

The material used in this study is a sheet of 316L stainless steel sheet. To quantify HE phenomenon of this material, tensile tests are performed on sub-size tensile samples. Testing conditions are: (i) under air, (ii) under hydrogen gas at 240 bar and (iii) thermally H₂ precharged samples. Tests are conducted to fracture using strain rate of 10⁻⁴ s⁻¹ and 10⁻⁵ s⁻¹. Tests interrupted before fracture were also performed for subsequent nondestructive ex-situ synchrotron micro-tomography examination. In-situ tomography tests were carried out with thermally hydrogen precharged samples. Damage evolution is quantified through ex-situ and in-situ tomography measurements carried out at Soleil Synchrotron.

Each post-mortem sample is additionally analyzed by classical SEM fractography to quantify the ductile to brittle transition, but not only. Results witness a significant effect of hydrogen on 316L stainless steel: there is a significant decrease in ductility and a moderate reduction of ultimate tensile strength. Hydrogen-atmosphere tested samples exhibit flat surface cracks of 80 to 100 µm depth. There is a coalescence zone between the surface cracks which exhibits a mixture of brittle damage features, ductile dimples and ductile shear features that could originate from the HELP mechanism. In addition, there are aligned damage features surrounded by ductile dimples for a strain rate of 10⁻⁴ s⁻¹. Their sizes and spacing is consistent with the presence of delta ferrite revealed by metallography and EBSD. Moreover, the potential effect of martensitic transformation on hydrogen embrittlement is investigated. In addition, gage length observation reveals a significant amount of surface cracks. Fracture scenario seems to be the result of a competition between HE of the surface, internal ferrite-related cracks, martensite transformation and ductile shear damage. For a strain rate of 10⁻⁵ s⁻¹, deeper brittle surface cracks are seen. Ductile damage features are also present at the center of the sample.

Effect of hydrogen on the passivity of steel: investigating the role of the surface and interfaces

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B8_5, Seminario 8 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

In the context of a growing hydrogen economy, we must confront a relevant number of challenges arising from hydrogen interaction with steel across various stages of production, storage, transportation, and utilization. While extensive research has been conducted on hydrogen embrittlement, the role of the passive oxide layer, which naturally forms on steel surfaces in both natural and controlled atmospheres, has received little attention. This layer serves a dual function: protecting against corrosion and potentially acting as a barrier to hydrogen ingress.

To investigate this, the interaction of hydrogen with the main components of steel oxides, namely Fe and Cr oxides, was studied. Fe-Cr alloys at different relative amounts are prepared by magnetron sputtering and subsequently in-situ thermally oxidized to simulate different steel oxides. Electrochemical hydrogen charging was performed using a custom flow cell within a glovebox, allowing hydrogen exposure on one side of the sample while maintaining an inert argon atmosphere on the other. This setup minimizes surface polarization and unintended modifications on the surface of interest, enabling the evaluation of hydrogen's effects on the oxide layer.

Post-charging, the samples are transferred under ultra-high vacuum conditions for analysis using both soft and hard X-ray photoelectron spectroscopy (XPS and HAXPES). The analysis focuses on determining the oxide layer thickness, composition, oxide/hydroxide phase distribution, the Fe³⁺/Fe²⁺ ratio within the oxide films, and the chemical states of elements at and near the oxide/alloy interface.

Additionally, hydrogen quantification and depth distribution within the thin passive layers were studied using Elastic Recoil Detection Analysis (ERDA). A custom electrochemical cell was designed for in-operando ERDA analysis during hydrogen charging, enabling measurements throughout the permeation transient.

This integrated approach offers new insights into hydrogen penetration, diffusion, and solubility mechanisms within steel surface layers, enhancing our understanding of hydrogen-steel interactions, contributing to the development of more durable materials for hydrogen-related applications.

Hydrogen induced softening and deformation mechanisms in nanoparticle reinforced CoCrFeNi

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B8_3, Seminario 8 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Hydrogen embrittlement poses a critical challenge for structural materials in energy infrastructure, particularly in emerging hydrogen-based technologies and storage systems, where material degradation can lead to catastrophic failures. This study investigates the influence of hydrogen charging on the mechanical behavior and deformation mechanisms of TiN and TiO₂ nanoparticle-reinforced CoCrFeNi medium entropy alloy (MEA) processed via laser powder bed fusion (LPBF). A characteristic LPBF microstructure consisting of alternating refined grain tracks and larger square grain pockets was obtained. Nanoindentation revealed that the as-processed composite exhibited minimal mechanical anisotropy, with hardness values of 3.55 ± 0.12 GPa in track regions and 3.51 ± 0.11 GPa in pocket regions, indicating homogeneous distribution of TiN reinforcement particles.

Electrolytic hydrogen charging was conducted under potentiostatic conditions (-1.2 V) for durations of 12 and 24 hours. Systematic nanoindentation mapping coupled with electron backscatter diffraction was performed on all the hydrogen charging conditions. Following 24-hour charging, thermal desorption spectroscopy detected 20 wt. ppm of hydrogen. The hydrogen-exposed surface showed a significant reduction in hardness to 3.05 ± 0.03 GPa, while the unexposed surface maintained 3.46 ± 0.19 GPa. High-resolution scanning transmission electron microscopy analysis combined with precession electron diffraction of subsurface deformation zones revealed distinct changes in deformation mechanisms. The uncharged state exhibited prevalent deformation twinning, whereas the hydrogen-charged condition displayed spatial heterogeneity in deformation features: well-defined subgrains with reduced dislocation content near the indent, and localized deformation twins in deeper regions.

These observations suggest a hydrogen-enhanced localized plasticity (HELP) mechanism, where hydrogen facilitates dislocation mobility and dynamic recovery processes. The spatial distribution of deformation features indicates complex interactions between competing mechanisms: enhanced dislocation mobility through HELP and increased propensity for twinning due to hydrogen-induced reduction in stacking fault energy. The presence of TiN nanoparticles appears to influence the distribution and evolution of these deformation mechanisms, potentially through their role as hydrogen trapping sites and stress concentrators. These findings provide new insights into hydrogen-microstructure interactions in nanoparticle-reinforced MEAs and demonstrate the potential of microstructural engineering for enhancing hydrogen embrittlement resistance in advanced structural materials.

Hydrogen-defect interaction in nanostructured iron samples

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B8_2, Seminario 8 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Understanding hydrogen embrittlement has been in the focus of metal research for many decades. Since the embrittling effect of hydrogen is most pronounced for high-strength grades (i.e., small structural sizes or multi-phase structures), the small (submicron) microstructural dimensions and their chemical and structural complexity (i.e., multiphase steels) makes a direct determination of the trapping sites and associated effects on the defect behavior challenging. This knowledge would however, be essential to understand failure mechanisms and derive effective design guidelines for hydrogen resistant materials. To reduce the chemical and microstructural complexity we therefore focus on hydrogen-defect interactions in nanostructured pure iron. This simple model material contains only grain boundaries and dislocations, but perfectly allows to reproduce the mechanical behavior of (nano) bainitic, pearlitic or martensitic steels. Deforming hydrogen charged nanostructured iron specimens thus allows for conclusions of a wide range of structural materials.

We will show by cyclic high-pressure torsion of pre-charged samples that hydrogen is homogeneously distributed in the specimen and does not favor strain localization nor enhances plasticity during cyclic loading. In fact, hydrogen seems to be located at grain boundaries and effectively pins them, stabilizing the nanostructure. For monotonic loading quite the opposite is observed. Deformation in the hydrogen charged samples becomes inhomogeneous and outstanding hardness (up to 11 GPa) and grain refinement (sub-10 nm grains) in these localized regions was observed. This implies that the effect of hydrogen on grain boundaries and dislocations depends not only on the material but also on the strain path applied.

Hydrogen effects on the scratch-induced deformation of pearlitic steel

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Hydrogen-induced degradation presents a significant challenge to materials and infrastructure in the context of hydrogen energy utilization. Hydrogen embrittlement in steels arises from interactions between solute hydrogen atoms and microstructural features. During production, transportation, and assembly, steel components inevitably develop surface scratches, which can become areas sensitive to hydrogen embrittlement. Pearlitic steel displays excellent mechanical properties, like tribological properties, due to its lamellar structure composed of alternating layers of ductile ferrite and brittle cementite. In this work, micro-scratch tests were performed on a pearlitic steel using an in situ backside hydrogen charging setup assembled on a standalone nanoindentation instrument. This allowed for the examination of scratch behavior during electrochemical hydrogen charging. The interactions between hydrogen and scratch-induced deformation under different scratch directions, that is, parallel to cementite lamella, perpendicular to cementite lamella, and inclined with cementite lamella were studied. The deformation response of ferrite-cementite interface varied across these directions. This work contributed to the understanding of hydrogen-induced damage in materials.

Boron segregation informed HE mitigation strategy in a two-phase lightweight steel

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B8_2, Seminario 8 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

In response to stringent regulations and challenges regarding weight reduction for fuel economy as well as the enhancement of crashworthiness performance for passenger safety in vehicles, advanced Fe-Mn-Al-C lightweight steels with specific high strength have garnered significant attention in recent decades. However, these alloys are prone to hydrogen embrittlement (HE) which hinders their application. The understanding of the operating mechanisms of HE and the development of effective strategies to mitigate HE are inevitably important. Here we studied the HE mechanisms and the effect of boron-doping on hydrogen-tolerant capability in lightweight steels featuring an austenite plus ferrite two-phase microstructure. We found the embrittlement in these alloys is driven by hydrogen-induced intergranular cracking along austenite-ferrite phase boundaries and hydrogen-induced transgranular cracking inside the ferrite phase. The boron-doped material demonstrates an enhanced hydrogen-induced intergranular resistance albeit with a reduced resistance to hydrogen-induced cleavage cracking within the ferrite phase. These effects are further elucidated based on a detailed comparison of damage behavior, the segregation of boron via atom probe tomography and the ab initio calculations. Those findings shed light on boundary conditions of different HE mechanisms in multiphase alloys as well as the effective mitigation strategies for HE.

Hydrogen Effects in Pre-Strained 316L Austenitic Stainless Steel Sheets

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B8_4, Seminario 8 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The maritime industry is actively investigating innovative technologies for the safe transportation and storage of liquid hydrogen (LH2), playing a crucial role in the shift toward a sustainable green economy. Material selection of storage tanks is a critical factor, given the extreme conditions required for LH2 containment (-253 °C, at atmospheric pressure). LH2 tanks utilize corrugated austenitic stainless-steel sheets due to their outstanding mechanical performance at cryogenic temperatures, superior resistance to hydrogen diffusion, and excellent weldability. However, the corrugation process induces pre-deformation in the material, significantly increasing its susceptibility to hydrogen embrittlement (HE) due to strain-induced martensitic (SIM) transformation. Controlling and understanding this transformation is essential for ensuring long-term reliability. This study aims to shed light on the link between SIM and HE of AISI 316L stainless steel, as a promising candidate material for LH2 applications. Specimens were subjected to uniaxial pre-strain at varying levels (10%, 20%, 30%, and 40%) to replicate the effects of corrugation process. Cathodic charging was employed to introduce hydrogen into the material efficiently, bypassing the prolonged exposure times required for natural diffusion. To analyze the phase transformations induced by pre-straining, metallographic techniques such as Electron Backscatter Diffraction (EBSD) and X-ray Diffraction (XRD) were employed. The influence of hydrogen was assessed through two key aspects: the amount of hydrogen absorbed by the material and its impact on mechanical properties. Thermal Desorption Spectroscopy (TDS) was used to quantify hydrogen absorption and correlate it to the fraction of SIM. Additionally, Slow Strain Rate Tests (SSRT) were conducted on cathodically H-charged specimens that contained a fraction of SIM from prior pre-straining. The insights gained from this research showed an increasing martensite fraction as pre-strain increased, despite the relative stability of 316L, which affected H absorption and ductility. These findings will contribute to the development of optimized materials and structural designs for LH2 storage and transportation, ensuring greater safety and reliability in future marine applications.

CABLE Twitchalloy: Design of a High Strength, High Electrical Conductivity and High Thermostability Aluminum Alloy

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B9_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Recycling of aluminum alloys is the best practice to reduce the carbon footprint of automotive aluminum products, however the aluminum scrap, “twitch”, is contaminated with impurity elements such as Fe and Si, and the cost of recycling techniques is significantly high. In parallel, the U.S. electricity delivery system undergoes changes to improve its reliability and resilience to extreme weather conditions. The design of a novel thermostable aluminum-based cable conductor for overhead transmission lines utilizing high volumes of aluminum twitch is a promising solution and a cost competitive way to recyclability. In the present study, CALPHAD-based ICME tools are employed for the design of an aluminum cable conductor with high strength, high electrical conductivity, and high thermostability via melt-spinning and high-temperature aging. A hierarchical system-based approach is adopted, and the thermodynamic calculations are aided by high-throughput DFT databases to design novel intermetallic compounds supporting new classes of aluminum alloys compatible with recycling of automotive scrap. The main design objectives are to maximize the electrical conductivity through the complete gettering of the impurity elements and maximize the precipitation strengthening through the formation of Q phase and the elimination of Si phase. Rapidly solidified specimens that utilize aluminum twitch were prepared, and electrical resistivity measurements using the 4-point probe method were carried out at room temperature. The calculations were validated experimentally, and the microstructures of the specimens were characterized via STEM and APT analyses.

Prediction of Porosity in CFRP Ultrasound Testing Using Deep Learning and X-ray CT

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B9_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Fast and reliable nondestructive testing (NDT) is critical for the carbon fiber reinforced polymer (CFRP) industry. NDT covers a range of techniques and plays a pivotal role in the development of novel materials by enabling the assessment of their properties and verifying the reliability of new manufacturing methods. During production, NDT is essential for quality assurance, ensuring that manufactured samples comply with required specifications. Additionally, NDT is invaluable for maintenance applications, allowing for the detection of defects caused by operational use. One key defect in CFRPs that can significantly influence mechanical performance is porosity. Porosity can lead to degraded mechanical properties and cause early catastrophic failure of parts, making its precise evaluation essential. The void volume fraction, which quantifies the percentage of a sample's volume occupied by voids, is a widely recognized metric for assessing porosity. Accurately measuring void volumetric fraction requires NDT techniques capable of high-resolution 3D data acquisition, such as X-ray Computed Tomography (XCT). While lab XCT offers unparalleled micron up to submicron resolution and detailed internal structure visualization, it is expensive, time-consuming, and demands strict experimental conditions. In contrast, ultrasonic testing (UT) is a highly efficient NDT method extensively used in the CFRP industry for its rapid diagnostic capabilities across varying sample sizes. However, UT faces limitations in resolution and clarity of internal structural representations compared to XCT. To bridge this gap, our research focuses on combining the efficiency of UT with the precision of XCT through artificial intelligence (AI). Specifically, we aim to leverage UT data to predict porosity metrics equivalent to those derived from XCT. We developed an end-to-end data pipeline, including automated data preprocessing and registration, and several deep learning models designed to predict the void volumetric fraction from UT measurements. So far, the best model has reached a R^2 score of 0.68. In this study, we present the comparison between model prediction and XCT data, to investigate the extent to which porosity prediction captures relevant porosity-related information. This allows to evaluate the potential of AI to enhance the precision of UT-based NDT.

Quantitative analysis on ML-DIC patch for daylight and dark mode strain measurement

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B9_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The Al-Zn-Mg-based 7xxx series aluminum alloy is widely utilized in aircraft as a structural material due to its excellent strength-to-weight ratio, fatigue properties, and superior corrosion resistance compared to the 2xxx series alloys. The A7050 alloy, known for its high strength, resistance to stress corrosion cracking, and fracture toughness, can be produced in rolled sheet form due to its low sensitivity to heat treatment, making it suitable for various aircraft structural components.

Detecting internal cracks within aircraft structures made from such materials poses a challenging task and overlooking them during inspections can lead to catastrophic accidents. To address this issue, various non-destructive testing methods have been investigated, among which the use of mechanoluminescent (ML) materials has been chosen. ML materials, a type of luminescent substance, can convert the luminescent intensity induced by mechanical stimuli such as tension, compression, torsion, and friction into measurable stress, which can then be further translated into strain by employed to perform comparative analysis between ML materials and strain.

Therefore, in this study, specimens fabricated from A7050-T7451 were intentionally introduced with randomly positioned, angled, and sized defects to simulate real-world conditions. ML and DIC images were captured during tensile testing, and each obtained image was meticulously examined and evaluated to analyze the presence of defects at the rear surface of the specimens.

Alloy design of γ' -strengthened CoNi-based superalloys with low crack susceptibility suitable for additive manufacturing

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B9_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

γ' -strengthened CoNi-based superalloys are more suitable for additive manufacturing (AM) than γ' -strengthened Ni-based superalloys due to their narrower freezing range and better weldability. In this study, a design methodology for CoNi-based superalloys suitable for additive manufacturing was developed by integrating machine learning (ML) with calculation of phase diagrams (CALPHAD) approach. This methodology comprehensively accounted for critical factors, including phase equilibrium, γ' volume fraction, γ' size, γ' solvus temperature, oxidation resistance, alloy density, and sensitivity to strain age cracking of CoNi-based superalloys. This approach enables an effective design of CoNi-based superalloys for additive manufacturing with low crack sensitivity. The results show that the designed alloy exhibited exceptional printability, minimal compositional segregation, and the ability to produce crack-free components with a relative density exceeding 99.99% on non-preheated substrates by selective laser melting (SLM). Furthermore, the designed alloy demonstrated an exceptional outstanding strength–ductility synergy. This study provides valuable technical insights for the engineering application of additively manufactured CoNi-based superalloys.

Machine-learning the thermodynamics of multi-principal element structural alloys through chemically embedded cluster expansions

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B9_1, Seminario 7 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Multi-principal element alloys are an emerging class of materials that are attractive candidates for structural, electronic and electrochemical applications. A systematic investigation of chemical space in such alloys is however untenable. Computational techniques, such as the cluster expansion methods, have proven to be useful tools in discerning alloy compositions with favorable properties and enabling a fundamental understanding of phase stability in multi-component alloys. However, the cluster expansion method remains difficult to deploy in alloy systems containing several chemical components. In conventional cluster expansions, the number of features scales polynomially with the number of alloying elements. The rapid increase in the number of features causes difficulties in parameterizing and evaluating conventional cluster expansions. Here, we introduce the embedded cluster expansion (eCE) formalism that mitigates this rapid growth in the number of features. Chemical similarities between elements are simultaneously learned during training to reduce the number of site-basis functions. We will then describe how eCE models can be deployed to build accurate thermodynamic models of refractory alloys containing up to 9 elements. We show that the eCE model can successfully reproduce ordering energetics of the alloy, requires a limited amount of data, and can robustly extrapolate ordering energies.

In-Situ Alloying through 3D printing of Ti-15Nb alloy and MMC of β Ti-42Nb/TiC

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β Ti alloys are considered for biomedical applications due to their mechanical properties, good biocompatibility and corrosion resistance. Based on that, Ti and its alloys have been applied as biomedical implants, especially the Ti-6Al-4V alloy. However, such alloy presents problems regarding cytotoxicity of Al and V elements related to neural disorder and Alzheimer's disease, although it presents good mechanical properties. Regarding orthopedic applications there is a considerable difference between elastic modulus of Ti and $\alpha+\beta$ alloys, from $E = 100$ to 110 GPa, and that of human bone, around $E = 30$ GP, having β Ti alloy lower $E = 50$ to 80 GPa closer to that of the bone. In this context, the metastable β alloy Ti-15Nb (% by weight) appears, which will be processed through laser powder bed fusion (LPBF) and arc melting, since this is free of cytotoxic elements and shows lower Young modulus. Another approach is LPBF of metal matrix composite (MMC) of β Ti-42Nb powder with micrometric graphite (C) addition for in-situ TiC precipitates formation for increase of hardness, mechanical strength and wear combined with slightly increase of elastic modulus maintaining in low levels. Characterization of LPBF β Ti-15Nb alloy and MMC of β Ti-42Nb with graphite (C) addition for in-situ TiC formation, were done by optical microscopy (OM), X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission (TEM) techniques, Vickers microhardness, and modulus of elasticity via excitation will be used. by impulse or nanohardness. Phase identification was done by X-ray diffraction (XRD), scanning (SEM) and transmission (TEM) electron microscopy coupled to ASTAR - automatic crystal orientation mapping (ACOM). hardness. The LPMF of β Ti-15Nb alloy formed $\alpha'+\beta$ microstructure, the Vickers microhardness and elastic modulus measured by nanohardness and impulse excitation technique were evaluated, showing suitable modulus of $E = 60$ GPa. The MMC of β Ti-42Nb + TiC resulted in Vickers microhardness of 215 to 239 HV and elastic modulus of $E = 57$ to 65 GPa for (Ti-42Nb alloy and MMC being suitable for bulk and coatings for biomedical implants, respectively.

Ternary NiTi-Nb eutectic alloys by laser powder bed fusion (LPBF): In situ phase formation by design of energy density

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C1_1, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 9:20 - 10:20

Alloying of niobium into the pseudoelastic NiTi alloy upon laser powder bed fusion (LPBF) of a eutectic stoichiometry was investigated under the impact of various volumetric energy densities. Specifically, the research examined the effects of volumetric energy density (VED) ranging from 56 to 89 J/mm³ on the potential in situ phase formation. The mechanisms behind the formation of these in situ phases, influenced by the applied VED during processing, were analyzed and compared with the results from micro-mechanical testing. To achieve this, nanoindentation testing was performed, and the resulting hardness distribution was mapped and correlated with microscopy findings related to the possible phase formations.

Novel directed energy deposited WC-Fe/Ni based wear resistant coatings for tillage tools

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The wear resistance of tillage tools depends not only on the coating process, but also on the properties of the powders and composites used. The microstructure and properties of Noval WC-Fe/Ni based composites produced by the arc thermal atomisation process will be highlighted. The influence of the atomised composites on the wear and mechanical properties of directed energy deposited coatings of tillage tools will be presented.

Development of Sustainable Fe-based Composite Powders for Highly Wear-Resistant Coatings

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C1_2, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 10:50 - 13:10

The automotive industry faces growing dependence on raw materials, which is caused by the rise of electromobility. In producing wear-resistant components and sheet metal forming tools, coating materials and processes are crucial for performance, sustainability, and lifespan.

This work focused on developing sustainable composite powders and innovative manufacturing processes for highly wear-resistant coatings. A novel Fe-based coating composition (Fe-Cr- X) was designed to reduce dependence on critical raw materials such as nickel, cobalt, and tungsten. A thermal arc atomization process was introduced, achieving an 80% efficiency for particles within the 40–150 μm range, without formation of hollow spheres, and lowering gas consumption by 15%. The microstructure and properties of the composites and the coatings will be presented.

Tribological Behavior of STS316L Sintered Bodies and Cu/STS316L Composites Fabricated via Binder Jetting Process

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The binder jetting (BJT) process is a promising additive manufacturing technique known for its high material selectivity and ability to create complex shapes. It enables the production of porous and composite materials through sintering and impregnation, techniques commonly used in powder metallurgy. STS316L powder is widely used in BJT due to its excellent weldability, corrosion resistance, and tribological properties. However, research on its tribological behavior is limited.

This study investigates the tribological properties of sintered STS316L bodies and Cu/STS316L composites fabricated using the BJT process. Sintering was performed at three different temperatures: 1100, 1200, and 1300°C. Tribological tests were conducted using the Pin-on-disc method, and friction coefficients along with wear marks were analyzed using scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS). The results showed that for STS316L, both the friction coefficient and wear mark size increased with the sintering temperature. In contrast, Cu/STS316L composites exhibited stable friction coefficients and smoother wear marks under all conditions. Microstructural analysis of the wear traces helped identify the underlying tribological mechanisms.

Application of Twin Wire and Arc Additive Manufacturing (T-WAAM) process for manufacturing of Invar 36 by in-situ alloying

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C1_2, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 10:50 - 13:10

Metal Additive manufacturing (AM), where metallic materials are added to the parts layer by layer, has attracted high attention over the last years due to its design freedom ability and short lead times. Among the metal AM processes are the so-called Directed Energy Deposition (DED) technologies, where a focused thermal energy source is used (laser beam, electron beam or electric arc) to melt materials as they are deposited. This research work analysed the possibility of creating the Invar 36 alloy using the DED-arc metal AM process or better known as WAAM (wire and arc additive manufacturing), more specifically in its Twin mode using two metallic wires as raw materials. The T-WAAM process is characterized by the use of two fully synchronized and independent power sources. From these two power sources two metallic wires are fed into a single torch, by means of two separate wire feeders, through two fully insulated contact tips. A single shielding gas nozzle is employed, and the two arcs generate a single weld pool. The possibility of isolating the power sources and at the same time their operation is synchronized increases the possibility of combining different synergistic curves, such as Cold Metal Transfer (CMT) mode, pulsed or other innovative synergistic curves. In this way, the deposition rate or welding speed can be doubled. In this work, the Twin-WAAM technology is used to obtain the Invar 36 alloy by mixing a steel and a Ni-Fe wires with in-situ alloying approach. Invar36 is an interesting material for skins in molds but its cost is high. With this manufacturing method it would be possible to manufacture steel parts with Invar 36 in desired areas by introducing tailored compositions in the manufacturing process. The microstructure and the mechanical properties of the in-situ manufactured Invar 36 alloy by T-WAAM has been investigated. The obtained results are compared with the ones obtained with commercial Invar 36 alloy wire manufactured by WAAM. The results revealed that there is a difference of 4-6% of the strength between the commercial Invar36 and the obtained T-WAAM alloy, been lower in the obtained alloy. The opposite is true for elongation, which is higher for the obtained alloy (10-15% higher than the commercial Invar 36).

Niobium alloy C-103 for high-performance space applications – first results with using Cold Spray Additive Manufacturing – CSAM

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C1_2, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 10:50 - 13:10

Space propulsion applications require lightweight materials that can withstand high stresses at elevated temperatures. Niobium has a very low density compared to other refractory metals but high strength, i.e. a high strength-to-weight ratio. The material also shows high thermal conductivity and a low ductile-to-brittle transition temperature. This low transition temperature is advantageous for space applications because it shows excellent resistance to high-frequency vibrations at cryogenic temperatures. Furthermore, C-103, a niobium, hafnium, and titanium alloys used for space propulsion applications, have a high melting point at around 2.350°C and show strong stability at elevated temperatures, too.

Currently, many investigations around C-103 material for in-space propulsion systems for satellites are happening in the space industry. This work shows the feasibility of Cold Spray Additive Manufacturing (CSAM) technology to produce a C-103 test part as a first step for future nozzle designs for different space applications. It is essential for the application to have as thin walls as possible to get down the take-off weight of the satellites. A tube of around 135 mm in length and 2 mm in wall thickness has been manufactured using CSAM. Secondly it will be presented a first Cold Sprayed nozzle with a length of about 600 mm and a diameter of about 500 mm and a wall thickness of around 1,5 mm only. The manufacturing process will be presented in detail, in pictures and videos. The work also shows the integration of Cold Spray equipment in a highly automated manufacturing environment, including automated mandrel manufacturing and machining capabilities.

It has been proven that C-103 can be sprayed with high deposition efficiency using cold spray technology. Deposition efficiency of around 92% with a 4 kg/h deposition rate was observed. Both properties make cold spray cost-effective for manufacturing in-space propulsion nozzles with C-103 niobium alloy. Furthermore, microstructural and mechanical properties of cold-sprayed C-103 have also been investigated.

Microstructure and Mechanical Properties of AlSi7Mg Alloy Deposited on Die-Casting Specimens by the L-DED Process

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Recent advancements in large-scale die-casting techniques, such as Giga Press, have garnered attention due to their potential to simplify automotive body manufacturing by eliminating the need for welding processes. This innovation reduces the number of components, streamlines processes, and enhances productivity. However, while the production of large components offers advantages, challenges arise regarding the handling and re-melting of defective products due to their substantial size. One potential solution to address defects or reinforce the structure of large die-cast components is the L-DED (Laser-Directed Energy Deposition) process. Despite this potential, studies focusing on the application of L-DED for aluminum alloys remain limited.

In this study, AlSi7Mg alloy powder was utilized to optimize the L-DED process. Mechanical property evaluations and microstructural observations were conducted on thin-wall specimens (90 × 40 × 4 mm). Subsequently, die-cast/L-DED joint specimens were fabricated by depositing AlSi7Mg powder onto die-cast specimens, and their mechanical properties and microstructures were evaluated. Results showed that as the deposition thickness (Z-pitch) increased, the occurrence of balling phenomena at the upper region of the specimens decreased, but wrinkling was observed. Furthermore, the mechanical property variations in the joint specimens increased with the Z-pitch.

Heat treatment of additive manufactured Ni-Fe-Cr-Based alloy 718: corrosion aspects

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C1_5, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 10:30 - 13:10

Alloy 718, a Ni-Fe-Cr-based superalloy, is extensively used in critical industries such as nuclear power, aerospace, and oil and gas, where high mechanical strength and resistance to corrosion are paramount. The alloy's exceptional performance under extreme environments makes it indispensable for components subjected to high stresses and corrosive conditions. With the increasing demand for efficient manufacturing and the need for substitutive parts, additive manufacturing (AM) offers a transformative alternative to conventional production methods. AM provides advantages such as reduced material waste, the ability to produce complex geometries, and shorter lead times, enabling the production of intricate components with tailored properties.

This study investigates the influence of solution annealing and double ageing heat treatments on the mechanical and corrosion performance of additively manufactured Alloy 718. While optimising mechanical properties has been the traditional focus, the corrosion resistance of AM-produced parts is equally critical, particularly for applications in the nuclear industry where component reliability is vital. The primary aim is to evaluate the effect of varying solution annealing and double ageing temperatures to identify optimum conditions that ensure superior corrosion performance without compromising mechanical strength. By systematically analysing the microstructural evolution, hardness, tensile strength, and corrosion resistance, this research establishes guidelines for tailoring heat treatment protocols for AM Alloy 718. The findings will contribute to enhancing the service life and reliability of critical components, reinforcing the role of AM in modern manufacturing and its potential to replace conventional production methods for high-performance alloys in demanding applications.

Defect Analysis through Process Monitoring in Screw Extrusion-Based metal 3D Printing

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study explores the detection and analysis of incomplete filling defects in screw extrusion-based metal 3D printing. In screw extrusion 3D printing, suboptimal process parameters—such as extrusion speed, jerk or acceleration—cause voids and unfilled areas in green parts. These defects, after debinding and sintering, lead to reductions in both tensile strength and elongation. Although process optimization can minimize such defects, identifying the precise parameter set depending on product geometries and feedstock materials typically requires nondestructive testing (NDT) of the final printed parts.

To address this challenge, we implemented a real-time process monitoring system that eliminates the need for extensive post-process NDT. During printing, a vision camera installed inside the 3D printer acquired grayscale image of each deposited layer. These images were converted to black and white images and underwent distortion and vignetting corrections to enhance accuracy in quantifying defect sizes and distributions. By comparing each processed image against the corresponding CAD image, we identified voids and partial infills within individual layers. Subsequently, we reconstructed a three-dimensional model from the stack of analyzed layer images, enabling early prediction of the extent of internal defects and their locations within the final product. To validate our monitoring approach, we compared vision-based defect images with computed tomography (CT) scans of the printed parts. The results demonstrated high consistency between the two methods, suggesting that in-process image acquisition can accurately locate internal defects without requiring external inspection tools. It seems that this work provides a practical, real-time strategy for optimizing printing parameters and enhancing quality assurance in screw extrusion-based metal additive manufacturing.

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Additive Manufacturing of CuCrZr Alloys for Nuclear Fusion Applications

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C1_3, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 14:30 - 16:30

CuCrZr alloy has significant potential for a wide range of fields, such as the nuclear and aerospace industries, due to its outstanding thermal and mechanical properties. Due to the high infrared laser reflectivity and high thermal conductivity of Cu, it remains a challenge to produce CuCrZr alloy using the Laser Powder Bed Fusion (LPBF) technique. In this study, CuCrZr alloy was produced using the LPBF method, and the optimum printing parameters were obtained. Heat treatments were applied to improve the strength and electrical conductivity of the additive-manufactured CuCrZr samples, and the mechanical, thermal, and electrical properties of the samples were examined. The results are presented by comparison for both as-built CuCrZr alloy and heat-treated CuCrZr alloy.

Grain growth and mechanical behaviour of a solid-state additively manufactured Mg-4Y-3RE alloy

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C1_3, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 14:30 - 16:30

Ultrafine-grained (UFG) materials exhibit high strengths due to grain boundary strengthening, but grains can grow rapidly if post heat treatment is required, making it challenging to achieve grain boundary and precipitation strengthening simultaneously. Grain growth stagnation at 525 °C (0.87 T_m, melting point) was observed in a Mg-4Y-3RE alloy fabricated by additive friction stir deposition (AFSD), a novel solid-state additive manufacturing technology. The AFSD processing produced a bimodal grain structure with UFG grains and coarse grains (around 10 microns). After solid solution treatment (SST) at 525 °C for 72 h, no noticeable grain growth occurred. The observed grain growth stagnation is attributed to Zener pinning by these thermally stable nanoparticles. Moreover, the mixture of coarse and UFG grains efficiently improved the ductility of the alloys compared to the corresponding casting and extruded samples. These new findings offer a novel approach to designing Mg alloys with exceptional thermal stability for high-temperature applications.

Application of Thermo-Calc's Additive Manufacturing Module for LPBF of Steel, Aluminium, and High-Entropy Alloys

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C1_3, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 14:30 - 16:30

Thermo-Calc has developed new models to predict thermophysical material properties with unprecedented accuracy, using the CALPHAD method. While the treatment of heat and fluid flow is state of the art in current FEM models, material properties are treated in a highly simplified manner. This gives us a unique possibility to address the solidification problem in AM, with the focus on a unified treatment of both process parameters and alloy dependent thermophysical properties. The first module for Additive Manufacturing, using this approach, was implemented in the Thermo-Calc 2023b release. The latest developments aim at creating a fully predictive module that requires minimal user input. This module automatically generates physics-based properties, including absorptivity and captures the transition from conduction to keyhole modes, including the impact of fluid flow.

This talk will give insight into these developments and their applications to process and materials optimization. Examples of the AM module applied to laser powder bed fusion (LPBF) processing of steel, aluminium, and high-entropy alloys are shown. Recent and ongoing developments, such as key-holing prediction and process maps, are demonstrated, along with simulations of precipitation reactions during heat-treatment of as-built structures using TC-Prisma and DICTRA.

Influence of PBF-LB and in-situ alloying on the microstructural features of refractory-based complex concentrated alloys

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C1_3, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 14:30 - 16:30

Refractory-based complex-concentrated alloys (R-CCAs), i.e. metallic materials relying on a multi-principal element alloying approach, are attracting increasing interest because of their promising high-temperature properties. Yet, these alloys are often difficult to manufacture, especially when they consist of elements with widely diverging melting points or miscibility gaps. Conventional casting has been linked, for instance, to coarse-grained microstructures and severe segregation phenomena, necessitating costly long-term homogenization heat treatments at high temperatures. In this work, we explore the potential of the metal additive manufacturing technique of Powder Bed Fusion – Laser Beam (PBF-LB) for the fabrication of fine-grained and homogeneous R-CCAs. In addition, by using a pre-mixed blend of elemental powders as feedstock material, we adopt the approach of in-situ alloying. Forming the respective alloy directly in the powder bed of the 3D printer, we make use of the small melt pools and high localized heat input inherent to the PBF-LB method, to create the best possible homogeneity in combination with a great freedom in selecting the respective alloy's chemical composition for further alloy development.

The present work focuses on the R-CCA alloying system Ti-Al0.1-Cr-Mo-Nb0.5 (in at.%). Different printing parameter sets were tested, varying, e.g., the laser power, scan velocity, hatch distance, layer thickness, and number of scan repetitions. Based on microstructural analyses including light-optical as well as scanning electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray diffraction, these parameters were correlated with the microstructural features of the printed parts. By assessing, in particular, the porosity, homogeneity, proximity to the desired chemical composition, and, if applicable, fraction of unmolten particles, several promising printing strategies could be derived. Eventually, the microstructures of the as-built parts were optimized further in selected short-term heat treatments. In this regard, in-situ high-energy X-ray diffraction experiments in a dilatometer setup at a synchrotron radiation source offered valuable insights into the microstructural stability and characteristic features of the prevalent phases. On the example of the alloying system Ti-Al0.1-Cr-Mo-Nb0.5, this presentation will critically discuss the advantages and pitfalls of employing PBF-LB and in-situ alloying in the development of R-CCAs.

Effect of solidification mode on the resulting microstructure of 304L steel produced with L-PBF

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C1_4, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 17:00 - 19:00

Laser Powder Bed Fusion (L-PBF) is not only renowned for its ability to produce intricate shapes and complex geometries, but it is also a powerful tool for tailoring and optimizing the microstructure of metallic parts. By precisely adjusting the process parameters, L-PBF enables fine-tuning of crystallographic textures, grain orientations and microstructural features, offering unprecedented control over material properties [1,2].

Austenitic stainless steels, such as the widely used 304L and 316L grades, can benefit significantly from this capability, as these alloys exhibit distinct deformation mechanisms, i.e., the Transformation Induced Plasticity (TRIP) and Twinning Induced Plasticity (TWIP), which are influenced by the crystallographic texture. As such, specific orientations can either promote or suppress these effects under different loading conditions, making site-specific microstructural tailoring a promising approach for enhancing mechanical performance [3].

This study investigates how the choice of atomization gas, i.e., nitrogen (N) versus argon (Ar), affects the microstructure of 304L stainless steel processed via L-PBF. Despite using identical processing parameters, the two powders exhibit significantly different microstructures due to variations in their solidification behaviors. N-atomized powder predominantly forms strongly textured, columnar grains with pronounced elemental segregation, following a primary γ -austenite with secondary ferrite solidification mode. In contrast, Ar-atomized powder produces less textured, equiaxed grains with a more uniform composition, adhering to a primary ferrite with secondary γ -austenite solidification mode.

In this study we employ operando synchrotron X-ray diffraction during L-PBF processing, which provides valuable insights into the critical role of solidification modes in shaping the final microstructure. The results are coupled with detailed electron microscopy investigations and thermodynamic calculations. The findings of this study underscore the importance of precise control over solidification conditions to achieve the desired microstructural characteristics in austenitic stainless steels.

[1] C. Sofras, J. Čapek, A. Arabi-Hashemi, C. Leinenbach, M. Frost, K. An, R.E. Logé, M. Strobl, E. Polatidis, *Materials & Design* 219 (2022) 110789. <https://doi.org/10.1016/j.matdes.2022.110789>.

[2] C. Sofras, J. Čapek, C. Leinenbach, R.E. Logé, M. Strobl, E. Polatidis, *Virtual and Physical Prototyping* 19 (2024) e2390483. <https://doi.org/10.1080/17452759.2024.2390483>.

[3] C. Sofras, J. Čapek, X. Li, C.C. Roth, C. Leinenbach, R.E. Logé, M. Strobl, E. Polatidis, *Materials & Design* 237 (2024) 112539. <https://doi.org/10.1016/j.matdes.2023.112539>.

Powder Reuse in Additive Manufacturing of Titanium Alloy: Effects on Corrosion Performance

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C1_4, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 17:00 - 19:00

Additive manufacturing (AM) of metal components is a transformative technology that currently shows the fastest growth rate than any other manufacturing industry. Compared to traditional manufacturing methods, it enables production of near-net shapes and complex geometries, often unachievable by any other way, as well as a significant reduction in material waste. The latter is particularly relevant to titanium components, where post-machining can lead up to 80% of material removed. Laser powder bed fusion (LPBF) is the most common AM technique for Ti. Metal powders are produced by costly and high energy-consuming atomization processes. Many manufacturers and end-users prefer to rely only on virgin powder to be able to avoid powder contamination or degradation and guaranty the adequate performance of the components. Nevertheless, there is also a considerable drive to reuse powders during AM as that presents economic and environmental benefits. There are several powder reuse strategies, including single batch and collective aging methods, top-up method and powder refreshing method. The procedure common to them all is sieving the non-consolidated powder between the builds to remove the agglomerates from previous runs, using the rest for the next run. When the sieved powder falls out of specifications, it is discarded. The reuse strategies are not standardized, i.e. the number of reuse cycles is not strictly limited and each manufacturer uses their own trial-and-error based know-how. It has been established that oxygen pick-up and other contaminant levels in powder increase and the powder density and flowability decrease with reusing cycles, all of that leading to increased porosity in the printed parts. However, manufacturers often do not know exactly to what extent powder reuse deteriorates the performance of the components.

The present work investigates corrosion performance of AM Ti6Al4V as a function of the number of powder reuse cycles. Specimens corresponding to cycle 0 (virgin powder) and 20 are characterized by common metallographic techniques, X-ray diffraction, SEM-EDS and optical profilometry pre- and post-corrosion. Corrosion resistance is evaluated using electrochemical impedance spectroscopy (EIS) and cyclic potentiodynamic polarization (PDP) tests. Two different corrosive media relevant to airspace and health applications were studied. Harrison's solution at 25°C and Hanks' solution at 37°C represented acid rain and physiological conditions, respectively. The effect of the powder reuse cycles on localized corrosion of Ti6Al4V is discussed.

Microstructure and Mechanical Properties Correlation of Additively Manufactured IN939 Superalloy

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This study evaluates the mechanical performance of IN939 superalloy, fabricated using Powder Bed Fusion-Laser Beam (PBF-LB) and subjected to post-process heat-treatment. The primary focus is understanding how heat-treatment affects the microstructural evolution and mechanical properties of IN939 for high-temperature aerospace and industrial applications. High-temperature tensile and compression tests at 850 °C for heat-treated samples are conducted to gather data on yield strength, ultimate tensile strength, and ductility. Microstructural analysis using scanning electron microscope (SEM) and electron backscattered diffraction (EBSD) reveals significant modifications in grain structure and phase stability due to heat-treatment, which are directly correlated with enhanced mechanical properties. The strain hardening behavior is assessed using the Hollomon and Ludwik equations, showing a decrease in the strain hardening exponent at 850 °C, indicating increased susceptibility to localized deformation. The results demonstrate that heat-treated IN939 exhibits substantially improved mechanical performance at 850 °C, with higher yield and tensile strength while maintaining adequate ductility. These improvements are attributed to refined microstructure and enhanced phase stability from heat-treatment. This study underscores the importance of optimizing heat-treatment parameters to ensure the alloy's reliability and effectiveness in high-stress, high-temperature environments.

Enhancing the Processability and Mechanical Properties of 2618 Al Alloy via Powder Functionalization for Additive Manufacturing

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C1_4, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 17:00 - 19:00

The application of Additive Manufacturing (AM) is rapidly expanding, enabling the creation of complex geometries unattainable with traditional technologies. Among AM methods, Laser Powder Bed Fusion (LPBF) is gaining prominence across various industries. However, existing alloys were designed for conventional manufacturing, presenting challenges in AM due to issues like solidification cracking and high-laser reflectivity. For instance, high-strength Al alloys like 2618 are prone to hot-cracking. One solution is modifying the chemical composition of the powders by introducing suitable alloying elements. The addition of Ti and B to form TiB₂ particles has proven to be an effective grain refinement strategy, reducing hot-cracking susceptibility. TiB₂ particles not only improve the processability of the alloy and enhance its strength, but they also significantly increase the elastic modulus of the material when added in considerable quantities. However, producing composite powders with a high ceramic fraction through gas atomization is challenging due to the reactivity of B with Ti, which causes early boride formation, nozzle clogging, and uneven particle distribution. An alternative approach involves modifying only the surface properties of the powder through powder functionalization. In this work, we propose a mixed powder configuration where the 2618 Al powder is pre-alloyed with Ti and B to promote the in-situ formation of TiB₂ particles. This approach is combined with a high-energy mechanical mixing method to functionalize the surface of the pre-alloyed powder with TiB₂ particles. The goal is to fabricate a Metal Matrix Composite (MMC) containing 7 wt% TiB₂, with enhanced LPBF processability. This high ceramic content is expected to increase the material's elastic modulus and improve its overall mechanical strength. The coated powder was processed by LPBF to produce bulk samples. These samples were heat-treated according to different schedules to investigate their effect on the microstructure and tensile properties of the MMC material. The microstructure was analysed using SEM, EBSD, and TEM to evaluate TiB₂ particle formation and distribution. The results showed that high-density printed composites were achieved, exhibiting homogeneous dispersion of TiB₂ and an absence of cracks. The borides effectively promoted heterogeneous nucleation of the α -Al phase, suppressing epitaxial growth and leading to a fine, equiaxed microstructure. Hardness and tensile tests were performed to assess the impact of TiB₂ formation and heat treatments on the alloy's strength and ductility. Results show significant enhancements in yield and ultimate strengths post-heat treatments, along with an increase in Young's modulus, despite a reduction in ductility.

Fatigue behavior of 316L stainless steel and polylactic acid joints fabricated exclusively via additive manufacturing

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C1_7, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 17:00 - 19:00

With the continuous advancement of multi-material additive manufacturing, the integration of dissimilar materials has gained increasing significance in both technological and industrial applications. This study investigates the adhesive-free joining of materials fabricated using distinct additive manufacturing techniques. Specifically, it focuses on the integration of 316L stainless steel, produced via Laser Powder Bed Fusion (LPBF), and polylactic acid (PLA), manufactured through Fused Filament Fabrication (FFF). The research emphasizes the design of tailored interface geometries and process optimization to enhance the bonding mechanism between these materials. The joining of 316L stainless steel and PLA presents substantial challenges due to their considerable differences in melting points, thermal expansion coefficients, and shrinkage behavior. A critical issue in this process is ensuring adequate filling of the interface geometries while mitigating polymer shrinkage during solidification which required meticulous fabrication planning. To address these challenges, various interface geometries were proposed, incorporating different cavity shapes and surface roughness characteristics to improve adhesion. The study systematically evaluates the influence of surface roughness, interface geometry, polymer integration within the metallic interface, and residual stresses through experimental tensile testing under both static and dynamic loading conditions. Tensile and fatigue specimens were designed and manufactured with a hybrid structure, consisting of half-metal (316L) and half-polymer (PLA) components along their length. Additionally, finite element analysis (FEA) was employed to develop a multi-physics thermomechanical transient model, enabling an assessment of thermal stress evolution at the 316L–PLA interface and its impact on principal stresses under tensile loading. By optimizing metallic component heating strategies, selecting suitable cavity geometries, refining interface roughness, and employing effective filling techniques, this study demonstrates the feasibility of achieving strong and durable joints exclusively through additive manufacturing, without the use of adhesives.

Development and Additive Manufacturing of an Al-Ni-Mn Alloy using Laser Beam Powder Bed Fusion (LB-PBF)

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C1_4, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 17:00 - 19:00

Additive manufacturing through Laser Powder Bed Fusion (LPBF) has revolutionised the production of complex geometries, particularly in lightweight materials such as Al-alloys. However, balancing mechanical performance and thermal stability in Al-alloys remains a challenge. In this study, a novel Al-Ni-Mn alloy system is designed to enhance the properties of Al-Ni alloys by incorporating Mn, a key element known for its high solid solution strengthening, utilising the high cooling rate in LPBF causes rapid solidification in improving the mechanical performance. Building upon previous work demonstrating significant improvements in Al-Ni alloys, this research explores the effects of varying Mn content to optimise the alloy's mechanical properties and thermal stability. The alloy design process integrates thermodynamic analyses, including Phase and Schiel diagram assessments, to predict and control phase stability and composition. The microstructural evolution of the alloys is characterised using advanced techniques such as SEM, EBSD, XRD, DSC, and TEM. Mechanical properties are evaluated through tensile and hardness testing, highlighting the role of Mn content in increasing the solid solution and improving material strength. Furthermore, the thermal stability of the alloys is assessed, focusing on their resistance to degradation at elevated temperatures. This work highlights the potential of Al-Ni-Mn alloys as a sustainable solution for LPBF applications, promoting efficient material usage and reduced environmental impact. It will contribute to developing next-generation Al-alloys with enhanced performance characteristics tailored for LPBF.

Development and processing of the Al 5356 aluminium alloy by additive manufacturing using wire laser-based DED technology (DED-LB/M)

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C1_4, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 17:00 - 19:00

Additive manufacturing (AM) is widely recognized as an innovative and revolutionary technology. Metal AM enables the manufacturing of parts with unique shapes and exceptional mechanical properties. The AM process is complex with numerous variants like temperature gradients, high cooling rates, which allows process parameter development for processing materials with tailored properties. Microstructure and mechanical properties of metal AM materials differ significantly from those produced by conventional methods.

Aluminium alloys are difficult materials to be processed by additive manufacturing due to its high energy reflectivity. Only few research studies about aluminium processing throughout DED-LB/M have been found.

In this work, the feasibility of processing the aluminium alloy Al 5356 (AlMg5Cr) by Wire Laser-based Directed Energy Deposition (DED-LB/M) technology has been carried out as the first stage of developing a new metal-polymer multimaterial family within the European funded “MULTHEM Project (Multimaterial additive manufacturing for lightweight and thermal management)” for applications mainly related to lightweight and heat dissipation.

In this process Al5356 welding wire has been used as feedstock. This approach offers a significant competitive advantage by employing an affordable material and reducing material waste compared to traditional machining methods.

The process window has been investigated to reach dense samples with a material densification up to 99.84 %. Microstructural analysis revealed a very fine microstructure composed of equiaxed grains between 3-5 µm and small precipitates homogeneously distributed. Microhardness measurements were performed in horizontal and vertical directions to study the anisotropy of the aluminium alloy developed. A microhardness measurement of 99 HV0.2 was obtained in the horizontal direction while a microhardness profile from 70 HV0.2 to 82 HV0.2 was measured from the surface to the bottom in a sample of 20 mm height. Higher microhardness values have been obtained compared to values from traditional joining methods (70-80 HV0.2) or WAAM studies (60-70 HV0.2).

Horizontal and vertical thin walls were also processed to machine cylindrical tensile samples according to ISO 6892 standard. Tensile strength values of 275 MPa and 262 MPa in the horizontal and vertical directions were obtained, respectively. These promising properties could lead to an innovative method for processing Al5356 alloy by wire DED-LB/M. Different geometries and thermal properties are also under evaluation.

Keywords: Directed Energy Deposition (DED), Wire Laser-based DED (DED-LB/M), Aluminium alloy, process parameters, microstructure, mechanical properties.

Study of Recyclability of Metal Powders, Debinding and Sintering in Binder Jetting

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C1_1, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 9:20 - 10:20

The recycling of metal powders, along with debinding and sintering, constitutes critical processes in the context of additive manufacturing using Binder Jetting technology. This study focuses on the analysis of powders for their recyclability and the optimization of debinding and sintering processes in industrial furnaces to achieve final parts with a relative density exceeding 98% for stainless steels 316L and 17-4PH.

The research emphasizes the characterization of recycled powders to understand their suitability for Binder Jetting. The study focuses on analyzing the oxide layer of the particles formed after various printing cycles using transmission electron microscopy (TEM). This analysis provides detailed insights into the thickness, composition, and distribution of oxide layers, which influence the recyclability and performance of the powders in the Binder Jetting process.

To further understand and refine the debinding and sintering steps, sintered parts are characterized using techniques such as SEM, EDS, EBSD, and XCT. Besides, a step sintering approach is also implemented to analyze the evolution of the sintering process and understand the mechanisms involved. This comprehensive analysis aims to enhance process reliability, parts densification, and to optimize material performance. Moreover, the microstructure of sintered parts subjected to different atmospheric conditions and temperature variations in industrial furnaces is analyzed and discussed. Using these non-optimized conditions sintered densities up to 98% are achieved. Additionally, work focuses on improving the cost-efficiency of these processes by exploring the use of specific controlled atmospheres, including vacuum and argon, to reduce expenses while ensuring the process is efficient.

Keywords: Metal Jetting, Additive Manufacturing, Sustainable Materials, Recycled Metal Powders, Debinding, Sintering.

Optimization of Binder Infiltration Mechanisms in Metal Jetting for High-Quality Stainless-Steel Components

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C1_3, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 14:30 - 16:30

Industries today increasingly demand advanced manufacturing techniques that revolutionize production while adhering to clean, energy-efficient practices. Metal Additive Manufacturing (MAM) has emerged as a transformative solution, enabling the creation of complex, customized products with improved efficiency, reduced material waste, and lower production costs. Among various MAM techniques, Binder Jetting, or Metal Jet technology, stands out for its scalability and production efficiency [1]. This powder-based method selectively applies the binder layer by layer to the powder to create intricate parts in the green state, which are subsequently post-processed through sintering to achieve the final product [2].

Binder Jetting addresses many scalability challenges in additive manufacturing, making it a viable option for large-scale production. However, achieving 100% density remains a key challenge to ensure the production of high-quality components. Stainless steels like SS316L and 17-4 PH, renowned for their exceptional mechanical properties, corrosion resistance, and strength, are widely used across industries such as aerospace, automotive, and medical devices. Despite their advantages, when processed via Binder Jetting, these materials often encounter inconsistencies in print quality [3]. Variations in green density, binder saturation, infiltration efficiency, and surface finish can lead to defects in the final part. These inconsistencies can lead to defects, affecting both the mechanical properties and the final part quality.

This study experimentally investigates binder infiltration mechanisms in metal powders and the binder under varying thermal conditions using advanced techniques such as confocal microscopy. The fluorescence behavior of binders will be utilized to visualize and analyze infiltration patterns, layer adhesion, and binder distribution. The temperature-dependent viscosity of the binder will be examined to understand its impact on infiltration efficiency. The study will also explore how these factors influence part density and overall print quality. The findings aim to provide a deeper understanding of binder-powder interactions and their effect on the quality of green parts, facilitating the optimization of process parameters to achieve consistent, high-quality components in large-scale Binder Jetting production.

Keywords:

Metal Additive Manufacturing, Binder Jetting, Powder Binder Interactions, Infiltration Mechanism, Green Density.

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Operando X-ray Investigation of Cracking in Copper-Steel Multi-materials

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C1_4, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 17:00 - 19:00

Additive manufacturing (AM) of multi-material alloy combinations is attractive for many industries that require a combination of material properties such as thermal conductivity, corrosion resistance and mechanical strength. However, the printability of these combinations can be hindered by macroscopic defects such as cracks. One such combination is copper-steel multi-materials that greatly suffer from cracking at the interface when processed using fusion-based additive manufacturing methods. Therefore, understanding the underlying mechanisms of cracking constitutes the first step towards obtaining sound copper-steel multi-material parts.

This study aims to reveal the mechanisms of cracking in copper-steel alloy combinations manufactured via fusion-based methods. For this aim, operando X-ray diffraction and imaging, as well as computed tomography techniques were employed during laser powder-bed fusion (LPBF) of CuCrZr and 316L stainless steel to gain a fundamental understanding on the events taking place at the onset of cracking. The miniature LPBF equipment developed at Paul Scherrer Institut (PSI), i.e. miniSLM, was employed in MS and P21.2 diffraction beamlines at the Swiss Light Source (SLS) in Switzerland and PETRA III in Germany, respectively. Moreover, ID19 beamline at the European Synchrotron Radiation Facility (ESRF) was utilized for operando X-ray radiography and computed tomography characterization. Operando X-ray experiments coupled with auxiliary characterization methods have shown that two main mechanisms are responsible for cracking at the interface between copper and steel. First, liquid-liquid phase separation between CuCrZr and 316L was observed upon melting, which led to the formation of species of vastly different freezing ranges and subsequently solidification cracking. Secondly, it was observed in operando X-ray radiography that cracking can occur either further away from the melt pools or right at the heat-affected zone next to the adjacent tracks. Scanning electron microscopy (SEM) characterization revealed that the second type of cracking stems from the copper segregation at the steel grain boundaries during solidification.

In the light of these findings, a new method for mitigating cracking has been proposed and experimented as proof-of-concept. The results have shown interfaces with greatly reduced cracking, although they were not completely eliminated. Nevertheless, the results provide a deeper understanding regarding the processability of copper-steel multi-materials using fusion-based methods, and hold promise for further optimization of multi-material components produced by fusion-based processes.

Microstructural characterization of aluminum samples fabricated by the Molten Metal Deposition additive manufacturing technology

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C1_9, Manuel de Falla Auditorium (Level +1), settembre 17, 2025, 14:30 - 16:30

Molten Metal Deposition (MMD) is a novel 3D printing approach that enables the fabrication of intricate geometries by continuous volumetric controlled stream of molten metal, such as aluminum, without the need for structural supports or post-processing operations like debinding and sintering. This method offers significant advantages in terms of efficiency and design flexibility. In this study, a 4xxx aluminum alloy, known for its combination of lightness properties and mechanical strength, was used as raw material. The inclusion of silicon plays a critical role in improving the molten metal's workability by reducing its viscosity, which facilitates the deposition of uniform layers, a key factor for achieving high-quality, intricate geometries. This study investigates the influence of process parameters on the defect formation and on the microstructure of single-wall rectangular samples in the as-built state. A Design of Experiment (DOE) approach was developed to assess the effect of variables such as nozzle temperature, substrate temperature, print speed, layer height, and trace width on defect formation and the microstructure of two different sample types with varying dimensions. The samples were subjected to conventional metallographic preparation followed by chemical etching with the Keller reagent to reveal their microstructural characteristics, which were then analyzed using Optical Microscopy (OM), Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS) to further assess chemical composition and morphology. Stereomicroscopy was then used to perform a surface analysis of the samples, including the characterization of surface waviness, aimed at understanding the quality of the material deposition process. Waviness between layers was examined to evaluate the cohesion between successive layers and to identify any interlayers defects. In addition, a detailed roughness analysis, both within each layer and between adjacent layers, was performed to further evaluate the surface quality and material behavior during the printing. Vickers microhardness tests were also conducted in order to investigate the mechanical properties along the growth direction of the samples. The results of this study provide crucial information on the potential of the innovative additive technology provided by ValCUN, highlighting the essential role of process parameters and their direct influence on the quality and performance of the final parts.

Blown-Powder Directed Energy Deposition (DED) of Inconel 625: process simulation and experimental validation

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C1_10, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 17:00 - 19:00

Blown-Powder Directed Energy Deposition (DED) is an advanced Additive Manufacturing (AM) technique widely used for producing complex, high-performance components, particularly in aerospace applications. The use of Inconel 625, a nickel-based superalloy, is essential for components subjected to extreme conditions, including high temperatures, mechanical stresses, and corrosive environments. Inconel 625 is known for its outstanding high-temperature strength, oxidation and corrosion resistance, and excellent fatigue and creep resistance, making it ideal for critical aerospace components like turbine blades and exhaust systems. However, the effectiveness of DED with Inconel 625 relies heavily on the properties of the powder feedstock, including granulometry, flowability, and interactions with the deposition nozzle. These factors are essential for ensuring uniform material delivery and precise deposition, which directly impact the quality and performance of the final parts. This study investigates both virgin and recycled Inconel 625 powders, characterized through Scanning Electron Microscopy (SEM), Energy Dispersive Spectroscopy (EDS), and X-ray Diffraction (XRD). The primary focus is on the impact of powder characteristic, such as particle size distribution and flowability, on the efficiency and quality of the deposition process. These properties were analysed in relation to the nozzle's performance, specifically how the powder's flowability affects deposition consistency and dimensional tolerance during DED processing. The correlation between the powder feedstock and the resulting mechanical and microstructural properties of thin-walled components was examined. Microstructural analysis, conducted via Optical Microscopy (OM) and SEM, were employed to assess key features such as grain structure, porosity, and phase formation and distribution. These characteristics are critical for ensuring the performance and reliability of the produced parts. To optimize the DED process, Finite Element Method (FEM) simulations were conducted on CAD models prior to printing to predict deformations and residual stresses that occur during deposition. The simulation results facilitated the optimization of component geometry to enhance printability and minimize distortions, with the methodology tailored for scalability to more complex geometries. The simulation accuracy was validated by comparing the virtual model with the printed geometry, using stereomicroscope measurements, which confirmed the FEM model's reliability in forecasting distortions.

The findings of this study emphasize the critical role of powder properties in the DED process and their direct influence on the quality and performance of additively manufactured aerospace components. By integrating powder characterization, process simulation, and microstructural analysis, this work provides valuable insights into optimizing material feedstock and process parameters, enhancing the efficiency and quality of components produced via additive manufacturing.

Characterization of the effect of copper addition on 316L Stainless Steel samples manufactured by Laser Powder Bed Fusion (LPBF)

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C1_5, Manuel de Falla Auditorium (Level +1), settembre 16, 2025, 10:30 - 13:10

Laser Powder Bed Fusion (LPBF) is one of the most attractive metal additive manufacturing technologies, receiving growing attention for fabricating parts without geometrical complexity restrictions linked to the layer manufacturing method. The production of the metal components by LPBF can result in mechanical properties comparable and sometimes superior to those of bulk materials, in terms of strength and ductility of the as-built parts. The AISI 316L austenitic stainless steel is one of the most widely used alloys in additive manufacturing, owing to its excellent properties such as corrosion resistance, high ductility and biocompatibility, making it very promising for structural and biomedical applications. Copper (Cu) addition generally enhances certain properties of stainless steel, such as antimicrobial activity and mechanical strength, while its impact on corrosion resistance can be complex and depends on its distribution within the base alloy, necessitating careful control of its distribution and concentration to optimize the desired properties. A Design of Experiment (DOE) approach was developed to assess the effect of variables such as laser power, scan speed, hatching distance, thickness and consequently the VED (Volumetric Energy Density) on the mechanical properties and microstructure of samples containing varying weight percentages of copper, produced using LPBF. Samples were subjected to conventional metallographic preparation, followed by electrochemical etching to highlight the microstructure. The samples were investigated using Scanning Electron Microscopy (SEM) and Energy Dispersive Spectroscopy (EDS) to assess the chemical composition and morphology. Optical Microscopy (OM) inspections were carried out to detect manufacturing defects, while X-ray Diffraction (XRD) was carried out to determine the distribution of the crystallographic phases in the samples. Vickers micro-hardness tests were conducted to investigate the mechanical properties on the XY plane and along the growth direction (YZ), aiming to assess potential variations between the central region and the edge areas, as well as between the bottom and top surfaces. Through detailed characterization and microhardness mechanical testing, the objective of this work is to identify the optimal process parameters and the appropriate amount of copper, in order to obtain the best compromise between microstructural properties and mechanical performance, while minimizing defects.

Effect of build orientation on the microstructure and corrosion properties of additively manufactured SS316L

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C1_9, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 14:30 - 16:30

This study investigates the effect of build orientation on the microstructure and corrosion behaviour of stainless steel 316L fabricated utilizing laser powder bed fusion (LPBF). Samples were produced at various inclination angles (40°, 50°, 60°, 70°, 80°, and 90°) using gas-atomized SS316L powder under an inert argon atmosphere. Microstructural analysis was performed using optical microscopy and scanning electron microscopy (SEM) to examine grain size, sub-grain cellular structures, and melt pool morphology. Residual stresses were measured via X-ray diffraction (XRD), while Vickers microhardness tests evaluated the mechanical properties. Corrosion performance was assessed through electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization (PDP) in borate buffer solution. Results show that build orientation strongly influences thermal gradients, leading to variations in microstructure, residual stress, and corrosion resistance. The 60° orientation demonstrated the best performance with fine, uniform columnar grains, minimal elemental segregation, and the highest charge transfer resistance (R_{ct}), indicating superior corrosion resistance. Conversely, orientations such as 50° and 90° exhibited high residual stress and greater susceptibility to localized corrosion. This research underscores the critical role of build orientation in optimizing the properties of LPBF-manufactured SS316L components for corrosion-resistant applications.

Spatter Formation Behavior Induced by Machining Chips in Hybrid Additive Manufacturing

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Metal additive manufacturing (AM) processes offer the advantage of rapid prototyping and part production without the need for molds. However, the resulting poor surface quality often requires post-processing. To address this challenge, hybrid AM systems have been developed, integrating laser powder bed fusion (LPBF) with three-axis computer numerical control (CNC) machining. Despite their benefits, machining operations inevitably generate byproducts such as chips, which may influence the AM process condition. In this study, we investigate the mechanisms of spatter formation, one of the major impurities in AM, induced by machining chips. It was observed that chips increase the oxygen concentration in the powder, thereby enhancing the Marangoni effect in the molten pool, which subsequently promotes spatter formation. Furthermore, Higher scanning speeds generally reduce spatter, but spatter has been shown to increase due to irregular powder size when there are machining chips in the powder. In conclusion, we proposed a method to achieve optimal process conditions in the hybrid AM. The findings of this study provide valuable insights into impurity formation in hybrid additive manufacturing systems and suggest strategies for optimizing process conditions to minimize defects.

Additive manufacturing of soft magnetic materials with Permalloy-80

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C1_5, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 10:30 - 13:10

Abstract

Recent advances in the understanding and control of manufacturing techniques such as physical-property-targeted additive manufacturing (AM) technologies have made considerable advances in many industries. AM technology was developed not only for polymers, but also for ceramics, metals, composites, amongst other materials. Here the use of laser powder bed fusion additive manufacturing methods are demonstrated as a production technique relevant to manufacture of magnetic shielding materials with Permalloy-80 (80% Ni, 5% Mo and the remaining is Fe) called Mu-metal [1,2]. Powder characterisation experiments such as powder morphology determination with SEM imaging and EDX analysis were carried out with a Hitachi TM3000 microscope. Particle size distribution analysis and powder flowability with hall flow meter tests were conducted to measure powder quality properties prior to additive manufacturing processes. Samples were manufactured with an M2 Cusin laser machine, orientated 45° to the build platform. Initially, simple geometries were printed such as cubes, tubes, rings, tensile strips (ASTM E8), etc. Microstructural characterisation of materials provided significant detail to determine material behaviour. As a result, printed parts were characterised in terms of both macroscopic magnetic and microstructural scales.

Currently, industry manufactures magnetic shielding assemblies with different thicknesses of Mu-metal sheets and bar stock using traditional manufacturing techniques such as rolling, bending, cutting, welding, etc. This research shows that the process of manufacturing magnetic shields additively with laser powder bed fusion can, in some circumstances, replace conventional manufacturing methods of magnetic shields. The economic feasibility of the manufacture of very complex on intricate shields is dependent on a large number of factors including cycle time, the number of disparate manufacturing operations required, geometric limitations, performance limitations, homogeneity limitations, mechanical integrity and robustness and material mass. The main objective of this research is to determine under which conditions it is appropriate to replace conventional manufacturing methods of soft magnetic structures with current additive manufacturing techniques and, more interestingly, identify utile geometries and structures which are currently unfeasible to manufacture using conventional techniques.

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Effect of substrate preheating on repairing Inconel 718 parts by Cold Spray Additive Manufacturing

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C1_10, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 17:00 - 19:00

Cold Spray Additive Manufacturing (CSAM) is a promising solid-state repair technique for high-performance materials such as Inconel 718® (IN718). However, the influence of substrate preheating on the deposition quality of IN718 coatings remains not completely explored. This study investigates the effect of substrate preheating on the microstructure, adhesion, and bonding mechanisms of cold-sprayed IN718 deposits, providing a viable alternative for repairing damaged IN718 components without altering their original microstructure.

Thick IN718 deposits were fabricated on IN718 substrates at three preheating temperatures: room temperature (RT), 250°C, and 400°C. The coatings were analyzed for porosity, microhardness, phase composition, and adhesion mechanisms at the splat-substrate interface. Bonding strength was also evaluated at varying deposit thicknesses and preheating conditions.

The results confirm that CSAM can effectively repair IN718 components without requiring bond coatings or extensive pre-processing, maintaining the feedstock's microstructure and phase composition. Substrate preheating significantly enhanced deposit density through two mechanisms: (i) increased plastic deformation due to substrate softening in the initial layers and (ii) the peening effect from subsequent particle impacts. Preheating also improved adhesion and cohesion, with the highest density (>99.9%) achieved at 400°C. Despite these improvements, microhardness remained unaffected by substrate temperature or deposit thickness.

These findings provide critical insights into optimizing CSAM processing parameters for IN718 repairs, reinforcing its potential as a sustainable and efficient alternative for restoring high-value aerospace and industrial components.

ODS Steels Produced by Additive Manufacturing for Materials in Harsh Environments

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Oxide dispersion-strengthened (ODS) steels are known for their superior mechanical properties at high temperatures and increased resistance to neutron irradiation embrittlement. These properties favour them for future applications as fuel cladding for next-generation nuclear systems and blanket materials for fusion power systems.

We aim to determine whether an ultrasonically gas-atomised precursor steel powder with the addition of oxide nanoparticles or a steel powder with smart surface oxidation, combined with consolidation techniques such as laser powder bed fusion (LPBF), can enhance the performance of ODS steel in extreme, high-temperature conditions. As a proof of concept, we have selected austenitic 316L stainless steel, which has good ductility, workability, and mechanical integrity at high temperatures. Y₂O₃ has been chosen as the nanopowder material to add to the matrix, as it has a higher ultimate tensile strength than other powders. As the project progresses and the strengthening mechanisms associated with the nano oxide dispersion are known, TiB₂ nanoparticles (with a higher melting point) will also be employed.

We prepare ODS steels by mechanical mixing in Turbula, followed by ball milling and LPBF processing. We perform microstructure characterisation, mechanical testing at elevated temperatures, corrosion tests, tribology tests, and Vickers' hardness. The morphology and phase composition of the resulting powders and LPBF samples are analysed using scanning electron microscopy (SEM) with an EDS and EBSD, respectively.

High-temperature profilometry-based indentation plastometry for nickel alloy development in additive manufacturing

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Developing new high-temperature alloys is a challenging and resource-intensive process, partly due to the high costs associated with traditional tensile testing. Standard methodologies require the fabrication of dogbone-shaped samples and specialized high-temperature tensile testing setups, significantly limiting the number of feasible experiments. To overcome these limitations, profilometry-based indentation plastometry at high temperatures (Hot-PIP) has emerged as an efficient alternative. Hot-PIP enables the extraction of stress-strain curves from small cubic samples ($<10 \times 10 \times 10$ mm) by analyzing indentation imprints created at temperatures up to 800°C. This technique reduces material consumption, shortens testing times, and facilitates rapid mechanical property assessment. In this study, we investigate the applicability of Hot-PIP for the mechanical characterization of Inconel 718-TiC alloy produced using a powder bed fusion-laser beam of metals (PBF-LB/M). The alloy is fabricated through in situ composite powder processing, introducing TiC to enhance high-temperature performance, and compared to pure Inconel 718. We evaluate the ability of Hot-PIP to infer key mechanical properties such as yield strength, ultimate tensile strength, and ductility, comparing the results against conventional high-temperature tensile testing data. The findings demonstrate the feasibility of Hot-PIP as a robust tool for rapid alloy screening in additive manufacturing, particularly for high-temperature material development. By offering a more accessible approach to mechanical testing, Hot-PIP may help streamline the evaluation of new alloys in additive manufacturing while reducing material and experimental costs.

Effect of surface roughness, defects, and residual stresses on the fatigue behaviour of additively manufactured metals

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

One of the main advantages of additive manufacturing processes, and especially of laser-based powder bed fusion (PBF-LB/M), is that it enables the production of topology-optimised and thus lightweight components. The materials produced via PBF-LB/M usually have a high monotonic strength due to their unique and fine microstructure. However, their fatigue strength is lower in relation to conventionally manufactured materials, which is mainly caused by the process-induced microstructural defects and the additively manufactured “as-built” surface layer, containing a rough surface topography and tensile residual stresses. Note that the “as-built” surface layer often shows a higher density of process-induced defects than the inner material volume.

Therefore, the objective of the presented work is to analyse the influence of the “as-built” surface on the fatigue behaviour of metals produced via PBF-LB/M. For this, specimens made of the austenitic stainless steel AISI 316L were examined in two different surface conditions, “as-built” and polished. To characterize the different surface conditions, the microstructure, the surface topography, and the residual stresses at the surface were analysed, showing huge differences in the surface roughness and especially in the residual stress state.

For both surface conditions fatigue tests were performed to determine the S-N curves. Subsequently, the fracture surfaces of the specimens were investigated to identify the crack-initiating defects. In accordance with previous work [Lehn24], based on the Varea approach the impact of the defects on the fatigue behaviour was assessed using a modified S-N curve, which further enables the consideration of the influence of process-induced residual stresses [Mura19].

These analyses showed that the “as-built” surface significantly reduces the fatigue life. However, considering the defect size and residual stresses at the surface by means of the Varea approach, both surface conditions show nearly identical S-N curves. Thus, these influencing factors were identified as the main reasons for the lower fatigue strength of the “as-built” surface condition, which is in accordance with previous findings for AISi10Mg [Lehn24]. Consequently, the results obtained indicate that the surface roughness is not the most limiting factor for additively manufactured metals.

[Lehn24] Lehner et al. (2024): doi.org/10.1016/j.ijfatigue.2024.108479

[Mura19] Murakami et al. (2019): doi.org/10.1016/C2016-0-05272-5

Laser powder bed fusion of AISI 4140 high strength low alloy steel: parameter optimization, microstructural and mechanical properties

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C1_5, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 10:30 - 13:10

Laser powder bed fusion is the predominant technique in metal additive manufacturing. It enables the production of intricate components with complex shapes by depositing metallic powders layer by layer, resulting in a nearly net-shaped final product. Experiments on single tracks were conducted to investigate the impacts of scan speed and laser power on the behavior of the tracks during laser powder bed fusion. For AISI 4140 steel, bead mode, the melt pool dimension, and the track stability were investigated. The laser power for the tracks was varied between 150 W and 400 W, while the laser scan speed ranged from 300 mm/s to 1400 mm/s. High porosity was seen at both high and low energy input densities. This was attributed to the presence of unmelted particles and keyhole pores, respectively. An increase in laser scanning speed results in the observation of discontinuities in the tracks. As the laser intensity increases, the depth of penetration of the bead also increases, indicating a shift in the bead morphology from conduction mode to transition mode or keyhole mode. This would lead to an increase in the occurrence of porosity flaws. The occurrence of balling can be elucidated by considering the Marangoni convection and the Rayleigh instability in relation to the flow of the molten material. Through the analysis of the track and bead morphology, a refined set of parameters was derived that can be utilized for printing specimens. A comparative study was conducted between additively manufactured and conventionally manufactured steel specimens. The examination of the additively manufactured specimens revealed the presence of martensite formation in the microstructure. Vickers hardness testing was performed in the vertical direction, starting from the bottom and moving towards the top. The hardness exhibited minimal variance, indicating a high degree of homogeneity. The mechanical properties and corrosion resistance of the additively manufactured specimens showed better and more promising results in comparison to the conventionally manufactured steel specimens.

Tungsten alloyed with varying carbon contents manufactured by Powder Bed Fusion – Laser Beam

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C1_5, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 10:30 - 13:10

In this study, carbon-prealloyed tungsten powders were manufactured by powder bed fusion – laser beam (PBF-LB) in a substrate plate temperature range of 550 °C to 1000 °C. The carbon contents of the alloys investigated ranged from 0.02 wt.% to 0.21 wt.%. Characterization of the specimens was performed for defects by optical microscopy (OM) and scanning electron microscopy (SEM) of metallographic cross sections, for microstructure by electron backscatter diffraction imaging (EBSD), and for mechanical properties by three-point bending strength or tensile strength.

In comparison to pure tungsten, the microstructure was refined and the epitaxial growth of grains was reduced. For lower carbon contents it was possible to reduce the amount of intergranular cracking and obtain samples without cracks in the inner regions, but surface cracks remained. By alloying with low amounts of carbon, the relative density as measured by optical density measurements increased to 99.9% with higher porosity at the surface areas where the cracks are located. For high carbon contents of 0.21 wt.% and small sample sizes 99.9% relative density and a crack-free microstructure was obtained. With increasing sample size, the thermal tensions and probability of lack-of-fusion defects increased, leading to 99.5% relative density and occurrence of cracking. The decrease in relative density can be attributed to the worsened powder spreading through increased adherence of the fine powder to the substrate plate at 1000 °C. The occurrence of cracks with increased sample size has a different origin than the cracks in pure tungsten or low carbon alloyed tungsten. While those are intergranular solidification cracks due to weakened grain boundaries, the cracks in tungsten alloys with high carbon contents are transgranular cold cracks due to thermal stresses and a lack of plasticity.

The defect mechanisms of tungsten-carbon alloys manufactured by PBF-LB are discussed and mechanical properties presented. This study is a significant step towards the production of defect-free tungsten components with mechanical properties that meet market requirements using PBF - LB.

Innovative chemically-assisted mass finishing processes for additively manufactured metallic components

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C1_10, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 17:00 - 19:00

Additive manufacturing (AM) is an emerging manufacturing technology allowing for the production of customized parts characterized by complex geometries, often presenting cavities and channels. Poor surface finishing of as-built components is an issue that frequently limits the applicability of this technology: the presence of surface defects and high roughness (average roughness R_a usually ranging between 5 and 30 μm) make surface post-processing necessary.

This study focuses on chemically-assisted mass finishing as effective process to polish AM components. Conventional mass finishing is a widely applied technology that promotes surface smoothing through the mechanical action of abrasive media that remove surface asperities. Chemically-assisted mass finishing is a newly developed approach relying on the combination of the mechanical action of media and the chemical action of etching solutions, allowing to increase material removal rate, treat highly rough surfaces and reach cavities and recesses poorly accessible by media. The effect of printing parameters, surface orientation, properties of the abrasive media, process time and composition of the etching solutions on surface roughness and morphology was investigated on samples with increasing geometrical complexity.

Tests were performed on AISI 316 L and Inconel 718 samples produced by Laser Powder Bed Fusion technology. Polishing processes were run in vibrating machines in wet conditions with ceramic or polymeric abrasive media characterized by different cutting efficiency. Chemical solutions composed by oxidizing species, pH regulators, passivating and complexing agents were added. Surface roughness was assessed by optical and by contact profilometry; surface morphology was observed by means of optical and electronic microscopy; 3D optical scans were used to evaluate material removal homogeneity. Treated components underwent compositional analysis (Energy Dispersive X-ray Spectroscopy and Glow-Discharge Optical Emission Spectroscopy) and corrosion tests.

Considering external surfaces, initial roughness (initial R_a ranging between 6 and 32 μm according to surface orientation) was reduced by more than 80% regardless printing orientation, reaching values lower than $R_a = 1,0 \mu\text{m}$ in most favorable printing conditions. On inner surfaces (inside the channels), roughness homogeneously decreased by about 60% along the entire length of the component. In both cases, chemically-assisted processes have proven to be more effective than conventional mass finishing and chemical polishing, resulting in lower roughness and more homogeneous surfaces. Based on corrosion tests, the investigated chemically-assisted mass-finishing processes did not alter the corrosion behavior of the components.

Additive Manufacturing of Hot Work Tool Steel Parts Using the L-PBF process

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C1_5, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 10:30 - 13:10

Additive manufacturing technologies are increasingly used in the metallurgical and machine industries. Due to the large possibilities of producing complex shapes without developing a series of manufacturing operations, they allow for additional optimization of production time and costs. In this work, the possibility of additive manufacturing of hot-work tool steels H11 (X37CrMoV5-1) and H13 (X40CrMoV5-1) as well as maraging steel MS1 (X3NiCoMoTi 18-9-5) was investigated using L-PBF technology with a laser in point-by-point mode. Based on the optimization, process parameters were selected to obtain acceptable quality prints from H13 and MS1 steel, introducing different amounts of energy into the material. Microscopic methods were used to characterize the produced materials, mechanical properties were examined, and the effect of heat treatment on the microstructure and properties of parts produced using the above technology was determined. In addition, the possibility of using a gas atmosphere and a laser beam for the controlled introduction of nitrogen into these steels was investigated. It was assumed that molecular nitrogen, present in a gas atmosphere, can be introduced into the pool of liquid metal by surface adsorption and subsequent decomposition into atomic nitrogen, which can form nitrides and carbonitrides during the solidification of steel. By controlling the time and size of the pool of liquid metal created using a laser beam, it was assumed that the amount of nitrogen introduced in this way could be controlled. The obtained research results show a new area of possibilities of additive manufacturing technology in the aspect of using gas atmospheres for local strengthening of 3D printed metals, which can open up new research directions for other materials.

Insights on Interface Features in 3D-Printed Multi-materials

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C1_5, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 10:30 - 13:10

Multi-material components, which integrate the properties of different materials within a single product, represent a major innovation in the industrial sector. This approach makes use of the unique characteristics of each material to enhance performance aspects such as mechanical strength, weight reduction, corrosion resistance, and thermal or electrical conductivity. However, integrating different metal alloys through additive manufacturing technologies remains challenging due to substantial differences in physical and metallurgical properties, which can compromise the quality and durability of multi-material interfaces. The study of interfaces in additively manufactured multi-material structures becomes thus crucial for understanding the mechanical, thermal, and chemical performance of the final component.

This research investigates the interfacial bonding mechanisms, defect formation, and property gradients that arise in additively manufactured multi-material samples obtained by coupling Ni-based, Fe-based, and Cu-based alloys. By using advanced characterization techniques (FEG-SEM, XRD, micro and nanoindentation) coupled with CALPHAD-based simulations, the microstructural and mechanical integrity of the interfacial regions were assessed. Results indicate that interface adhesion is influenced by printing parameters, material compatibility, and thermal history.

This study contributes to the development of high-performance multi-material AM components for applications ranging from automotive to aerospace, electronics, and medical devices.

PBF-LB of a non-weldable Ni-base superalloy CM247LC: from conventional to non-conventional parameters

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C1_2, Manuel de Falla Auditorium (Level +1), septiembre 15, 2025, 10:50 - 13:10

Additive manufacturing (AM) of the non-weldable γ' -strengthened Ni-base superalloy CM247LC via powder bed fusion – laser beam (PBF-LB) faces significant challenges due to its susceptibility to both solidification cracking during fabrication and strain age cracking during post-processing heat treatments. Solidification cracking arises from thermal stresses and interdendritic strain accumulation in the final stages of melt pool solidification, while strain age cracking (SAC) is driven by residual stresses from PBF-LB and γ' precipitation during heat treatment. This study integrates multi-faceted approaches to mitigate these issues, combining process parameter optimization, novel scan strategies and microstructure control.

Initial work focused on optimizing laser parameters (power, speed, hatch spacing) to minimize porosity and cracking. Low line energy density (<0.2 J/mm) and strong melt pool overlap (50–80%) reduced solidification cracking by promoting shallower melt pools and minimizing thermal gradients. Residual stress analysis via X-ray diffraction revealed that volumetric energy density (VED) directly correlates with residual stress magnitude, emphasizing the need for lower VED parameters to alleviate SAC. This is however not a possible solution as processing with lower VEDs lead to higher fraction of lack of fusion indicating the need to find other ways to solve the SAC problem. SAC Electron Backscatter Diffraction (EBSD) identified $<100>$ -textured columnar grains in crack-resistant samples, suggesting grain orientation reduces high-angle grain boundaries that are susceptible to solidification cracking.

Building on these findings, novel scan strategies were explored to address residual stress limitations. Reducing laser stripe width from 5 mm to 0.2 mm lowered the crack density by promoting $<100>$ texture and reducing residual stresses by 30%. A demonstrator component manufactured with 0.2 mm stripes survived post-build heat treatment without strain age cracking, unlike components with conventional 5 mm stripe width. Additionally, other strategies such as in-situ remelting strategies showed promise in minimizing solidification cracking with some promise to mitigate SAC.

Ongoing work investigates the role of advanced scan strategies (e.g., laser beam shaping) to have better microstructure control to suppress both the forms of cracking. Results underscore that CM247LC's processability requires tailored approaches distinct from weldable alloys like IN718, with grain structure and texture playing pivotal roles in defect mitigation. These insights provide a framework for alloy and process designers to advance AM of crack-prone superalloys, balancing parameter optimization, scan strategy innovation, and microstructural engineering to achieve robust, high-performance components.

EFFECT OF PRINTING PARAMETERS ON THE MICROSTRUCTURE OF BLUE LASER DIRECTED ENERGY DEPOSITION OF A CuCrZr ALLOY

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C1_6, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 14:30 - 16:30

Copper-based alloys are extensively used in the nuclear, aerospace or injection molding industries due to their conductivity and corrosion resistance. Among them, the CuCrZr alloy, is a precipitation-hardened copper alloy which offers balanced properties such as relatively high strength, elevated softening temperature, and enhanced creep rupture strength. Directed Energy Deposition (DED) is a versatile additive manufacturing process capable of rapidly depositing high-performance materials. It enables efficient production of large parts, complex geometries, and component repairs, while offering precise control over material properties and supporting cost-effective, sustainable manufacturing through the repair and remanufacturing of components. Nevertheless, the manufacturing of copper alloys by laser DED remains challenging due to their high reflectivity to the conventional infrared laser (IR). IR radiation is reflected by copper at room temperature by up to 95%. Furthermore, the high thermal conductivity of copper alloys causes rapid heat dissipation during DED, resulting in anisotropic microstructures, and difficult control of residual stresses that may cause geometric distortions or promote cracking. Also, differences in heat dissipation along the building direction during DED manufacturing, result in heterogeneous properties and microstructures, which could limit the direct application of DED without costly post-processing heat treatments. Blue lasers sources provide an absorptivity of about 13 times higher than the IR in copper alloys. They offer greater manufacturing efficiency and flexibility, i.e., are gaining significant interest. This study investigates the effect of blue laser parameters used in laser wire DED and of the baseplate temperature on the microstructure formation of CuCrZr. Microscopy and synchrotron X-ray diffraction were used to analyze microstructural evolution along the building direction for developed printing strategies.

XCT image analysis for characterizing 3D printed thermomagnetic materials in energy harvesting applications

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C1_6, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 14:30 - 16:30

A critical amount of industrial energy input is lost as waste heat, and this amount peaks just above room temperature. The aim of this work, which is part of the ITN Heat4Energy project, is to develop a technology to convert this low-grade waste heat into electricity through a thermomagnetic generator based on Faraday's law of induction. To this end, water-flowable thermomagnetic elements will be developed both in the laboratory and by the industrial partner to be used as heat exchanger components in the demonstrator. The extrusion and post heat treatment process of the developed parts may introduce various defects that have an impact on their heat transfer efficiency, magnetic and mechanical properties.

Here, the non-destructive characterisation technique of X-ray computed tomography (XCT) is used to evaluate the morphology of the developed components and to identify trends that contribute to the improvement of material performance in the demonstrator. In specific, XCT image analysis enables the 3D visualisation of the developed 3D printed structures. Using DragonFly software, scalar quantities such as internal porosity, total surface area and void fraction are estimated for each sample. More specifically, image segmentation using the Otsu's thresholding method combined with morphological operations on multiple 2D XCT image slices, contributes to the estimation of the mean 2D void area of each slice and the distribution of the mean 2D void area as a function of z-coordinate along the printing direction.

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[3] You, X., Maschek, M., van Dijk, N.H.H. and Brück, E., 2021. Magnetic Phase Diagram of the $\text{Mn}_x\text{Fe}_{2-x}\text{P}_{1-y}\text{Si}_y$ System. *Entropy*, 24, p.2.

Microstructure and Mechanical Properties of Laser Powder Bed Fusion Processed NiTi SMAs: A Comparative Study of Different Feedstock Powders

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C1_6, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 14:30 - 16:30

NiTi shape memory alloys (SMAs) are known for their unique superelasticity (SE) and shape memory effect (SME) and are extensively used in aerospace, biomedical and actuator applications. Additive manufacturing (AM), particularly laser powder bed fusion (LPBF) process, has the ability to produce complex geometries with a high buy-to-fly ratio, and superior shape memory and mechanical properties compared to conventional routes. In this study, blended and pre-alloyed forms of NiTi powders with similar particle size distribution ($D_{50} = 39 - 40 \mu\text{m}$) were considered to compare the efficiency and performance of the respective printed parts. A noticeable difference in costs and availability of the two feedstocks are the main motivation behind the study. A one-on-one comparative study for LPBF process parameter optimization using the two forms of powders is the main objective of this work.

Firstly, both form of powders was characterized for morphology and shape memory properties before printing. The powders exhibit a spherical shape. Using LPBF, defect-free, high-density cubes were fabricated by varying laser power and scanning speed while keeping hatch spacing, layer thickness and scanning strategy printing parameters constant. The highest density achieved was 99.16% for pre-alloyed powder and 90.25% for blended powder. Differential scanning calorimetry (DSC) revealed single-step phase transformation in both printed parts with distinct transformation temperatures. X-ray diffraction (XRD) analysis confirmed different phase formations (B19 and B2) in the optimized cubes. Microstructural variations were observed along and perpendicular to the build direction for both printed parts. Hardness analysis showed that the optimized blended powder cube had higher hardness than the pre-alloyed cube. This difference is due to secondary phase formation, particularly Ni_2Ti phase in blended printed part, which degrades functional performance. However, pre-alloyed NiTi exhibits superior SME and SE properties. This study clearly identified the influence of powder type on LPBF processing, mechanical properties and functional behavior of NiTi SMAs. It is inferred that improving the density and powder characteristics of blended powder could enhance its printability using LPBF for various applications.

Tensile and Low-Cycle Fatigue Behavior of Laser Powder Bed Fused Inconel 718 at Room and High Temperature

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C1_10, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 17:00 - 19:00

The nickel base superalloy Inconel 718 (IN718) is the most commonly used Ni-based superalloy for high temperature structural applications for its remarkable strength, as well as creep, fatigue, and corrosion resistance up to 650 °C. While IN718 has traditionally been employed as cast or wrought material, is difficult to machine because of its high strength and toughness. The additive manufacturing of IN718 components made by metal AM has thus gained extensive attention to produce expensive near-net shaped components of high-temperature alloys such as IN718 for it saves material and costs in processing and machining steps.

Among all metal additive manufacturing (AM) technologies, laser powder bed fusion (PBF-LB/M) is the most widespread, IN718 being one of the most common alloys produced. However, high cooling rates associated to the PBF-LB/M process, hinders the primary strengthening phases γ'' and γ' to form, as these cooling rates induce a dislocation cellular substructure at which walls forming Laves phases bind segregating Nb, Ti and Mo. Many of the therefore needed heat treatment strategies can then promote Laves phase transformation into the stable δ phase along the cell and grain boundaries. Laves and δ phases, as well as grain boundary primary carbides may have adverse effects on mechanical properties. The mostly needle-shaped δ phase was namely found to have a detrimental effect on creep rupture life while no direct effect on LCF fatigue life was evident.

In this work room- and high-temperature (650 °C) tensile and low-cycle fatigue behaviors of PBF-LB/M IN718 is investigated in the four-step heat treated state and compared wrought IN718. The microstructure of both materials is characterized across length scales via microscopy methods. The elastic and yield properties are comparable at both test temperatures while tensile strength, ductility, and strain hardening capacity are lower for the PBF-LB/M IN718 material. Its fatigue life at room temperature is slightly lower than that for the wrought material, which is reversed at 650 °C. The cyclic stress response for both materials is marked by cyclic softening that is more pronounced at higher test temperatures. Multiple secondary cracks form at high strain amplitudes, at both room and high temperatures. High testing temperatures specially enhance crack formation at the transitions of regions between elongated grains and columns of stacked grains with ripple patterns in the PBF-LB/M material. Additional to this behavior, pronounced crack branching and deflection indicate that the cracks are controlled by sharp micromechanical gradients.

Microstructural characterisation and thermophysical analysis of additively manufactured scrap aluminium alloys for circularity of material

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C1_6, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 14:30 - 16:30

Aluminium alloys are exceedingly applicable engineering materials. Their very good mechanical and corrosive properties make them a highly sought-after material in automotive and aerospace industries. Accounting that, a huge amount of end-of-life aluminium alloy products is being recycled every year. Even though the energy required for the production of fresh aluminium is much higher (~95%) than that needed for its recycling, a considerable amount of high-grade engineering alloys still goes unrecycled every year. Thus, recycling of end-of-life scrap is necessary to meet the demand and to reduce energy consumption. In this research, we experimentally verify a computer-based rapid alloy development approach that predicts novel alloys purely based on mixing of automobile and aircraft aluminium waste fractions without refinement. The alloys 2024-T3 and Al-Si piston scraps were melted and cast in certain ratios to obtain three mixtures with varying content of silicon and other influencing elements. The ingots were cut into discs, ground to a thickness of 0.4 mm using 240P abrasive paper. A 3D-printer built at German Aerospace Centre (DLR) called MARS-M was used for laser re-melting by scanning straight lines on the discs. This treatment created melt pools which were investigated for their susceptibility to solidification cracking. Microstructural analysis with Scanning Electron Microscope (SEM) involved determining existence of strengthening and detrimental phases and precipitates, absence of solidification cracking or micro-cracks. Thermophysical analysis consisted of melting and solidification temperatures, enthalpy, specific heat and thermal diffusivity determination with Differential Scanning Calorimetry (DSC) and Laser Flash Analysis (LFA). After the analyses, a suitable mixture was powdered with ultrasonic atomiser and printed with MARS-M at DLR and SiMaP's 3D-printer at ESRF with different ranges of parameters. The results of two different printers were analysed for their microstructural characteristics involving elemental compositions and phases identification by SEM. Tomography results obtained at ESRF were analysed for porosity quantification and hot tearing in the printed material. Thermophysical properties, presence and formation of different phases were determined to understand the thermal behaviour of the material.

DED-LB/Mp additive manufacturing of a G91 steel using atomized and mixed commodity powders

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Among all additive manufacturing (AM) technologies, Directed Energy Deposition, DED, is preferred due to its ability to produce relatively large parts requiring minimal tooling and relatively little secondary processing. In addition, DED processes can be used to produce components with composition gradients, hybrid structures with different materials and microstructures and to repair or add features on pre-existing components. But, probably one of the main interests for some industries is the potential to fabricate spare parts on demand as in the case of the Energy sector. In this sector, G91 ferritic-martensitic alloy is of specially interest due to its stability at high temperatures and creep strength. However, this material does not exist as powder feedstock and parts are not conventionally made using pulvimetallurgy routes.

In this work, we have optimized and printed by Laser Beam Directed Energy Deposition using metallic powder (DED-LB/Mp) several coupons using an atomized G91 alloy in a robot cell consisting in a KUKA industrial table and robot with a PERMANOVA laser head equipped with a FHG-IWS continuous nozzle and a 8kW COHERENT fibre laser. A GTV powder feeder was used to blow the powder carried using an argon flow. On the other hand, a pre-mix of commodity powders (H13 and SS430L) as prepared using a Turbula mixer with a composition close to the G91 one. With this pre-mix, also tracks, overlaps and coupons have been printed and compared with the original alloy. Macro and microstructural observations were made using Optical Microscopy (OM) to assess both quality and microstructure, revealing no noticeable porosity nor cracks for both materials. The microstructure was also studied using Scanning Electron Microscopy (SEM) to detect intermetallic and or segregations on different regions of the coupon. The resulted microstructure present different morphologies and phases depending on the printing parameters and the type of alloy. Finally, mechanical properties using microhardness, tensile and small punch tests (SPT) were obtained. A noticeable increase in resistance was detected in the mixture as a consequence of the higher content of carbon

Effect of long annealing heat treatment on the microstructure evolution and mechanical behaviour of LPBD Ti-6Al-4V alloy

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C1_6, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 14:30 - 16:30

The Ti-6Al-4V alloy is well known for its good mechanical properties, lightweight, and corrosion resistance. Laser Powder Bed Fusion (LPBD) additive manufacturing technique allows to produce complex geometry parts, as required in aeronautical, space, and medical industries. As built parts are very brittle because of its martensitic microstructure. To enhance the mechanical properties, such as ductility, post-built heat treatments are needed [1]. In this work, the effect of long isothermal heat treatments on the microstructure and resulting mechanical properties was studied. For this purpose, LPBD samples were fabricated. These samples were subsequently exposed to different thermal programs in the range of 750°C (14 hours) to 970°C (3 hours). Both, longitudinal and transversal crossed sections of the samples, have been analysed by scanning electron microscopy to study the microstructural changes in the sample series. Moreover, the hardness and elastic modulus of the samples were obtained by nanoindentation to investigate the mechanical properties evolution under the different thermal treatments. Besides that, dilatometry tests were performed on the samples, and the Avrami equation was fitted to represent the kinetics of the transformation (evolution of α and β fractions) at different temperatures. The main results are related to the microstructure coarsening (increment in the α phase particle thickness) with the temperature increment of the heat treatment.

References:

[1] A.D. Boccardo, Z. Zou, M. Simonelli, M. Tong, J. Segurado, S.B. Leen, D. Tournet, Martensite decomposition kinetics in additively manufactured Ti-6Al-4V alloy: In-situ characterisation and phase-field modelling, *Materials & Design*, Volume 241, 2024, 112949.

Dynamic Chemical Milling for Enhancing Internal Surface Quality of LPBF-Manufactured Scalmalloy Components

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In recent years, the additive manufacturing of metal parts using Laser Powder Bed Fusion (LPBF) has gained significant traction in high-performance industries such as biomedicine and aerospace due to its ability to produce complex geometries with high precision. However, a major limitation of this technology is the relatively poor surface quality of the fabricated parts, which can negatively impact their functional properties, including wear resistance, corrosion resistance, and fatigue life. To address this issue, various post-processing techniques, such as mechanical polishing, shot blasting, and chemical or electrochemical treatments, are commonly applied to improve the external surface finish. However, enhancing the surface quality of internal features, especially in complex geometries produced via LPBF, remains a significant challenge due to limited accessibility and the lack of effective treatment methods.

This study presents preliminary findings on the development of a novel dynamic chemical milling methodology specifically designed to improve the internal surface finish of Scalmalloy alloy parts produced by LPBF. Scalmalloy, an advanced AlMg-based alloy developed by Apworks for aerospace applications, offers high strength and lightweight properties, making it a prime candidate for additive manufacturing. An experimental setup was designed to facilitate the controlled circulation of an etching solution within the internal cavities of the parts, ensuring uniform material removal. The etching solution, composed of NaOH, Na₂S, and triethanolamine, was formulated based on established aerospace industry practices for aluminum alloy chemical milling. This study systematically investigated the influence of chemical concentration, treatment temperature, and exposure duration on surface roughness while minimizing unintended reductions in wall thickness. The results provide insights into optimizing the process parameters to achieve significant improvements in internal surface quality, thereby enhancing the overall performance and reliability of LPBF-manufactured Scalmalloy components for critical aerospace applications.

Probing the Influence of HfC Nanoparticles on the Crack-Free Fabrication of CMSX-486 Nickel-Based Superalloy via Laser Powder Bed Fusion

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C1_7, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 17:00 - 19:00

The CMSX-4 single-crystal Nickel-based superalloy is widely employed in the aerospace industry due to its exceptional oxidation resistance and mechanical properties at high temperatures. The use of Additive Manufacturing (AM), particularly Laser Powder Bed Fusion (L-PBF), presents significant challenges in fabricating this alloy due to the poor weldability and high susceptibility to cracking. To address this, the present work explores a novel in-situ incorporation of Hafnium Carbide (HfC) nanoparticles as a strategy to enable a successful LPBF processing of CMSX486. The findings reveal that adding 2 wt.% HfC nanoparticles improved weldability and enabled the fabrication of a fully dense nanocomposite, at an optimal laser energy density of 83.33 J/mm³. By combining HfC nanoparticles incorporation with heat input control, this approach fully suppressed both solidification and solid-state cracking, reducing the cracking density from 9.2 mm/mm² to an almost negligible 0.15 mm/mm². Synchrotron X-Ray Diffraction (S-XRD) confirmed that HfC remained stable within the microstructure, acting as a reinforcing secondary phase without altering the γ/γ' lattice structure. The dislocation entanglement near HfC particles was analysed using Bright Field (BF-TEM) to indicate their role in pinning the grains/cells boundaries. The Dark Field (DF-TEM) imaging revealed that the γ/γ' eutectic phases are formed along the cell's boundaries in CMSX-486. Energy Dispersive X-ray Spectroscopy (EDX-TEM) identified the modification in elemental segregation and depletion at the cell's boundaries. These nanoparticles also induced a 50% refinement of the solidification cell's structure, further suppressing the elemental segregation and the embrittlement caused by gamma prime contents. Additionally, the impact of post-processing treatments, including jet-cooling Hot Isostatic Pressing (HIP) and Double Ageing (DA) on the gamma prime evolution and defects mitigation was investigated. These findings establish a groundbreaking framework for extending AM capabilities to single-crystal Ni-based superalloys, thereby unlocking pathways for their integration into high-performance aerospace applications.

Strategies for enhancing TiNbTa alloys via laser powder bed fusion processing: Effects of layer thickness, scanning speed, and remelting

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C1_7, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 17:00 - 19:00

This study investigates the optimization of laser powder bed fusion (L-PBF) parameters for manufacturing Ti-Nb-Ta alloys, aiming to improve production speed, material properties, and reduce porosity. The focus was on achieving columnar grains with a $\langle 001 \rangle$ crystallographic texture while analyzing the effect of varying printing parameters across different sample sizes. Two compositions of pre-alloyed Ti-Nb-Ta powders were utilized: Ti-20Nb-6Ta and Ti-35Nb-6Ta (wt.%), both processed under controlled conditions to assess their microstructural and mechanical responses. Characterization included scanning electron microscopy, uniaxial tensile testing, hardness testing, and X-ray fluorescence. Initial experiments used a 30 μm layer thickness, 80 μm hatch space, and varying scanning speeds (400, 700, 1000 mm/s) and laser powers (100, 200, 300 W) to assess melt pool behavior. A 67° rotation between layers promoted directional effects with melt pools around 200 μm in size and the greatest depth at the edges. Based on this, the layer thickness was increased to 150 μm for full fusion. To mitigate these issues, additional strategies were implemented, including reducing the scanning speed to 400 mm/s and applying a remelting step. While remelting effectively reduced porosity and enhanced fusion, it nearly doubled the production time, making it unsuitable for high-throughput manufacturing. Therefore, the optimal parameter set – 400 W laser power, 400 mm/s scanning speed, 80 μm hatch spacing, 150 μm layer thickness, and 1 mm stripe, without remelting – provided a balance between material quality and production efficiency. This configuration resulted in low porosity levels ($<0.1\%$) and acceptable fusion quality. The Ti-20Nb-6Ta and Ti-35Nb-6Ta alloys exhibited yield strengths of around 840 MPa and 600 MPa, respectively, exceeding those in existing literature. Hardness values were 281 HV for Ti-20Nb-6Ta and 218 HV for Ti-35Nb-6Ta. The study emphasizes the importance of optimizing L-PBF parameters to balance material performance and production efficiency.

In-Situ Lamination during 3D Printing of High Silicon Steel

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C1_7, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 17:00 - 19:00

Theorists, experimentalists, and industrialists have all acknowledged that further improvements of electrical steel (ES) magnetic properties with the current chemical composition and manufacturing routes is extremely challenging. However, to enable the prevailing vehicle and aircraft electrifications revolution, further developments in materials and electrical machine design are required. Today, additive manufacturing (AM) unlocks opportunities for novel machine designs and production of higher Si steels than previously available via standard manufacturing routes. However, challenges around their inferior magnetic properties remain to be overcome. Here, the in-situ lamination during 3D printing of 6.5%Si steel is demonstrated. The in-situ steel lamination via “Coating and Fusion” was conducted through a combination of powder coating and printing strategies that enabled a production of a near net shape laminated high Si steel. The Ar atomised 6.5 wt% Si steel powder was coated with Fe-(Mn,Zn) ferrite by sol-gel auto-combustion method and with SiO₂ by sol-gel method for comparison purposes. Various Ferrite/ES and SiO₂/ES ratios were explored to determine the desired coating thickness. The coated powder was fused in the ProX300 Laser Powder Bed Fusion to build successive and insulated layer by layer of high Si steel. The study highlights the need for extensive optimisation of coating compositions, thicknesses, and scanning strategies to refine the process. While in-situ lamination was successfully achieved, the coating layers were non-uniform and discontinuous. Preliminary results suggest that coating 6.5% Si electrical steel with (Mn_{0.8},Zn_{0.2}) Fe₂O₄ improved its magnetic properties compared to conventionally printed 6.5% Si steel.

Real-Time Insights into Microstructure Evolution in Laser Powder Bed Fusion Using Operando Neutron and X-ray Diffraction

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C1_8, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 10:30 - 13:10

Additive manufacturing (AM) has transformed modern materials processing, enabling the fabrication of highly complex structures with remarkable efficiency. Among the various AM techniques, laser powder bed fusion (LPBF) is particularly notable for its ability to produce intricate metallic components. The process relies on a high-energy laser to selectively melt fine metal powders, followed by rapid solidification. However, the extreme thermal gradients and fast phase transformations inherent to LPBF present challenges in controlling microstructural development, residual stress distribution, and defect formation. Gaining a deeper understanding of these evolving phenomena is key to optimizing processing conditions and enhancing material properties.

In recent years, operando neutron and synchrotron X-ray diffraction have emerged as powerful methods for capturing real-time microstructural changes occurring within and around the melt pool during laser-based AM processes. These advanced techniques offer crucial insights into phase transitions, thermal effects, and stress evolution—factors that ultimately dictate the final performance of AM-produced materials.

Achieving meaningful operando measurements requires specialized experimental setups that not only mimic industrial AM conditions but also integrate seamlessly with synchrotron and neutron beamlines. This presentation showcases the developments at the Paul Scherrer Institute (PSI) aimed at overcoming this challenge. A series of miniaturized, AM-compatible setups have been designed and implemented at beamline facilities, enabling real-time studies of LPBF processes.

Demonstrations of these setups include case studies where operando X-ray diffraction provides detailed tracking of phase evolution and thermal behavior across various alloys and multi-material systems. Neutron diffraction and Bragg edge imaging reveal critical insights into the development of residual stresses in bulk components. Fast X-ray imaging provides insight into cracking mechanisms and chemical mixing at the interface of multi-materials.

By directly observing transient phenomena as they occur, these techniques not only enhance our understanding of LPBF process dynamics but also generate valuable experimental datasets for refining computational models. Ultimately, these findings contribute to improving AM process control, optimizing material properties, and increasing the reliability of additively manufactured components.

Accelerating Thermal History Predictions in Additive Manufacturing with Artificial Intelligence.

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C1_12, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 17:00 - 19:00

In the scope of understanding the factors controlling the defects that commonly appear in the microstructures of materials produced by Additive Manufacturing (AM), a first step is the prediction of the thermal history at which the material is subjected by means of different printing parameters. The extremely large number of different combinations of printing parameters (laser power, hatch distance, laser scanning speed...) adds to the different printing geometries which also can vary the influence of such printing parameters. Its computation by means of Finite Element Modelling is the logical choice, but is time consuming and cannot be used in large computational optimization processes.

This work therefore aims at developing a fast and accurate predictive methodology to calculate temperature history during the AM process. First, a Finite Element Method (FEM) model was developed to extract thermal profiles at key points for Selective Laser Melting processes, optimized for computational efficiency for many different combinations of the printing parameters. Subsequently, different Machine Learning (ML) methodologies are tested as predictive models to determine the most robust approach. The models employed include several Tree-based methods and Deep Learning methods (i.e., Neural Networks). These models were fed with the generated dataset, yielding optimal predictive outcomes for both Extremely Randomized Trees (ERT) and Feedforward Neural Networks (FNN) with very good performance. Additionally, by leveraging Long Short-Term Memory (LSTM) networks, the study has enabled the prediction of thermal profiles for any point within a wide variety of scanning strategies. This was achieved through the innovative use of "Constrained random walks" (CRW), an approach specifically developed to train ML models for predicting thermal profiles across diverse scanning strategies and printing geometries.

The results demonstrate that it is viable to develop models based on ML for predicting thermal profiles in AM for a large variety of printing parameters and strategies, offering quasi-instantaneous predictions with minimum error as compared to the computationally expensive FEM simulations.

4D printing of buckling-induced architected Fe-based shape memory alloys, microstructure and mechanical behavior

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C1_12, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 17:00 - 19:00

This study focuses on buckling-induced architected materials (BIAMs), a class of materials engineered for enhanced functionality and efficiency by manipulating geometry and base material. Existing metallic BIAMs exhibit a trade-off between energy dissipation and geometrical recoverability, limiting their applications. This research introduces 4D printing of buckling-induced architected Fe-based shape memory alloys (BIA Fe-SMAs) of a designed and optimized geometry using finite element (FE) simulations by Wire-Arc Additive Manufacturing (WAAM). Material characterization, heat treatment, and compression tests of the printed parts from low-alloy carbon steel and Fe-SMA were carried out to assess energy dissipation and geometrical recoverability. The results of the compression tests are using to refine the parametric design of a larger-scale BIAM, which will be printed and tested to evaluate its suitability for practical applications.

To achieve this, single pulse WAAM process parameters were first optimized by printing several single-layer samples of low-alloy carbon steel and Fe-SMA. Various path strategies were then investigated, including back-and-forth layer deposition, zigzag printing, continuous and discontinuous printing of walls and Tee-joint connections. The printed dampers using the optimized strategy were tested using Digital Image Correlation (DIC) to evaluate their mechanical performance.

In the following, in addition to microstructure analysis and hardness testing, the shape memory properties (shape memory effect and pseudoelastic) of BIA Fe-SMAs were first analyzed systematically for the entire dampers and then individually for Tee-joint connections, sinusoidal profiles, and walls.

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Effect of Surface Finish and Heat Treatments on the Mechanical Behaviour of WE43 Alloy Lattice Structures Fabricated by Laser Powder Bed Fusion

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C1_7, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 17:00 - 19:00

Laser Powder Bed Fusion (LPBF) is an advanced additive manufacturing technique that uses a laser to selectively melt metallic powder particles layer by layer, enabling high customisation in 3D component production. It allows for intricate geometries unattainable by traditional methods like casting or machining, optimising structures by reducing weight and material waste.

Magnesium alloys have significant potential in industries such as biomedical and transportation. They are the lightest structural material, with a density of 1.8 g/cm³, which gives them high specific properties. In the case of the WE43 alloy, the presence of rare earth elements in its composition allows it to be heat-treatable, enabling modifications to its mechanical and electrochemical properties.

In this study, compression specimens of WE43 alloy were fabricated using Laser Powder Bed Fusion (LPBF), and two heat treatments, T5 and T6, were applied. To compare the effect of these treatments on mechanical behaviour, the microstructures (as-built, T5, and T6), microhardness, and surface finish of the samples will be analysed.

The as-built alloy has a hardness value of 83 HV, which is 23% higher than that of the sample fabricated by non-additive processes. The T5 treatment results in a 20% increase in hardness compared to the as-built samples, while the T6 treatment yields values equivalent to the as-built ones. This phenomenon is related to a change in the proportion of β' precipitates and is accompanied by a decrease in ductility. The microstructure has been analysed using optical microscopy, scanning electron microscopy (SEM), and transmission electron microscopy (TEM), as well as an EDS compositional analysis to evaluate the evolution of precipitates, the composition of different phases, and changes in grain size.

Regarding compression behaviour, taking the as-built sample as a reference, the T5 treatment shows higher strength. This effect is due to the precipitation of phases as a result of aging. In the case of the T6 treatment, greater ductility is observed compared to the previous cases, as the solution treatment eliminates secondary phases and precipitates formed during fabrication.

Heat treatments of 17-4PH stainless steel produced by binder jetting: tailored cooling rates for performance repeatability

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C1_6, Manuel de Falla Auditorium (Level +1), settembre 16, 2025, 14:30 - 16:30

Binder jetting has emerged as a key additive manufacturing technology, enabling the production of geometrically complex components from various metallic alloys. Nonetheless, the multistep nature of the process introduces a large variety of independent parameters which could affect the properties of the printed components, thus limiting the performance repeatability for the same material supplied by different producers.

This study explores the microstructural evolution and mechanical response of 3D printed 17-4PH martensitic stainless steel subject to tailored thermal treatments. The aim is to understand the interplay between processing and mechanical properties to design heat treatments capable of achieving repeatable performance regardless of the powder chemical composition, the binder jetting printing system and the sintering route (temperature/duration), thus facilitating the adoption and commercialization of printed components in the highly demanding biomedical sector.

A comprehensive description of the microstructure is obtained by SEM equipped with EDX and EBSD, aided by the detection of reverted austenite formation by XRD. Phase evolution description is clarified by CALPHAD modelling of equilibrium and precipitation phenomena. Hardness values are collected at the macro- and micro-scale through Rockwell C and Vickers indenters to determine the contribution of different phases. Tensile testing (ASTM E8/E8M) is performed on as-sintered and heat treated samples to evaluate the variation and strength and ductility at subsequent manufacturing stages.

For 17-4PH stainless steel, the as-sintered materials exhibited a continuous δ -ferrite network within a martensitic matrix, with Cu-rich phases localized within the ferritic regions, and solution annealing was found to redistribute alloying elements more homogeneously and reduce the continuity of the ferritic network. Different mechanical properties, especially tensile strength and hardness, can be achieved by aging at different temperatures and times, according to standardized procedures (e.g. H900 and H1150 from ASTM A564/A564M – 19a). The only available control parameter was the cooling rate: water quenching, air cooling and nitrogen-assisted cooling after solution annealing and aging were analyzed to understand whether specific combinations could produce constant and satisfactory mechanical performance regardless of the specimens production route.

This investigation highlights the critical role of thermal processing strategies in enhancing the microstructure and mechanical performance of binder jetted metallic alloys. The findings underscore the importance of solution annealing, which removes undesired secondary phases obtained during sintering, and fast cooling rates preventing the uncontrolled precipitation of copper after solution annealing, thus allowing an optimal tuning of the mechanical strength by aging.

Sustainable processing of metal components by material extrusion additive manufacturing technique and concentrated solar energy

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Material extrusion additive manufacturing (MEX) enables the design and production of complex metal components, optimizing their physical, mechanical and/or thermal properties, with wide applicability in numerous industrial sectors. It is considered a sustainable technology as it minimizes waste generation and natural resources consumption, thanks to its high material utilization rate, without compromising quality and functionality of the final product. MEX is based on a three-stage PDS (Printing-Debinding-Sintering) methodology: the first step involves 3D-printing using filaments composed of binder system and metal powder, then the polymeric content is removed, and, finally, the parts are sintered at high temperatures during prolonged times. The final sintering stage is the most energy-demanding, so the exploration of new clean energy resources and the development of more efficient energy utilization strategies should be prioritized at this stage.

Concentrated Solar energy (CSE) is proposed as a clean, renewable, and non-polluting energy resource that is highly efficient for high-temperature materials processing. In this context, this research studies the feasibility of using CSE in the sintering of metallic components obtained by advanced additive manufacturing techniques. Concentrated solar energy through a low-cost Fresnel lens installation was used in the sintering stage of metal parts produced via MEX in a novelty methodology defined as PDSS (Printing-Debinding-Solar Sintering).

Optimal PDSS processing parameters were established for H13 tool steel, Inconel 625 nickel-based alloy and copper components. Density measurements, SEM microscopic analysis and mechanical characterization were carried out at the different stages of the processing in order to evaluate the porosity and properties of as printed, debinded and final parts. It has been demonstrated that the use of CSE in the sintering stage lowers treatment temperatures and shortens manufacturing times thanks to the activator effect of solar radiation in diffusion processes, reducing total costs and environmental footprint. Furthermore, solar sintered metal components achieved competitive relative density properties up to $\approx 95\%$, as well as adequate dimensional accuracy compared to conventional material extrusion additive manufacturing. Finally, different components with relatively complex geometries and specific applications have been designed and processed via PDSS.

Solar reactive sintering applied in Additive Manufacturing and Powder Metallurgy to process multi-material components

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C1_7, Manuel de Falla Auditorium (Level +1), septiembre 16, 2025, 17:00 - 19:00

Multimaterials are becoming increasingly relevant in sectors such as the energy and aerospace industries due to their ability to combine advanced thermal, chemical, and mechanical properties into a single component, enhancing performance, durability, and operational safety. Among them, copper aluminides stand out for their applicability in heat dissipators, tribological components, and aircraft engine parts. This study analyzes the synthesis and processing of multimaterials based on intermetallic compounds through powder metallurgy and additive manufacturing. In the powder metallurgy method, laminated metallic materials are processed from mixtures of elemental copper and aluminum powders, activated using concentrated solar energy. Three experimental configurations have been designed: multilayer Cu/Al/Cu systems, multilayer systems with a reactive intermediate layer (Cu with 15-30-50 wt.% Al), and Cu-Al powder mixtures with 15, 30, and 50 wt.% Al. Prior to solar treatment, the samples, in the form of 16 mm diameter disks, were compacted at 200 MPa. On the other hand, multimaterials are obtained via additive manufacturing, using filaments composed of metallic powder (Cu and Al alloy) and PLA as a polymeric binder, which undergo a debinding cycle followed by sustainable solar sintering. In both processes, a Fresnel lens is used as a solar concentrator, capable of multiplying the incident solar radiation up to 2644 times, reaching a power density of $\sim 260 \text{ W/cm}^2$ in a 16 mm diameter focal point.

The processed multimaterials are characterized using X-ray diffraction (XRD), optical microscopy, and scanning electron microscopy with EDX analysis (SEM-EDX), and Vickers hardness testing. The powder metallurgy results reveal the synthesis of copper aluminides with different stoichiometries, low porosity, good metallurgical bonding between layers and minimal dimensional distortion after cooling. Similarly, 3D-printed parts exhibit excellent adhesion between layers during printing, proper binder removal, and high densification after solar processing. In both methods, solar reactive sintering activates highly exothermic reactions between Cu and Al, promoting the formation of intermetallic compounds through SHS (Self-propagating High-Temperature Synthesis) processes.

Microstructure, mechanical and thermal properties of copper – steel multimaterials fabricated by laser direct energy deposition

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Copper – steel multimaterials combine the excellent electrical and thermal conductivity of copper with the high mechanical properties of steel. Compared to conventional joining techniques, additive manufacturing enables the fabrication of complex multimaterial components with precise control over internal material distribution. However, the manufacturing of copper – steel parts presents significant challenges due to the poor solubility between Cu and Fe and the large discrepancy in thermal conductivity and expansion coefficients, often leading to the development of large thermal stresses and the formation of solidification cracks.

This investigation is focused on the characterization of copper – steel multimaterial parts produced via laser direct energy deposition, using a system equipped with multiple hoppers for the simultaneous deposition of different powders in controlled weight ratios. Pure copper and AISI 4130 low-alloy steel powders were used for the in-situ fabrication of distinct blend compositions, which serve as the building blocks for a possible functionally graded structure: 100% 4130, 75% 4130 – 25% Cu, 50% 4130 – 50% Cu, and 25% 4130 – 75% Cu. The samples were characterized through X-ray fluorescence and diffraction, optical and scanning electron microscopy, microhardness, indentation plastometry, and laser flash analysis to determine their chemical composition, microstructural features, and mechanical and thermal properties.

As-built parts exhibited peculiar macrostructure morphologies resulting from Fe-Cu liquid phase separation and Marangoni effect. A recursive macrostructure comprising Cu and Fe regions alternating as matrix and dispersed phase at different length scales was observed for 50% 4130 – 50% Cu composition. Large thermal stresses and scarce terminal liquid at the end of solidification led to the formation of cracks in the samples with 75% 4130 – 25% Cu composition, whereas the abundant terminal liquid in 50% 4130 – 50% Cu and 25% 4130 – 75% Cu allowed microcrack backfilling, resulting in sound parts.

The formation of interconnected Cu regions in 50% 4130 – 50% Cu and 25% 4130 – 75% Cu samples led to ~50% and ~200% higher thermal diffusivity compared to the base steel, respectively. Fine martensitic constituents, supersaturated solid phases with finely dispersed precipitates, and the interaction between hard Fe and soft Cu domains contributed to high strength and ductility in 50% 4130 – 50% Cu parts. Heat treatments improved the strength and hardness of 100% 4130 samples due to the formation of tempered martensite, while 50% 4130 – 50% Cu samples softened due to Cu recrystallization and Cu/Fe diffusion from supersaturated phases.

Additively manufactured high-strength and heat-resistant eutectic aluminum alloys

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Aluminum alloys are widely utilized in lightweight structural applications due to their favorable strength-to-weight ratio and excellent corrosion resistance. However, in additive manufacturing, conventional high-strength aluminum alloys exhibit a pronounced susceptibility to solidification cracking, significantly limiting their processability and applicability. Moreover, these alloys suffer from severe mechanical degradation at elevated temperatures, as the precipitate phases undergo rapid coarsening and lose their strengthening efficacy. Consequently, there is a pressing need to develop novel alloy design strategies that mitigate cracking susceptibility while ensuring superior thermal stability and mechanical performance in high-temperature environments. This work presents a novel Al-Ni-Fe-Zr eutectic alloy, designed using thermodynamic principles and non-equilibrium solidification modeling to optimize both printability and mechanical performance. Fabricated via laser powder bed fusion, the alloy with finer grains in the horizontal and vertical planes, refined by Zr-induced nucleation, significantly reduces microstructural anisotropy. The alloy achieves an as-built yield strength of 339.9 MPa and ultimate tensile strength of 560.9 MPa, attributed to its refined ~300 nm cellular microstructure with high-volume fractions of stable Al₃Ni eutectics. Thermal exposure at 350 °C for 100 h demonstrated the alloy's excellent resistance to coarsening, indicating its thermal stability. In-situ synchrotron X-ray diffraction, analyzed via the Williamson-Hall method, revealed significant dislocation accumulation in the as-built state. Aging led to partial dislocation recovery, suggesting a moderate relaxation of internal stresses. Nanosized L1₂-Al₃Zr precipitates with coherent interfaces further enhanced the yield strength to 391.4 MPa after aging at 300 °C for 6 h and contributed to high-temperature interface stability. These findings highlight the potential of the Al-Ni-Fe-Zr alloy for high-performance applications in environments where long-term thermal stability and mechanical integrity are crucial.

A new stainless steel with microstructural and compositional gradient by selective laser melting

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Additive manufacturing (AM) is driving metallurgists to design new alloys and complex microstructures. One of the main restrictions of AM is that, in general, it is not intended for a subsequent thermomechanical process, which motivates the study of alternative hardening methods based on pure heat treatments.

This work proposes the design and manufacturing of a new stainless steel by selective laser melting, in line with the following alloying and microstructural strategies: Nickel content reduction and mechanical composite behavior conferred by a layered structure. The intrinsic heat treatments during the manufacturing process will be explored in order to achieve a controlled microstructural refinement, and, consequently, improved mechanical properties.

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Influence of laser powder bed fusion on the microstructure and thermoelectric properties of CuNi

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C1_9, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 14:30 - 16:30

Thermoelectric materials enable the direct conversion of thermal energy into electrical energy and vice versa, offering a promising approach for energy harvesting and active cooling in various applications. However, the conventional manufacturing of such materials restricts the geometrical complexity, involves long process chains and leads to significant material losses. Additive manufacturing offers a solution for a potential broader application of thermoelectric devices, by enabling the direct fabrication of complex, customized structures. At the same time a reduction of material consumption and production time can be achieved as well as controlling the microstructure. However, applying additive manufacturing to synthesize thermoelectric materials still requires considerable research regarding processability and material properties. Furthermore, developing eco-friendly, non-toxic and earth-abundant thermoelectric materials that are competitive for specific applications are becoming increasingly important.

The present contribution investigates the additive manufacturing of an earth abundant CuNi alloy by laser powder bed fusion (PBF-LB/M). Through optimized process parameters development, highly dense bulk samples were successfully produced. Furthermore, PBF-LB/M enables specific tailoring of the microstructure, i.e. regarding grain size and morphology, by adjusting the process parameters as detected by optical microscopy, scanning electron microscopy (SEM), electron backscatter diffraction (EBSD) and X-ray diffraction (XRD). This process optimization enables the modification of thermoelectric properties, such as electrical and thermal conductivity as well as the Seebeck coefficient, to meet the demands of advanced applications.

Microstructure Analysis and Micro-Mechanical Properties of Cu-based Metallic Glass between Different Scanning Strategies by Laser Powder Bed Fusion

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C1_8, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 10:30 - 13:10

With advancements in additive manufacturing (AM) technology, researchers have identified that the high cooling rates and small-scale molten pool characteristics inherent to this process offer a viable pathway for fabricating bulk metallic glasses (BMGs). By precisely controlling processing parameters based on the energy density equation, molten pools in the Laser Powder Bed Fusion (LPBF) process can be systematically stacked, enabling the formation of fully dense final components.

Despite the theoretical advantages of LPBF for BMG fabrication, two primary challenges remain. First, the densification of printed structures is highly sensitive to process parameters, including laser power (P), scanning speed (v), hatch distance (h), and layer thickness (t). These four parameters collectively define the energy density, which governs molten pool behavior. Optimizing these parameters is critical to achieving a homogeneous arrangement of molten pools within the material, thereby maximizing densification. Second, the formation of a heat-affected zone (HAZ) due to heat conduction around the molten pool poses a significant risk to maintaining the amorphous structure. If the printed amorphous alloy is reheated beyond its glass transition temperature (T_g), crystallization may occur, compromising the material's desirable properties.

To address these challenges, this study introduces a repetitive scanning strategy. In the initial scan, a lower energy input partially melts the metal powders, creating a porous structure that enhances heat dissipation and mitigates the impact of the HAZ. A subsequent scan with higher laser energy then fully melts the porous structure, ensuring densification while minimizing crystallization risks.

Microstructural analysis revealed that the two scanning strategies produced distinct phase separation morphologies. Furthermore, nano-indentation testing demonstrated that these variations in scanning strategy led to differences in micro-mechanical properties across different regions within each molten pool. In conclusion, this research focuses on comparing the effects of single-pass and repetitive scanning strategies on microstructural evolution and micro-mechanical performance, providing insights into optimizing LPBF parameters for BMG fabrication.

Microstructural Evolution and Mechanical Performance of Heat-Treated LPBF 17-4PH Stainless Steel:

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Additive Manufacturing (AM) processes, particularly Laser Powder Bed Fusion (LPBF), have revolutionized the production of complex metallic components. Among various materials, 17-4PH stainless steel has gained significant attention due to its excellent combination of strength, hardness, and corrosion resistance. However, the rapid solidification conditions typical of LPBF processes lead to unique microstructural features that differ from conventionally manufactured parts, requiring specific post-processing treatments to achieve optimal properties.

This study investigates the influence of various heat treatment parameters on the microstructural evolution and mechanical properties of LPBF-manufactured 17-4PH stainless steel. Despite significant research in this field, contradictory results are often reported in literature regarding microstructural features obtained under as-built condition and optimal post-processing conditions. The inert gas used during the manufacturing process has been also reported to affect microstructural features under as-built condition. A comprehensive experimental campaign was conducted combining multiple characterization techniques, including optical microscopy, Scanning Electron Microscopy (SEM) and X-Ray based techniques to analyze the phase transformations and precipitation phenomena. Mechanical properties were evaluated through Vickers microhardness measurements. Different heat treatment cycles were tested to identify the optimal processing window for achieving desired microstructural features and mechanical performance.

Building upon the optimized heat treatment parameters, lattice structures were fabricated and mechanically characterized through compression testing. This application-oriented phase of the research demonstrates the potential of properly heat-treated LPBF 17-4PH for lightweight structural applications. The results provide valuable insights into the relationship between processing parameters, microstructural evolution, and mechanical behavior of LPBF 17-4PH, contributing to a better understanding of this widely used but complex material system.

Design of thermal treatments and composition evaluation of bio-compatible HEA Ti 3DP alloys based on computational thermodynamic approach

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The design of titanium-based high-entropy alloys (HEAs) for biomedical applications presents a significant challenge, particularly when considering the complex thermal histories associated with additive manufacturing (AM) processes. This work leverages advanced computational tools to investigate the microstructural evolution and mechanical properties of a range of Ti-HEA compositions subjected to diverse AM thermal cycles. By integrating computational modeling with experimental validation, this study aims to establish a robust framework for selecting optimal HEA compositions and developing tailored post-AM heat treatments to achieve the desired combination of biocompatibility, strength, and ductility for demanding biomedical applications.

Post-processing effects on surface integrity of C300 subjected to different finish machining conditions.

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Additive Manufacturing (AM) techniques have attracted much attention due to the capability to produce unique and complex geometries with high productivity rates. Selective Laser Melting (SLM) is one of the most widely used techniques due to its versatility with various materials. It allows the production of complex three-dimensional parts, the production of functional components and is economically viable [1]. As a result, SLM are becoming increasingly used in several industries as in the aerospace, automotive or biomedical industries [2]. Nevertheless, one of the limiting factors of AM processes is the part surface quality closely related to service performance and durability. Therefore, the as-produced metallic AM parts cannot be used directly, and subsequent post-treatments are required. In this work, the influence of different finish electrical discharge machining (EDM) strategies to improve the surface integrity quality and mechanical properties of a C300 maraging steel with a simple geometry was studied. Damage characterization of the machined subsurface was analysed in terms of microstructural changes and micromechanical behaviour.

Surface integrity of both AM and AM machined samples were characterized on surface and cross-section view. A combination of nanoindentation techniques and advanced microscopy techniques including, 3D Optical profilometry, scanning electron microscopy (SEM-EDX) and electron backscattered diffraction (EBSD) were used to study the effect of the post-processing strategy on both the surface and the subsurface levels. Results are presented in terms of micromechanical changes (hardness and elastic modulus) and micro-damage discerned at the edge of the post-processed surface.

The results from these tests will allow for the prediction of the most effective post-processing methods to enhance the mechanical performance of additive manufactured components. Additionally, this study will offer valuable guidance for future advancements in the field, particularly in optimising the mechanical properties of components with inhomogeneous microstructures commonly found in additive manufacturing.

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In-situ x-ray imaging of porosity control by power modulation during additive manufacturing by the directed energy deposition technique.

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In-situ synchrotron X-ray imaging has been used to directly observe the behaviour and mechanisms of porosity formation during directed energy deposition laser additive manufacturing of a nickel based superalloy material. The flow pattern established in the melt pool can be observed to entrain the porosity and allow coalescence into larger pores. Disrupting the flow pattern by applying modulation to the laser power allows porosity to escape while also minimising the size by preventing coalescence. This behaviour has been observed via X-ray radiography. The variation of these effects under different modulation frequencies and wave patterns can be used to develop optimised deposition procedure and provide data to physical models, to achieve good quality additively manufactured items of such materials.

Innovative FeCr alloys SOFC/SOEC Interconnectors processed by advanced processing technologies leveraging master alloy concept

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This study assesses innovative FeCr alloys designed for interconnectors in solid oxide fuel cells (SOFC) and solid oxide electrolyzer cells (SOEC). Using Crofer22 APU as a reference, novel alloys were developed for powder injection molding (PIM) and material extrusion (MEX) additive manufacturing, seeking improvement in performance with scalable and cost-effective processing routes. These alloys incorporate controlled additions of cobalt, manganese, and copper into a Fe-30Cr matrix using the master alloy approach to optimize thermal expansion, oxidation resistance, and mechanical strength. Both PIM and MEX processing were optimized to ensure defect-free fabrication of complex interconnectors. The feedstock formulation was carefully adjusted to achieve homogeneous powder dispersion and optimal flowability. Injection parameters were refined to minimize defects such as warping and residual stresses. Similarly, MEX processing involved fine-tuning extrusion parameters, including temperature, layer adhesion, and infill density, to enhance shape retention and reduce porosity. For both techniques, debinding strategies were optimized to prevent carbon residues, employing a two-step thermal and solvent-based approach that ensured complete binder removal without compromising dimensional stability. Sintering was conducted at 1320 °C, leading to near-full densification and a uniform microstructure with finely dispersed precipitates. The impact of exposure to in-service conditions, including high temperatures and oxidizing/reducing atmospheres, was evaluated through detailed microstructural characterization and phase analysis using scanning electron microscopy (SEM) and X-ray diffraction (XRD). Mechanical performance was assessed via microhardness and bending tests, comparing as-sintered specimens with those subjected to simulated operating environments. By addressing critical manufacturing challenges this research enhances the viability of advanced FeCr alloys for interconnector applications, supporting the development of more efficient and durable components for sustainable energy technologies.

Effect of static recrystallization on the anisotropy of mechanical properties of Inconel 625 additively manufactured by LPBF process

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The post processing heat treatment which significantly reduces the anisotropy of mechanical properties of additively manufactured (AM) materials is currently gaining attention. Due to the fact that static recrystallization occur in Laser Powder Bed Fusion (LPBF) Inconel 625 without any plastic deformation, the heat treatment involving recrystallization might be applied for reduction in mechanical properties anisotropy. Therefore, the aim of this work was to determine the influence of static recrystallization of Inconel 625 LPBF on the mechanical properties and its anisotropy.

The repetitive melting and solidifying of the melt pools during the LPBF process generate a high residual stress level and high dislocation density in AM Inconel 625. Such material subjected to high-temperature annealing may recrystallized. The static recrystallization temperature and the recrystallization kinetics of Inconel 625 is LPBF process parameters correlated, whereas different microstructure is obtained after the processes with different sets of parameters. The samples for this experiment were manufactured using the LPBF machines with the laser beam spot size equal to 35 μm (AYAS 120LM) and 55 μm (SISMA MySint100). After manufacturing, the samples were annealed in a temperature range of 900-1200°C for 5 to 90 minutes. Such approach allowed determine the recrystallization temperature and its kinetics for materials obtained in two different printers. Subsequently, the heat treatment routs allowing achieve different level of recrystallized microstructure (approx. 50 and >90%) were designed to determine the effect of recrystallization on the mechanical properties and its anisotropy.

The microstructure of annealed samples was examined using light and scanning electron microscopy. The fraction of recrystallized grains was estimated from the grain orientation spread (GOS) determined by the EBSD analysis. The mechanical properties was evaluated in the tensile test.

The results of the study indicate that the static recrystallization temperature for both variants of Inconel 625 LPBF samples is between 950 - 1000 °C. Some differences in recrystallization kinetics are observed for Inconel 625 LPBF manufacture on AYAS and SISMA machines. Annealing at 950 °C for 90 min involved partial recrystallization of Inconel 625 LPBF-AYAS (~35 %) whereas more significant changes are observed in Inconel 625 LPBF-SISMA (~52%). The heat treatment, which trigger recrystallization, causing a significant reduction in the anisotropy of the mechanical properties of Inconel 625 LPBF, in parallel increases the plastic properties of the samples.

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High-temperature oxidation behavior of Inconel 625 superalloy processed by additive manufacturing

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Inconel 625 is a nickel-based superalloy that stands out for its excellent mechanical and resistance to oxidation and corrosion properties. Thanks to these characteristics, it is widely used in sectors such as power generation, the aerospace industry and the petrochemical industry, where parts are exposed to high temperatures and various corrosive environments or fluids. In these conditions, Inconel 625 components are susceptible to oxidation and corrosion problems and, therefore, deterioration or loss of functionality and safety in service.

In this work, the technology FFF (Fused Filament Fabrication) of additive manufacturing, also known as FDM (Fused Deposition Modeling), is used to produce Inconel 625 parts. This technique has demonstrated the possibility of obtaining metal parts in a much more economical, simple and safe way than other conventional and advanced manufacturing methods. A detailed study of high-temperature oxidation has been carried out to evaluate the mechanisms involved and the effects of oxidation on these components. The Inconel 625 parts manufactured using FDM have been exposed to temperatures of 850, 900, 950, 1000 and 1100 °C for times up to 96 hours, using both a muffle furnace and thermogravimetry equipment. After these tests, the oxidation constant has been calculated and the oxides formed on the surface have been characterized by X-ray diffraction and optical and scanning electron microscopy.

By studying the results obtained and carrying out a bibliographic review and comparison, it is demonstrated that fused filament additive manufacturing technology is a viable and economic alternative for the manufacture of Inconel 625 parts, which allows obtaining fully functional parts with potential for applications at high temperatures where materials with high resistance to oxidation and mechanical properties are required.

AM2C3 Twinning Project: Development of Al-based Metal Matrix Composites for Laser Powder Bed Fusion Additive Manufacturing

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The AM2C3 – Additive Manufacturing and Advanced Materials Competence Centre is a Horizon Europe Twinning project designed to establish a regional hub for cutting-edge research in metal additive manufacturing (AM) and advanced materials. The project brings together expertise from leading European institutions to develop high-performance materials tailored for aerospace, space, and high-value industrial applications. At full deployment, AM2C3 will serve regional SMEs by providing customized materials solutions, supporting New Space companies—the emerging private space industry driven by disruptive business models and independent innovation. As part of the University of Cyprus (UCY), the project will also build local expertise in high technology readiness level research, bridging materials science with industrial-scale implementation.

One of AM2C3's core research activities focuses on the development of next-generation high-strength aluminum alloys, optimized for Laser Powder Bed Fusion (LPBF) additive manufacturing. The project explores novel Metal Matrix Composites (MMCs) based on Al2618+, a Zr-modified aluminum alloy known for its improved processability in AM. Going beyond existing solutions, AM2C3 integrates nanoparticle reinforcements via mechanical alloying, aiming to enhance microstructural stability, mechanical performance, and high-temperature resistance. These reinforcements act as heterogeneous nucleation sites, refining the grain structure, reducing columnar grain growth, and mitigating hot cracking. Additionally, their presence contributes to load transfer strengthening and grain boundary stabilization, leading to improved hardness, wear resistance, and overall mechanical response.

Preliminary results demonstrate a homogeneous dispersion of reinforcements within the Al2618+ matrix, validating the feasibility of this novel Al-MMC approach for LPBF. Initial processing trials suggest promising densification behavior, with reduced porosity and enhanced microstructure compared to unmodified Al2618+. These advancements will broaden the AM processing window, making high-performance aluminum alloys more accessible for industrial adoption.

Microstructure and mechanical properties of additive manufactured 18Ni-maraging steel after two-step aging treatment

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Additive manufacturing (AM) is an advanced technology used for the manufacture of products that have intricate shapes and complex inner geometries. In commercial metallic material field, various metallic materials have been investigated to use AM processing. The microstructural features such as grain size and precipitates will differ profoundly from those obtained by casting, heat treatment and forming processing, which is resulted from the rapid heating and cooling rates during AM. Therefore, the evolution in microstructure of metallic materials fabricated AM with post-treatment can give an opportunity to discover the enhanced mechanical properties of the metallic materials. In this study, the maraging steel powder with mean particle radius of 36 μm have been used in AM experiment. The specimens with bulk cuboidal shape were fabricated with the optimized laser power and scanning rate conditions. The as-built specimens were composed of α' martensite phase in applied AM condition. The density of as-built specimens reached $\sim 8.03 \text{ g/cm}^3$, which is almost similar to the full density of maraging steel. The as-built specimens was aged at two different temperatures to form nanoscale precipitates in the α' martensite matrix. From the systematic microstructural analysis, it was found that the formation of nanoscale precipitates and its volume fraction depend on the aging temperature and time. After single aging treatment at 733 K exhibited Ni_3Ti type nano-precipitates. On the other hand, the specimens aged at two different temperatures contained two types of nano-precipitates. The microstructural evolution achieved by two-step aging treatment revealed an improved mechanical properties than the specimen aged by single aging treatment. Moreover, the processing time for aging treatment was reduced by two-step aging treatment. From these results, it is suggested that the optimized microstructure and mechanical properties of 18Ni-maraging steel can be achieved by modulating the aging treatment condition.

Altering microstructure and enhancing mechanical properties during additive manufacturing of Ti-6Al-4V via in-process laser heat treatments

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In this work, we have explored in-process laser-based heat treatment (LHT) as an alternative to post-process heat treatments such as annealing, in order to alter the hcp α' / α and bcc β phase content in additive manufactured Ti-6Al-4V. To that end, three samples were manufactured with a laser metal deposition machine, a directed energy deposition technique, with the laser operating at 300 W. The reference sample was not subjected to any LHT. For the remaining two samples, each deposited layer was subjected to either an LHT at 100 W (LHT100) for one sample or an LHT at 300 W (LHT300) for the other, without powder addition.

LHT100 showed an overall improvement in the strength/ductility trade-off. Whereas LHT300 resulted in a lower strength but a much higher ductility and toughness than the other samples. In order to understand the origin of these differences in the mechanical response, the contribution of each of the microstructural features and internal strains to the overall mechanical response is studied in detail. A combined analysis via synchrotron X-ray diffraction, scanning electron microscopy and transmission electron microscopy of the as-built samples revealed that the differences in between the different types of hcp phase fractions between the three samples has the dominant contribution to the difference in their mechanical response. These results, which will be presented in this talk, demonstrate the potential of in-process LHTs for altering microstructures and tailoring mechanical properties.

Correlation between Process Parameters and Microstructure of Nano- to Micro-Particle-Reinforced 3D Printed Aluminum Matrix Composites

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Lightweight materials are widely applied in aerospace, construction, and automotive applications. Introducing high specific strength materials is a promising way to achieve weight loss. Meanwhile, the 3D printing process is equally important due to its capability to realize complex lightweight designs. However, aluminum alloys such as Al-6061 and Al-7075 are challenging to be printed due to the hot cracking issue. Among the aluminum alloys, scalmalloy (Al-4.49Mg-0.71Sc-0.51Mn-0.27Zr-0.07Fe-0.03Si alloy, Al-Sc alloy) was developed to overcome the hot crack issue during the laser powder bed fusion (LPBF) process. In our previous study, the nano to micron-sized defects, such as the precipitate-free zone or unmelted powders, were successfully eliminated with the assistance of Al/MgI. In this study, in-situ synthesis and ex-situ addition were introduced to accomplish the simultaneous strengthening of precipitation and dispersion. Sc was added to the Al-Mg alloy to precipitate the Al₃Sc nanoparticles during the solidification. At the same time, SiC particles were mixed with the Al-based alloy powders and would remain after 3D processing due to the higher melting temperature of SiC. The relationship between the microstructure evolution and process parameters, including the 3D printing process and heat treatment, was explored.

Coupling a continuous wave laser with a scanning electron microscope; use to improve mechanical behaviour of additive manufacturing 316L stainless steel

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C1_9, Manuel de Falla Auditorium (Level +1), septiembre 17, 2025, 14:30 - 16:30

Novel and vanguard fields like additive manufacturing (AM) require dedicated solutions to reach their full potential. In order to research the extreme heat processes involved in metal AM, a new coupling between a continuous wave laser and an environmental scanning electron microscope (SEM) was developed [1]. The laser parameters can be varied in a wide range that includes those used in metal AM techniques like laser powder bed fusion (LPBF) and laser-based direct energy deposition (LDED). The SEM allows to characterise in situ the processed materials in vacuum or controlled atmosphere.

This device was used to study the effect of lasering the surface of an LDED 316L stainless steel with LPBF parameters [1]. The state before and after lasering was characterised with SEM (secondary electrons, backscatter electron, electron backscatter diffraction), transmission electron microscopy and mechanical testing (static and fatigue). A one order of magnitude microstructural refinement was achieved, with significant mechanical behaviour improvement. These results showcase the capabilities of the laser SEM device, that also include great prospects for simulation research, which can gain significantly from the data provided by it [2,3].

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Manufacture of tailorable biodegradable Mg/Zn multimaterial by additive friction stir deposition; microstructural and interfacial characterisation

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C1_11, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 14:30 - 16:30

The development of biodegradable materials for the medical sector can bring substantial improvements in numerous applications. An example of this is bone implants. However, it is difficult to create a material that matches bone properties adequately and consistently during the healing process. A combination of Mg and Zn could assemble the advantages of both, that is, rapid degradation and elastic modulus similar to that of bone for Mg, which limits the stress shielding effect, and slow degradation and moderate strength for Zn.

Manufacturing a viable multimaterial with a good interface can be difficult. Additive friction stir deposition (AFSD) is an appropriate solution in this case. This solid state fabrication process has the potential to allow for tailoring the interface thickness and the structure of the intermetallic compounds (IMC) therein.

In this study, a Mg/Zn multimaterial was produced by AFSD from WE43 Mg alloy substrate and cast Zn-Mg alloy bar feedstock. Extensive microstructural analysis including XRD, EDS, EBSD, 3D FIB-SEM and TEM allowed to characterise the multimaterial, with a focus on the interface, which exhibits a 3-layer IMC structure of Mg+MgZn, MgZn₂ and Mg₂Zn₁₁. Significant plastic accommodation was also found in the interfacial IMC layer. The obtained results are promising for the manufacturing of tailorable multimaterials with enhanced interfacial bonding for biodegradable applications.

Laser Powder Bed Fusion of Crack-Susceptible AISI M2 Tool Steel: From Process Parameter Development to Industrial Validation — A Comparative Study of Additively and Conventionally Manufactured Components

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

AISI M2 high-speed tool steel is extensively used in the forging and tooling industry due to its exceptional hardness and wear resistance. However, its conventional manufacturing route, which includes casting, forging, complex multi-step heat treatment, and diamond-tool-based hard machining, is both time- and cost-intensive. Additive Manufacturing (AM), specifically Laser Powder Bed Fusion (LPBF), offers a transformative alternative by enabling near-net-shape fabrication with rapid solidification and intrinsic layer-by-layer thermal cycling. This approach can potentially eliminate the need for extensive post-processing, such as prolonged heat treatments and hard machining.

Nevertheless, processing AISI M2 via LPBF remains highly challenging. The high carbon content (~1 wt.%) and complex alloy chemistry lead to poor weldability, causing crack formation, delamination, and high residual stresses due to the formation of hard and brittle martensitic and carbide phases. This work focuses on developing a robust LPBF process parameter set to fabricate crack-free AISI M2 components. A comprehensive parameter optimization strategy was employed to suppress cracking and produce defect-free builds.

The additively manufactured components were characterized using a suite of microstructural techniques including optical microscopy, SEM, EBSD, TEM, and XRD, along with mechanical testing such as hardness, tensile, and compression tests, benchmarked against conventionally manufactured counterparts. Finally, both sets of components underwent industrial cold forging trials to evaluate tooling life and failure mechanisms under real service conditions.

The study demonstrates the feasibility of producing crack-free AISI M2 tool steel via LPBF and establishes its potential to replace conventional manufacturing for high-performance tooling applications, significantly reducing processing time, cost, and energy consumption.

LOW- VELOCITY IMPACT PERFORMANCE OF 3D PRINTED CONTINUOUS FIBRE REINFORCED BIOINSPIRED COMPOSITES STRUCTURES

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This study proposes the development and mechanical characterization of bioinspired composite material structures based on Bouligand-type helicoidal architectures, processed using Fused Filament Fabrication (FFF) additive manufacturing technology. These structures can be found, for example, in the exoskeletons of various crustaceans and insects. It has been observed that such structures enhance the mechanical properties of the material, particularly its toughness and impact resistance. FFF-based additive manufacturing is a highly promising technology for polymeric materials and presents an alternative to conventional techniques due to its ability to create functional structures with complex geometries.

In this work, thermoplastic matrix composite structures reinforced with continuous carbon fibre were manufactured. The primary goal was to characterize the mechanical behaviour, specifically the toughness and low-velocity impact resistance, of bioinspired helicoidal composite structures reinforced with continuous fibre, depending on the reinforcement arrangement through the thickness. Additionally, the effect of a post-processing technique, hot compression, was analysed to reduce the porosity inherent to the manufacturing process. Mechanical characterization was performed using standardized ASTM D3039 tensile tests and ASTM D790 three-point bending tests. Furthermore, interlaminar shear strength (ILSS) tests were conducted in accordance with ASTM D2344 standards to analyse the effects of porosity, matrix-fibre interaction, and layer-to-layer interaction on the interlaminar behaviour for each configuration. Finally, Charpy impact resistance tests were performed according to ASTM D6110 for the different helicoidal configurations. The fracture surfaces were then analysed using scanning electron microscopy (SEM) and optical microscopy.

Advances and challenges in direct additive manufacturing of Al₂O₃ and ZrO₂-based Eutectic Ceramic Oxide

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Introduction

Al₂O₃-based directionally solidified eutectic ceramics have garnered significant interest over the past decades due to their exceptional high-temperature strength retention and creep resistance compared to metal alloys, as well as their superior oxidation resistance and microstructural stability relative to other ceramics. For these reasons, they have been identified as some of the most promising candidates for ultra-high-temperature structural applications. From a processing perspective, oxide eutectic composite ceramics have been produced through various solidification methods. However, these methods are often unable to achieve fine microstructures or fabricate large or complex-shaped components. To address these limitations, additive manufacturing (AM) presents a promising alternative for the production of monolithic and complex-shaped ceramic parts with fine and homogeneous microstructures.

The aim of this study is to evaluate the feasibility of using L-PBF technologies for the production of Al₂O₃-based eutectic ceramics.

In the initial phase of the study, the focus was on characterizing and optimizing the particle size distribution (PSD) of eutectic Al₂O₃-ZrO₂ based granules for use in various laser powder bed fusion (PBF) technologies. Initial characterization, performed using SEM imaging and laser granulometry, assessed the PSD, average particle size, and distribution width of the engineered batches. Subsequently, the optimized ceramic powders, with tailored size distributions, morphologies, and compositions, were selected for specific applications in L-PBF (fiber laser) and L-PBF (CO₂ laser) technologies. The addition of graphene to the studied compositions enabled an evaluation of its impact on laser beam absorption.

Acknowledgement

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Advancing Sustainable Filtration: Integration of 3D Printing and Graphene Oxide-Based Composites

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

3D printing, or additive manufacturing, enables the construction of three-dimensional objects from digital models, such as CAD files. This technology stands out for its versatility, allowing the creation of complex and customized geometries difficult to achieve with traditional methods. It is widely applied in engineering, medicine, and industrial design [1]. Among the 3D printing methods, fused filament fabrication (FFF) uses thermoplastic filaments like PLA, a material valued for its practicality and low cost. Graphene, in turn, is notable for its exceptional properties, such as high mechanical strength, electrical conductivity, and the ability to form ultrathin films. In filter membrane production, its nanoparticulate structure provides high selectivity and efficiency. When oxidized, graphene oxide (GO) exhibits functional groups that introduce active chemical radicals, enhancing its interaction with elements such as heavy metals [2][3]. The integration of 3D printing and PLA-GO composites shows promise in developing advanced solutions for filtering organic and inorganic compounds. Structures made from PLA-GO filaments processed by FFF have demonstrated high efficiency in removing heavy metals like lead and cadmium, commonly found in industrial waste [3]. A commercial PLA filament with graphene from VOOLT3D was used. Characterization revealed GO peaks via Raman spectroscopy and the presence of nanometric structures, such as flakes and loose tubes on the surface, using scanning electron microscopy. Additionally, X-ray diffraction has been conducted to confirm the GO quality. The performance evaluation procedures includes filtration kinetics studies and adsorption isotherms. Optimizing manufacturing parameters, such as infill and layer thickness, and refining annealing conditions like temperature and time, this study lays the groundwork for the development of advanced filtration materials with enhanced heavy metal adsorption capabilities.

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Voxel-level control in stereolithography 3D printing: Achieving dual properties from a single material

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C2_2, Andalucía II Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

SLA (stereolithography) 3D printing, despite significant advancements, typically uses a single material per print job. Recent developments try to overcome this limitation and allow multi-material printing through different mechanisms: exchanging the vat, inkjet deposition, or by varying the curing parameters. These approaches often introduce new complexities and limitations. Our work presents a novel approach to SLA 3D printing utilizing a single printing formulation with a “switchable monomer”, which changes its functionality based on the printing parameters. Depending on the monomer state at different temperatures and irradiation conditions, its polymerization behavior is changed. This leads to significant variations in obtained material properties such as the degree of stiffness, young’s modulus and translucency. To employ this novel material system in 3D printing, we introduce tailored software that enables 3D modelling and printing at varying reaction conditions (temperature, irradiation) at the level of individual voxels. During the printing process, the temperature and irradiation strategy are adjusted based on the desired properties of each voxel within the current layer, ensuring precise control over the final material properties.

To demonstrate the feasibility of this approach, we create hybrid materials with spatially varying properties. This enables the fabrication of functionally graded structures that are predefined at the level of individual voxels. Contrary to previous achievements in the field of multi-material polymerization, this technology does not rely on the degree of curing, which is unstable over time in the presence of residual monomers due to post-polymerization and hence leads to deteriorating property-differentiation over the use time of the printed object. Furthermore, the property variation is not restricted to just gradient materials but can be switched discreetly between two states and independently of the printing direction. This level of finely graded control opens up new possibilities for design for additive manufacturing. Together with the tailored voxel-based modelling we exploit this for shape-memory 3D printing (4D printing) of the multi-material objects, which could be employed in soft robotics applications.

Our research contributes in the field of multi-material printing by demonstrating a new material chemistry concept, “switchable monomers”, alongside a complete software solution for modelling and printing with voxel-level property control.

3D Printing of bio-based polymeric composites obtained by vat-photopolymerization technology containing biofillers

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C2_2, Andalucía II Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Bio-based polymers coming from renewable sources are emerging to replace the traditional plastics derived from fossil sources, because they offer easy processing, fulfill technological and durability requirements, guaranteeing improved properties such as biocompatibility, lower costs and environmental impact. At the same time, additive manufacturing (AM) technologies have been emerging as greener alternatives to production technologies for polymeric materials. 3D printing is considered a rapid prototyping tool due to its high printing accuracy, low raw material uses and wastes, and the ability to realize printed objects with complex geometry and good dimensional stability for many application fields, such as automotive, packaging and biomedical.

Among the different 3D printing technologies, vat-photopolymerization (VP), represents an easy method for obtaining accurate objects by 3D printing. It is a light-based technology, which allows to obtain high printing resolution and good level of shape complexity of the printed parts. During the process, the build platform is immersed into the liquid photocurable resin and, thanks to the UV light, the resin in the vat can be photocured and transformed in a uniform layer of solid material according to the previously designed CAD model. The process goes on until the desired object is complete.

The present research work aims to develop novel bio-based composites containing biofillers by using the Liquid Crystal Display (LCD) 3D printing technology.

Acrylate epoxidized soybean oil (AESO) resin was used as photocurable polymer matrix, isobornyl methacrylate (IBOMA) was used as reactive diluent, and phenyl bis (2,4,6-trimethylbenzoyl) phosphine oxide (BAPO) was employed as radical photoinitiator. Different kinds of fillers were used to prepare the final composites deriving from agro-wastes corn and wine by-products, and biochar coming from cellulose pyrolysis.

The composites were obtained by dispersing the different fillers within the AESO-based matrix and 3D printed via LCD. Then, the specimens were fully characterized from thermal, morphological, and mechanical point of view. Several 3D printed parts were successfully realized showing very complex structures and improved final properties in terms of elastic modulus, ultimate tensile strength, and glass transition temperature due to the reinforcing effect induced to the presence of the filler's particles, without significant effects on the thermal stability.

ACKNOWLEDGMENTS

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Towards In-Situ Pre-Programming of Transformation Characteristics in Shape Memory Polymers During Fused Filament Fabrication

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C2_1, Andalucía II Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Shape Memory Polymers (SMPs) have gained significant attention in industrial applications due to their ability to transform shapes and recover their original form in response to external stimuli, such as heat. Their integration with 3D printing, particularly Fused Filament Fabrication (FFF), enables the fabrication of complex, morphing structures with spatially controlled properties. SMPs exhibit the Shape Memory Effect (SME) by transitioning between rubbery and glassy phases, governed by their glass transition temperature (T_g). This transition is influenced by reversible polymer bonds, which are affected by thermal, chemical, and mechanical treatments during manufacturing. Effective application of SMPs requires precise programming of their shape memory characteristics to ensure controlled transformation. While prior research has modified SMP properties through material composition changes, reinforcements, and post-processing, recent efforts focus on embedding material programming within the manufacturing process. FFF facilitates this by allowing localized control of material properties through process parameters such as extrusion temperature, speed, and infill geometry. However, the specific impact of extrusion temperature on T_g and shape memory programming remains unclear. This study aims to optimize SMP programming by tuning T_g and pre-programmed transformation strain without altering the material composition or using reinforcements. Through experimental thermal and thermomechanical testing, coupled with thermal-structural modeling, the study investigates how extrusion temperature influences SMP behavior, enhancing control over shape memory properties. This allows the imparting of multiple shape memory properties into printed SMP parts to realize complex shape-morphing behaviors during the manufacturing stage and without requiring a programming stage before applying those parts.

Additive Manufacturing of Gradient Polymer Nanocomposite Structures Using SLA 3D Printing

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Additive manufacturing offers unique opportunities for fabricating complex structures with tailored material properties, and stereolithography (SLA) 3D printing has emerged as a promising technology for fabricating customized materials with tailored mechanical performance. This study presents an innovative approach for producing gradient structures using SLA 3D printing, employing photopolymer resins reinforced with nanoparticles. The method involves systematically varying the concentration and distribution of nanoparticle reinforcements within the resin matrix during printing, resulting in a controlled gradient of material properties across the 3D-printed structures. Our approach enables the design of mechanical gradients that mimic natural tissue interfaces, offering improved stress distribution, durability, and mechanical resilience. We investigate the influence of nanoparticle type, concentration, and gradient profile on mechanical properties such as stiffness and strength. Through a series of mechanical tests, including tensile and compressive testing, we demonstrate the significant enhancement in mechanical performance achieved by leveraging this gradient design. Additionally, the underlying mechanisms contributing to the improved properties are discussed. This work introduces a novel strategy to advance the field of SLA 3D printing, showcasing the potential for functional gradient materials in high-performance applications such as medical devices, structural components, and energy-absorbing materials.

Tailoring the Microstructure of 3D printed pieces by incorporating Cellulose Nanofibers into the PLA-based formulations containing Inorganic Phases

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In recent years, manufacturing technology has undergone a remarkable transformation due to the invention and expansion of additive manufacturing (AM). Among its most promising applications, AM enables the development of complex, efficient and stable structures using ceramic, polymeric, metallic, or composite feedstocks. Within the broad spectrum of 3D printing techniques, fused filament fabrication (FFF) has garnered significant interest for its suitability in printing composite materials while ensuring good applicability.

In this work, FFF was employed to fabricate specifically designed structures using a PLA matrix in which functional phases were added (e.g., TiO₂, CuO, hydroxyapatite) to create advance 3D printed pieces. The proposed patterns were digitally designed to maximize surface area exposure to the surrounding medium, enhancing their functional performance. But also, cellulose nanofibers, obtained through a biorefinery process (that allow to valorize local agri-food wastes), were incorporated into the PLA/inorganic formulations to further enhance the microstructural surface area. Following fabrication, the physicochemical, structural, and functional properties of the composite membranes were characterized.

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Development of physical vapour deposition coatings for weathering protection of additive-manufactured polymer substrates

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C2_3, Andalucía II Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The main barrier to the application of disruptive additive manufacturing (AM) is the limited range of materials currently printed using these techniques. Some common materials typically processed by fused filament fabrication (FFF) are high molecular weight polylactic acid (PLA) and acrylonitrile-styrene-butadiene (ABS). The development of new polymeric base materials, such as acrylonitrile-styrene-acrylate (ASA), with better mechanical and UV resistance properties and the use of protective surface coatings have recently emerged as alternatives to overcome these problems.

In this work, protective metallic coatings (Ti6Al4V and 316 stainless steel) of approximately 500 nm of thickness were deposited by physical vapour deposition (PVD) on additive-manufactured ASA substrates. Pulsed DC magnetron sputtering (p-DCMS) and high-power impulse magnetron sputtering (HiPIMS) techniques were used. The conformal deposition of the coatings and the analysis of the mechanical properties, in particular, the evaluation of the local residual stresses without the use of a reference, were carried out using the Focused Ion Beam - Digital Image Correlation (FIB-DIC) ring-core milling technique [1]. The dual beam FIB-SEM performed an annular trench on the samples, isolating a central island. SEM observation of island surface while the trench is further deepened enabled the measurement of the stresses using digital image correlation (DIC) analysis, as the material undergoes gradual stress relief. The optical properties of the coated AM substrates (total and diffuse reflectance) were evaluated by UV-Vis-NIR spectroscopy. UV-Vis-NIR results showed an increase of the total reflectance of coated samples both in the UV (+15%) and NIR region (+35%). The higher reflectance properties enhance the UV and heat resistance of the material. The changes observed in the mechanical and optical properties, before and after exposure to UV-A and UV-B irradiation, simulating weathering conditions will be also discussed in the presentation.

In conclusion, using protective PVD metallic coatings on additive-manufactured polymers improves the resistance to degradation by UV radiation and weathering extending the life of AM parts exposed to ambient conditions. Studies made by FIB-SEM-DIC analysis in combination with finite element simulation assess the conformability and local residual stress of the coating/AM substrate interface.

Fiber-Reinforced Photopolymers - Additive Manufacturing of High-Performance Composites

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C2_2, Andalucía II Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Stereolithography based additive manufacturing technologies has enabled the fabrication of a wide range of materials for creating complex and highly individualized products. For some applications, the overall (thermos)mechanical properties of these photopolymers limits the performance. However, to further increase the mechanical properties, this work is exploring the possibility of fiber reinforcement for photopolymers to use in high-performance materials.

A 3D printer based on the digital light processing (DLP) process (used wavelength $\lambda = 385$ nm, pixel size 50 μm) was used to produce fiber-reinforced photopolymers. Glass fibers with varying length and aspect ratios were employed as reinforcement, integrated into a (meth)acrylate-based photopolymerizable matrix. Fiber orientation within the printed samples was controlled, with options including semi-random orientation or alignment in the direction of applied load. The fiber orientation and content can be adjusted on a layer-by-layer basis. Fiber sizing is a critical component in composite manufacturing as the sizing has a great influence on the mechanical properties. With appropriate sizing for both the glass fibers and photopolymeric matrix material, the adhesion between fiber and matrix can be significantly enhanced.

The 3D-printed photopolymer composites were tested with respect to their (thermo)mechanical behaviour. The influence of fiber content, orientation and location on the (thermo)mechanical properties of photopolymer composites were investigated using tensile testing and dynamic mechanical analysis. Tensile tests and dynamic mechanical analysis revealed significant improvements with fiber reinforcement. Tensile strength increased by over 44 %, and the glass transition temperature exceeded 90 °C. Notably, the storage modulus exhibited a 3.5-fold enhancement. Furthermore, light and scanning electron microscopy analysis of fracture surfaces provided valuable insights into fiber-matrix adhesion and revealing failure mechanisms, including fiber pull-out and matrix cracking.

Continuous fiber reinforcing lithography-based additive manufacturing

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C2_3, Andalucía II Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Stereolithography (SLA) is an additive manufacturing (AM) process known for producing components with highest precision and smooth surface quality. However, the material properties of the photopolymers commonly used in SLA are often insufficient for demanding technical applications.

The integration of glass fibers offers a promising approach to enhance stiffness, strength and creep performance of SLA-fabricated components.

Particularly, the selective use of continuous fibers is of significant interest, as it allows for the customization of material properties based on the geometry, loading type, and direction of the applied forces. This individual adapted reinforcement strategy enables the production of high-performance components for specialized applications.

To integrate continuous fibers during the printing process, specific mechanical and design requirements must be addressed in the SLA machine architecture. This study presents the development of a lithography-based additive manufacturing system using digital light processing (DLP) technology. The system is equipped with a novel module that enables the precise embedding of continuous glass fibers into the geometry of the printed component along defined contours.

The presented work details the machine's fiber deposition process, focusing on the precision placement of fibers within the photopolymer matrix. Various glass fiber deposition strategies are investigated to assess their influence on the mechanical properties of the resulting structures. Experimental results highlight the significant improvements in component performance due to the reinforcement material and provide insights into the optimal integration of continuous fibers within SLA processes.

This work advances the capabilities of SLA for engineering applications by combining the precision of photopolymerization with the superior mechanical properties of fiber-reinforced composites. It opens new avenues for producing high-strength, stiff, and application-specific components, pushing the boundaries of additive manufacturing in material science.

RHEOLOGICAL BEHAVIOR OF ZEOLITE PASTES REINFORCED WITH GRAPHENE FLAKES FOR 3D PRINTING OF MEMBRANES WITH POTENTIAL APPLICATION AS GAS SEPARATION

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Zeolites are crystalline aluminosilicates characterized by an open-cavity structure consisting of micropores and channels, formed by three-dimensional tetrahedral units of SiO_4 and AlO_4 . This study aims to investigate the potential of these cavities for gas separation membranes. Membrane technology is widely used for the physical separation of CO , CO_2 , and H_2 mixtures during CH_4 reforming. Additionally, 3D printing has shown great promise in fabricating zeolite/graphene flake (GF) composite membranes with tailored configurations and hierarchical porosity. This is achieved through the successive layer deposition of optimized hydrogel inks containing varying solid contents (40–60 vol.%) and additives such as surfactants, plasticizers, and binders to enhance rheological properties for effective 3D printing. Furthermore, the incorporation of graphene flakes (GF) with Faujasite-type (FAU) zeolite enhances packing density and consequently the viscosity of hydrogel inks, which can significantly improve both mechanical properties and surface area of the resulting membranes. In this study, a 3% (wt./vol.) alginate-based hydrogel was prepared in distilled water at 60 °C, after 0.5–1.0% (wt./vol) of GF solution were homogenized under magnetic stirring for 24 h. After that, commercial zeolites 13 X (ZEO-13X) powder was added to hydrogel with a suitable amount of bentonite (2.5–5 wt.%), as plasticizer, methylcellulose (0.5–1.5 wt.%), as thickener and PEG poly(ethylene glycol) (1–5 wt.%), as lubricant, to prepare inks. Hydrogel inks were homogenized under stirring at 250 rpm for 10 min, followed by rheological characterization, aiming to establish correlations with printability. A rotational rheometer (Haake Viscotester iQ) was used to determine the flow curves, and an oscillatory rheometer (Anton Paar MCR 92) was used to determine the yield strength and viscoelastic behavior. All inks exhibit pseudoplastic behavior, with a content of 1.0% (wt./vol.) of GF being identified as the most suitable for decreasing the viscosity of the ink for the manufacture of 3D membranes.

Advancing 3D Printing with Vacuum Technology: Process Optimization, Material Properties, and Hybrid Manufacturing

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C2_2, Andalucía II Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

In recent years, 3D printing under high vacuum conditions ($<10^{-2}$ mbar) has gained increasing scientific interest, offering new possibilities for advanced manufacturing. This cutting-edge approach holds significant potential for space and in-orbit manufacturing, the production of high-performance polymers, and the fabrication of hybrid material combinations, such as those used in biomedical applications.

The vacuum environment provides unique advantages, including enhanced heat flux control for printed parts and significantly reduced heating power requirements. Additionally, integration of a vacuum arc-based coating process into the polymer extrusion process allows for in-situ surface modifications, further expanding its capabilities.

This presentation will first outline our extensive research into 3D printing in vacuum, addressing current challenges and proposing solutions to optimize the process. We will focus on temperature management strategies (including sensor integration and heating mechanisms) and examine the critical electrical and mechanical design considerations necessary for successful vacuum-based printing.

We will then explore the mechanical properties of printed components, discuss potential slicing software optimizations, and evaluate the hybrid approach of combining 3D printing with in-process coating techniques. Finally, we will present key applications and challenges associated with this novel manufacturing process, paving the way for future advancements in vacuum-enabled additive manufacturing.

Characterization of highly filled PLA-based composite filaments with silica and alumina for desiccant applications

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C2_1, Andalucía II Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Additive manufacturing via material extrusion (MEX) enables the direct, single-step fabrication of complex geometries. Recently, this technology has explored for the production of desiccant elements for air treatment systems. To achieve this, composite materials with high water vapor adsorption capacity are required.

This study explores the incorporation of adsorbent ceramic materials into polylactic acid (PLA)-based composite filaments. Two types of filaments were analysed, containing 20 wt% silica and 20 wt% activated alumina, respectively, both known for their high adsorption capacity. The objective of this work is twofold: first, to evaluate the water vapor adsorption capacity of the novel materials; and second, to characterize their thermal and mechanical properties. The filaments were analysed using thermogravimetric analysis (TGA) to verify the actual silica and alumina content. Adsorption-desorption isotherms (N₂, 77 K) were obtained to assess the porosity and surface area of the materials. Finally, standardized specimens were manufactured using MEX and their tensile and flexural properties were tested according to ISO 527 and ISO 178 standards.

TGA results confirmed silica and alumina contents of 19.4 wt.% and 19.3 wt.%, respectively. Furthermore, both composites exhibited thermal stability up to 255 °C (PLA-Silica) and 235 °C (PLA-Alumina), setting an upper limit for their printability. The N₂ adsorption-desorption isotherms revealed a substantial increase in surface area compared to pure PLA, with BET surface area enhanced by 4200% (PLA-Silica) and 1700% (PLA-Alumina). This increase in porosity resulted in a maximum N₂ adsorption capacity 1800% and 550%, respectively, higher than that of pure PLA.

Regarding mechanical properties, tensile tests demonstrated a reduction in maximum tensile stress of 63% and 30% for PLA-Silica and PLA-Alumina specimens, respectively. Flexural tests revealed a similar trend, with decreases of 62% and 27% in maximum flexural stress for PLA-Silica and PLA-Alumina, respectively.

Overall, the incorporation of ceramic fillers significantly enhances the adsorption capacity of PLA-based composites, demonstrating their potential for applications requiring efficient moisture removal. While mechanical properties are reduced compared to pure PLA, this limitation is not critical for passive desiccant applications. These findings provide valuable insights into the feasibility of high-filled composite filaments for MEX-based additive manufacturing, particularly in adsorption-driven engineering applications.

Interpenetrating phase composites with complex geometries: pressureless infiltration of alumina-based systems

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C2_3, Andalucía II Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Additive manufacturing (AM) has transformed material design, enabling complex geometries and overcoming the limitations of conventional processing techniques. Among AM methods, binder jetting offers a scalable and cost-effective route for producing high-precision ceramic components with open porosity, paving the way for applications such as interpenetrating phase composites (IPCs). These IPCs exhibit a unique 3-3 connectivity that combines the intrinsic properties of ceramics and metals to achieve an optimal balance of hardness, wear resistance, toughness, and ductility.

This study focuses on the binder jetting of alumina preforms as a foundational step for fabricating ceramic- and metal-matrix IPCs. A comparative analysis of spherical feedstocks prepared by plasma spheroidization is performed to evaluate the influence of multimodal particle size distributions on preform resolution, packing density, and overall print quality. Key parameters influencing the evolution of open porosity during thermal debinding and sintering are investigated, with processing temperatures reaching up to 1750 °C.

To demonstrate the feasibility of this manufacturing route, alumina preforms with optimized porosity are infiltrated with copper under oxidizing conditions and aluminium in a nitrogen atmosphere. The resulting IPCs are characterized for their microstructural integrity and mechanical performance. Techniques such as scanning electron microscopy, x-ray diffraction, and ball-on-disk wear testing are employed to assess the relationship between preform properties, composite microstructure, and mechanical behaviour.

The outcomes highlight the potential of binder jetting for producing complex geometries at scale while maintaining precise control over porosity and material distribution. This approach advances the development of multifunctional composites and aligns with ongoing efforts to address challenges in AM, including process robustness, scalability, and the qualification of materials for industrial applications in challenging environments, as high temperature, corrosive media and severe mechanical stresses.

APPLICATION OF 3D PRINTING TECHNOLOGY TO CERAMIC WASTE RECYCLING

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In a context of industrial transformation, additive manufacturing or 3D printing has established itself as a key technology within Industry 4.0, with particular interest in areas such as civil engineering and the biomedical sector. However, the availability of raw materials remains a challenge. In this regard, the use of waste as a source of materials represents a sustainable and highly relevant alternative. Unlike polymer-based 3D printing, which is well studied, the printing of ceramic and metallic materials, especially those derived from waste, still presents significant challenges and research opportunities. This study focuses on the fabrication of ceramic parts through 3D printing, using industrial waste. Additionally, organic waste will be employed as plasticizers to improve material consolidation and extrusion. The research will address the formulation of suitable mixtures for 3D printing, considering the necessary rheology and plasticity for optimal part manufacturing. Key process variables will be analyzed, such as extrusion speed, material deposition thickness, and the influence of different binder and ceramic waste combinations. Subsequently, the printed parts will be sintered and characterized to evaluate their physical properties, such as porosity and density. This investigation aims to contribute to the development of new solutions in additive manufacturing, promoting the valorization of industrial waste and sustainability in the production of ceramic materials.

Evaluation of properties of PA 12 used in the Multi Jet Fusion printing process after reprocessing in an extruder.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
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The multi jet fusion (MJF) printing process is a variation of the powder fusion process, which uses a polymeric matrix applied in the form of a jet and fusing and detailing agents that are fused by the action of infrared radiation. Among the polymeric materials used in the MJF process, PA 12 (polyamide) dominates almost the entire market due to its easy and flexible processing. During printing, only a minority of powders are sintered during the cycle, approximately 10%, the remaining powder must be reused in other cycles or can be recycled. In this sense, this work evaluated the properties of PA 12, originating from the MJF printing process, when subjected to reprocessing in a twin screw extruder and thus predict its behavior in mechanical recycling. For this purpose, this polymer was reprocessed 5 (five times). At each extrusion cycle, the polymer fluidity index was measured, characterized by thermogravimetry (TG) and Fourier transform spectroscopy (FTIR). The samples subjected to extrusion showed an increase of approximately 300% in the fluidity index value. This result follows a tendency of increasing as the number of reprocessing cycles increases, which can be associated with the polymer degradation process in the presence of humidity and temperature. The spectra obtained by FTIR indicated a reduction in the intensity of the peaks of some chemical groups present in the polymer with the number of reprocessing cycles, which implies a lower concentration that the species absorbs. The TG results indicated that the thermal stability of the polymer was maintained with the reprocessing cycles, however the amount of final residue is greater, which indicates a greater amount of degraded material. The behavior observed from the characterizations performed indicates fragility of the material to the mechanical recycling process.

Thermal Shock-Resistant Cordierite Ceramics: A Breakthrough for Aerospace Optics

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C2_3, Andalucía II Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The aerospace industry constantly drives innovation, demanding materials with unparalleled mechanical strength and functional performance. While ceramics offer promising solutions, their inherent low fracture toughness and thermal shock resistance present significant challenges. This study explores the potential of graphene as a transformative reinforcement material to overcome these limitations. The development of cordierite ceramics, renowned for their superior thermal shock resistance, reinforced with reduced graphene oxide (rGO), is investigated.

Using Pellet Material Extrusion (Pellet MEX), a cutting-edge manufacturing technique tailored for creating complex geometries with rapid prototyping and low production volumes, an aerospace prototype specifically designed for optical applications was successfully fabricated. To achieve fine dimensional precision, green-state machining was employed, significantly improving geometric tolerances and surface quality. This work demonstrates the viability of integrating advanced ceramic composites with innovative manufacturing and post-processing techniques, meeting the aerospace industry's high standards for performance, precision, and reliability.

Inkjet printing of PVDF-TrFE thin films: influence of solvent and annealing conditions on piezoelectric properties

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), settembre 17, 2025, 13:10 - 14:30

Among organic piezoelectric materials, poly(vinylidene fluoride-co-trifluoroethylene) (PVDF-TrFE) is a highly versatile polymer that, beside high piezoelectric and ferroelectric properties, also presents high biocompatibility, chemical resistance and thermal stability [1]. Moreover, its ability to be deposited in the form of thin films via advanced manufacturing techniques like Inkjet Printing (IJP) makes it even more suitable for the next generation of flexible sensors and energy harvesters [2]. Indeed, IJP is based on the controlled deposition of droplets of an ink containing the material of interest and this approach is characterized by intrinsic properties of customizability, scalability, and cost-effectiveness.

The use of IJP, however, implies the use of fluid inks, where PVDF-TrFE is dissolved in suitable solvents. On this note, it is important to analyze and understand how solvents, necessary for the printing process, affect ink's printability and piezoelectric properties. In fact, PVDF-TrFE gains its piezoelectric properties thanks to a specific crystalline phase, called β -phase, whose formation can be favored or suppressed by some organic solvents and by annealing the layer after the printing process [3].

The present work aims at studying and comparing, for the first time, how different solvents affect the printability, the β -phase content and the polarizability of PVDF-TrFE thin layers obtained via IJP. Additionally, this work aims at determining if the annealing process can be avoided, by selecting a proper solvent, without loss of performance, further reducing time and costs of productions. To these aims, test samples are produced by inkjet printing silver electrodes and thin PVDF-TrFE-based active layers on Kapton as substrate. The active layers are printed using four different inks, containing the same amount of PVDF-TrFE dissolved in four different solvents and solvents' combinations: Dimethyl Sulfoxide and Methyl Ethyl Ketone (DMSO/MEK with 70/30%wt.), Dimethyl Sulfoxide (DMSO), Cyclopentanone (CP), and N,N-Dimethylformamide (NN-DMF). Following the printing process, samples are analyzed exploiting a special combination of Raman analysis and Piezoelectric Force Microscopy (PFM), first to assess the β -phase content present in each sample and then to assess its polarizability.

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Influence of Printing and Bed Temperature on the Mechanical Strength of Simple PLA Filament Joints

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C2_1, Andalucía II Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Fused deposition modelling (FDM) 3D printing is widely used in prototyping and manufacturing due to its accessibility and versatility. However, the mechanical properties of printed parts are highly dependent on process parameters. This study focuses on evaluating the mechanical strength of a single joint between PLA filaments and how it is affected by printing temperature and bed temperature. To quantify the strength, tensile tests were performed on specimens printed with varying temperature settings. The results indicate that both printing temperature and bed temperature significantly influence the interlayer adhesion and overall mechanical performance of the joint. Higher extrusion temperatures generally improve filament fusion, leading to stronger joints, whereas bed temperature plays a crucial role improving adhesion during the first layers of printing. Understanding these effects is essential for optimizing printing parameters to enhance the mechanical integrity of PLA structures.

4D-printing of nacre-inspired ceramic-polymeric composites

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C2_1, Andalucía II Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Additive manufacturing of shape memory polymers has attracted significant attention due to their broad potential in applications across fields like biomedicine and aerospace. However, their mechanical properties, particularly stiffness and strength, limit their utilization. In this study, we demonstrate a novel fabrication approach where ceramic platelets and vitrimers' monomers are printed instead of polymers to produce nacre-inspired responsive ceramic-polymeric composites. Printing of monomers instead of polymers offers two main advantages: processing at room temperature since no polymer needs to be melted and yet adequate direct writing viscosity despite the high ceramic platelets' solid load. Upon extrusion during the direct writing printing process, solvent evaporation induces polycondensation of the monomers, forming a vinylogous urethane vitrimer in between the ceramic alumina platelets. The resulting composites feature a covalent adaptable network (CAN) after this polymerization during printing, which enables rapid and efficient self-healing, reshaping, and shape memory capabilities without significant mechanical loss. Moreover, they exhibit up to 3.3 and 26.7 times higher tensile strength and stiffness, respectively, compared to the unmodified vitrimer. The proposed strategy represents a straightforward, direct-write 4D-printing method that operates under ambient conditions for the fabrication of smart responsive ceramic-polymeric composites with shape memory capabilities.

Structural optimization of Fused Filament Fabricated components with biomechanical optimization methods

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C2_1, Andalucía II Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Additive manufacturing processes have evolved from rapid prototyping to the production of directly usable components. Extrusion-based processes such as Fused Filament Fabrication (FFF) enable fast and, for smaller quantities, cost-effective productions. FFF can create complex geometries, by extruding filament strands layer by layer.

The limitation of the technology is the low mechanical strength due to the layered structure. Print strands result in orthotropic properties, with strength and stiffness highest along print directions and decreasing in deviating directions. In order to design highly robust components without over dimensioning, it is not only necessary to take the anisotropy through the layered structure and the printing patterns into account, but also to optimize the printing paths themselves.

Computer Aided Internal Optimization (CAIO) is a method inspired by tree growth that aims at optimizing the internal structure of materials. Based on the Finite Element Method (FEM), CAIO iteratively rotates the orthotropic axis of each finite element in local principal normal stress directions and thus aligns the directions of maximum material strength and maximum load. For the example of a perforated plate subjected to a unidirectional tensile load, a FEM analysis was performed. The local orthotropy orientation, calculated by CAIO was translated into printing paths and demonstrators were fabricated in PLA using an FFF printer. Applying this optimization and compared to industry-standard printing patterns with the same amount of printed material, an increase in tensile strength of up to 28% was realized. In addition, the Soft Kill Method (SKO) was used to optimize the topology. The SKO method aims to optimize components for maximum stiffness and strength while minimizing material usage and thus component mass. The method is based on the biomechanical principles found in bone growth, where mineralization and demineralization controlled by mechanical stress vary structure and stiffness. By applying SKO to the FFF printed parts, a reduction in weight of 25% was realized. Even though the material usage was reduced, an increase in tensile strength of 5%, compared to industry standard prints, was achieved. Compared to standard patterned specimen of the same mass, an increase in breaking load of almost 70% was accomplished. The results of both methods show significant improvement in tensile strength of Fused Filament Fabricated parts. This suggests a strong potential for applying CAIO and SKO in optimized manufacturing of highly robust components.

Optimizing printing orientation for improving mechanical performance in multi-material 3D printing: a dual material and interface criterion approach

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C2_1, Andalucía II Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

In the era of Industry 4.0, where the focus is increasingly on innovative materials, multi-material 3D printing is garnering significant attention. As its name implies, this technology enables the combination of several materials within a single structure, thereby offering enhanced possibilities in design and functionality. However, the poor mechanical performance of the interfaces between materials can compromise the reliability and durability of the final part, despite the physico-chemical compatibility of the constituent materials. This study focuses on polymer parts fabricated by Fused Deposition Modeling (FDM).

First, we highlighted the role of print orientation on the morphology of the interface, notably its effective contact area and mechanical strength. On the other hand, the literature demonstrates that print orientation is a crucial parameter affecting the mechanical performance of FDM-manufactured parts. Thus, there exists a trade-off between the mechanical performance of the individual materials and that of the interfaces in order to optimize the overall integrity of the part. The present study proposes an approach to manage this trade-off effectively.

Two complementary failure criteria were employed to determine the optimal print orientation angle. The first, the Tsai-Wu criterion, is applied solely to the different materials of the part and takes into account the stresses in all directions to address the anisotropy of the printed material. The second criterion, developed specifically in this work, targets the interface by decoupling the normal and tangential stresses on the two types of interfaces at the layer scale: overlapped and adjacent. Its formulation is based on tensile and shear tests designed to characterize the various parameters of both criteria.

These two criteria were subsequently evaluated by comparing the predictions between analytical predictions and experimental mechanical tests. The results, obtained notably on a PLA/PLA material combination, demonstrate that this approach provides excellent predictive capability relative to the experimentally measured values, thereby validating the robustness of the method. These findings pave the way for an improved design of multi-material parts fabricated by 3D printing.

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These two criteria were subsequently evaluated by comparing the predictions with numerical simulations and experimental mechanical tests. The results, obtained notably on a PLA/PLA PETG/TPU & PETG/PC material combination, demonstrate that this approach provides excellent predictive capability relative to the experimentally measured values, thereby validating the robustness of the method. These findings pave the way for an improved design of multi-material parts fabricated. by 3D printing.

Design, manufacturing and development of piezoelectric PLLA-ZnO nanocomposites by 3D printing

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C2_2, Andalucía II Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The main objective of this research is the synthesis of nanoparticles for coordination with bio-based polymers for developing composite materials with improved piezoelectric properties that are flexible, more sustainable and efficient for new applications in potentially disruptive related technologies, such as wireless sensor networks and bio-implanted medical devices.

For this purpose, two materials with piezoelectric properties are used, which, through their coordination in a bionanocomposite achieve a higher electrical response. These materials are poly-L-lactic acid with medical grade purity (PLLA) and zinc oxide nanorods. From 2D WAXS, DSC and electron microscopy analysis of 3D printed bionanocomposites we could deduce that the piezoelectric morphology of PLLA is both influenced by the filler and the processing parameters (1,2,3,4).

This observation allows us to address one of the main challenges in the fabrication of piezoelectric materials and devices, which is to achieve a structure and arrangement that favors the piezoelectric response of the produced devices. This challenge has been overcome by 3D printing, through which it has been possible to orient both the polymeric chains of the matrix and the nanoparticles inside it, achieving a high electrical response potentially suitable for implantation and cell growth activation. Both the elongation and the orientation of the printed material are key to increase the final piezoelectric response of the device (4.7 pC/N), for which the 3D printing conditions have been optimized to achieve thin and flexible films that are adaptable to different structures using specialized 3D printing equipment in the medical sector (5).

Acknowledgements

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Negative Poisson ratio glass/ceramic metamaterials by two-photon polymerization

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C2_2, Andalucía II Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Metamaterials with multiple anisotropic properties, including negative Poisson's ratios, negative thermal expansion, negative modulus, high strength and stiffness, and double-negative acoustic properties, hold significant promise for applications such as medicine or civil engineering. However, most are based on polymers or metals, with limiting performance at very high temperatures. At the same time, it is difficult for traditional ceramic processing, such as powder sintering, to process complex metamaterial structures or ceramic components.

Two-photon polymerization (TPP) enables the fabrication of intricate 3D objects by scanning a laser beam within a volumetric body, without relying on a conventional layer-by-layer approach as in traditional stereolithography (SLA). A combination of a galvano-scanner and a micropositioning system provides precise control over the manufacturing process, resulting in true net-shape components. TPP is particularly advantageous for producing high added value ceramics with nanoscale structures, making it highly relevant for nanotechnology applications such as microfluidics, micromechanics, and microelectronics.

In this study, hybrid organic-inorganic resin systems were used as precursors, consisting of photocurable polymers and fumed silica. The resin mixtures exhibited high transmittance in a broad spectral range (400–1000 nm), making them compatible with femtosecond lasers operating at different wavelengths.

Auxetic metamaterial geometries were 3D printed by TPP and underwent thermal treatment in air to gradually eliminate the organic fraction and sinter the silica particles, resulting in homogeneous glass/ceramic components. Microstructural characterization of the printed objects was performed using scanning electron microscopy (SEM) coupled with energy-dispersive X-ray spectroscopy (EDS). Shrinkage and geometrical accuracy were assessed via image analysis.

The mechanical performance of the printed structures was evaluated by nanoindentation before and after thermal treatment at different temperatures, to validate the effect of lateral contraction upon axial compression.

This research was co-funded by the German Research Foundation (DFG) under the Walter Benjamin Program, project code STO 1296/2-1.

Additive Manufacturing of Porous Structural Ceramic Supports via Aqueous-Based Direct Ink Writing: Rheological Considerations and Integration of Functional Phases

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C2_3, Andalucía II Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Additive manufacturing (AM) has significantly expanded the design possibilities for ceramic based components, offering possibility to produce structures with more complex geometries. Among the various AM techniques, Direct Ink Writing (DIW) is particularly well-suited for the cost-effective fabrication of complex ceramic structures. That is, this technique enables the manufacturing of structures with hierarchical porosity distribution with complex mass flow pathways which are critical for advanced applications such as energy conversion and heterogeneous catalysis. The implementation of aqueous-based systems in DIW presents numerous advantages, particularly in terms of environmental sustainability and cost efficiency. However, achieving high-fidelity printed structures requires precise tailoring of the paste formulation, particularly its rheological behavior, as well as stringent control over drying conditions to prevent structural defects.

Thus, the rheological properties of aqueous-based ceramic pastes must be meticulously optimized to ensure stable extrusion, shape retention, and defect-free layer stacking. The presentation will provide the insights on the optimization of these pastes that must exhibit shear-thinning behavior. In particular, solid loading, surfactant selection, pore former integration and binder interactions will be discussed. Practical details, such as drying control of printed structures will be addressed.

Examples post-processing modifications of these porous structural ceramic supports will be presented, such as reactive surface functionalization and hierarchical porosity engineering through in situ synthesis of meso-micro porous materials. Some cases of deployment of these structures in high-performance environments, such as energy conversion and heterogeneous catalytic systems will be discussed.

DEVELOPEMENT OF PVD DIFFUSION BARRIERS AGAINST CARBON DIFFUSION DURING SPARK PLASMA SINTERING

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C3_2, Andalucía I Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The elaboration of metallic parts by powder metallurgy techniques such as Spark Plasma Sintering (SPS), represents a relevant alternative to conventional manufacturing processes [1]. This technology allows the elaboration in a single stage of dense and high-performance materials with high mechanical properties [2,3]. The powder inserted into a mold is densified by the simultaneous application of Joule heating and uniaxial pressure. The sintering duration is limited, due to the use of high heating and cooling rates (of the order of several hundred of °C·min⁻¹) [4,5]. One of the major problems during SPS of metallic powders is the carbon diffusion from the graphite tooling (punches and die), and/or from the graphite foils inserted between the powder and the tools, to the powder. If the carburization is not blocked, it can lead to a degradation of the sintered material properties and to the formation of a surface composition gradients. Up to now, only few studies addressed this issue [6].

In a previous work [7], it has been demonstrated that a titanium coating (about 1 µm thick) deposited by Physical Vapor Deposition (PVD) on the graphite foil was efficient in avoiding carburization of pure iron during sintering. In the present study, thermodynamic simulations were performed using the ThermoCalc® DICTRA module in order to select new promising barriers. It was noted that Ti, Zr, Hf, Ta, and W are good candidates to slow down carbon diffusion. The synergy of these five elements was tested. A TiZrHfTaW-HEA (High Entropy Alloy) coating was deposited by PVD on the graphite foils. SPS tests were performed using a pure iron powder, to assess the efficiency at preventing carbon diffusion in a simple metallic substrate. The coating stability and the coating/substrate interfacial elemental diffusion were carefully investigated by SEM-EDS, and completed by phase identification using XRD. Very promising results were obtained, showing the relevance of this kind of HEA system.

This study was performed in the frame of the ANR OEDIPUS project (ANR-23-CE08-0028).

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A Colloidal Processing Approach to improve the Photocatalytic Performance of TiO₂-CuO Heterojunctions

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C3_1, Andalucía I Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

This research proposes an innovative solution to overcome the existing agglomeration issues that usually take place during the blending of semiconductors constituting n-type/p-type heterojunctions with photocatalytic activity.

As alternative to conventional synthesis methodologies (e.g., sol-gel, co-precipitation, impregnation) and/or the dry mixing procedures, a colloidal processing strategy was addressed to promote higher dispersion degree among the involved species. Colloidal chemistry provides a straightforward approach to achieving highly homogeneous composite materials in well-dispersed systems by controlling key parameters such as pH, ionic strength, and the addition of specific additives.

To this end, a comprehensive study of the colloidal stability of commercial TiO₂ and CuO nanopowders was conducted using zeta potential measurements. Based on the surface charge characteristics of both starting materials, a stable charge balance was achieved in suspensions, where electrostatic interactions promoted intimate surface contact between the TiO₂ and CuO nanoparticles, facilitating the formation of the desired heterojunction.

The resulting heterojunctions were optimized by preparing mixtures in different ratios of TiO₂:CuO (1:0.10, 1:0.25 and 1:1), and a comparative study of mixing methodologies, both wet and dry procedure, was performed. All composite materials were characterized in terms of their optical, physicochemical, and photocatalytic properties using UV-Vis absorption spectroscopy, XRD, SEM-EDS and De-Nox activity measurements.

Acknowledgements

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On the pressureless sintering of B₄C with Si aids at low temperature

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C3_1, Andalucía I Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The feasibility is investigated of fabricating boron carbide–SiC composites by low-temperature pressureless sintering of B₄C with Si aids. Firstly, it is demonstrated on powder compacts with different Si aids (5–30 vol%) that low-temperature conventional pressureless sintering is not viable. Secondly, it is demonstrated on the same compacts that fast pressureless sintering is not viable either. And thirdly, it is demonstrated on powders of the model composition B₄C with 20 vol% Si aids that fast pressure-assisted sintering is viable at low temperature if a threshold pressure is applied. All these findings are explained considering that molten Si is a short-lived transient phase that reacts rapidly with B₄C to form SiC and a B-rich boron carbide, so external pressure is needed for it to be spread quickly and efficiently throughout the entire porous microstructure before being consumed.

Characterization of oxygen and nitrogen in SA508 steel powder in the vacuum induction melting gas atomization (VIGA) process

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C3_2, Andalucía I Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Metal powder, as a unique form of metallic feedstock, has been extensively used in structural applications through powder metallurgy (PM) and the emerging field of additive manufacturing (AM). Vacuum induction melting gas atomization (VIGA) is a widely applied method for producing metal powders due to the efficiency and recovery rate. However, the influence of the atomizing conditions not only on the oxygen and nitrogen content but also on the composition of surface and internal oxides remains unclear, especially of the different powder size.

The present study provides a comprehensive characterization of the oxygen and nitrogen content in SA508 powders of varying sizes, produced using Ar and N₂ gases during the atomization process. The relationship between powder size and impurity elements, such as oxygen and nitrogen, was systematically analyzed. Results indicate that the specific surface area and surface oxidation layer significantly influence the total oxygen content in the powder samples. Consequently, the composition and thickness of oxide layer on the powder surface were evaluated through XPS analysis, and the mechanism of the formation of surface oxide layer was investigated using thermodynamic calculations. The correlation between powder size and oxide layer thickness was also explored, as it is critical for understanding and optimizing the properties of metal powders.

Furthermore, non-metallic inclusions such as Al₂O₃, MnSiO₃, and MnS, were characterized in terms of their type and size using SEM. Thermodynamic software calculations elucidate the formation and evolution of the inclusions, offering critical insights for metal powders. These findings are essential for enhancing the production of high-performance powder metallurgy components through the Hot Isostatic Pressing (HIP) process.

High-performance Powders via Powder2Powder Ultrasonic Atomization

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C3_1, Andalucía I Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Current methods for the production of spherical powders restrict the development of custom particles with tailored chemical compositions. This challenge is even greater when the input material is already a powder. The proposed Powder2Powder ultrasonic atomization process based on plasma melting allows to change the particle size, morphology and form an alloy in-situ.

During processing the liquid, in contact with a surface vibrating at ultrasonic frequencies, forms standing capillary waves that lead to the ejection of fine droplets. As the amplitude of these waves increases, the wave crests can reach a critical height where the cohesive forces of the liquid are overcome by the surface tension, leading to the ejection of droplets from the wave tips.

The material in the form of powder was used to prepare custom alloy from the powder blend which was melted in the plasma stream and atomized from the sonotrode. The obtained material was used in laser powder bed fusion to print high entropy alloy. Additional case studies will be presented using other out-of-spec additive manufacturing feedstocks.

Evaluating and optimizing the plastic additive pelleting process with a single-die press

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C3_1, Andalucía I Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Plastic additives are key components in plastic material. They are essential for protecting the polymers from thermo-oxidation during plastic manufacture and enhancing the properties of the final plastic product, i.e. color, durability, etc. Typically produced in powder or granule form, they are pelletized for efficient handling, transportation, and processing. Pelletization, i.e., the compression of powders into pellets, is an important process in several industries, including animal feed, pharmaceuticals, wood, and food production. Pellets are often produced in ring die pellet mills. Since pelletization in such mills is a large-scale continuous process, optimization of the process conditions with extensive trials is infeasible. Alternatively, a single-die pellet press can be used as a representative model to study the pelleting process offering a low-cost lab-scale testing. The single-die presses have been extensively used to optimize pelletization in feed and wood industries, offering insights into key parameters such as compaction pressure, energy consumption, and pellet properties.

Our study investigates whether single-die presses can similarly be applied to optimize the pelletization process of plastic additives. We observed that while compaction pressure plays an important role in forming the pellets, process temperature is a critical parameter for the pellet quality. If the temperature is too low, the material remains in its powder state; if it is too high, then the material turns into a paste. Hence, achieving and maintaining appropriate process temperatures is vital for ensuring pellet integrity. For some formulations, required hardness and durability could not be achieved even at relevant temperatures. This was due to the material sticking to the compression rod resulting in inconsistent pellet formation further complicating the process. Another challenge that arises in the plastic additive pelleting process is that one of the components in the additive blend acts as a binder, directly influencing the process temperature across all compositions. Therefore, this study showcases the importance of optimizing the process parameters and, binder properties, to achieve consistent pellet quality. Since further work is needed to adapt this methodology for a wider range of formulations, we incorporated simulations to complement our experiments. By validating our experimental findings through simulations, we were able to pave a path for optimizing the pelletization process across diverse formulations.

Performance evaluation of new polymer additives for technical ceramic shaping processes

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C3_1, Andalucía I Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The manufacturing of complex ceramic components faces persistent challenges in powder processing and shaping techniques. This study introduces an innovative approach combining freeze granulation and robocasting, addressing key challenges in colloidal processing and powder functionalization through novel polymer additives[1][2].

High-purity alumina powder (Al_2O_3 , 8.1 m²/g) serves as a model material for developing this new processing methodology. The investigation focuses on nine distinct polymers. Aqueous ceramic suspensions (30-50 vol% solid loading) were formulated using these novel polymer additives, following an optimized dispersion protocol.

The research evaluates powder characteristics and suspension behavior through comprehensive rheological analysis. Critical process parameters in freeze granulation, including suspension flow rate and air pressure, were optimized to control granule morphology and size distribution. The relationship between processing parameters and powder compact properties was investigated under varying pressing conditions (2-300 MPa), with particular attention to microstructural development.

A key innovation of this work lies in the strategic integration of freeze granulation as a pre-processing step for robocasting feedstock preparation. This novel approach enables the creation of functionalized powder granules with pre-incorporated dispersants, binders, and plasticizers, significantly simplifying subsequent paste preparation for additive manufacturing.

Results demonstrate the successful development of ceramic granules suitable for both granulation and robocasting processes. This processing route shows promising results in terms of powder flowability, and printability, offering new opportunities for manufacturing complex ceramic components.

Study of the Manufacturing Differences in Recycled Material Produced from Mixed Waste Using Different Methods.

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B7_11, Federico García Lorca Auditorium (Level 0), septiembre 18, 2025, 10:30 - 13:10

Fabrication methods are one of the main factors influencing the properties of materials, as well as their potential industrial applications. The viability of different manufacturing methods for the same materials provides versatility for various uses and facilitates industrial adaptability, allowing a broader range of industrial installations to be adapted for the production of the new material. Therefore, comparing the properties of the same material manufactured using different methods is particularly important, as it highlights the advantages and limitations of each approach.

In the present study, a comparison of the properties of Construction and Demolition Wastes (CDW) mixed with industrial wastes in different proportions has been conducted using two manufacturing methods. Physical and mechanical properties have been analyzed in materials produced by molding and uniaxial compaction, both of which were consolidated through sintering at the same temperature for each method. Density, porosity, contraction and tensile strength have been tested for the different series and manufacturing methods.

Influence of pressure on the electrical resistivity of a metal powder mass under compression

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In this work, a simple mathematical model is proposed to describe the variation of the electrical resistivity of a mass of metallic powder subjected to increasing compression. To date, this study has not yet received an answer that is fully satisfactory for a variety of powders and at the same time is mathematically simple. The current trend, more interested in other strategies of massive computation or AI prediction, does not seem to explore this traditional way of acquiring knowledge, which has, however, obvious advantages as it leads to a direct and clear understanding of the relationships between microstructure properties. In this work, a simple expression with few empirical parameters is proposed that allows fast and reliable predictions. The model is validated with experimental curves acquired in tests with commercial metal powders.

Opportunities of material extrusion 3D printing technology for producing advanced meso-structured steels with improved properties

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C3_2, Andalucía I Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Mesostructured composite steels with hierarchical patterns offer a promising route to achieving unique combinations of mechanical properties in advanced engineering components. By modifying both the pattern and composition in these mesostructures, it is possible to fine-tune the structural behaviour of steels, enhancing the balance between strength and toughness while improving damage tolerance. Additive manufacturing, particularly material extrusion (MEX), presents a viable approach for fabricating these complex structures. However, due to processing constraints, multi-material printing of metallic alloys remains a significant challenge. Addressing these challenges requires a thorough investigation into key manufacturing factors, starting with developing and optimising feedstocks tailored for multi-material applications.

This study explores the use of MEX for fabricating multiphase steel composed of 316L and 17-4PH stainless steels. The effects of particle size distribution and solid loading on feedstock rheology and printability are examined, as these parameters are critical to ensuring process reliability. Additionally, the dimensional shrinkage of both materials is evaluated as a function of solid loading to achieve a similar contraction rate after sintering, which is essential for minimizing thermal stresses and preventing warping or structural defects in the final parts. Through the optimization of process parameters, defect-free components with consistent shape retention were successfully produced.

Beyond processing considerations, microstructural and mechanical characterization revealed a synergistic deformation behaviour among phases, with a beneficial transition of properties at the interface due to compositional and microstructural gradients. Furthermore, the potential formation of a galvanic pair between the two stainless steels is investigated through corrosion resistance assessments, providing insights into the electrochemical compatibility of the material system.

Alternative processing method for fabrication of amorphous/nanocrystalline FINEMET alloy

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C3_2, Andalucía I Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

FINEMET is a nanocrystalline soft magnetic alloy with high permeability, low core loss and good thermal stability making it ideal for high-frequency transformers, inductors for power electronics, EMI suppression components and magnetic sensors. The fabrication process of FINEMET involves rapid solidification followed by controlled heat treatment to form its nanocrystalline structure. However, rapid solidification requires an extremely high cooling rate ($\approx 10^6$ K/s) and any deviation can lead to devitrification and degrading the final properties. Moreover, the final product are very thin and mechanically fragile ribbons (20-30 μm), which makes manipulation and further processing difficult. In this paper, mechanical alloying, an alternative powder metallurgy manufacturing method of FINEMET, will be used. Pure elemental powders were mixed to give the desired FINEMET composition and alloyed for different milling times in high energy attritor mill. After 40 hours of milling, a mixture of amorphous and nanocrystalline powder was obtained. Size distribution and granulometric curves were obtained by laser diffraction, the structure and amorphisation progress was characterized by X-ray diffraction, scanning electron microscopy and transmission electron microscopy. The crystallization process of amorphous/nanocrystalline powder was followed by differential scanning calorimeter.

The influence of high-temperature high-pressure spark plasma sintering (HPHT/SPS) parameters on the initiation moment of the exothermic reaction in Ni-Al

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

As part of the undertaken scientific activity, the sintering process of intermetallics from the Ni-Al system with a molar ratio of nickel and aluminum of 1:1, 2:1 and 3:1, respectively, was optimized. Sintering with simultaneous application of pressure and temperature was carried out using a globally unique HPHT/SPS hybrid device equipped with a Bridgman-type chamber. Using this device, it is possible to heat with high-frequency pulse current in order to achieve very high temperatures. Sintering of powder, placed in special containers, ensuring uniform pressure and temperature distribution, was carried out in the pressure range of 2÷7GPa and temperatures of 873K-1473K. The applied sintering parameters made it possible to produce materials characterized by a high degree of compaction (88-100%). The influence of high pressure and temperature on the moment of occurrence of the exothermic reaction was demonstrated, different for individual alloys. High pressure causes this moment to be shifted to higher temperatures. Therefore, depending on the HPHT/SPS test parameters at which a given sinter was produced, a single, two or multi-phase microstructure is observed (XRD, EDS-SEM analysis). The conducted research and analyses allowed to determine the optimal sintering parameters: pressure and temperature for which a specific microstructure is obtained. It was additionally shown at what parameters of the powder mixture and sintering parameters the exothermic reaction is initiated. The produced materials are characterized by Young's modulus up to 210GPa and hardness up to 715HV1. Abrasive wear resistance tests conducted in the Ball-On-Disc system have shown that the materials are characterized by high resistance to this type of wear. Corrosion resistance tests of selected samples in 0.1M H₂SO₄ acid showed that their stationary potential values were stable for 24 hours of measurement. The samples did not show a tendency to selective or pitting corrosion. The corrosion potential values were very close to those obtained for pure Ni and increased slightly with time, indicating the high stability of the passive layers produced. As a result of the tests of strength properties conducted in a wide range of temperatures and strain rates, the brittle nature of most of the sinters produced was confirmed. In the compression test at room temperature, significant strength of up to 3GPa was achieved (NiAl 2:1) and decent deformations of 10-25%. In the tensile test, at room temperature, the samples were quickly torn off. At higher temperatures, deformations of the order of 60% were achieved for individual samples.

Densification, microstructure and properties of ZrB₂ particle reinforced copper matrix composite by spark plasma sintering

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), September 17, 2025, 13:10 - 14:30

Copper matrix composites are materials whose use requires excellent mechanical properties as well as high electrical or thermal conductivity. Mechanical properties can be effectively improved by adding a ceramic reinforcing phase to the copper matrix. Crucial aspect in the design of copper matrix composites is to produce a material with good mechanical properties and good conductivity. Spark Plasma Sintering (SPS) is an advanced manufacturing technology that enables the production of very dense composite materials. This study focuses on the effect of sintering temperature (850°C, 900°C, and 950°C) and pressure (20 MPa and 35 MPa) and amount of reinforcing phase on the microstructure and properties of copper matrix composites. The composites with various zirconium diboride contents (5-20 wt%) were synthesised by ball milling and successfully consolidated using Spark Plasma Sintering (SPS). The relationship between the change of ZrB₂ content and physical, mechanical, electrical, corrosion and tribological properties was studied. Scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) were used to analyse microstructure evolution in copper matrix composites.

The density of the sintered composites was measured by Archimedes' principle. Vickers microhardness and compression tests at room temperature were carried out to investigate the mechanical properties. The electrical conductivity of the samples was determined using a the four-point method. Ball-on-disc method was carried out to study the wear behavior of based composites. The corrosion behaviour was examined in an environment of H₂SO₄ using electrochemical techniques. Experimental data showed that the properties of Cu–ZrB₂ composites depended significantly on the SPS sintering conditions. The optimal sintering temperature was 950°C with a pressure of 35 MPa. Composites exhibited a high degree of consolidation. The relative density of the sintered composites is in the range of 95-97%. The results showed that the higher content of ZrB₂ in the copper matrix is responsible for the improvement in Young's modulus, hardness and wear resistance with the reduction of the conductivity and corrosion resistance of sintered composites.

Revealing fretting wear resistance mechanism under liquid lead-bismuth eutectic of Cr-Al-C composite coatings fabricated by laser cladding

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Laser cladding technology was utilized to construct Cr-Al-C coatings on the surfaces of service materials. Through the fretting wear test in liquid LBE, the fretting wear behaviour of Cr-Al-C composite coatings under different fretting working conditions was studied to elucidate the characteristics of the coating's sub-surface components, chemical composition distribution, morphology, crystalline orientation, and micro-structure after the fretting wear, so as to reveal the protection mechanism of coatings against fretting wear in liquid LBE. Results show that the coating mainly consists of diffuse Cr₂AlC phase, interdendritic Cr₇C₃ phase and dendritic Cr-based solid solution. The wear resistance of the coating is 4.25 times that of the 316 stainless steel substrate at a test temperature of 320 °C, the wear resistance of the coating was 33 times that of the 316 stainless steel substrate at a test temperature of 450 °C. The oxidized layer can block the direct contact between the material and the friction partner and reduce the wear, while also preventing the infiltration of LBE and the dissolution of the base metal elements. In addition, the Cr₂AlC in the coating possesses good self-lubricating properties, which can also effectively reduce wear; the coating's Schmidt factor is statistically distributed between 0.41-0.5, with a high capacity for plastic deformation, which effectively improves the resistance to fretting wear damage of materials. The presence of carbide effectively impedes the movement of dislocations, dislocations stacked around it and can not make it fracture or deformation, thus playing a certain role in strengthening. This study provides a theoretical basis and foundation for the protection design of heat transfer tubes in steam generators.

Growing TiN/TiB superlattice thin films via multi-cathode DC magnetron sputtering

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C4_5, Picasso Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Transition metal borides like TiB₂ are known to exhibit excellent hardness and strength as well as extremely high thermal stability. Like other ceramics, fracture toughness and brittleness in general are considered weak points that limit their use in certain applications. While hexagonal TiB₂ is the thermodynamically stable version of Ti-borides, ab-initio calculations indicate the existence of a metastable face-centered-cubic TiB with supposedly low stacking fault energy, potentially supporting the enhancement of plasticity through the formation of mechanical twins upon deformation.

We report the deposition of TiN/TiB superlattice thin films via physical vapor deposition (PVD), with TiN acting as a stabilizer for the formation of the metastable TiB phase. Cross-sectional transmission electron microscopy (TEM) reveals well-defined multilayer structures with coherent interfaces, while X-ray diffraction (XRD) highlights the superlattice effect contributing to the films' mechanical strength. We give a comprehensive overview of the material design, fabrication techniques, and the interplay between structure and properties, highlighting not only the possibility of using the template effect to stabilize otherwise unstable phases but also showcasing a superior combination of strength and ductility through nanotwinning effects.

Hydrophobic and Ice Adhesion Properties of Aluminium Samples with Surface Modification Mimicking Scallop Shell Structures

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C4_8, Picasso Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

With the rapid rise in heat pump installations in recent years, the issue of icing on aluminum samples used in air sourced heat pump systems has gained significant attention. Ice formation on the heat exchanger located on the outside of the building reduces the efficiency of heat transport; moreover, it results in increased energy consumption and maintenance costs. Thus, developing aluminum samples with anti-icing properties has become an important research direction. Inspired by the surface structure of scallop shells, we propose using laser technology to create scallop shell-like structures on aluminum sheet surfaces to optimize their hydrophobic properties, so that the ice on the sample surface can be easily separated or slide off more easily after melting.[1]

In this study, we first measured the surface characteristics of untreated aluminium samples, including ice adhesion, as well as static and dynamic contact angles. These initial results served as a baseline for comparison. Subsequently, we applied Direct Laser Interference Patterning (DLIP) to replicate the ridged structures of scallop shells on the aluminium surface and conducted the same tests on the laser-treated samples. The results demonstrated that the static contact angle of the aluminium samples significantly increased after laser treatment, indicating a notable enhancement in hydrophobicity. The ice adhesion force varied depending on the laser treatment method and showed a consistent decrease with repeated measurements.

To better understand the impact of laser treatment on surface morphology, detailed observations were performed using scanning electron microscopy (SEM). Furthermore, we applied a dip-coating process with a PDMS solution to fill the cavities within the DLIP-generated ridges. This approach not only reduced ice adhesion by minimizing the anchoring points between the ice and the DLIP-structured surface but also maintained high contact angle values. Our findings revealed that the laser-treated aluminium surfaces exhibit regular ridged structures that closely mimic the surface features of scallop shells.

This study verifies the effectiveness of bioinspired structures in enhancing the hydrophobic surfaces and demonstrates the great potential of laser technology in surface engineering. It expands the boundaries of biomimetic materials science and provide a basis for optimizing heat pump performance with potential for widespread industrial application.

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Oxide-Based Preceramic Polymers for Dual Protective Coatings on Cast Aluminum Structures: Enhancing Corrosion Resistance in Heat Transfer Applications.

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study investigates the development of advanced anticorrosive ceramic coatings through an innovative approach that combines multiple protective technologies. Specifically, polymer-derived ceramic (PDC) coatings were applied using Durazane 1800 onto surfaces pre-treated with plasma electrolytic oxidation (PEO). The research focused on optimizing the coating process by incorporating a 70% functionalized alumina nanopowder into the Durazane 1800 matrix, followed by curing the coatings under controlled air atmosphere conditions. Initial experimental results demonstrated significant promise in achieving highly effective ceramic coatings with enhanced durability. To assess the performance, the coated samples underwent rigorous testing in a corrosive environment (the corrosive medium is $\text{MgCl}_2 \cdot 6\text{H}_2\text{O}$) over 25 cycles, with periodic measurements of mass to monitor material degradation. Remarkably, almost no detectable mass change was observed across all samples after completing the 25 cycles, underscoring the exceptional corrosion resistance and stability of the developed coatings. These findings suggest a robust and reliable solution for protecting metallic surfaces in challenging environments.

Acknowledgments:

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Reactive Magnetron Sputtered Cr_{1-x}Ta_xN and Cr_{1-y}Nb_yN coatings: Microstructure and mechanical properties

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C4_2, Picasso Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Nitride films based on refractory metals can exhibit unique properties which make them suitable candidates in wear resistant applications. The model systems chosen for this study are Cr_{1-x}Ta_xN and Cr_{1-y}Nb_yN coatings with various Ta or Nb contents ($0.105 \leq x \leq 0.727$, $0.106 \leq y \leq 0.458$). They were synthesized by reactive magnetron sputtering utilizing a combinatorial experiment in thin film deposition. We used a segmented circular target consisting of two half plates of pure Cr and Ta or Nb for the deposition at 250 W DC target power, 0.4 Pa pressure with a mixture of Ar and N₂ (31:23, 41.5:16 and 54.5:5), 0 V substrate bias and $\approx 150^\circ\text{C}$ substrate temperature. The gas mixture was adjusted to achieve nearly stoichiometric nitride coatings. Polished steel substrate samples of 10x10x1 mm³ were placed in a horizontal line opposite to the target. Thus, we obtained different Cr_{1-x}Ta_xN and Cr_{1-y}Nb_yN coatings with various Ta or Nb content in a single deposition experiment.

The elemental composition of the coatings was determined by electron probe micro analysis and their phase composition was characterized by X-ray diffraction. Based on these results and according to the atomic concentrations of Cr and Ta or Nb, the coatings can be classified as follows:

1. All coatings are crystalline.
2. All XRD reflections exhibit a similar shape and suggest that all coatings grow in a single-phase fcc (face-centered cubic) solid solution structure.
3. The solid solution (Cr_{1-x}, Ta_x)N exists in a range $0.105 \leq x \leq 0.727$ while the solid solution (Cr_{1-y}, Nb_y)N is found in a range $0.106 \leq y \leq 0.458$.

Transmission electron microscopy and scanning electron microscopy analyses will resolve the microstructure further.

Mechanical properties of the coatings were studied by micro-indentation. The hardness and Young's modulus of the Cr_{1-x}Ta_xN and Cr_{1-x}Nb_xN in dependence of their Ta or Nb content and as well of the pure CrN and TaN or NbN coatings will be discussed. It was found that both the Cr_{1-x}Ta_xN and Cr_{1-y}Nb_yN coatings have a higher hardness than pure CrN. For Cr_{1-x}Ta_xN, the hardness values range from 1789 to 1952 HV and for Cr_{1-y}Nb_yN from 1244 to 1777 HV.

Applications of surface treatments obtained by ion implantation techniques

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Ion implantation is a sophisticated surface engineering technique that utilizes ionized atomic species accelerated to high energy in a vacuum environment. This method is used to introduce accelerated particles into the surface of a substrate. Unlike conventional coatings, this process allows the atoms to penetrate the substrate at the sub-surface level. This unique feature avoids the risk of delamination, an issue often encountered with traditional surface coatings. Like other surface treatment processes, ion implantation can improve the corrosion resistance, wear resistance, hardness, electrical conductivity, bioactivity, and antibacterial effect of materials compared to their pristine forms. As it is a surface modification technique, the bulk properties of the substrates are retained. In addition, one of the most valuable advantages of this low temperature surface treatment technique is that the concentration and depth distribution of the implanted ions can be strictly controlled by adjusting the processing parameters.

In this work, Plasma Immersion Ion Implantation (PIII) and Metal Vapor Vacuum Arc (MEVVA) ion implantation techniques have been used for surface functionalization of metallic and polymeric materials.

In the field of dental implants and keratoprosthesis, bactericidal surface treatments on titanium have been developed by co-implantation of silver and copper ions using a MEVVA ion source. Antibacterial activity against *S. aureus*, *E. coli* and *P. aeruginosa* has been demonstrated, as well as resistance to the formation of a biofilm composed of the bacteria *F. nucleatum*, *P. gingivalis* and *A. actinomycetemcomitans*. Fungicidal activity against *C. albicans* has also been validated.

Finally, in the field of hard PVD coatings, an improvement in the adhesion strength of AlCrSiN coatings deposited on WC-Co substrates implanted with Ti and Cr species by PIII has been demonstrated. This improvement is attributed to the introduction of residual stresses in the substrate, which increases its fracture toughness and load bearing capacity.

Optimizing the heat treatments for electroless Ni-P nanocomposite coatings: the impact on mechanical properties and tribological behavior

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C4_9, Picasso Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Electroless Ni-P coatings with high phosphorus content (≈ 11 wt.%) are widely used in the energy production industry to protect steel components from extreme environmental attack. However, the deposition process can lead to hydrogen entrapment within the coating, causing significant embrittlement and reducing mechanical resistance. Improvement of properties and durability of coatings can be achieved by two approaches: (i) incorporating functional second-phase particles and (ii) applying heat treatments for dehydrogenation and crystallization. This study investigates the manufacturing and characterization of Ni-P nanocomposites reinforced with Al_2O_3 and ZrO_2 nanoparticles and subjected to various heat treatment schedules, focusing on how dehydrogenation affects coating microstructure and protective properties

Coatings were reinforced with varying concentrations of nanoparticles and underwent dehydrogenation at 200°C for 2 hours and annealing at 400°C for 1 hour, applied individually or in sequence to assess their effects on coating performances. Microstructural changes were analyzed by SEM and XRD. Hardness, elastic modulus and fracture toughness were evaluated through instrumented indentation tests, wear resistance and mechanisms were investigated by ball-on-disc tests with an Al_2O_3 counterpart.

Microstructural analysis revealed that the amorphous structure of the coatings remained unaltered with nanoparticle inclusion, although ZrO_2 provided better dispersion than Al_2O_3 and, accordingly, higher microhardness. Dehydrogenation improved coating hardness by facilitating initial grain growth, while annealing at 400°C induced the formation of nanometric Ni_3P precipitates, resulting in +120% hardness compared to unreinforced Ni-P coatings.

Nanocomposite coatings exhibited higher fracture toughness compared to unreinforced Ni-P due to the crack deflection mechanisms. No detectable differences in hardness and microstructure were detected after heat treatment at 400°C for 1h with or without prior dehydrogenation and, as expected, fracture toughness dramatically decreases; however, the dehydrogenated coatings exhibited higher KI and lower Young's modulus.

ZrO_2 -reinforced coatings exhibited enhanced wear resistance, with wear tests highlighting the critical role of dehydrogenation in reducing both the coefficient of friction (-14%) and the wear rate (-97%) when performed prior to annealing at 400°C for 1 hour. Wear track analysis revealed that non-dehydrogenated samples primarily failed by complete coating delamination, with abrasion identified as the dominant wear mechanism. In contrast, dehydrogenated samples displayed significantly improved durability, attributed to the formation of a protective oxide layer, which effectively enhanced the overall wear resistance of the coatings.

The present findings underscore the synergistic benefits of nanoparticle reinforcement and tailored thermal treatments, highlighting the critical role of dehydrogenation and offering practical solutions for improving the durability in demanding engineering applications.

Plasma-Assisted Fabrication of Metal Oxide Nanostructures Using Phthalocyanines and Porphyrins: A Route to Functional Porous Layers

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C4_10, Picasso Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Developing innovative methods for nanostructural control is key to designing advanced materials with superior properties.[1] In such a context, plasma-activated deposition has shifted from compact thin films to controlled nanoscale materials, including nanoporous layers, low-dimensional carbon, and complex one-dimensional structures.[2,3] These methods offer scalability, low deposition temperatures, wide substrate compatibility, precise compositional control (including doping), and morphological precision (microstructure, texture, alignment).[2,3] However, a critical limitation is the scarce availability of volatile metalorganic and metal halide precursors for nanoscale deposition.

This study establishes the bases for a vacuum and plasma-supported methodology for fabricating metal-oxide nanostructured layers with controlled microstructure using metal phthalocyanines and porphyrins as precursors.[4–6] Key strengths of this method are its ample general character from the point of view of the material composition and microstructure, mild deposition and processing temperature and energy constrictions, and compatibility with the direct deposition on processable substrates and device-architectures. Leveraging commercially available metal porphyrins and phthalocyanines, we developed metal oxide layers including CuO, Fe₂O₃, TiO₂, VO_x, and ZnO with morphologies ranging from compact to porous films as well as low dimensional nanostructures such as 2D networks, nanowires or nanocolumns. The synthesized layers demonstrate potential in energy applications, particularly optical and optoelectronic technologies.

ACKNOWLEDGEMENTS

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Functional coatings: from gas phase synthesis to applications

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C4_8, Picasso Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Functional coatings based on highly filled particulate metal-dielectric nanocomposite films exhibit unique properties with a wide range of applications. To explore collective interactions between the particles, we control particle separation at the nanometer scale using vapor phase deposition, a scalable approach that offers excellent control over the filling factor and other properties. For the deposition of functional polymer thin films, we employ initiated chemical vapor deposition (iCVD) to prevent the decomposition of functional groups. Examples include highly stable electrets for electret microphones and magnetoelectric sensors, 3D superhydrophobic coatings, nanoscale gradient copolymers, and strain-invariant conductors for soft robotics.

In fabricating nanocomposites, nanoparticles can form during gas phase co-deposition via self-organization or through high-rate gas aggregation cluster sources, which provide independent control of filling factor and size, as well as in situ monitoring and control of alloy nanoparticle composition. Recent examples of nanocomposites include plasmonic meta-materials, photoswitchable molecular plasmonic systems, memristors, memsensors, and self-organized nanogranular networks for neuromorphic electronics. Additionally, we have explored nanoscale synergistic effects of plasmonics and photocatalysis, such as photoinduced enhanced Raman spectroscopy (PIERS).

Surface modification of titanium components for motorsport industry by diffusion treatments

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C4_11, Picasso Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

BOZZA ABSTRACT PER EUROMAT 2025

Surface modification of titanium components for motorsport industry by diffusion treatments

In the motorsport industry, the choice of material for manufacturing the heat-resistant components often fall on titanium alloys. Nevertheless, one of the most common problems of titanium alloys is fretting. [1]

Fretting is a complex phenomenon that occurs at the contact interface subjected to cyclic loading. In the case of titanium components, fretting can be particularly problematic because induces fatigue wear.[1]

Currently, carburizing is the predominant treatment employed to enhance the fatigue strength, [2] however, this process is time-consuming and expensive due to the exploited process to diffuse carbon on surface, i.d PVD.

Therefore, the objective of this study is to identify different surface treatment to improve the wear resistance properties inherent within titanium alloys.

To address these challenges, the idea is to develop a new surface treatment that carburize titanium oxide surfaces instead of titanium itself, thank to knowledge that the diffusion rate of carbon in TiO₂ is significantly higher.[3]

Two different titanium alloys have been investigated: Titanium Grade 2 and Grade 5 (Ti6Al4V alloy) . Samples have been coated by controlled oxidation processes, that is anodization, to provide oxide layers with tailored properties. Subsequently the oxidized specimens are performing carburizing, exploiting different process parameter, such as different temperatures. The diffusion of carbon into the oxide layer to form a carburized surface, has been evaluated with the aim to form a uniform and well-adhered carburized layer. Chemical, physical and preliminary mechanical tests were carried out on samples. In details: optical microscopy, a SEM – EDS analysis, a microhardness and nanoindentation test, scratch test and XRD analysis.

The results show that the oxidation thickness was among 2–3-micron layer and the coating composition, structure, and elemental distribution were composed of three different forms of oxide: anastasio, rutile and amorphous phase.

Furthermore, pin-on-disk tests will be conducted on the carburized surface to evaluate the wear resistance of the treated specimens. The wear behavior, coefficient of friction, and surface morphology will be analyzed to assess the effectiveness of the treatment in reducing wear resistance.

The results prove the possibility to overcome the limitations inherent in traditional carburizing processes. Through controlled oxidation and subsequent cementing, we anticipate the formation of a carburized surface with improved wear resistance and reduced fretting-induced damage.

[1] DOI: <https://doi.org/10.1520/STP10766S>

[2] DOI: <https://doi.org/10.3221/IGF-ESIS.58.13>

[3] DOI: <https://doi.org/10.3390/pr12010102>

Effect of Sputtering Conditions and Post-Deposition Treatment on Structure and Properties of CrZrNbN Thin Films

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C4_6, Picasso Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Protective coatings are increasingly valued for their exceptional resistance to corrosion, oxidation, and wear. Chromium-based thin films have emerged as a primary choice due to their commendable properties since their development in the 1990s. However, the demand for enhanced performance under more challenging conditions necessitates improvements in wear and oxidation resistance. Thus, CrN and CrAlN thin films require further enhancement through innovative approaches. This study investigates the effect of sputtering parameters, such as nitrogen flow rate, discharge power and substrate temperature, on the structure, mechanical properties and oxidation behavior of CrZrNbN thin films. These films were produced via reactive high-power impulse magnetron sputtering of a single CrZrNb (40:30:30) target in argon-nitrogen mixtures. Analysis using energy-dispersive X-ray spectroscopy, X-ray diffraction, X-ray photoelectron spectroscopy, and Raman spectroscopy demonstrates that precise controlling the sputtering parameters, as well as variations in the oxygen content (ranging from trace amounts to significant levels), can significantly alter the phase compositions (from solid solutions to novel crystalline phases). In addition, microscopy analysis (scanning electron microscopy and atomic force microscopy) revealed a significant influence of these parameters also on the morphology of thin films. The resulting phase changes, combined with a multilayer oxygen-induced design, can enhance the hardness, tribological properties, oxidation resistance, and self-healing capabilities of CrZrNbN thin films. The findings of this study may serve as a foundation for the development of smart surfaces featuring multifunctional thin films.

ZrN-Cu coating by hybrid magnetron sputtering for maritime applications

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C4_3, Picasso Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Maritime transportation is a central player in the worldwide economy. Problems with marine shipping always directly impact the final price of merchandise. Currently, this industry deals with two significant issues: biofouling and corrosion. Both represent maintenance and operating costs increasing. The ban imposed on tributyltin paint, the most used product to fight these problems, seeking a multifunctional solution was open. Magnetron sputtering could represent a big step forward in solving this inconvenience. The present work aims to gather the desired characteristics in one surface: antibiofouling action, corrosion resistance, and mechanical reliability. A ZrN-Cu nanostructured coating was obtained through hybrid magnetron sputtering technology, employing DCMS and HiPIMS simultaneously under a reactive atmosphere (Ar + N₂). Stainless steel 316L was utilised as substrate. Different techniques assessed the fundamental features of the coating (SEM, EDS, XPS, XRD, TEM, EELS). Zone of inhibition tests and quantification of colony-forming units (both with *Cobetia marina*) were employed to evaluate the antibiofouling action. Electrochemical impedance spectroscopy (up to 30 days) and potentiodynamic polarisation measurements were conducted in a 3.5 wt. % NaCl solution to assess the corrosion resistance. Likewise, nano-indentation, scratch tests, and tribology measurements established the mechanical characteristics of the coating. The results demonstrate that Cu diffusion to the surface and the presence of CuO species provoked the antibiofouling action, regardless of the activation mechanism (electrochemical or chemical). Cu²⁺ Ionic releasing (ICP-OES) after 24 h did not represent a toxic agent for *C. marina*. Also, the deposition method effectively limits the influence of Cu over ZrN properties (i.e., anticorrosion and mechanical reliability) due to the increase of compactness provoked by HiPIMS. With coating activation, the mechanical properties of the coating diminished, though the corrosion resistance increased. These findings represent a viable alternative for the marine industry, replacing other harmful products in ship components.

Patterned slippery surfaces for efficient and consistent fog harvesting

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C4_4, Picasso Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Currently, water shortages are one of the most serious social crises that threaten human life. Notably, in moist air, numerous microdroplets exist in fog, from which many creatures are capable of collecting water in clean and efficient ways. Inspired fog harvesting materials have been developed for efficient water collection in recent decade. The fog harvesting surfaces were mostly focused on (super)hydrophobic surfaces which are beneficial for water transportation, however, such surfaces are unstable in fog flow environment and thus difficult to realize long-term stable applications. Both the water collection efficiency and stability are significant for applications of fog harvesting materials. Here, four kinds of surfaces, including superhydrophobic surfaces, lubricant-infused slippery surfaces, liquid-like slippery surfaces and smooth solid surfaces, are investigated by simple method for long-term fog harvesting. The effect of surface structure and wettability on fog harvesting efficiency/stability and the corresponding mechanisms are systematically discussed. At the same time, by learning and cooperating from the fog capture, droplets coalescence, water transportation and collection of multiple creatures, a series of hybrid surfaces are prepared through optimizing surface structures and patterns. As a result, synchronously improved fog harvesting stability and efficiency are realized. For the most excellent surface, it is highly stable during 30-day test and the daily water collection efficiency can reach 90 L m⁻² day⁻¹; and the transparent patterned surface is able for large area fabrication assisted by printing technology. Moreover, a simple device is developed by integrating the patterned surface and a solar evaporator. A cooperative mechanism between fog harvesting surface and solar evaporator is preliminarily verified, and efficient vapor condensation efficiency and vapor collection efficiency are achieved, providing new ideas for the development of water collecting technology in future.

The change in tribological properties of aluminum thin films deposited by magnetron sputtering with an additional cooled anode

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C4_3, Picasso Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

In this work we studied the effect of adding an anodic plasma to DC magnetron sputtering discharge; we demonstrated that the anodic plasma could generate additional argon ions in the magnetron discharge. Aluminium thin films were deposited on glass substrates, and the anodic plasma was generated by a cooled graphite electrode. The changes in the two plasmas were studied by optical emission spectroscopy (using an Avantes AvaSpec-DUAL spectrometer). In particular, we studied the effect of the anode position (from 5 cm to 8 cm) respect to the cathode and the temperature of the anode (cooled and uncooled electrode). Finally, we studied the changes in the hardness and wear resistance, obtained by scratch tests (NANOVEA ST-500), of the deposited film, as a function of experimental parameters: argon gas pressure (from 5 to 15 mTorr), magnetron sputtering voltage (250 V) and anode voltage (80, 100 and 120 V) applied, as well as deposition rates measured by optical profilometry.

Tailoring Zr-Cu-based thin-film alloys by W and Nb additions: from metallic glasses to supersaturated solid solutions

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C4_2, Picasso Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Zr-Cu-based thin-film metallic glasses (TFMGs) have emerged as a promising class of materials due to their exceptional properties such as high glass-forming ability, superior elastic strain limit, enhanced hardness and plasticity. Moreover, these TFMGs offer the potential to be combined with nanocrystalline materials (transition metals or metal nitrides) to create heterogeneous dual-phase nanocomposite structures and thus achieving a better balance of toughness and hardness and/or unlocking new functionalities.

Therefore, this study explores the effect of gradual addition of W (negative mixing enthalpy with Zr but positive with Cu) and Nb (positive mixing enthalpy with both Zr and Cu) on microstructure and properties of Zr-Cu-based thin-film alloys. Two film series, W-Zr-Cu and Nb-Zr-Cu, were prepared by magnetron sputtering technique, keeping Zr:Cu as 1:1 and gradually varying the W and Nb content in the respective series.

A systematic investigation revealed that W and Nb additions have a significant impact on microstructure and other properties of the films. The films remain amorphous with smooth surfaces (roughness < 2 nm) up to 65 at.% of W or Nb, displaying vein-like features typical of metallic glasses upon fracture. W-Zr-Cu films with 67 at.% W are characterized by a combination of featureless structures (amorphous-like) close to the substrate and thin columns in the upper part of the film. Films with even higher W contents grow in a V-shaped columnar microstructure corresponding to the bcc α -W crystalline structure. Nb-Zr-Cu films with 70 at.% Nb clearly exhibit a dual-phase structure with thin columns surrounded by vein-like features. Further increase in the Nb content above 70 at.% leads to the formation of a crystalline structure with parallel columns and very small voids. These voids tend to vanish with increasing Nb content. A gradual increase in hardness and reduced Young's modulus is observed with increasing W content for the amorphous W-Zr-Cu films and the crystalline films show an enhancement in hardness of up to 15% compared to films with pure W due to solid solution hardening. In the case of Nb-Zr-Cu films with up to 70 at.% Nb, the hardness remains nearly constant. However, further addition of Nb results in a decreased hardness and this reduction might be attributed to a less dense structure of the films.

Results of ongoing analysis and experiments on W-Zr-Cu and Nb-Zr-Cu films based on ZrCu will also be presented, providing new insights into the material's phase transitions, mechanical strength, and electrical properties.

Amorphous Al₂O₃ Thin Films: The Influence of Alloying Elements on Dielectric Properties at High Temperatures

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C4_6, Picasso Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Aluminium oxide (Al₂O₃) is a widely recognized insulating material used as a thin film in various applications. This material obtains several polymorphs and features also an amorphous state, providing high oxidation resistance and excellent thermal stability. One significant advantage of amorphous-grown PVD films is typically their lack of pinholes and fewer diffusion paths for charge carriers. Research into the use of insulating Al₂O₃ thin films is ongoing in multiple fields, including as a dielectric substance in electronics, semiconductor applications, and energy storage. Therefore, exploring economically and sustainably viable deposition techniques for growing insulating Al₂O₃ thin films is essential.

The study examines how alloying Al₂O₃ thin films with silicon and yttrium-zirconium (YZr) affects the thermal stability of the amorphous state, aiming to prevent any phase transitions up to 1200 °C. To achieve this, Si and YZr were incorporated into the used target materials. Amorphous Al₂O₃ thin films have been synthesized using a reactive Modulated Pulse Power (MPP) process carried out in mixed Ar/O₂ atmospheres on a custom-developed sputter system (equipped with 3-inch targets). The formation and evolution of the amorphous state have been studied using in-situ X-ray diffraction (XRD) over a temperature range from room temperature to 1200 °C. Scanning and transmission electron microscopy (SEM) has been employed to assess the deposition rate and morphology of the coatings. Additionally, in-situ impedance spectroscopy has been used to investigate changes in electrical properties across various temperatures. For this procedure, photolithography has been utilized to deposit titanium/platinum (Ti/Pt) electrode pads for electrical characterization. The chemical composition of the films was determined using X-ray photoelectron spectroscopy (XPS), which also helped to examine the bonding nature of the elements present in the films.

Enhancing Metal-Polymer Interlocking by Optimizing the Geometry of Micro-Pins

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study aims to enhance metal-polymer interlocking by optimizing the geometry of micro-pins fabricated on metallic substrates. Polymeric materials, such as PEEK and Trogamid, will be bonded to metal surfaces through axially symmetric, mushroom-shaped interlocking structures produced using Directed Energy Deposition (DED). By varying pin geometry—specifically size, shape, and surface distribution—their impact on interlocking strength is expected to be evaluated. Potential failure mechanisms will be analyzed, including polymer rupture, pin fracture, and separation caused by excessive shear forces. A mathematical model will be developed to predict these failure mechanisms, providing a tool for designing optimal interlocking structures. The model will enable the design of optimum interlocking structures for metal-polymer interfaces, while separation tests are expected to yield data on force-displacement and stress values.

A novel MTES/polysilazane hybrid polymer coating for corrosion protection of stainless steel substrate

Dr. Yolanda Castro¹, Dr. Emilia Merino¹, PhD Parisa N. Moghaddam², Dr Milan Parchovianský², Dr. Alicia Durán¹, Dr. Amir Pakseresht²

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

A novel MTES/polysilazane hybrid polymer coating for corrosion protection of stainless steel substrate
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Keywords: Polysilazane, corrosion, stainless steel, thin films

Polysilazane is an attractive candidate of coating materials due to its good adhesion properties to most substrates and its great potential to be modified and to obtain tailored properties for a variety of applications [1] [2]. In this work, the hybrid coating based methyltriethoxysilane (MTES) and poly(methylvinyl)silazane (Durazane 1800) was synthesized by sol-gel route to improve corrosion resistance and lifetime of stainless steel substrate. The MTES/polysilazane solution was synthesized using tetra-n-butylammonium fluoride (TBAF) and n-butyl acetate (NBTA), and was deposited on stainless steel by dip coating method. The structure and thermal stability of hybrid sol were investigated by Fourier transform infrared (FTIR) spectroscopy and thermogravimetric analysis (TGA). FTIR studies demonstrated that the incorporation of MTES to polysilazane backbone the integrity of polysilazane was preserved. Based on Field emission electron microscopy (FESEM) analysis, crack-free, smooth, and homogenous hybrid coatings were obtained on stainless steel. The corrosion resistance of MTES/polysilazane and polysilazane coatings are studied by electrochemical impedance spectroscopy (EIS) and potentiodynamic polarization techniques. The preliminary results confirmed that the synthesized hybrid coatings can be a good option to improve the corrosion resistance of the stainless steel substrate in 3.5 wt% NaCl solution.

Acknowledgments:

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Mechanical properties and adhesion of $W_{1-x}Al_xB_{2+z}$ coatings

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C4_2, Picasso Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

The quest for advanced materials with outstanding properties has brought tungsten borides into the spotlight, thanks to their exceptional hardness, thermal stability, and resistance to wear. The crystallographic structure of these materials is crucial in shaping their physical, mechanical, and antioxidation behavior. Notably, borides doped with aluminium have emerged as a standout option, exhibiting excellent mechanical and antioxidation characteristics [1]. These materials hold significant potential for use as protective coatings that can remain stable under high-temperature conditions.

To achieve the desired material structure, a novel magnetron deposition technique was used, integrating direct-current magnetron sputtering (DC) with High Power Impulse Magnetron Sputtering (HiPIMS). The films were deposited using two distinct targets: AlB_2 (DC) and $WB_{2.5}$ (HiPIMS). Mechanical testing demonstrated exceptional hardness (~30 GPa for aluminum doping below 10% atomic). As the aluminum content in $W_{1-x}Al_xB_{2+z}$ coatings increased, a slight decrease in density and hardness was observed.

The experimental findings were compared with theoretical values derived from DFT calculations. All $W_{1-x}Al_xB_{2+z}$ structures examined using DFT were confirmed to be both mechanically and thermally stable. The experimentally measured hardness values surpassed those predicted by DFT, highlighting the notable impact of aluminum doping.

Due to the use of hard coatings mixed with a soft substrate, it is important to achieve good adhesion. Coatings were applied to nitrided steel QR90 with tungsten interlayer. For this purpose, the films were subjected to two methods of adhesion measurement: scratch testing and laser spallation.

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Investigation of coating properties in cold-sprayed Ni-base superalloys post processing – long term heat treatment and hot isostatic pressing

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C4_11, Picasso Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Cold spraying (CS) is extensively employed to fabricate protective coatings, such as Inconel 718 (IN718), owing to its remarkable efficacy in challenging environments. Although the technique has significant versatility but owing to the problem of porosity inclusions in coatings, parts are often subjected to post-processing treatments. This research examines the impact of such post-processing on IN 718 cold-sprayed coatings onto IN 718 substrates. The post-processing techniques employed are Hot Isostatic Pressing (HIP) and prolonged heat treatment of the IN 718 coating with the aim to examine their influence on the microstructure and mechanical properties of CS coatings addressing the challenges related to coating integrity. The CS IN718 coating was heated to 1150°C and then subjected to an isostatic pressure of 120MPa for 4 hours for HIP treatment, while the long-term heat treatment involved exposure to 750°C for 168 hours. The HIP treatment resulted in superior mechanical properties due to the combined effect of recrystallization, twins and MC carbides. Concurrently, it diminished the work-hardened microstructure via recovery, evidenced by a reduction in dislocation density within the coating. The alterations in coating microstructures resulted in an approximate 200 percent increase in the cohesive strength of the coating following HIP-ing. The application of long-term heat treatment significantly decreased the porosity levels of the coating from approximately 4% to 0.8%, signifying an enhancement in the metallurgical bonding among the individual splats. Precipitation hardening, resulting from the formation of intermetallic phases (γ'' and δ) and MC carbides, alongside a decrease in material ductility, collectively contribute to this phenomenon. In general, both the post processing techniques resulted in improvement of coating strengths. In addition to an increased cohesive strength, the HIP-ed coating additionally demonstrated a notable plastic region, in contrast to the heat-treated coating. Ultimately both post-processing techniques altered the microstructures of the coating, leading to enhanced cohesive strength and ductility. This presentation will offer a comprehensive discussion of all notable findings related to the benefits derived from post-processing treatments of CS coatings.

The Influence of Ethanol-Fueled HVOF Deposition Parameters for 316L based coatings

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The thermal spray process is widely utilized across industries to deposit metallic or non-metallic coatings on prepared surfaces, enhancing properties such as corrosion and abrasion resistance. The High Velocity Oxygen Fuel (HVOF) thermal spray process, known for producing coatings with low porosity, low oxide content, and high substrate adhesion, employs liquid fuels like ethanol and powder feedstock delivered through a converging-diverging Venturi nozzle. Ethanol, a relatively recent advancement in liquid-fuel technology, has shown promise due to its safety, efficiency, reduced oxygen consumption, and minimal emissions of toxic fumes and particulates. This study focused on 316L based coatings, an austenitic nickel-chromium stainless steel powder (Fe 17Cr 12Ni 2.5Mo 2.3Si 0.03C). Coatings produced with this material are dense, bright, and exhibit exceptional resistance to corrosion, wear, and impact, as well as tensile strength, making them ideal for applications requiring corrosion resistance, solid particle erosion protection, and dimensional restoration. The experimental design employed a Taguchi L9 orthogonal array to analyze the influence of four factors: working distance, mass flow of combustion gases, combustion stoichiometry, and powder feed rate, each analyzed three levels. Calibration curves were developed to correlate RPM settings with powder feed rates, ensuring precise parameter control. The findings aim to enhance the understanding of the relationships between process parameters, coating microstructure, and performance. To characterize the coatings and compare the effects of different process parameters, the following analyses were conducted: optical microscopy, scanning electron microscopy (SEM), Vickers microhardness, analysis of the porosity and oxide area fraction, and fracture toughness. To evaluate the significant difference between levels were used the Tukey test. The optimal coatings are expected to exhibit lower porosity, lower oxide content, higher microhardness, greater thickness, and higher toughness. The results indicate that porosity was significantly influenced by the mass flow rate, while the oxide content showed no significant influence from any of the parameters analyzed. Microhardness was significantly affected by the standoff distance, whereas the coating thickness was influenced by the combustion stoichiometry and powder feed rate. In contrast, fracture toughness showed no significant relationship with the evaluated parameters. The parameter levels that contributed to improved coating properties were the two highest levels of standoff distance, the highest mass flow rate, the lowest levels of stoichiometry, and the highest powder feed rate. In summary, small variations in standoff distance and stoichiometry did not significantly affect the results, highlighting the robustness of the process under these conditions.

Novel interface-engineered nanolaminated Al-X / AlOH thin films towards superior mechanical properties and thermal stability

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C4_10, Picasso Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Recent deposition advances allow interface-engineered multi-layered Al-X- / AlOH (25 / 1 nm) thin films by a combination of physical vapour and atomic layer deposition. These allow systematic evaluation of grain boundary complexion engineering and the unique crystalline / amorphous interface on mechanical properties and thermal stability. Annealing at low homologous temperatures allows rather segregation enrichment at interfaces than grain growth. Thermal stability was investigated based on lateral grain growth— out-of-plane growth being limited by 1 nm AlOH interlayers. Mechanical testing by nanoindentation and micropillar compression at multiple strain rates allowed mechanical property analysis of the high-strength Al-X / AlOH multilayer thin films with nanoindentation hardness of more than 5 GPa. Ultimately, high-resolution analysis by transmission electron microscopy and atom probe tomography allowed the enhanced properties to be linked to interface decoration and secondary phases that hinder dislocation and grain boundary movement.

Nanocomposites based on transition metal borides and silver in view of mechanical and antibacterial properties

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C4_7, Picasso Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Transition metal borides are becoming increasingly popular due to their unique properties. They are outstanding not only for their very high hardness and fracture resistance, but also for their considerable chemical and thermal stability. Silver, on the other hand, is valued as an antibacterial material due to its unique biological properties. The combination of these two materials may enable the development of an innovative super-hard composite with antibacterial properties.

In this study, it was decided to create Ag/WB2.5, Ag/W0.84Ti0.16B2.5 nanocomposites and compare their properties to the individual composite components. The silver coating was produced by pulsed laser deposition (PLD), while the WB2.5 and W0.84Ti0.16B2.5 coatings were produced by high-power pulsed magnetron sputtering (HiPIMS). Subsequently were carried out a series of necessary tests for the realisation of the work's topic. The microstructure and surface morphology were characterised using a scanning electron microscope (SEM) with chemical composition analysis (EDS) and an optical profilometer. The observations revealed that the silver particles are uniformly covered by a coating of tungsten borides. This contributed to a reduction in the roughness of the composite compared to a layer composed of pure silver (Ra of about 100 nm).

In order to determine the mechanical properties, hardness tests, adhesion of the coatings by scratch-test and wear resistance by abrasion in reciprocating motion were tested. As a result of the presence of the silver film, the wear resistance increased compared to the coating composed of W0.84Ti0.16B2.5.

The biological properties of the materials were assessed by a test in a liquid suspension of *Staphylococcus Aureus* bacteria (Gram-positive bacterium). The samples were incubated in a greenhouse at 37°C for a specified time and then analysed for changes in the number of bacterial colonies.

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Innovative plasma nitriding process of a biomedical grade CoCrMo alloy by High Power Impulse Magnetron Sputtering

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C4_5, Picasso Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Medical implants are requested to meet stringent requirements to ensure their safety and reliability over long periods within the human body. Cobalt-Chromium-Molybdenum (CoCrMo) alloys are widely used in this field due to their excellent mechanical properties, corrosion resistance and biocompatibility. However, concerns about ion release and wear debris from implants [1], especially in Metal-on-Metal (MoM) applications, highlight the need for improved surface treatments to mitigate tribocorrosion effects and enhance implants durability. Surface engineering such as the application of protective coatings or nitriding treatments can reduce the effects of wear and corrosion as well as material release, addressing challenges like adhesion failure and wear debris generation in service. Surface conversion treatments, as nitriding and carburizing, are effective alternatives to coatings for improving tribocorrosion resistance of biomedical implants, enhancing mechanical strength, wear, and corrosion resistance, and can be tailored to meet specific implant requirements. Plasma nitriding, a recent and versatile technique, offers energy and cost efficiency, shorter treatment duration, and improved nitrogen uptake compared to traditional methods. Among plasma treatments, those based on magnetron sputtering technology appear particularly attractive, such as HiPIMS-based (High Power Impulse Magnetron Sputtering) low-pressure nitriding [2], which promotes superior nitrogen diffusion at lower temperatures, reduces oxygen interference and allows duplex treatments with the following application of protective coatings. The present study uses the HiPIMS discharge in an innovative way to perform a plasmochemical surface treatment on a CoCrMo alloy, modifying the target materials exploited to sustain the plasma, to affect nitrided layer properties. Among the target materials, i.e. Cr, Ti, Mo and Ta, molybdenum demonstrates the best overall performance, facilitating the formation of the desired γ N phase without the presence of secondary phases, enhancing mechanical properties and chemical stability. The nitriding process results in an increase in hardness, up to 18 GPa, which is significantly higher than that of the untreated CoCrMo alloy (~6 GPa). Moreover, the nitriding environment has been investigated, by changing the H₂/N₂ flow ratio in the chamber during the HiPIMS process. It has been demonstrated that all nitrided samples exhibit a positive shift in corrosion potential values in Ringer's solution, indicating improved corrosion resistance, reduced wear rate and smoother wear scars, compared to pristine samples, thus balancing wear and corrosion resistance effectively. These results highlight the potential of tailored plasma processes for biomedical applications. [1] N. Espallargas et al, Wear 332–333 (2015) 669-678 [2] P. Hovsepian et al, Materials Letters 313 (2022) 131782

Design of an innovative cathodic arc source with high deposition rate and low macroparticles generation

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C4_3, Picasso Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Within the group of PVD techniques, Cathodic Arc Evaporation technique stands out for its performance, which is characterized by an almost 100% ionized, high-energy plasma. Its versatility, lower economic cost compared to other deposition techniques and ease of industrial scaling have led to massive industrial implementation for the production of coatings and thin films of various types. One of the disadvantages of the cathodic arc technique is the generation of macroparticles due to the arc discharge on the cathode surface. This fact can be an important technological limitation in cases where a good surface finish, low friction coefficient or good wear and corrosion resistance is required. Traditionally, this problem has been solved by using magnetic filters to separate the macroparticles from the plasma ions. However, this solution is associated with a significant reduction in the deposition rate, which makes it difficult to implement on an industrial scale. On the other hand, to reduce the costs of the coating process, cathodic arc sources that allow a high deposition rate are required.

In this work, an innovative cathodic arc source was designed to achieve a deposition rate of up to 20 microns/hour with an 80% reduction in macroparticles. To increase the deposition rate, a high current pulsed source (100-500 A, 10-20000 Hz) was used to generate the arc discharge between the anode and cathode. On the other hand, aimed to reduce the generation of macroparticles, an optimized magnetic field configuration around the cathode has been obtained by means of Finite Element Method (FEM) simulation, which allows to induce a fast and homogeneous movement of the arc on the cathode surface. Standard transition metal nitride (CrN, AlTiN) hard coatings obtained using this source show excellent surface finish and improved mechanical properties in terms of adhesion and hardness.

Impact on the B/Ti-ratio on microstructure and mechanical properties of DCMS and HiPIMS TiB₂±z thin films

Mr. Ludwig Enzlberger¹, Mr. Thomas Astecker¹, Dr. Alexander Kirnbauer¹, Mr. Tomasz Wojcik¹, Mr. Maximilian Podsednik², Prof. Andreas Limbeck², Dr. Szilard Kolozsvári³, Prof. Paul Heinz Mayrhofer¹

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C4_5, Picasso Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Titanium diboride is widely known as a superhard material achieving an indentation hardness of 40 GPa and beyond. Coatings of TiB₂ produced by DC magnetron sputtering are typically in the superstoichiometric regime regarding the B/Ti-ratio in a range of TiB_{2.4} to TiB_{3.5}. This surplus in Boron is attributed to a different radial distribution of Boron and Titanium during the deposition process and forms a B-rich tissue phase which is highly relevant for the material's mechanical properties.

A reduction of Boron content in the coating would thus mean a reduction of tissue phase formed and consequently a clear change in e.g., hardness or fracture toughness. Earlier works have already shown an increase in fracture toughness (measured by microcantilever bending) of DC-sputtered TiB₂ when reducing the B/Ti-ratio from 4.4 to 2.1. There have also been reports of even higher fracture toughness in understoichiometric TiB_{1.43} produced through HiPIMS and measured by cube corner indentation, although films grown by DC showed a decrease in KC with decreasing B-content.

In the current work, we aim to show how the mechanical properties of TiB₂ change when crossing the stoichiometric point by DC and HiPIMS sputter deposition. The stoichiometry of DC-grown films is controlled by placing pieces of pure Ti along the race track of the target, while in HiPIMS mode it is controlled by varying the pulse on-time as well as adding pieces of Ti. The films are analysed through XRD and SAED for structural information, ICP-OES to determine the B/Ti-ratio as well as SEM and TEM for microstructure. Hardness and Young's Modulus are measured by nanoindentation while KIC values are determined by cube corner indentation and microcantilever bending to investigate the influence of stresses.

Development of surface treatments and coatings for the corrosion protection of bipolar plates of PEM fuel cells and electrolyzers

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

PEM electrolyzers are essential for the production of green hydrogen as they use renewable electricity to split water into hydrogen and oxygen with high efficiency. Their compact design, fast response time, and ability to operate under variable conditions make them key to enabling a sustainable hydrogen economy. On the other hand, PEM fuel cells are a promising candidate to replace internal combustion engines in today's transport applications. However, in both cases, there are some aspects related to their performance, durability and cost that limit their effective implementation. These technical limitations are mainly associated with the durability of the metallic bipolar plates, a crucial component of PEM fuel cells and electrolyzers.

Stainless steel and titanium alloys are suitable materials for the manufacture of bipolar plates for PEM fuel cells and electrolyzers, respectively. In the case of PEM fuel cells, stainless steel bipolar plates can be produced cheaply, easily and on a large scale in the form of thin sheets by means of forming processes. However, their corrosion resistance is not high enough to withstand the acidic and humid environment under which a PEM fuel cell operates. This fact increases the interface contact resistance and contaminates the proton exchange polymeric membrane, thus reducing the energy efficiency of the cell. In the case of PEM electrolyzers, titanium bipolar plates face several corrosion-related challenges: (i) surface passivation due to the formation of a passive oxide layer (TiO_2), which can increase contact resistance and reduce electrical efficiency; (ii) aggressive environment due to acidic and high potential operating conditions; (iii) hydrogen embrittlement, which can compromise their structural integrity over time.

In both cases, a solution to these problems involves the application of electrically conductive coatings with good corrosion resistance. In this respect, PVD (Physical Vapor Deposition) coatings (e.g. noble metals, transition metal nitrides and carbides, and amorphous carbon-based coatings) have been extensively studied in recent years.

In this work, the preparation and characterisation of carbon-based coatings obtained by PVD cathodic arc evaporation is presented. In addition, the development of corrosion resistant surface treatments obtained by Metal Vapor Vacuum Arc (MEVVA) ion implantation has been explored.

The effect of the acid content and the electrical parameters in the dry-anodising process of Ti6Al4V

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Titanium has low density, high strength to weight ratio and excellent corrosion and wear resistance. When titanium is suspended in an electrolytic bath as an anode and a current is passed through the bath, oxygen is produced at the anode Surface. This oxygen combines with the titanium to form titanium oxide. The interference taking place between the oxide and light results in the appearance of colors on the metal surface and oxides with different thickness generating different colors. This passive oxide film formed on titanium surface is responsible for its high corrosion resistance. Thus it has wide range of applications in aerospace, automotive and biomedical industries. This presentation presents a dry-anodizing technology by using DryLye® Technology. In this sense, the thickness, voltage and current density effect of the acid content is evaluated by different advanced characterization technique. The direct and indirect coating thickness measurement of the anodize layer by using the Focused Ion Beam and reflectometry techniques, respectively; highlight that the anodize thickness layer does not depend on both the acid content and the applied electrical parameters, yielding a homogeneous value of around 60 nm.

Kinetics and Mechanisms of Stripping HVOF Coatings (Inconel 625 and Inconel 625 + 40% CrC) Using Drylyte® Technology

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C4_9, Picasso Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

The stripping process and kinetics of two high-velocity oxy-fuel (HVOF) coatings—Inconel 625 and Inconel 625 + 40% CrC—were studied on carbon steel and AISI 316 stainless steel substrates using Drylyte® Technology. The removal rate, surface morphology evolution, and electrochemical behavior during the stripping process were analyzed.

The Drylyte electrolyte-based process demonstrated effective material removal, with significant differences observed between the two coatings. Inconel 625 exhibited a higher removal rate than the composite Inconel 625 + 40% CrC due to the presence of chromium carbide, which increased coating hardness and reduced dissolution kinetics. For both coatings, the stripping rate was higher on carbon steel compared to stainless steel, attributed to the different electrochemical behavior of the substrates.

Kinetic analysis revealed that the stripping rate followed a mixed mechanism involving electrochemical dissolution and mechanical particle detachment. The activation energy for material removal was estimated to be higher for the Inconel 625 + 40% CrC coating, confirming its greater resistance to stripping. Surface characterization after stripping showed minimal substrate damage, confirming the selectivity of the Drylyte process.

In conclusion, the Drylyte® Technology presents an efficient and controlled method for stripping HVOF coatings, with stripping kinetics strongly influenced by coating composition and substrate type. The findings provide valuable insights for optimizing the removal of thermally sprayed coatings in industrial applications.

Biocompatible multilayer system for the degradation control of an additively manufactured WE43 alloy

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C4_8, Picasso Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Mg alloy WE43 is one of most relevant alloys for bioimplants due to its good mechanical properties and biocompatibility. Additive manufacturing (AM) techniques such as powder bed fusion (PBF) have paved the way for fabrication of orthopaedic implants with complex internal and external geometries with excellent mechanical properties, unachievable by other means. However, the main problem that prevents the wider use of Mg-based implants is the control of their degradation rate. Plasma electrolytic oxidation (PEO) is based on the growth of an oxide layer by means of high voltages (300V – 600V) and eco-friendly electrolytes that can improve the corrosion resistance and enhance the bioactivity of the structure. The combination of PEO with other coatings in a hybrid system can be employed to control the degradation rate of biomedical devices. This study focuses on the development of a multilayer system on an AM WE43 scaffold comprising a PEO layer in combination with hydroxyapatite (HAp) and polycaprolactone (PCL). The role of HAp is to promote bone growth and PCL is used as a carrier of a fluoroquinolone that exhibit antibiotic and corrosion inhibition properties. The scaffolds were characterized by optical and scanning electron microscopy (SEM), X-ray diffraction (XRD), energy dispersive X-ray spectroscopy (EDS) and transmission electron microscopy (TEM). The drug-loaded coating was characterized by SEM, EDS, XRD and their roughness was measured using optical profilometer. Electrical impedance spectroscopy (EIS) measurements on drug-loaded coated scaffold in Hank's solution at 37°C were performed up to 3 days. The fluoroquinolone release into Hank's solution was measured by means of ultraviolet-visible spectroscopy (UV-VIS) and correlated with corrosion resistance of the coated system. The corrosion of a bare alloy in the presence of fluoroquinolone was also studied. The results revealed that both PEO and HAp layers were able to uniformly cover the struts of the scaffold even within the recesses of difficult access. The role of the coating in corrosion modulating effect of quinolone on AM WE43 Mg alloy scaffold is highlighted.

Superfast stripping of DLC coatings from WC-Co cutting tools using a Low-Energy High-Current Electron Beam.

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Diamond-Like Carbon (DLC) coatings are extensively applied to enhance the durability and cutting efficiency

of Hard Metal (HM) cutting tools, particularly under demanding operating conditions. Over time, these tools inevitably develop defects and wear, requiring their disposal. To extend their lifespan through resharpener and reuse, an efficient decoating process is essential. In the present research, a vacuum plasma technology is implemented to tackle the issue of cutting tools decoating, with an eye on avoiding

the use of harmful chemicals in the process. Low-Energy High-Current Electron Beam (LEHCEB) [1] was employed to remove DLC coatings from WC-Co₂ milling inserts. Pulsed irradiation by LEHCEB allows to completely evaporate the carbon coating from the substrate by exploiting the fast (10^9 K/s) induced thermal gradient and the lowered sublimation point of the coating at the vacuum working pressure. The

electron accelerating voltages were 20, 25 and 30 kV, with an associated energy density of 2.5, 3.3 and 4.9 J

cm⁻², respectively. The number of pulses were 5, 10 and 20, with a 0.2 Hz repetition frequency. The working

pressure ($1.8 \cdot 10^{-4}$ Torr) and the ionized gas (Ar) were kept the same. Stripped substrates were then reground, recoated and tested to demonstrate the full regeneration of the cutting tools. Samples were characterized in terms of surface morphology by Scanning Electron Microscopy (SEM, Zeiss EVO 50P). Chemical microanalysis was performed by Energy-Dispersive X-Ray Spectroscopy (EDS, Bruker Quantax 200

spectrometer). The crystalline structure was assessed by X-Ray Diffraction (XRD, PANalytical EMPYREAN

PW1830. Coating thinning was assessed by Raman Spectroscopy on DLC and X-Ray Fluorescence on TiN.

Vickers microhardness was assessed by instrumented indentation at different loads (Helmut Fischer, HVX100).

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Pulsed Electron Beam Irradiation of AlSi alloys as Pretreatment to Grow Modified Anodic Oxide Layers

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C4_2, Picasso Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Aluminum alloys play a crucial role in several engineering fields, like aviation, aerospace, automotive, construction and marine industries. They are employed thanks to their low density, high strength-to-weight ratio, excellent electric and thermal conductivity, good castability and machinability, and easy recycling. In aluminum-silicon alloys, the content of Si usually varies between 4 and 25 wt. % and other alloying elements, such as Cu, Mg, Mn, and Fe, may be added in smaller amounts to improve the mechanical properties of the alloy [1]. In order to improve the corrosion resistance and the surface mechanical properties, anodic oxidation is usually employed to form a protective coating. However, the anodizability of Al-Si alloys is strongly influenced by the presence of alloying elements, that make the achievement of a homogenous and durable anodic layer a challenging task. The presence of coarse silicon structures, in particular, causes the formation of a highly defective anodic oxide in which unoxidized regions, gas-filled porosities and cracks are frequently encountered [2]. In the present work, the Low-Energy High-Current Electron Beam [3] is employed for surface modification of Al-Si alloys as a pre-treatment for anodic oxidation. In this way, thanks to the rapid melting and solidification induced on the metal surface by the electron beam irradiation, the redistribution of silicon can be achieved, obtaining a small and fine dispersion. In particular, the influence of different energy densities (2-5 J/cm²) and different number of pulses (4-32) was investigated. Oxides were produced by anodic oxidation in H²SO₄, at 0°C for 15, 30 and 45 minutes. Surface and cross-sectional morphology were investigated using a Zeiss EVO 50VP SEM equipped with a Bruker Quantax X-ray spectrometer for EDS chemical microanalysis. The crystalline structure was characterized by X-ray diffraction in Bragg-Brentano (BB) configuration utilizing a PANalytical EMPYREAN PW1830 diffractometer. Vicker microhardness and elastic modulus were assessed by a Helmut Fischer HVX100 at different loads. The electrochemical behavior of coatings was characterized by Linear Sweep Voltammetry and Electrochemical Impedance Spectroscopy with a Solartron Modulab XM ECS potentiostat in 3.5% NaCl solution at room temperature.

[1] doi.org/10.1088/1757-899X/1107/1/012116

[2] doi.org/10.1002/adem.202101480

[3] [doi.org/10.1016/S0257-8972\(99\)00604-0](https://doi.org/10.1016/S0257-8972(99)00604-0)

Nanostructure engineering and properties enhancement of Cu-based films by Zr and Ta alloying

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C4_5, Picasso Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Nanocrystalline Cu films exhibit unique mechanical properties due to the increased surface area of grain boundaries. However, this structural state creates excess free energy leading to low thermal stability. Our study addresses this challenge through targeted alloying of magnetron sputtered Cu films with low content of Zr and Ta. The mutual immiscibility and large atomic size mismatch between Cu and Zr or Ta have the potential to influence grain boundary chemistry and structure implying grain boundary engineering approach. Magnetron sputter deposition, in turn, represents a non-equilibrium technique widely used for reproducible preparation of thin films with a variety of structural states, including both thermodynamically stable and metastable structures.

Nanocrystalline Cu-rich Cu-Zr and Cu-Ta films were deposited from two separate targets of the base metal (Cu) and alloying element (Zr or Ta) under identical technological conditions with a fine composition variation. The effects of Zr and Ta alloying on the structure, surface, mechanical, and electrical properties were investigated using X-ray diffraction, electron microscopy, atomic force microscopy, indentation, and the four-point probe method. Additionally, non-equilibrium atomic-scale growth simulations of Cu-rich Cu-Zr and Cu-Ta films were conducted to provide information not achievable experimentally.

The results show that alloying with Zr and Ta significantly influences the microstructure and anisotropy of the films, which leads to a notable structural refinement and a reduction of the average grain size from 220 nm in unalloyed Cu to below 100 nm with Zr or Ta alloying. A systematic investigation shows that during film deposition, a redistribution of alloying atoms occurs between the grain interior and grain boundaries resulting in the formation of a complex microstructure. As a result, the alloyed films exhibit hardness values between 3.2 and 4.2 GPa, exceeding the 2.5 GPa measured for the unalloyed Cu film. The electrical resistivity increases with increasing content of the alloying elements, primarily due to electron scattering by solute atoms and additional scattering at the grain boundaries. However, the as-deposited alloyed Cu films exhibit a favorable combination of hardness and electrical conductivity that is comparable to or better than reported values in literature.

Our findings demonstrate that precise alloying with Zr and Ta, combined with non-equilibrium conditions of magnetron sputter deposition, is an effective approach for modifying the structural state of the Cu films, optimizing their mechanical, electrical, and surface properties, and offer insights that can be applied to other comparable binary systems in the development of nanocrystalline metallic films.

Study on Microstructure and Mechanical Properties of Nanoparticle-Coated Maraging 300 for Iron-Based MMCs

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C4_6, Picasso Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Metal matrix composites (MMCs) are promising materials due to their high specific strength, hardness, wear resistance, and relatively low density, making them widely used in civil engineering, aerospace, electronics, and automotive industries. Although Ti- and Al-based MMCs have excellent performance, their high cost and limited availability restrict their use in general industrial applications. In contrast, iron-based MMCs have attracted attention due to their lower cost, good mechanical properties, high thermal stability, and wide applicability. In particular, particle-reinforced iron-based MMCs with additives such as Al_2O_3 , Y_2O_3 , and TiC have shown great potential for high-performance materials by providing uniform microstructures and improved mechanical strength.

However, conventional casting and powder metallurgy methods for fabricating particle-reinforced MMCs often face challenges in achieving uniform dispersion of nanoscale reinforcement. Strong van der Waals forces between nanoparticles cause agglomeration, leading to non-uniform distribution in the matrix, which can reduce mechanical performance. Additionally, traditional mixing and sintering processes may result in particle growth and microstructural segregation, limiting the full benefits of reinforcement.

To overcome these challenges, this study applied powder metallurgy techniques by coating Maraging 300 powder with nanoscale ceramic particles to produce an iron-based MMC. The microstructure and mechanical properties of the composite were analyzed using X-ray diffraction (XRD), scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), electron backscatter diffraction (EBSD), microhardness testing, and compression testing. This research provides insights into the effects of nanoparticle dispersion and reinforcement mechanisms in iron-based MMCs.

Optical emission spectroscopy of deposition process of W-Al-B coatings obtained by HiPIMS/DCMS hybrid technique

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Tungsten borides because of their properties, like hardness and thermal stability, may be a potential alternative to traditional superhard materials (diamond and cubic boron nitride) or typical materials for tool coatings (TiN, TiAlN etc). Tungsten borides can be furtherly enhanced by alloying with various metals. In this regard, addition of aluminium can increase oxidation resistance of diboride-based materials [1].

High power impulse magnetron sputtering (HiPIMS) technique is already well-used for deposition of high quality coatings. Flux of highly energetics species have a significant influence on deposited coatings and its properties. Due to this, plasma behaviour during HiPIMS should be extensively studied.

In this work we present the study of deposition of W-Al-B thin films by HiPIMS/DCMS technique. WB_{2.5} and AlB₂ targets were co-sputtered in various parameteres of WB_{2.5}-HiPIMS/AlB₂-DCMS. Plasma behaviour was investigated via optical emission spectroscopy to obtain intensities and distribution of atoms and ions of tungsten, aluminium and boron. Due to lower deposition rate of dual than single magnetron set-up it was very important to perform examination of plasma plume behaviour. Mechanical properties were evaluated by nanoindentation technique, microstructure was observed using scanning and transmission electron microscopy (SEM, TEM). Chemical and phase composition were measured by ToF-ERDA and X-ray diffraction (XRD), respectively.

Addition of Al into WB₂ structure lowered the hardness of deposited films form 29 to 17 GPa at ≈ 0.7 Al/(W+Al) atomic ratio. Crystalline coatings were only obtained for Al/(W+Al) ratio between 0.05-0.2.

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Unravelling solid self-lubrication mechanisms of B₂O₃ in TiB_{2±z} and WB_{2±z} based thin films

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C4_2, Picasso Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Transition metal borides (TMBs) represent a highly promising family of materials for functional coatings due to their abundance, cost-effectiveness, and exceptional mechanical properties. These include a high melting point, hardness of up to 60 GPa, excellent chemical and thermal conductivity, and outstanding resistance to wear. TMBs have distinct self-lubricating properties due to the formation of boron oxide, which helps to reduce friction. The temperature plays a significant role in the formation of boron oxide. However, the fundamental mechanisms behind this tribo-reaction are not yet fully understood, especially concerning TMB-based thin film materials.

Understanding the oxidation behavior of physical vapor deposited TiB_{2±z} and WB_{2±z} thin films is essential for comprehending their friction and wear properties in high-temperature tribo contacts. Tribological tests reveal that sputter deposited super-stoichiometric TiB_{3.5} exhibits a significantly lower friction coefficient (~0.25), roughly half compared to that of sub-stoichiometric TiB_{1.67}, tested at 500°C. This reduction is attributed to the higher oxidation rate of super-stoichiometric TiB_{3.5} and the presence of B-rich tissue phases at the column boundaries. Similarly, α-WB_{2±z} coatings also exhibit self-lubrication properties. However, they tend to stabilize in the sub-stoichiometric form, resulting in reduced amounts of boron available for oxidation.

Additionally, we conduct an in-situ investigation of the oxidation process in sub- and super-stoichiometric TiB_{2±z} and WB_{2±z} thin films using elastic backscattering spectrometry (EBS). This technique provides detailed depth profiles of the chemical composition over a temperature range from room temperature to 800°C. The oxidation data are further correlated with tribological, XPS, XRD, and TEM analyses, offering new insights into the lubrication mechanisms of boron oxide in TMB thin films across a wide temperature range.

Wetting properties of titanium surfaces tuned by duplex treatments combining nanosecond laser treatment and chemical functionalization

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 15, 2025, 13:15 - 14:30

Duplex treatments combining different processing methods open up a wide range of possibilities for modifying the surface properties of materials. In the case of titanium, nanosecond laser treatments have demonstrated their ability to induce a surface oxidation layer whose stoichiometry and properties depend on treatment conditions [1-2]. The covalent grafting of organic molecules onto the surface of titanium oxide films [3-4] opens up interesting prospects for controlling the hydrophobicity and biocompatibility of titanium surfaces, as well as for developing self-cleaning surfaces, sensors, photocatalytic supports, etc. [3].

The aim of the present work is to tune the wetting properties of metallic titanium by laser-assisted surface oxidation followed by chemical functionalization to produce hydrophobic to superhydrophobic surfaces.

A Q-switched and frequency-doubled Nd:YAG green laser (KALUTI) operating at 532 nm and delivering 5 ns pulse duration was used for laser treatments on CP-Ti plates. They produced a saw-tooth patterned surface covered by an oxidized surface layer containing mainly TiO₂-anatase [5]. The chemical modification of laser-treated surfaces with octylphosphonic acid (OPA) in form of tetrahydrofuran (THF) or boiling water solutions was performed. The effect of concentrations of modifier going from 0.01 to 100 mM on the resulting organic load, layer structure and contact angles was investigated. The duplex-treated surfaces were characterized by SEM-EDS/WDS, XPS, XRD and Raman spectroscopy.

OPA solutions in THF were found to give rise exclusively to monolayer formation (16 ± 5 Å), with surface coverage completed at a phosphorus concentration of around 4.8 at.% according to XPS results. Concentrated OPA solutions in water produced an additional layer of titanium (IV) octylphosphonate, bringing the total thickness of the organic layer to 37 ± 11 Å at a maximum phosphorus concentration of approx. 8 at.%.

Despite the different nature of the organic layers, all surfaces containing at least 2.2 at.% P showed a similar static contact angle of around 155°. Based on dynamic contact angle measurements, superhydrophobic behavior was confirmed for surfaces bearing a full OPA monolayer and titanium phosphonate (IV) overlays.

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Study on the Electrochemical Characterization of Multi-component Dimensionally Stable Electrodes for Copper Electroplating in PCB Manufacturing

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Dimensionally stable electrodes (DSEs), as substitutes for conventional copper anodes, enable precise fine-pattern formation in copper electroplating for PCB circuits. The use of DSEs in PCB electroplating requires high energy efficiency and durability. DSEs are typically fabricated by coating one or more noble metal oxides onto the titanium substrate due to their electrochemical performance and stability. During the PCB electroplating process, oxygen evolution reactions at the anode decompose organic additives in the electrolyte, reducing electrolyte stability and hindering fine-pattern formation. Therefore, research on the fabrication of noble metal coatings for DSEs is required to enhance electroplating performance and electrolyte stability. In this study, noble metal coatings with high current efficiency and reduced organic additive decomposition were fabricated by depositing metal oxides such as iridium, ruthenium, and tantalum in various compositional ratios, followed by optimization of oxidation heat treatment conditions. The composition and surface morphology of the DSE were characterized using field emission scanning electron microscopy (FE-SEM) and energy-dispersive X-ray spectroscopy (EDS or EDX). Electrochemical reactions were analyzed using a potentiostat, and the decomposition characteristics of organic additives were evaluated by cyclic voltammetry stripping (CVS). The copper electroplating process was performed using a sulfuric acid-based electrolyte containing a suppressor, an accelerator, and a leveler of organic additives at a current density of 50 mA/cm² for 60 minutes, and the decomposition rate of organic additives in the electrolyte was measured. The decomposition rate of the suppressor showed minimal dependence on the DSE composition, whereas the accelerator exhibited a higher decomposition rate with increasing Ir content in the DSE coating layer.

Hierarchically Structured Catalysts Via Additive Manufacturing For Emerging Applications

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Additive manufacturing (AM), or 3D printing, has emerged as a revolutionary technology in catalytic applications, offering unprecedented advantages over traditional manufacturing methods. This innovative approach enables the creation of customized electrocatalysts with complex geometries, tailored porosity, optimized active surface and formation of nano-micro levels hierarchical structures. Additive manufacturing opens new frontiers in the field of catalysts, electro-chemical reactions and in the manufacturing of their reactors and peripherals that were previously impossible to achieve.^{1,2} Key advantages include unparalleled design flexibility, rapid prototyping capabilities, material efficiency, and the ability to create highly customized structures with enhanced surface area-to-volume ratios.

The unique benefits of AM in electrode manufacturing extend beyond traditional production limitations, allowing for the integration of multiple materials, cost-effective small-scale production, and precise structural optimization.^{3,4} By enabling the creation of intricate electrode designs with minimal material waste, this technology accelerates research and development processes while providing unprecedented opportunities for innovation in electrochemical applications.

In this work, novel architectures were developed using state-of-the-art powder sintering technologies in additive manufacturing, including Powder Bed Fusion Electron Beam (PBF-EB), Powder Bed Fusion Laser Beam (PBF-LB), and Multi Jet Fusion (MJF). These advanced techniques enabled the successful manufacturing of a wide range of metallic and non-metallic structures. The fabricated components underwent optimized surface modifications through chemical, electrochemical, and thermal treatments to create hierarchical catalytic structures. Furthermore, these metallic structures were thoroughly validated in various electrochemical and photoelectrochemical applications, such as water splitting, electrochemical nitrate reduction, and other related applications.

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Decoating process by using the DLyte® Technology of TiAlN/TiSiN and AlCrSiN coatings: insights from chemical analysis using XPS measurements

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C4_4, Picasso Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

TiAlN/TiSiN and AlCrSiN are advanced coatings employed in a wide range of industries due to their remarkable properties, including enhanced wear resistance, hardness, and excellent high-temperature performance. One of the most used applications is in cutting tools, since they provide an increase in tools' life under service like working conditions.

However, over time the used parts degrade and need to be reconditioned. In that sense, stripping or decoating process is a key point in order to remove the coating and re-coat again to reuse the cutting tool. In addition, decoating process can be used to remove defective coatings produced during the production process, and restore the initial substrate of the tool. Currently on the market, the decoating process for the TiAlN/TiSiN and AlCrSiN can be conducted though chemical (such as acid etching or chemical stripping) or with physical methods (e.g., laser ablation or plasma stripping). However, in both cases substrate could be affected, and as a direct consequence the surface integrity is deteriorated. In the particularly case of cemented carbide (WC-Co) tools, this effect is magnified, since the metallic Co binder undergoes corrosion in acidic or even neutral mediums.

Within the aforementioned information, recently, a new technology can be employed to decoat materials without damaging the substrate and being able to preserve the geometries. In this regard, through this presentation the DLyte® Technology will be employed to decoat TiAlN/TiSiN and AlCrSiN coatings deposited over WC-Co material. Furthermore, the thickness of the coating removed along the decoating time will be investigated by using the focused ion beam technique (FIB) in order to determine the decoating kinetics for ternary (TiAlN/TiSiN) and quaternary (AlCrSiN) systems.

In addition, as chemical analysis plays a pivotal role in order to understand the process and to control de substrate integrity, X-ray Photoelectron Spectroscopy (XPS) analysis thought the entire decoating process has been conducted. During the decoating process, XPS provides information about the superficial chemistry, identifying the coating's removal elements, and detecting any contaminants or oxidation that may occur. This surface-sensitive technique can be used to track the reduction in signals corresponding to coating elements (e.g., Ti, Al, Cr, Si) as the process of the decoating process by using the DLyte® Technology progresses. This real-time monitoring ensures that the coating is completely removed without damaging the underlying material.

Design and Investigation of DC Magnetron Sputtered TiN/TaN superlattice structures

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C4_2, Picasso Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Thin films based on transition metal nitrides (TMNs) are versatile materials suitable for a broad range of applications. Cubic NaCl-type titanium nitride (TiN), in particular, is a paradigm coating material with excellent mechanical properties. Tantalum nitride (TaN) offers intrinsic ways of tuning mechanical performance via its metastable cubic phase (NaCl-type): providing access to a wide range of stoichiometries and (beneficial) lattice defects, including stacking faults, which may hinder the onset of crack initiation and propagation.

Contrarily to TiN, ab initio calculations indicate the ability of TaN to nucleate mechanical twins and activate twinning-induced plasticity effects. To verify and complement these predictions, we deposited TiN and TaN in the form of superlattice coatings (alternating nano-layers) via unbalanced DC magnetron sputtering. Thereby we take advantage of the TiN template effect and generate numerous interfaces, providing a basis for subsequent analysis of stacking fault and twinning activities in TiN/TaN superlattices, as well as related interface effects. The combined micro-structural analysis using XRD and SEM reveals the expected nano-layered structure of the TiN/TaN coatings, while mechanical tests corroborate the enhancement of hardness and fracture toughness (superlattice effect). In the long run, the insights gained from this study contribute towards a comprehensive knowledgebase for the design of materials with unique property combinations.

Innovative Cold Spray Solutions for Composite Substrate Metallization

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C4_10, Picasso Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Metallization of composite substrates enhances their electrical conductivity making them suitable for advanced applications such as aerospace. Methods like Physical Vapor Deposition, Electroless Plating, and Thermal Spraying offer varied advantages but also face challenges, such as thermal degradation, limited adhesion, and environmental concerns. Cold Spray (CS), is a Thermal Spray technology that involves high-velocity particle deposition without melting the powder material while forming a coating, minimizing thermal impact. This makes it particularly suitable for temperature-sensitive substrates like carbon fibre-reinforced polymers (CFRPs).

This study aims to enhance the adhesion in CFRPs metallization by combining Arc Wire Spray for interlayer deposition with CS for top-layer coating. This technique also solves the challenges like erosion and cost -efficiency. Various interlayer materials, including Zn, Al, Zn/Al alloys, Cu, Brass (Cu/Zn), and combinations, were deposited via Arc Wire to enhance bonding between the composite substrate and the metallic coating. Al and Cu powders were then applied as the top layer using CS. Experimental evaluations assessed coating thickness, porosity, adhesion strength, and electrical conductivity, targeting aerospace industry requirements for lightning protection and electromagnetic interference shielding.

Results show that interlayer selection plays a crucial role in improving adhesion, reducing delamination, and enhancing electrical performance. Additionally, top-layer coatings further improved electrical conductivity, making the metallized CFRPs more effective for advanced applications. The combination of AWS and CS enables superior adhesion and performance, demonstrating the potential of combining different thermal spray techniques for composite metallization. Future work will focus on optimizing process parameters, enhancing material compatibility, and exploring scalable industrial applications.

Helium-assisted deposition of Cu-doped TiO₂ for Conductometric Hydrogen Sensing via DC Magnetron Sputtering

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C4_6, Picasso Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

This study presents a novel helium-assisted sputter deposition method for Cu-doped TiO₂ conductometric sensors, intending to enhance the active surface area through microstructure modification, thereby improving sensing capabilities. This is achieved by careful optimization of discharge parameters, while the working gas consists of a mixture of argon, helium and oxygen. Partial replacement of argon with helium leads to the formation of structured porous films. The influence on the sensing response and the possible explanation of the effect in helium-rich working gas are discussed.

Cu-doped TiO₂ films were fabricated using conventional DC magnetron sputtering, utilizing a circular titanium target with an adjacent copper strip in carefully controlled working gas mixtures of argon, helium, and oxygen, maintaining a total pressure of approximately 520 mPa. Helium was introduced as a replacement for part of argon in the working gas mixture of argon and oxygen. After deposition, samples were annealed at 400 °C in ambient air to crystallise and stabilize the films for hydrogen sensing. A series of different helium concentrations was prepared, varying the helium content from 0% to 95% in the working gas. The glancing angle deposition (GLAD) technique was applied to enhance the films' active surface area. The copper doping was chosen to make the films more conductive since the undoped titania films are nearly insulating.

X-ray diffraction patterns revealed the effect of helium on film microstructure:. Films deposited under helium exhibit both anatase and rutile phases, whereas films deposited without helium show only the anatase phase. Scanning electron microscope observation reveals a grain size reduction with increasing plasma helium content. Nevertheless, the most pronounced effect was the distinct change in the structure, which appears highly porous for the films prepared with helium. Conductometric sensing was carried out using a four-point probe, demonstrating that helium usage leads to a 600% increase in sensor response for Cu-doped TiO₂ films (maximum He vs 0% Helium).

This paper further discusses the He-induced effects leading to microstructure modification. The discharge with He-rich working gas specifics is also mentioned. The effect of the GLAD is also presented.

Low-temperature plasma-assisted carburizing of additively manufactured 316 L steel

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C4_11, Picasso Room (Level -2), settembre 18, 2025, 17:00 - 19:00

Austenitic stainless steels are used in several industrial sectors (chemical, energy, biomedical, pharmaceutical, etc.) due to their excellent corrosion resistance, however, they suffer from low hardness and wear resistance. To improve these characteristics without detrimental effects on corrosion resistance, the 316L steel, manufactured by Laser Powder Bed Fusion (L-PBF), was subjected to a plasma assisted carburizing process at 475 °C. The temperature is suitable to avoid the precipitation of $M_{23}C_6$ carbides and η , χ and σ phases.

The work aimed to optimize the more relevant process parameters, namely the composition of plasma gas mixture (CH_4 plus H_2), and the treatment time. In a first stage the effects of different amounts of CH_4 (0.5, 1, 2, 2.5 and 4 %) in the gas mixture were examined by keeping constant the time (7 hours) of treatment. The samples were characterized by Light Microscopy (LM), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), X-ray Diffraction (XRD), Raman Spectroscopy (RS), X-ray Photoelectron Spectroscopy (XPS), Glow Discharge Optical Emission Spectroscopy (RF-GDOES), and Vickers micro-hardness tests. The results evidenced that the mixture consisting of 2.5% CH_4 + 97.5% H_2 is the most effective: the surface hardness (547 ± 27 HV) becomes more than double if compared to the one of original material (245 ± 3 HV). Surface hardening is due to the formation of a C-enriched austenite (S-phase) with thickness of ~ 20 μm . S-phase resulted covered by a very hard and brittle diamond like carbon (DLC) over-layer of ~ 2 μm that fractures and detaches during tribological tests and these abrasive particles increase the wear rate.

Therefore, in the second stage of the research the treatment time has been changed step by step to find the conditions for forming the S-phase without the DLC over-layer. The best trade off, in terms of surface hardening and wear resistance, is the treatment with 2.5% CH_4 + 97.5% H_2 for 90 minutes, resulting in a wear rate of ~ 20 times lower than that of the same material before plasma carburizing treatment.

Investigation of the nanostructure of TiSiN coatings using high resolution methods

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C4_1, Picasso Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

Owing to its excellent mechanical properties TiSiN is commonly used as hard protective coating in cutting applications. However, the nanostructure of TiSiN is controversially debated and the detailed investigation is a challenging task, requiring the application of advanced high resolution characterization techniques such as transmission electron microscopy and atom probe tomography (APT). While APT would be a valuable method to illuminate the local elemental distribution with close to atomic resolution, peak overlaps of Si and N in the mass spectrum do not allow for an unambiguous differentiation, resulting in poor elemental accuracy and imaging precision. In the present work, different approaches to improve both, elemental accuracy and imaging precision are shown. In addition, the nanostructure of magnetron sputter deposited as well as cathodic arc deposited TiSiN coatings is illuminated, showing the effect of varying Si content and deposition parameters on the evolving structure.

Design of superhydrophobic transparent surfaces by laser and fluorine-based functionalization with anti-fogging and anti-icing responses

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C4_8, Picasso Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Glass surfaces used for outdoor applications are partially hydrophilic, making them particularly susceptible to ice-accretion, fog, and contaminants. These events hamper maintaining long-term transparency and an easy cleaning of architectural and cover elements, such as glazing, photovoltaic panels, outdoor optical systems and sensors. This makes the control of the wetting properties of structural glass a topic of the utmost importance and high interest for many industrial applications. However, surface modification procedures such as functional coatings and/or the microscale surface texturing for controlling the wetting behavior inevitably entails optical changes and possibly transmittance losses. Therefore, keeping a high transparency while providing a robust water repellence to transparent systems is a key challenge for the surface engineering community. The endeavour is even more demanding for situations and systems operating in harsh environments at low temperatures and high humidity conditions.

In this work, we present a new strategy to get a precise control over the hydrophobicity of transparent substrates, while preserving as much as possible their optical properties. The approach combines laser patterning with a mild chemical surface functionalization to achieve superhydrophobicity, anti-icing, and anti-fogging responses. A precise parametrization of the femtosecond UV laser treatments on borosilicate glass, whereby pattern geometry, scanning cycles, and motif dimensions, have been systematically changed, lead to a controlled variation of surface morphology, as characterized by the resulting percentage of the laser-treated area and surface roughness. The developed microstructure proved suitable for hosting fluorinated molecules devoted to the enhancement of the hydrophobicity while preserving the optical transmittance. Moreover, superhydrophobic laser-patterned transparent glass has been shown to have an anti-fouling behaviour upon interaction with biological simulating agents. Water condensation experiments carried out by environmental scanning electron microscopy have confirmed a remarkable anti-fogging performance of the laser-treated glass surface, whereas freezing delay time measurements, as well as ice adhesion tests in a pull-off configuration, have demonstrated the extraordinary anti-icing capacity of the laser patterned transparent substrates and their stable behaviour even after 5 freezing/thawing cycles.

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Laser Surface Treating WSC Coatings to Optimize WS₂ Crystallization-to-Carbon Phase Graphitization

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C4_3, Picasso Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

WSC coatings i.e. WS₂ phase immersed in an amorphous carbon matrix, provide low friction and wear in several environments (e.g. humid air, vacuum, dry N₂, etc.), attributed to WS₂ phase crystallization and basal plane reorientation along sliding, together with a high structural integrity, mainly attributed to the harder amorphous carbon. However, before WS₂ is able to provide a stable low CoF, a running-in period with unstable CoF is generally unavoidable, especially when sliding against soft materials (e.g. rubber), for which contact stresses are low. Spatially precise laser energy inputs could potentially allow for local crystallization of the WS₂ phase in surface regions, with little structural degradation (e.g. by graphitization) of the amorphous carbon matrix. However, given the multitude of laser systems and input parameters that can be varied during the process, laser treating a new material typically entails the need for time-consuming trial-and-error iterations before the process is easily understood and controllable. Therefore, we set out to find if a single laser parameter could govern WSC phase transformations at specific thresholds. WSC coatings with ~50 at. % of C were thus deposited by magnetron sputtering and subsequently treated with a fiber laser, and an adequate interplay between the most relevant input parameters (found to be the peak power, pulse duration and repetition rate) was reached, with five final treatment conditions (WSC-IR1 to WSC-IR3*) obtained from independently varying each of the latter. Different experimental techniques were then employed to help identify phase transformations, namely: i) optical microscopy, 3D optical profilometry, white light interferometry and calotests to study morphological and cross-sectional features; ii) Raman spectroscopy and nanoindentation to study the level of structural and mechanical transformations, including its spatial variation along treated spots (center, edges, and in-depth). Average power, power density, energy per pulse and fluence were estimated for each treatment condition, as they are known to describe certain laser-matter interaction phenomena in other materials. Increasing each of the latter, treated regions darkness, diameter (10-23 μm), heights (29-118 nm), transformed depths (0.07-0.17 μm), degree of amorphous carbon graphitization and WS₂ crystallization concomitantly increased (former seems to occur at slightly lower exposure thresholds, though almost concurrent with the latter), with mechanical properties like the hardness and elastic modulus reducing little (~3-4.5 GPa compared with ~5-6 GPa in non-treated zones), such that mechanical integrity of the coating should remain high.

Plasma etching-controlled microstructure and optical properties of ZrN Coatings on ABS for automotive applications

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C4_7, Picasso Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Zirconium nitride (ZrN) coatings of 750 nm thickness were deposited on plasma-etched acrylonitrile butadiene styrene (ABS) substrates using low-temperature direct current reactive magnetron sputtering. Argon plasma etching time and pressure were varied from 2 to 8 minutes and 0.4 to 1.5 Pa, respectively, under a -70 V bias. Plasma etching modified the substrate's surface reactivity, roughness, and hydrophilicity, leading to an increase of the total surface free energy (up to 50.2 mN/m). X-ray diffraction analysis showed that etching parameters influenced the coating's texture, with a predominant [111] orientation and a [200] texture emerging at 5 minutes of etching under 1.5 Pa pressure. Optimal etching (5 min at 0.4 Pa) resulted in ZrN coatings with a smooth surface, golden hue, high lightness ($L^* \approx 74\%$), and 62% total reflectance. Higher etching pressures (1.5 Pa) produced glossier coatings with fewer pinholes but introduced minor reflectance loss due to stress-induced cracking. Peel tests confirmed strong adhesion across all samples. These findings underscore the importance of plasma etching in optimizing both the functional and aesthetic properties of ZrN coatings, highlighting their potential for decorative automotive applications.

Assessing hydrogen diffusion in ceramic PVD coating materials

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C4_6, Picasso Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

The introduction of hydrogen-based energy production, storage, and conversion technologies requires materials that can withstand hydrogen's unique and reactive properties. A key concern is the durability of structural components, particularly issues like hydrogen embrittlement and corrosion in fuel cell and electrolyzer technologies. These factors are crucial as we transition to green and sustainable energy sources. Specifically, the interaction of hydrogen with the uppermost micrometers and the microstructural features of materials will significantly influence their performance. Thus, employing physical vapor deposition (PVD) coating materials to protect and enhance material surfaces will be essential for a wide range of future applications.

Degradation mechanisms related to hydrogen occur at multiple length scales, involving different strategies for exposure or treatments. These strategies are typically divided into the two hydrogen-related material research worlds: (i) electrochemical degradation setups and (ii) and non-electrochemical treatments as a collective term for pressure/gas-related setups. Nevertheless, the broad field of hydrogen-related applications is increasingly merging. Consequently, the different degradation strategies primarily focus on electrochemical test setups as they are highly versatile.

Therefore, in this study, the interaction of hydrogen with well-known protective coating materials such as TiN, CrN, ZrN, or TiAlN and AlCrN is described by an electrochemical Devanathan-Stachurski permeation setup. Different sets of these ceramic coating materials have been deposited on ferritic steel sheets through sputter and arc-evaporation technologies with varying deposition parameters. Subsequently, the coatings have been electrochemically loaded, and parameters such as diffusion coefficients, permeability, or permeation reduction factors are estimated. These results are correlated with the coatings' microstructural appearance before and after hydrogen testing using a set of diverse high-resolution techniques such as SEM, TEM, XRD, and micro-mechanical testing methods.

Correlation of ab initio methods with experimental phase exploration of TM-Al/Si-C thin film materials

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Thin films, consisting of Transition Metal Carbides (TMCs), are known for their remarkable thermal stability, with melting points reaching up to 4000 °C, and their excellent mechanical properties, including exceptional hardness. These properties make Physical Vapor Deposited (PVD) TMCs indispensable materials for challenging applications in the aerospace and tooling industries. Nevertheless, their limited oxidation resistance inspires the alloying of strong oxide formers such as Al and Si to improve their high-temperature performance. Setting the focus on metastable, fcc-structured, TM-X-C (TM = Ti, Zr, Hf, Ta, W and X = Al, Si) solid solutions, Density Functional Theory (DFT) was used in order to access the metastable solubility trends, by the means energy of formation and unit cell distortion. In a second step, these theoretical findings are correlated with an experimental approach in which over 260 different compositions within these ten material systems are grown by combinatorial magnetron sputtering. Phase formation, mechanical properties, and oxidation resistance are subsequently analyzed by X-ray diffraction, nanoindentation (CSM method), and Transmission Electron Microscopy (TEM) for selected states. The comprehensive analysis of structure-property relationships of these ternary TMC thin films provides crucial insights into the so-far relatively unexplored phase space and opens up opportunities for advanced applications.

The Role of Substrate Roughness and Chemical Composition in HiPIMS-Coated Cutting Tools

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C4_1, Picasso Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

The European Union's target of reducing greenhouse gas (GHG) emissions by 55% until 2030 has driven innovations in the mobility sector, leading to the development and application of lightweight alloys and composite materials. This transition is essential for achieving environmental targets; moreover, the efficiency and cost-effectiveness of machining processes of the new materials under development within the mobility sector remain equally important. In this context, a more efficient machining process for these hard-to-cut materials is essential, which can be achieved through the development of advanced cutting tool materials, the optimization of tool geometry, or through modifications in coating design, aiming to improve tool performance, service life and increase retooling time. This is particularly challenging, as the tools must combine wear and oxidation resistance at high temperatures without compromising their toughness, in order to withstand demanding machining conditions.

In the present work, multilayer thin films with different compositions – including TiN, TiAlN, TiSiN, AlCrN and/or ZrN – were deposited through High-Power Impulse Magnetron Sputtering (HiPIMS), on polished and unpolished Si₃N₄-based cutting tools, to assess the substrate roughness and chemical composition influence on structural, morphological, adhesion and wear properties of the ceramic multilayer coatings. With thickness values ranging between 1.5 and 2.5 µm, these films were thoroughly characterized. The structure and morphology of the thin films were analyzed by SEM/EDS, along with roughness measurements, and mechanical properties assessed through adhesion and wear tests. Overall, preliminary results indicate that both substrate surface roughness and coating composition significantly impact multilayer deposition. Unpolished samples exhibit higher roughness values, leading to uneven material deposition and, consequently, less consistent thickness values. These differences in surface roughness, along with the coating composition, also pose a great influence in the adhesion and wear properties of the coatings. Nevertheless, the surface roughness does not seem to affect the presence of defects on the coating topography or the adhesion between layers.

A Materials Science Approach to the Analysis of Ion Diffusion Effects in Barley Seed Surfaces Treated with an Air Plasma Discharge

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C4_9, Picasso Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Plasma in agriculture is a current application area of surface engineering which is generating much interest from both fundamental and applied perspectives and because of its high impact on seeding efficiency and environmental sustainability. Plasma treatment of seeds contributes to enhance the germination rate, promoting early plant deployment, and providing protection against pathogen detrimental actions. Current studies often link these positive effects to biochemical alterations affecting seed metabolism and genetic factors controlling seeds germination and young plants growth. In this study, we focus on the analysis of the redistribution of ions in the interior of barley seed surface layers when they are subjected to a cold air plasma treatment. For this purpose, we apply a Materials Science approach involving the use of scanning electron microscopy combined with Energy Dispersive X-ray spectroscopy and depth profiling analysis using X-ray photoemission coupled with gas cluster sputtering. Moreover, we have developed a Monte Carlo model accounting for the positive ion migration in the interior of seeds upon their exposure to a plasma. These tools are compatible for the description of similar ion migration effects taking place during the processing and use of a large variety of materials (e.g., membranes, ionic solids, etc.).

Additionally, we explore the impact of plasma exposure on the lixiviation of ions through the seeds' hull when they are immersed in water. The findings reveal that the superficial layers of the seed hull (up to approximately ~100 nm in depth) exhibit a notable enrichment of K⁺ and Ca²⁺ ions, accompanied by alterations in the O/C and N/C atomic ratios. These observations were further corroborated by electron microscopy and fluorescence analysis of seed cross-sections. Meanwhile, the Monte Carlo model, which simulates the electrostatic interactions between the negative charge accumulated at the seed surface due to plasma exposure and the positive ions present within the seed interior has provided some clues to understand the migration mechanism in this system. It has been also demonstrated that plasma-treated seeds exhibit more efficient ion lixiviation when immersed in water compared to untreated seeds. Notably, a significant concentration of NO₃⁻ anions was detected in the leachate, which is attributed to secondary reactions between nitrogen species incorporated into the seeds during the air plasma treatment and reactive oxygen species generated at the seed surface. These findings are discussed in the context of their potential use to improve seed germination capacity and a more robust plant growth.

Electrical insulation properties of reactive grown AlN thin films at high-temperatures

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Aluminum nitride-based ceramics are known for their insulating properties and high thermal conductivity. Their range of applications is vast, whether as structural components or thin films. As the electrical conductivity is highly depended on the temperature, the mobility of charge carriers at elevated temperatures causes distinct challenges for insulating thin film materials.

Therefore, in this study the growth of insulating AlN thin films via PVD and their electrical insulation up to 750 °C is studied. For the growth various reactive PVD techniques have been used, including magnetron sputtering (DCMS), high-power pulsed magnetron sputtering (HIPIMS), and pulsed magnetron sputtering (PMS). For all depositions a 3" Al target was used in mixed Ar/N₂ atmospheres. Phase formation has been examined using XRD, while the deposition rate and film morphology were investigated through SEM and TEM. The insulating properties of the coatings were analyzed using in-situ impedance spectroscopy, with measurements taken from room temperature to 750°C. The experiment was conducted using Pt/Ti lithography pads.

The electrical properties are influenced by the morphology of the film, with the densest HIPIMS grown films exhibiting the highest electrical resistance over temperature. Nevertheless, the influence of impurities, such as O₂, plays a significant role in reducing the insulating properties of the films.

Characterization of antifouling efficiency, mechanical and chemical properties of polydimethylsiloxane Fouling Release coatings

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The increasing demand for sustainable marine coatings has driven research toward non-toxic solutions for protecting bronze propellers from biofouling and corrosion. Conventional biocidal antifouling systems, while effective in reducing microbial adhesion, are subject to stringent environmental regulations due to their ecological impact. As a result, silicone-based fouling-release coatings have emerged as a promising alternative. However, these systems often suffer from suboptimal mechanical properties and adhesion issues, leading to detachment over time. Additionally, their long-term antifouling performance requires further optimization to match that of traditional antifouling coatings. This study evaluates the performance of environmentally friendly fouling-release coatings, with a particular focus on the role of polydimethylsiloxane (PDMS)-modified topcoats in enhancing biofouling release while maintaining adequate mechanical properties. The research explores key formulation parameters of the silicone topcoat, including the influence of catalysts, silicone oils, and functional additives. A comprehensive characterization approach is adopted, involving scratch testing, profilometry, protein adhesion and toxicity assessments, crosslinking density evaluation, and in situ monitoring of biofouling growth on immersed coated panels. Additionally, Fourier-transform infrared spectroscopy (FTIR) and scanning electron microscopy (SEM) are employed to analyze the structural and chemical characteristics of the coatings. The findings provide valuable insights into the development of high-performance fouling-release coatings with improved durability and antifouling efficiency.

Innovative Copper-Based Electrocatalysts: Harnessing 3D Printing for Sustainable Nitrate Management in Drinking Water

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Nitrates are naturally present in the environment. However, anthropogenic activities, particularly the widespread use of fertilizers in intensive agriculture, have led to a significant increase in nitrate levels in both aquifers and soils. This excessive nitrate contamination of groundwater systems poses serious environmental risks, such as eutrophication, and can also threaten human health.

The United States Environmental Protection Agency (EPA) has established a maximum contaminant level (MCL) for nitrate in potable water at 10 mg L⁻¹ necessitating the development of effective nitrate removal strategies for drinking water treatment.¹

Copper and its alloys have demonstrated considerable promise in electrochemical applications, particularly for the electro-reduction of nitrates.² The utilization of additive manufacturing (AM) techniques, specifically 3D printing of metallic electrodes with various surface modifications, offers potential enhancements in electrochemical processes by increasing the active surface area.³ In this context, powder bed fusion (PBF) systems, employing electron beam melting (EB-PBF) as the energy source, are frequently utilized for 3D printing of metallic structures.

This study investigates the development and performance of innovative copper electrodes manufactured by Electron Beam Powder Bed Fusion (EB-PBF) technology. These electrodes undergo subsequent electrochemical and thermal modifications to enhance their catalytic properties. This work evaluates the effectiveness of these modified electrodes by comparing them with unmodified 3D-printed copper electrodes and conventional copper foil, all tested under identical conditions. The performance of these electrodes is assessed as electrocatalysts in the reduction of nitrate to ammonia, a process with substantial potential for fertilizer production.

Following a comprehensive analysis of the parameters influencing the electrochemical reaction, we successfully scaled up operations using a novel, custom-designed electrochemical cell. This cell features fabrication through Multi Jet Fusion technology, utilization of polyamide-based materials, and scaled-up electrodes with surfaces reaching up to 200 cm² of geometric area. Employing various electrochemical techniques on the modified 3D copper electrodes yielded exceptional performances, achieving over 99% nitrate reduction and up to 90% conversion to ammonia within a 3-hour timeframe. These findings underscore the potential of additive manufacturing technologies in revolutionizing the design and production of advanced electrochemical systems. The demonstrated scalability opens new avenues for industrial applications, particularly in sustainable fertilizer production and environmental remediation, highlighting the promising intersection of advanced manufacturing techniques and electrochemical engineering.

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Concentrated Solar Energy for the elaboration of VC-reinforced steel as a sustainable alternative to conventional arc melting

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This work is part of an integrated research project targeted to investigate the feasibility of optimising a novel “solar surface treatment” process for the elaboration of carbide-based hardfacing layers with acceptable microstructure and satisfactory performance under harsh operating conditions. For this purpose, Concentrated Solar Energy (CSE) was applied for the fabrication of thick surface layers, composed of a dispersion of μm -sized vanadium carbide reinforcing particulates within the metallic matrix of St 37-2 common steel. All “solar” experiments were carried out in the solar furnaces of Plataforma Solar de Almería (Spain). Typical such campaigns involve (a) pre-deposition of a specific volume of the reinforcing particles onto steel substrates, (b) positioning of the materials system in a closed jar, onto a thermal insulating Al_2O_3 support, ensuring the continuous flow of Ar inert gas and (c) exposure of the materials system to CSE and dwell at surface temperature above the melting temperature of the substrate (1.540°C) for given time. Under these conditions, the solar radiation is concentrated solely on the area covered by the black pre-deposited powder and the heat is transferred to the underlying steel resulting in its melting during exposure, whereas the ceramic reinforcement remains unaffected due to its higher melting temperature ($>2.800^\circ\text{C}$). VC particulates are immersed into the melting pool and after solidification the requested composite layer is formed on the top of the steel substrate, having a thickness that depends on the dwell time at surface temperature higher than 1.540°C . Subsequently, the microstructure of the CSE-obtained surface layers was characterised by means of microscopy and X-ray diffraction, and their operation performance was evaluated during sliding wear tests and exposure to corrosive environments. The findings were compared with the corresponding ones concerning similar bulk composites fabricated via conventional arc melting that was applied for the elaboration of nm-sized vanadium carbide dispersions within a stainless steel matrix. The potential and limitations of both the CSE and the arc melting processes were evaluated using as criteria the performance of the respective composites, as well as the initial size of the reinforcing ceramic particles and the steel grade of the matrix.

During the last two decades, Concentrated Solar Thermal Systems as the one proposed here were extensively studied and found successful implementation in the field of energy applications. The present attempt is focused to transfer relevant scientific findings to other potential applications like of materials engineering and “Green Metallurgy”.

High-Temperature Concentrating Solar Technologies for direct surface processing of metallic parts

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Surface modification, as a sub-field of Surface Engineering, targets on enhancing the performance and longevity of metallic parts that operate under severe environments that involve wear, abrasion, erosion and cavitation. Addressing these issues is crucial as industries strive towards sustainable solutions amidst global climate concerns. In particular, there is an increasing interest to develop new routes based on renewable energy sources that would be a reliable and efficient alternative to conventional surface modification processes of metals. The work presented here aims at the application of high-temperature Concentrating Solar Technologies for processing of metallic parts. Since 2014, a series of such “solar” campaigns implemented at Plataforma Solar de Almeria (Spain) by the authors’ groups, which were targeted to the direct elaboration of wear-resistant composite surface layers, led to the proof-of-concept that, indeed, concentrated solar energy can be a promising renewable energy solution for the direct surface processing of metallic parts.

The project TWINSOLARSURF (“Twinning for solar energy-driven surface engineering of metallic parts”), a Horizon Europe-funded project that started in October 2024 and will last 3 years, capitalizes on these promising scientific results and aims to contribute to the development of a novel ecosystem in the frame of “Green Metallurgy” and in general of “Green Manufacturing”. The consortium will work on an exploratory project on the research playground of surface processing of metallic materials for use in aggressive environments e.g. wear, abrasion, erosion and high temperature. In particular it will pursue the parallel development of ultra-hard as well as thermal barrier coatings (TBCs). The former will be elaborated on steel substrates via concentrated solar thermal energy; the latter will be targeted to protect metallic ducts carrying the heat transfer fluids in such solar thermal plants from excessive solar irradiation retarding their sensible heating beyond critical temperatures and mitigating the consequences of temperature overshooting. In parallel the partners will work together on a strategic plan for co-developing a space of excellence via a capacities’ building programme, sharing knowledge, integrating expertise and skills and delving into new research avenues. The overall approach is fully linked to the European Green Deal strategy for green industrial technologies of the future, further penetration of renewable energies and building the skilled research personnel capable of addressing the global societal, political and environmental challenges of our future ecosystem.

Influence of Mo on the mechanical and tribological properties of DCMS and HiPIMS deposited TiB₂+z thin films

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Transition metal borides (TMBs) represent a highly promising family of materials for functional coatings due to their abundance, cost-effectiveness, and exceptional mechanical properties. These include high melting temperatures, hardness of up to 60 GPa, excellent chemical and thermal conductivity, and outstanding resistance to wear. Theoretical predictions by density functional theory assessing the elastic constants revealed that the formation of ternary Ti-Mo-B₂+z might be a suitable approach to gain a less brittle character. In addition, Mo is also known to form self-lubricating phases such as MoOx (Magnéli phases), which typically helps to reduce friction.

To study the effect of Mo on TiB₂+z three different target compositions were used for the non-reactive growth of ternary Ti_{1-x}MoxB₂+z thin films: TiB₂/MoB 95/5 mol%, TiB₂/MoB 90/10 mol%, and TiB₂/MoB 80/20 mol%. The binary TiB₂+z system was deposited with a TiB₂/C 99/1 wt.% target. In addition, direct current magnetron sputtering (DCMS) and high-power impulse magnetron sputtering (HiPIMS) were employed to investigate the influence of different deposition techniques.

The structural and mechanical properties of the coatings were characterized by a wide variety of methods, such as scanning electron microscopy, X-ray diffraction analysis, and nanoindentation. The chemical composition was determined by inductively coupled plasma optical emission spectrometry and elastic recoil detection analysis. To verify the suggested enhancement on the brittle behavior of Ti_{1-x}MoxB₂+z, fracture characteristics, such as KC and KIC, have been determined by cube corner indentation and in-situ micro-mechanical bending tests, respectively. Furthermore, tribological tests were conducted at room temperature and high temperatures of up to 600 °C to investigate the influence of Mo on the friction coefficient and wear mechanisms.

Functionally graded laser deposition to overcome fabrication challenges in Tribaloy™ T800 hardfacing on stainless steel

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C4_7, Picasso Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Laser additive manufacturing by directed energy deposition (DED) of hard and brittle materials presents significant challenges. Tribaloy™ T800 (Co-17.5Cr, 28.5-Mo, 3.6Si in wt.%), a cobalt-based alloy, exhibit exceptional wear and corrosion resistance, however, its laser deposition to produce hardfacing coatings poses difficulties due to its limited ductility. The rapid cooling rates inherent to additive manufacturing, gives rise to significant thermal contraction strain which can lead to fabrication cracking and delamination in part due to high volume fraction of brittle Laves phase (~60 vol%) and low fracture toughness ($20 \text{ MNm}^{3/2}$) of the material. To address these challenges, a functionally graded T800 (FG-T800) is developed via in-situ alloying by blending the Tribaloy powder with stainless steel 316L (SS316L) powder. Alloying T800 with Fe and Ni reduces the proportion of the primary Laves phase and enhances the Laves-Co-solid solution eutectic aggregate, improving the toughness of the alloy at the expense of hardness. This understanding is leveraged to fabricate a four-layer 2mm thick clad, comprising a T800 top layer with successive layers of pre-blended T800-SS316L powders in ratios of 9:1, 3:1, and 3:2. This graded structure achieves a spatial variation in composition, microstructure, and mechanical properties along the build depth. The FG-T800 clad retained superior surface hardness (903 HV5) and wear resistance ($1.4 \times 10^{-5} \text{ mm}^3 \text{N}^{-1} \text{m}^{-1}$), comparable to monolithic T800 deposit, while exhibiting significantly improved toughness in the interior regions. Serial sectioning along the build direction revealed a progressive reduction in fabrication cracks while approaching the clad-substrate interface. This improvement is attributed to the gradual incorporation of SS316L, which modifies the Laves phase morphology and distribution, reducing brittleness while preserving the tribological advantages of T800 at the surface. The study demonstrates the potential of functionally graded laser cladding to mitigate cracking in hard and brittle materials, enabling the fabrication of robust, high-performance coatings for demanding applications.

Influence of thermal treatments and UV irradiation on anisotropic TiO₂ architectures prepared by oblique angle deposition

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C4_10, Picasso Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

The development of advanced surface treatments is essential for enhancing material properties and introducing new functionalities. This is particularly critical in applications requiring efficient light capture in challenging environments, such as photodetection and solar energy. In these cases, coatings must not only optimize optical performance but also exhibit additional features, such as tunable wetting properties, to ensure long-term efficiency.

In this context, this study - conducted in collaboration between the Pprime Institute, the company Safran (France), and the University of Seville (Spain) - aims to enhance the performance of imaging devices in the visible and near-infrared spectrum by developing porous titanium dioxide (TiO₂) films with controlled columnar architectures. These films are fabricated using electron beam evaporation combined with the oblique angle deposition (OAD) technique, enabling precise control over porosity and morphology through deposition angle adjustments. This structural control allows fine-tuning of the refractive index, a key factor in the optical design of photonic systems, such as antireflection coatings and polarimetric filters, integrated into essential optical components.

By carefully adjusting deposition parameters, highly anisotropic nanostructures can be achieved, which are crucial for obtaining significant linear birefringence, a critical property for high-performance polarimetric filtering. To further optimize this characteristic, this research will investigate the effects of thermal treatments at different temperatures on the nanostructure, including morphology, crystalline structure, and overall optical properties of the TiO₂ films. Additionally, to explore the potential for antifogging and self-cleaning functionalities, the study will analyze how thermal treatments influence wetting behavior. Finally, the impact of ultraviolet (UV) irradiation on these properties will also be examined, assessing its potential as a tool for further controlling surface characteristics.

Electrodeposition of nickel-matrix nano-composite coatings for tribological applications from REACH compliant electrolytes

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C4_9, Picasso Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

For years, chromium trioxide CrO_3 has been used for hard chromium plating, guaranteeing wear resistance due to its outstanding tribological properties. However, the use of highly concentrated CrO_3 solutions and the formation of hexavalent chromium species is hazardous for human health. In fact, chromium trioxide is classified as carcinogenic (category 1A) and mutagenic (category 1B). Since 2013, it has been listed as a Substance of Very High Concern (SVHC) in Annex XIV of the REACH authorization list by European Chemicals Agency (ECHA) [1].

The most recent achievements in new tribo-coatings suggest that nickel-based layers constitute a viable alternative to hard chromium plating, both in the form of alloys (NiP, NiW) and nickel-matrix nano-composites. Regarding the latter, two types of particles can be embedded within the nickel matrix: hard ceramic particles (B_4C , Al_2O_3) and solid lubricant particles (graphene, MoS_2), which confer high hardness and low friction coefficient, respectively [2].

Nickel plating, nevertheless, introduces safety issues that must be addressed. Boric acid (H_3BO_3), routinely added to the plating solution as a pH buffer, must be replaced since it has been nominated as a SVHC candidate. According to the harmonised classification and labelling (ATP20) approved by the European Union, boric acid may damage fertility and the unborn child [1] and can be potentially substituted with different organic compounds, such as citric, succinic or malonic acid.

The need to operate in a more sustainable and human-centred way, following Safe and Sustainable by Design (SSbD) principles, brings to the development of REACH compliant formulations for the electrodeposition of functional coatings based on nickel. In this context, the MOZART project, founded by the European Union, has the ambitious purpose of assisting the fulfilment of REACH requirements to deposit nickel-matrix nanocomposite coatings for wear reduction or self-lubrication [3].

In the framework of the MOZART project, the present research aims at developing a nickel nano-composite coating deposited from an innovative boric acid-free REACH compliant solution. Hard nanoparticles are dispersed in such electrolyte in order to improve the wear resistance of the electrodeposited material. The morphological and tribological properties of the resulting composite coatings are characterized and compared to those of typical hard chromium layers.

[1] European Chemical Agency, <https://echa.europa.eu/en/home>

[2] R. Karmakar et al., *Met. Mater. Int.* 27, 2134–2145 (2021)

[3] European Union, MOZART Project, Grant Agreement 101058450, <https://www.mozart-project.eu/#>

Laser micro-textured aluminium metallic surfaces for self-cleaning and stickers anti-vandalism urban furniture applications.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The development of new materials with improved properties and new functionalities is a permanent challenge for the industry to obtain differentiating products or products with high added value. In the case of urban furniture, such as bike parking, bins, bus shelters..., the most common innovation trends focus on aesthetic design improvements. Important aspects such as self-cleaning and stickers anti-vandalism are generally not taken into account what rapidly interfere on the furniture appearance and force to do costly maintenance works. Most studies and actual solutions for urban furniture protections are mainly focused on the application of functionalized coatings with anti-adhesive and hydrophobic properties. However, these coatings life time is relatively short and oblige to periodic maintenance works with the consecutive associated costs.

Laser patterning is a promising method to achieve a direct surface modification on metals, due to the potentially high fabrication speeds, low waste and a single-step processing (1-3). Moreover, as the micro-textured surface is carried out in the metal substrate itself, the surface properties reached last for a long time.

This work reports the surface modification of Aluminium AA60-61, using several micro-textured patterns, to develop superhydrophobic and anti-adhesive properties by means of a solid-state pulsed Nd-YAG nanosecond laser with the 1064nm wavelength (Rofin).

Directly after fabrication, the samples show a hydrophilic behavior but gradually become superhydrophobic over time with the maximum contact angle of 158,6° being achieved after 60 days, exhibiting a self-cleaning property. This wettability modification has been explained by a surface oxidation of the aluminium.

Furthermore, the micro-textured pattern has been successfully developed to ensure an anti-adhesive property, facilitating an easy and perfect removal of the stickers.

Overall, this work demonstrates a cost effective, direct write, environmentally friendly and fast processing method to modify wettability of aluminium metals for anti-vandalism applications.

- (1) "Laser textured superhydrophobic surfaces and their applications for homogeneous spot deposition" Van Duong Ta et al., Applied Surface Science 365 (2016) 153–159.
- (2) "Fast wettability transition from hydrophilic to superhydrophobic laser-textured stainless steel surfaces under low-temperature annealing" Chi-Vinh Ngo et al. Applied Surface Science 409 (2017) 232–240
- (3) "Nanosecond laser textured superhydrophobic metallic surfaces and their chemical sensing applications" Duong V. Ta et al. Applied Surface Science 357 (2015) 248–254.

SiZY-Coat: Silicon-Zirconium-Yttrium coatings for graphitic materials

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Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Major disadvantage of carbon-matrix composites is their susceptibility to oxidation, which can occur at temperatures above 400°C in atmospheric air. Therefore, for applications in oxidising environments, it is standard practice to deposit oxidation-resistant SiC coating or to convert carbon matrix into a carbide material following the reactive melt infiltration (RMI) approach with pure Si. Despite its well-established position, described technology is not without its drawbacks. These include a decrease in the protective values of the SiC-coating over time or a significant increase in the density of the composite by converting carbon into SiC.

In this paper we present the ambition of the "SiZY-Coat" project, which is to explore the feasibility of synthesising a new type of multiphase protective coating that conditions oxidation resistance at high temperatures while maintaining an attractive low density of the starting material. The coating is obtained by RMI of porous graphitic material surfaces with eutectic Si-10Zr alloy in the presence of Y₂O₃ nanopowders. This approach provides an opportunity to study numerous high temperature phenomena occurring during the process, such as the influence of surface roughness on wetting kinetics or the adopted process parameters on the oxidation resistance of the coatings. The preliminary results presented facilitate the wider application of RMI methods for the production of advanced oxidation resistant coatings for carbon based materials.

Comparative Assessment of Plasma and Gas Nitriding on Air-Hardening Ductile Steels

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C4_11, Picasso Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Steel components subjected to dynamic loads are susceptible to wear and oxidation. The relative movement between contacting surfaces under such loading conditions can trigger various wear mechanisms, including abrasion and adhesion. Additionally, dynamic loads can induce surface damage and deformation, exposing new material to the environment and accelerating oxidation. Nitriding is one of the thermomechanical treatments to overcome these disadvantages. The notable improvement in the properties of steel parts after nitriding is primarily due to increased surface hardness, internal stress, and chemical changes within the treated region.

While nitriding can be performed using different techniques, plasma nitriding provides several distinct benefits. Gas nitriding, which utilizes ammonia as the nitrogen source, is a well-established method for enhancing surface properties. However, plasma nitriding, where nitrogen gas is ionized by applying a high voltage between the furnace wall and the steel component acting as the cathode, offers several advantages. Specifically, plasma nitriding facilitates a faster process due to the accelerated formation of the nitrogen concentration gradient compared to gas nitriding. Additionally, plasma nitriding eliminates the production of harmful by-product gases, making it a more environmentally friendly option. These differences highlight the potential for plasma nitriding to deliver superior performance in terms of process speed, environmental impact, and surface property enhancement for AHD steels.

A recent innovation introduces a new class of martensitic steels that achieve their final properties through air cooling directly from the forging heat. These air-hardening ductile (AHD) forging steels, alloyed with approximately 4 wt.% manganese, develop a uniform martensitic microstructure without the need for quenching and tempering, significantly lowering CO₂ emissions. With the first commercial melts of these steels now available, interest in their performance across various applications is increasing.

This study compares the plasma and gas nitriding performance of newly developed sustainable AHD steels. Within this scope, a comprehensive characterization study, including mechanical and chemical analyses, was conducted following plasma and gas nitriding processes carried out under similar process parameters. Electron Probe Microanalysis (EPMA) and X-ray Diffraction (XRD) were utilized for elemental analysis and to identify phase formations within the nitrided layers. The results revealed that plasma and gas nitriding yielded comparable hardness values at around 1000HV. Given that the mechanical and chemical properties after nitriding were similar, plasma nitriding emerges as a more advantageous option due to its environmental benefits and time efficiency.

Operational properties of Mn_{1.9}CuFe_{0.1}O₄ protective coatings deposited on ferritic stainless steels of different Cr content for SOC application

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C4_7, Picasso Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

The technology of solid oxide electrochemical cells (SOC) is attracting a huge scientific interest because it seen as the most efficient green technology for generating hydrogen or electricity, with a high commercialization potential. Therefore it requires further material development to prolong the failure-proof operation time and to reduce its cost. One of the key components of a SOC stack is the interconnect, that has a role to conduct electrical current between adjacent cells and serve as a separator for the air and fuel zones. It is exposed to high temperatures (~700°C) and corrosive factors (oxygen, hydrogen, steam), which dictate the choice of material: ferritic stainless steel (FSS). This generates challenges such as the growth of oxide scale and the evaporation of chromium compounds that poison the air electrode. To mitigate it, protective coatings made of spinel-structured oxides are used. The state-of-art coating materials rely on critical raw materials, specifically Co. The presented approach is using Cu-based coatings, which seems promising concerning price, conductivity, and sustainability. Moreover, the common usage of specially designed steel Crofer 22APU for small scale studies is hampering the up-scaling. Since only a single producer offers this material, its price is high, and its availability is limited.

The aim of the study was to investigate Co-free coatings deposited on four generic types of FSS differed in Cr content (15-18 wt%) for their potential application as interconnect. Steel samples were subjected to different pre-oxidation procedures and coated with a 15-30 µm layer of Mn_{1.9}CuFe_{0.1}O₄ powder by colloidal processing. The sintering procedure was adjusted to technical aspects of possible implementation for full scale interconnects and allowed to obtain layers of 20% porosity. Obtained samples were then subjected to ASR measurements in temperature range 620-750°C, with 200h hold at 700°C. SEM/EDS was used to analyse the surface of oxide scales, the surface and cross-section of the protective coatings before and after the sintering, as well as post-test. Special focus was given to the intermediate layers formed at the interface between the steel and the coating. The results indicate that K41 steel is the most perspective for applied studies and that Mn_{1.9}CuFe_{0.1}O₄ powder can offer desired properties of the coating.

Acknowledgments:

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Sintering Response of Columnar Thermal Barrier Coatings Deposited by Solution Precursor Plasma Spray (SPPS) Technique

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C4_7, Picasso Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Yttria-Stabilized Zirconia (YSZ) Thermal Barrier Coatings (TBCs) are widely used to protect gas turbine components from high-temperature oxidation and creep degradation. However, prolonged thermal exposure can lead to sintering, phase transformations, and cracking in the TBC, degrading its mechanical integrity by altering the elastic modulus and fracture toughness. Sintering is particularly critical for columnar coatings, which are engineered for high in-plane strain tolerance to mitigate the risk of delamination under thermal cycling. Recent studies on Axial Feed Solution Precursor Plasma Spray (SPPS) have shown promise for producing such columnar YSZ coatings while addressing the sedimentation issues of Suspension Plasma Spray (SPS) and the high costs of Electron Beam Physical Vapor Deposition (EB-PVD). In EB-PVD YSZ coatings, high-temperatures sinter the columns together, drastically reducing the strain tolerance. Since columnar SPPS-YSZ coatings have only been reported recently, their sintering response has not been widely investigated yet.

In this talk, we will provide a systematic assessment of the microstructure and mechanical property evolution of columnar SPPS-YSZ TBCs upon thermal exposure. Hastelloy disk specimens coated with SPPS-YSZ are subjected to 1150°C in air for 50-200 hours. Microscopy is used to quantify key microstructural changes that influence mechanical properties, including column density, vertical crack density, porosity, and thermally grown oxide (TGO) formation at the TBC/Hastelloy interface. Additionally, Rietveld refinement of X-ray diffraction (XRD) data is performed to analyze TBC degradation through phase transformations from stabilized tetragonal zirconia to the monoclinic or cubic phases. The second part of the talk will focus on the mechanical property evolution with increasing thermal exposure duration. The elastic modulus and hardness is measured at two length scales, using a nanoindenter and an instrumented-microindenter, while the toughness is assessed using the Palmqvist method. The observed behaviors are compared with those in SPS and EB-PVD columnar coatings reported in the literature. Our findings provide key insights into the microstructure-property correlations in SPPS-YSZ TBCs and their post-sintering delamination resistance.

Smart Coatings Through Sol Gel Microencapsulated Additives

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The microencapsulation of active substances for inclusion in smart surface coatings is currently proposed as a novel technique to protect their integrity and functionality, so that their activity does not take place until the capsule shell is opened upon receipt of a stimulus. Metallic corrosion continues to be a current problem in the industry as it is a degradation process that occurs naturally and inevitably. Among the methods available to prevent this phenomenon, the application of coatings is the most convenient alternative. However, their use entails other problems such as cracking or degradation, so they must be repaired, since any crack or defect would cause corrosive substances to reach the metal surface. Nowadays, it is necessary to find new solutions to solve corrosion problems located in inaccessible sites, such as off-shore facilities, to reduce maintenance costs. For this reason, the use of self-healing coatings, based on the use of additives, is considered in recent times as the most innovative option. Direct doping with these additives has been widely studied but has some disadvantages, such as easy leaching from the matrix or reaction with some of its components and consequent loss of efficiency. Isocyanates are the most promising self-healing reagents as they do not require a catalyst, however, their encapsulation is hampered by their high reactivity. In this work, isolation of these compounds was carried out efficiently by microencapsulation. Most examples in the literature are based on the introduction of these capsules in epoxy resins but few and very recent are the examples where they are introduced in sol gel matrix for self-healing coating of a galvanized steel. Here we describe the encapsulation technique of interesting additives by sol gel technology, synthesizing “microcontainers” of these compounds to achieve a more prolonged effect and isolate the inhibitor from the coating matrix. In addition, these microcapsules are dispersed in a new sol gel coating formulation specially designed for galvanized steel to increase its corrosion resistance and provide it with self-repairing capabilities.

On the other hand, microencapsulation of liquid lubricants contained in a rigid silica shell is also studied in this work, together with their integration in a coating matrix. In this manner, another type of smart coating was designed, in order to act as a self-lubricating material when these capsules are deposited by dispersion in certain coatings. Its application on the design of energy-efficient machinery offers a solution to reduce energy consumption.

DEVELOPMENT OF WEAR-RESISTANT SURFACES BY DEPOSITION OF SOL-GEL COATINGS DOPED WITH Co_Ni NANOPARTICLES

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Surface wear degradation is one of the main causes, together with fatigue and corrosion, that frequently obliged the replacement of equipment parts, increasing maintenance labors and the associated economic cost.

Surface wear degradation is usually partly solved by the application of anti-wear coatings with low coefficient of friction directly on the component parts and techniques based on vacuum processes (CVD and PVD) allow the growth of conformal and dense layers. Indeed, different kinds of coatings based on nitrides (TiN, CrN), carbides (TiC, CrC, W₂C, WC/C), oxides (mainly Al₂O₃), molybdenum disulfide (MoS₂) and diamond-like carbon (DLC) have been widely investigated showing great properties of resistance and adhesion. In the last two decades ceramic coatings (e.g. SiO₂, ZrO₂ or Al₂O₃), with interesting mechanical and corrosion resistant properties, have also been developed using sol-gel technology. Indeed, the sol-gel is a promising alternative to the deposition by vacuum techniques since the deposition parameters, including composition, are easily modified what allow to develop low-cost coatings (1).

The nanotechnology advances have enabled the development of innovative sol-gel formulations with improved tribological properties. Results have been reported in which a Al₂O₃_sol-gel matrix doped with MoS₂ nanoparticles (15-25 vol%) has led to the development of a coating with a very low friction coefficient ($\mu = 0.02$) and minimal wear rate. It has also been shown that small amounts of SiC nanoparticles (5 vol%) improve the anti-wear properties of alumina. Just as anti-wear sol-gel layers developed with Al₂O₃, Ni doped TiO₂ films have been successfully obtained (2).

This work reports the experimental results obtained after the surface modification of galvanized steel DX51D+Z with different coatings of SiO₂_sol-gel/Ni₂O₃_nanoparticles or SiO₂_sol-gel/Co₂O₃_nanoparticles. In all tests the unmodified steel tribological response has been improved, achieving a reduction of 35% in the friction coefficient and a wear rate decrease of 20%. Finally, the current research will be expanded, with the aim of going on with the investigation of the anti-wear effect of other doping agents.

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(2) Pereira, N.F.S., Reis, B.C.M., Dos Santos, A.J. et al. Tribological assessment of the SiO₂ coating deposited by sol-gel process toward cutting tool coating. *Int J Adv Manuf Technol* 2023, 126, 487–503.

Assessing the anticorrosion efficiency of functionalized hybrid sol-gel coatings for environmentally-friendly passivation of galvanized steel

Dr. Lucía Florentino¹, Mrs Verónica Maestre Peña¹, Mrs. Marta Prado García¹, Dr. Olga Conejero Iglesias¹

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The use of hexavalent chromium-based conversion coatings for corrosion protection of galvanized steel and other metals has been widespread due to their exceptional corrosion resistance and self-healing properties. However, the toxic and carcinogenic nature of hexavalent chromium has led to its restriction in many countries. In response to these concerns, silane technology has emerged as a promising alternative. Among the silane-based solutions, sol-gel coatings have shown particular promise in enhancing corrosion resistance when applied to metallic surfaces.

The sol-gel process involves creating an oxide network through hydrolysis and condensation reactions of various precursors in a liquid medium. These coatings can be synthesized using either inorganic or organic precursors, each offering unique characteristics. To harness the benefits of both precursor types, researchers have developed hybrid coatings that incorporate organic components into the inorganic matrix. This innovative approach yields coatings with distinctive properties in terms of morphology, size, and multifunctionality, resulting from the synergistic interaction between organic and inorganic components. These hybrid coatings effectively combine the durability and chemical resistance of inorganic materials with the flexibility and functionality of organic compounds. As a result, they demonstrate enhanced performance in various applications, including corrosion protection, wear resistance, and surface modification.

This research focused on the synthesis of hybrid sol-gel coatings under varied experimental conditions. The process involved the hydrolysis of 3-(Glycidoxypropyl) methyl diethoxy silane (GPTMS) and tetraethyl orthosilicate (TEOS). To improve coating thickness and mitigate stresses during curing, polyvinylpyrrolidone (PVP) and polyethylene glycol (PEG-6000) were incorporated into the formulation. Furthermore, various corrosion inhibitors were added to the sol-gel matrix in different concentrations in order to enhance the anti-corrosion properties and extend the coating's durability. These inhibitors included ZnO and ZrO nanoparticles, as well as lanthanum and zirconyl nitrate. The application of the sol-gel film to galvanized steel plates was accomplished using the dip coating technique. To assess the corrosion resistance of the coated samples, salt spray tests were conducted.

The corrosion resistance of galvanized steel was substantially improved, with the onset of white rust delayed by over 264 hours. This marked enhancement in protective performance demonstrates the efficacy of the developed coating system in significantly extending the durability of the galvanized steel substrate under corrosive conditions.

Hybrid Highly-Porous Photonic Structures for Photocatalysis Fabricated by Atomic Layer Deposition

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C4_10, Picasso Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Harnessing the wide spectrum of solar energy for photocatalysis holds a promise for sustainable pollutant abatement with titanium dioxide (TiO₂) being a benchmark material due to its stability and photocatalytic efficiency when exposed to ultraviolet light (UV). Nevertheless, as TiO₂ is mostly activated by UV-radiation, the rest of the solar spectrum radiation remains unutilized, i.e. is “wasted”. Moreover, pure TiO₂ presents a high carrier charge recombination rate, hindering the catalyst efficiency. Earlier studies have focused on material modifications or semiconductor heterojunctions to widen the radiation range towards utilizing of a wide range spectrum in TiO₂’s photocatalysis. Light absorption and interaction can however also be tailored via (nano)structuring of the material systems, such as in the case of inverse opal photonic crystals (i-PhC). These highly ordered 3D structures are able to tailor light-matter interactions due to their structural photonic stopband (PSB), which when in combination with photoactive materials can enhance the generation of free charge carriers due to the activation of the slow photon amplification effect. To further optimize photocatalytic efficiency, semiconductor heterojunctions can be engineered within the i-PhC structure. In this talk, I will present the challenges and developments regarding the fabrication of hybrid TiO₂-Fe₂O₃ i-PhCs by multilayer atomic layer deposition (ALD). Our results reveal that the complete functionalization of TiO₂ i-PhCs with Fe₂O₃ increase the photocatalytic activity through the slow photon amplification effect and semiconductor heterojunction formation, where a maximum photocatalytic activity of 1.38 ± 0.09 per hour is observed for the i-PhC with a 16 nm-2 nm TiO₂-Fe₂O₃ bilayer. These results greatly outperform the pure TiO₂ i-PhC, highlighting the potential of hybrid i-PhCs macroporous structures for efficient water pollutant removal, as well as the advantages of precise nanostructuring and heterojunction engineering by ALD.

Tribological testing and crystallographic analysis of high hardness, ultra-low friction Mo-S-C thin film coatings with self-assembling tribolayers

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Transition metal dichalcogenides (TMD) are a group of materials that are well-known for their low friction properties. The weak van der Waals forces between layers of covalently bonded atoms gives rise to easy shear and can therefore provide very low friction. These materials, however, have low hardness, meaning that in their pure form they display high wear rates. To improve their material properties, TMD coatings can be deposited with a doping element, which leads to the production of amorphous coatings with significantly increased hardness and density.

Although the as-deposited amorphous coatings do not initially feature the crystals responsible for the ultra-low friction properties of pure TMDs, the application of frictional forces has been found to lead to the creation of crystalline regions, or a 'tribolayer'. It has been shown via sliding wear tests that these coatings display an initial coefficient of friction (COF) of around 0.3, which rapidly reduces and can reach steady state values of as low as 0.025 at room temperature.

Molecular dynamic simulations were used to model the process of tribolayer formation to find the optimal carbon content that should provide the maximum hardness whilst still allowing for the creation of the tribolayer. This composition was then used to deposit the Mo-S-C coatings studied in this project. The coatings were deposited via magnetron sputtering, a physical vapour deposition (PVD) process, via high power impulse magnetron sputtering (HIPMS).

The coatings were tribologically tested using a linear reciprocating tribometer. A range of sliding conditions were used: applied load ranging from 5-20N, sliding frequency ranging from 1-20Hz and sample temperature ranging from 20-150°C. The tribological results showed COF ranging from 0.035 to 0.05.

The wear tracks were analysed using scanning electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS), and Raman spectroscopy to search for crystalline regions within the wear tracks as evidence of tribolayer formation. Most of the wear track remained amorphous, however an area of crystalline MoS₂ was discovered. High resolution transmission electron microscopy was also employed to investigate the layer adhered onto the ball used in the wear tests, in which MoS₂ platelets were found although no compact tribolayer was present.

MECHANICAL AND WEAR PERFORMANCE OF HYBRID POWDER COATINGS: THE ROLE OF CURING CONDITIONS

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C4_9, Picasso Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Keywords: Powder coatings, curing conditions, epoxy-polyester, mechanical properties, wear resistance.

Powder organic coatings have gained significant attention as a sustainable alternative to conventional liquid coatings due to their solvent-free formulation, which eliminates volatile organic compound (VOC) emissions [1]. In addition to their environmental benefits, these coatings exhibit high efficiency, durability, and excellent corrosion resistance. Most of them are composed of thermosetting resins (epoxy, polyester, hybrid, polyurethane, or acrylic), curing agents, pigments and performance-enhancing additives, which collectively determine their mechanical and chemical properties [2]. The curing process is one of the most important factors in achieving a high-performance painted system, as it directly influences the adhesion, hardness, and flexibility of powder coatings, wear resistance and environmental degradation [2]. Improper curing, whether under-curing or over-curing, can lead to inadequate mechanical integrity and reduced protective capabilities. To date, some studies have investigated the curing behavior of nanoparticle-functionalized epoxy or polyester [3] powder coatings; however, no studies on epoxy-polyester hybrid coatings have been reported in the literature. Therefore, this study aims to systematically evaluate the influence of temperature and curing time on the properties of a hybrid epoxy-polyester organic powder coating applied to carbon steel substrates.

The curing process was carried out at 4 different temperature-time combinations: 160 °C for 18 min, 170 °C for 10 min, 180 °C for 10 min, and 180 °C for 15 min. The effect of these curing conditions was analyzed focusing on polymer crosslinking (measuring the glass transition temperature, T_g), aesthetic properties (gloss), roughness, hardness and wear resistance.

The main results indicate that lower curing temperatures with longer curing times lead to a decrease in T_g and hardness, as well as reduced wear resistance, suggesting incomplete crosslinking. On the other hand, high-temperature curing results in a higher T_g, hardness and wear resistance. Regarding the aesthetic properties, high temperature enhances the gloss. Based on the results, the optimal curing range for the studied coating was determined to be 180 °C for 10–15 min, achieving a balance between mechanical performance and wear resistance, due to optimized crosslinking. These results contribute to the optimization of curing processes in powder coatings to enhance their durability and protective capabilities in different applications.

References:

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- [2] X. Lv, et. al. Prog. Org. Coat., 200 (2025) PAG.
- [3] M. Fernández-Álvarez, et. al. J. Mater. Res. Tech. 9 (2020) 455–464.

The morphology of the INCONEL 686 alloy and WC powder mixtures after mechanical synthesis dedicated for the Cold Gas Spraying process

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In this work, the mixture of Inconel and WC powders was subjected to the mechanical synthesis process to produce composite powders used as the starting material for spraying coatings using the CGS method. This work, which presents results concerning the morphology of the Inconel 686 superalloy, focuses on a detailed analysis of the powder particles formed during mechanical alloying. The influence of the grinding time and the weight ratio of powders on their morphology and crystallite size was examined. Three powder mixtures were prepared with different Inconel 686 - WC weight ratio (10, 30 and 50 wt.% WC). Inconel 686 was mainly in the form of spherical particles with a diameter of approximately 50 μm . In raw state, analyzed tungsten carbide powder had irregular shapes, the particle size was approximately 1-3 μm , with tended to agglomerate. During the process of mechanical alloying (MA), the powder particles were subjected to a strong collision with the balls in the ball mill, which causes their strong deformation. As a result, the fine and hard WC particles were embedded in the surface layer of the Inconel particles, forming a composite surface coating of the Inconel particles. The powders were investigated before and after the process of mechanical synthesis using the Scanning Electron Microscope and the X-ray Diffraction methods. The mixing time and proportion of powders have a significant effect on their morphology and the degree of grinding. The crystallite size of the pure Inconel686 particles, varied from 30 nm (in the initial state) through 18 nm (after 2 h of milling) to 15 nm after 10 h of milling. At 10% WC content, the crystal size changed from 25 nm to 19 nm after 2 and 10 hours of milling, respectively. Moreover, a significant fragmentation and deformation of Inconel particles, which take the form of a plate with an irregular shape and sharp edges were observed after mixing time longer than 6 h. In the mixture of powders with a high content of WC (50 wt.%) no fragmentation and no significant change in the shape of the Inconel particles were observed at the same time of grinding in a ball mill. Inconel 686 particles with embedded WC particles are very attractive for the CGS spraying process applications, especially as uniform and stable matrix structure in sprayed coatings that increase wear resistance.

Multifunctional Coatings for Harsh Environments

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¹Department of Engineering Physics, Polytechnique Montréal, Montréal, Canada

C4_3, Picasso Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Materials exposed to extremely demanding environments in applications such as aerospace, automotive, mining, petroleum and consumer products, continue to face increased technological, environmental and economic challenges, especially since the performance of modern equipment, systems and components is pushed to and beyond their limits. This frequently leads to material deterioration accelerated by excessive wear, erosion, tribo-corrosion, and other mechanisms related to surface damage, resulting in increased operation and maintenance costs, decreased efficiency, premature failure, and compromised safety in the case of critical applications.

A good understanding of materials deterioration processes allows one to develop appropriate strategies to protect technologically relevant substrates taking into account the complete life cycle of the component. Advanced nanostructured coatings call for an “ideal” combination of mechanical, elasto-plastic, tribological, corrosion, thermal and other characteristics. Such requirements can only be satisfied by using specifically tailored coating architectures while considering nanocomposite, nanolaminate, multilayer and graded layer systems. Specifically, the combination of multiple coating types obtained by different complementary processes (called “hybrid” coatings) provides much promise for combined functional characteristics including multifunction, adaptive or smart performance.

Throughout the talk, I will illustrate the relationships that exist between the microstructure, the mechanical properties and the tribological performance of protective coatings by presenting different examples of coatings used in three areas: aerospace, manufacturing and energy.

From passive to active structurally controlled optical coatings for energy and eyewear applications

Dr. Bill Baloukas, Mr. Martin Crouan, Dr. Oleg Zabeida, Prof. Jolanta Klemberg-Sapieha, Prof. Ludvik Martinu

C4_8, Picasso Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Control of energetic interactions at the surface of the growing thin films allows one to selectively adjust their micro- and nanostructure. This is particularly important when synthesizing optical films by vapor-based techniques such as reactive sputtering (including HiPIMS), evaporation (including Glancing Angle Deposition), Plasma-Enhanced Chemical Vapor Deposition, Atomic Layer Deposition and Gas Agglomeration Cluster formation. As a result, this has become increasingly attractive for judicious fabrication of nanostructured optical filters with controlled film porosity, crystallinity, anisotropy, plasmonic effects and other features of both passive as well as active (dynamic – e.g., electrochromic or thermochromic) coating materials with new functionalities.

This presentation will illustrate the progress and new opportunities in structurally controlled optical coating systems such as high-performance low-emissivity and smart windows for energy saving in the building sector, energy control in satellites, ophthalmic lenses and enhanced vision, and other optical coating devices.

Pulsed laser interference heating of FeSiB ribbons - Structure and properties characterization

Dr. Agnieszka Radziszewska¹

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Pulsed laser interference heating (PLIH) is a technique that allows regular distribution of micro- and nanostructures on the surface of various materials. It is characterized by high efficiency, precision, and resolution, which leads to improvement of material properties, such as magnetic, biomedical, mechanical, optical, or tribological properties. PLIH allows for precise impact of energy on a precisely defined area of the material surface, which makes this technique very promising for use in fields such as electronics, energy, biomedicine, or nanotechnology. Under the influence of pulsed laser heating, a fine-crystalline structure of the material can be obtained because of the occurrence of rapid cooling and a high crystallization rate. This works in favor of modifying the structure of thin surface layers of the material, minimizing thermal deformations, and enabling precise control of the thickness of the processed layers. PLIH is based on the phenomenon of interference of two or more coherent laser beams, which leads to the formation of periodically distributed micro-areas on the surface of materials. Many industries are looking for new materials with improved properties, including magnetic materials, such as FeSiB alloys with the addition of, e.g. Cu and Nb. The aim of the research is to improve the magnetic properties of these materials while maintaining their mechanical properties by heating thin surface layers of FeSiB alloys. The use of the PLIH technique, including laser surface annealing, has the following functions: to accelerate the process of creating a nanocrystalline structure, increase crack resistance, reduce production costs, and significantly improve process efficiency. This work presents the structure and changes in the properties of the material subjected to laser interference surface heating.

Study of ceramic materials by magnetron sputtering for barrier properties in paper-based food packaging

Dr. Mariana Marques¹, Americo Cunha¹, Joana Pimenta¹, Miguel Coelho²

¹CeNTI, Famalicao, Portugal, ²RAIZ, Aveiro, Portugal

C4_5, Picasso Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

The growing worldwide challenge with plastic waste management requires an urgent investigation into sustainable packaging alternatives. The use of paper with bio-barrier properties in food barrier packaging solutions, namely flexible packaging, cups, lids, straws, and capsules, emerges as a solution to tackle this problem. Furthermore, this transformation is essential to accomplishing the objectives of the Green Deal, guaranteeing an efficient transition to a climate-neutral and eco-friendly economy. By acknowledging this, the present work proposes and explores the integration of ceramic thin films through magnetron sputtering (PVD technology) onto paper substrates to improve their barrier properties against oxygen, water vapour, and oil. PVD coatings can be deposited as a first layer on the paper (monolayer), with additional coatings applied by other technologies like spray-coating, screen-printing, knife-coating, layer-by-layer, extrusion coating, and other solutions (multilayer). Hybrid multilayers, combining multiple coating technologies, represent a significant innovation and provide the capability to integrate diverse functionalities to enhance the overall paper-product performance. To assess the effectiveness of these hybrid multilayers, tests for grease resistance, oxygen transmission rate (OTR), and water vapor transmission rate (WVTR) were performed. Additionally, a study to evaluate how the thickness of the ceramic thin film affects the barrier qualities is undergoing. In fact, the film thickness achieved with PVD deposition is rather low and may not be enough to completely cover the porosity of the paper, which impacts the barrier effect. Thus, this comprehensive study is fundamental to understanding the effect of the PVD films in both the monolayer approach and within the overall multilayer system.

The current study was developed within the scope of the Agenda “From Fossil to Forest-Sustainable Packaging and Products to Replace Fossil Plastic” [C644920945-00000036| Project nr. 8], financed by the RRP-Recovery and Resilience Plan under the Next Generation EU from the European Union.

Optimization of solution composition and parameters for electrophoretic deposition of SiO₂ coatings on NiTi alloy

Mrs. Barbara Rynkus¹, ph.D. Anna Taratuta¹, ph.D. Karolina Goldsztajn¹, Mrs. Julia Kolasa¹, ph.D. Ada Orłowska¹, ph.D. Magdalena Antonowicz¹, Mrs. Karolina Szawiraacz², prof. Roman Major², ph.D. Przemysław Kurtyka², prof. Marcin Basiaga¹

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Nickel-titanium (NiTi) alloy is widely used in medicine, especially in cardiology, due to its unique properties such as shape memory effect and superelasticity. However, its biocompatibility and corrosion resistance remain challenges, especially in biological environments. In order to improve these properties, surface modification was carried out by coating silicon dioxide (SiO₂) by EPD method (electrophoretic deposition) using polyethylenimine (PEI) as an electrolyte component.

In this study we analysed the effects of various concentrations of PEI in the electrolyte and deposition parameters, such as current voltage and process time, on the morphology and uniformity of the coatings. The EPD process was carried out in a suspension of SiO₂ nanoparticles in ethanol with PEI at various concentrations. The coatings were deposited at varying voltages and deposition times to determine the optimum conditions for forming a coating with a homogeneous structure and strong adhesion to the substrate.

The obtained coatings were structurally and chemically characterised using scanning electron microscopy (SEM) and EDS spectroscopy. Electrochemical tests were also performed to assess corrosion resistance in simulated body fluids. In addition, a biological evaluation was carried out to determine the biocompatibility of the produced coatings. The results of the tests showed that the use of PEI at the appropriate concentration improves the homogeneity of the coating and increases its adhesion to the NiTi surface. The results indicate that electrophoretic deposition of SiO₂ coatings using PEI as an electrolyte additive is an effective method to improve the biomaterial properties of NiTi alloy.

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Stress evolution during thin film growth: in situ studies of interface reactivity and structure formation at the nanoscale

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C4_5, Picasso Room (Level -2), septembre 16, 2025, 10:30 - 13:10

The issue of stress in thin films and functional coatings is a persistent problem in materials science and technology that has congregated many efforts, both from experimental and fundamental points of view, to get a better understanding on how to deal with, how to tailor, and how to manage stress in many areas of applications.

In this talk, I will present the recent advances in our understanding of stress evolution during polycrystalline metal film growth, based on in situ and real-time diagnostics. These include simultaneous measurements of stress, structure and morphology of the growing layer using a combination of wafer curvature and X-ray scattering (XRD and XRR/GISAXS). In particular I will show the importance of interface reactivity on the intrinsic stress of nanoscale systems used in micro- and opto-electronics applications.

Two different systems will be showcased: the growth of ultrathin Ag layers on weakly interacting substrate (SiO_2) and the growth of silicide (germanide) compounds that spontaneously form at the interface during growth of Mo, W or Pd on amorphous Si (or Ge). For the former case, the impact of reactive plasma ($\text{Ar}+\text{N}_2$) on the nucleation and coalescence stages of Ag islands will be discussed. The presence of N species adsorbed on the substrate surface not only improves the wetting of Ag but also leads to incomplete coalescence, and as a result to the formation of a continuous Ag layer at lower nominal thickness. By selective deployment of N_2 we could tailor the Ag growth morphology without compromising the optical and electrical properties, which is key for the design of ultrathin Ag layer as transparent conductive electrodes. For silicide layers, our findings uncover a thickness-dependent crystallization process during growth associated with the development of tensile stress. In the case of W-Si alloys, a wide range of stress state (compressive or tensile) is observed depending on the phase and texture formation.

Overall, our real-time and in situ methodology makes it possible to disentangle different origins of stress build-up (interface formation, phase formation, grain growth, and texture) on the nanoscale.

Research on medical Ni-Ti alloy with ZrC coatings deposited by PVD technique

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The studies were conducted on Ni-Ti medical shape memory alloy, with characteristic temperature of $30 \pm 5^\circ\text{C}$. To deposition of ZrC coatings on Ni-Ti and Si alloy substrates, one of the PVD techniques was used, the reactive magnetron sputtering method in an atmosphere of a mixture of argon and acetylene gases. The coatings were deposited under different conditions, the acetylene flow rate was changed in the range of 1.5-6.3 sccm, the substrate polarization bias voltage was changed in the range of -10 to -100V and the temperature in the range of 200 - 400°C.

Phase and chemical composition tests (XRD, XPS, EDS) were carried out, the structure (SEM) of the coatings was examined. The hardness and the E module were tested using the load-unloading method, internal stresses and adhesion (scratch test, Rockwell test) were determined. Tribological tests (ball-on-disk) of ZrC coatings and substrates were carried out in combination with an alumina counterspecimen. XRD and XPS analyses confirmed that the coatings contained ZrC phase crystallites. The highest hardness of ZrC coatings (26.1 GPa) was significantly higher than the hardness of Ni-Ti alloy (2.3 GPa). Scratch tests and Rockwell tests indicated good adhesion of ZrC coatings to Ni-Ti alloy substrates. The dry friction coefficient of ZrC coatings against alumina counterspecimen was many times lower (0.1-0.3) compared to Ni-Ti substrates (0.96). Coatings deposited at acetylene flow above 3.5 sccm showed wear indicator values one order lower than Ni-Ti substrates. EDS chemical composition analyses of the surfaces of friction pairs were carried out after ball-on-disk tribological tests. The structure and properties of ZrC coatings produced by the reactive magnetron sputtering method indicated the possibility of using them to coat, for example, endodontic tools made of Ni-Ti alloy. Initial comparative operational tests of files without coating and coated with ZrC coating were conducted.

The studies showed that the use of ZrC coatings increases their hardness and resistance to wear of Ni-Ti alloy substrates, while maintaining good adhesion. Therefore, ZrC coatings produced by the reactive magnetron sputtering method can be used in various fields of technology and medicine to increase the durability of objects/tools made of Ni-Ti alloy.

Ultrafast high-temperature sintering of B₄C with Si aids

Dr. F. J. Martínez-Vázquez¹, Dr. Pedro Rivero², Dr. Víctor Zamora³, Dr. Ángel Luis Ortiz³

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C5_1, Z4 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

Boron carbide ceramics are very attractive because of their combination of super-hardness and ultra-lightness. They are commonly sintered by techniques involving pressure and high temperatures, often by Spark Plasma Sintering. In this study, the ultrafast high-temperature of B₄C with SiC aids was investigated. The effect of the proportion of Si aids, green bodie compaction, and sintering temperatures and times were studied, demonstrating that relative densities close to 90% can be achived and thefore that UHS is preferable to pressureless-SPS. Implications of this work are discussed.

Straightforward design of 3D structured SiC objects via a granule-derived FDM technology of polycarbosilane-based formulations

Dr. Samuel Bernard¹, Dr Maxime Cheype, Mr Dorian Sazarin, Prof. Pateloup Vincent

¹Cnrs-ircer, Limoges, France

C5_2, Z4 Room (Level -3), septembre 15, 2025, 10:50 - 13:10

There is a trend toward more performant or competitive materials with the objective to improve the efficiency of actual systems and to repel technological boundaries. Silicon Carbide (SiC) attracts strong interests due to its properties targeted for future materials and technologies especially in aerospace. Inherent difficulties to the traditional techniques for manufacturing such dense materials with a complex geometry can be overcome by the development of new manufacturing approaches and the deployment of synthetic paths where chemistry of materials and ceramic science are combined rationally. The Polymer-Derived Ceramics (PDC) route offers great opportunities in material sciences when combined with 3D printing. Here, the aim of this talk is to introduce a straightforward design approach consisting in tailoring the extrusion ability of polycarbosilanes to fit with a granule-based fused deposition modeling process and form after a two-step heat-treatment process at a relatively low temperature 3D stoichiometric SiC and derived composites parts.

WC based cermets with low additions of Ni

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C5_2, Z4 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

There is an increasing interest in substitute Co in the traditional WC-Co cermets compositions owing to its carcinogenicity and for being considering as a strategic material due to its limited supply. The most studied alternative metals were Fe and Ni or combinations of Co-Fe-Ni. Iron is abundant, non-toxic and low-cost raw material, but shows low wettability with the WC grains and a poor corrosion resistance. However, nickel has a better wettability with the WC grains, that is crucial to obtain a good joining and full densification during sintering, as well as a better corrosion resistance in use.

The metal to ceramic ratio in the composition is a compromise between the thermomechanical properties of the carbide and the sintering conditions. Low metal contents on the composite will provide low corrosion rate and a better response at high temperature. Colloidal processing of the starting powders allows a homogeneous distribution of low amounts of metallic particles with the WC powders, also if they have a variable quantity and very different sizes. The high distribution of the metallic particles promotes a uniform liquid state sintering, even with the low amount. As a result, the metal acts as a sinter-aid to achieve full densification, without being detrimental for the carbide properties.

Little research has been done about WC compositions with low Ni content sintered by conventional methods due to the difficulties in achieve full densification. Therefore, in this study, low amount of Ni was used as a sinter-aid in the WC cermet, thanks to the previous colloidal processing of the powders, achieving a high densification. First, samples were conventionally shaped and different conventional sintering conditions were studied. Density, microstructure and mechanical properties were compared to decide the best sintering condition. Furthermore, in view of use these compositions in additive manufacturing, microstructure and post-processes were optimized to improve densification after the de-binding and sintering stages.

Development of ceramic photocurable slurries with metal precursors for the fabrication of functional materials by Digital Light Processing

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C5_2, Z4 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Since the early stages of additive manufacturing (AM), one of the key objectives was the fabrication of multimaterials. Using Digital Light Processing (DLP), when the material is the same but differs in characteristics (e.g., particle size), changing the slurry exhibit minimal difficulties. However, when printing with two different materials, a cleaning step should be incorporated to avoid cross-contaminations. Moreover, if a layered material is desired, the problems/limitations are much less than if a multimaterial is desired in each layer.

In the case of functional materials, other limitations may appear, such as light absorption. In many cases, it is not possible to print the materials (for example: black powders, TiO₂, etc.), and new alternatives are necessary to produce ceramic functional materials by 3D printing.

In this work, we propose the use of a photocurable slurry of a structural ceramic like SiO₂, with different metal precursors to fabricate functional materials. Slurries with different solids contents and metal precursor concentrations were prepared. The influence of the metal precursors nature on the stability of the slurries, printing parameters, and thermal treatments was studied. Finally, the obtained functional materials were characterised and evaluated.

2D materials-based nanostructured interfaces for advanced membranes and porous materials synthesis for application in energy and environment

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C5_1, Z4 Room (Level -3), septembre 15, 2025, 9:20 - 10:20

Porous ceramics are of great importance for various applications in energy, catalysis, filtration and refractory applications. Achieving rational design of polymer- derived ceramics (PDC) with hierarchical porosity has been made possible with the use of porogen agents, direct foaming or (nano)casting. However, these approaches often suffer from complexity and limited control over the desired porous architectures. Here, we describe an innovative method for fabricating porous ceramics monoliths by combining the preceramic polymer route and the Pickering emulsion method. The emulsions were prepared using a SiOC precursor and stabilized with modified graphene oxide (GO) nanosheets. The effects of formulation and the chemical parameters on the final properties of Pickering emulsions will be discussed. As a proof of concept, the monoliths have been used as electrode materials for electrochemical energy storage in Li-ion batteries (LIBs). Following a similar strategy, new process for the preparation of porous polymeric filtration membranes, of great interest in the context of green technologies development, has been developed. In that case, the formation of the porosity of the polymeric membranes results from Pickering emulsion templating involving hexagonal boron nitride (h-BN) nanosheets as stabilizer. In addition, Other examples Finally, some tailoring strategies susceptible of improving 2D materials membrane separation performances will be presented, including the development of laminar membranes prepared from 2D MoS₂ nanosheets for enhanced desalination performance. In a similar vein, another part will be dedicated to the use of 2D clay membranes for organic solvent nanofiltration (OSN) applications, by intercalating cations into the interlayer of the nanosheets, which significantly improves the stability and molecular sieving properties of the membranes.

From the 1st order phase transition in cristobalite to a compact high-temperature stable chemically stabilized ceramic

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C5_4, Z4 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

The limits of the applicability of fused silica in HT processes due to the material properties are well known. However, the use of fused silica at temperatures $> 1300^{\circ}\text{C}$ is limited by the deformation and crystallization of the material. In case of crystallization, cristobalite precipitates and during cooling a first-order phase transition, which runs parallel to a steep decrease in volume, appears. This phase transition leads to material failure. Reflecting on these properties and in connection with the good thermal shock resistance of cristobalite in the temperature range between $300\text{--}1600^{\circ}\text{C}$, the idea arose to develop a technology for the production of a material that combines the very good thermal shock resistance of fused silica with the good deformation resistance at high temperatures ($> 1300^{\circ}\text{C}$) of cristobalite by making use of the mechanism of chemical stabilization of the high-temperature phase of cristobalite (β -cristobalite) down to room temperature, which has already been mentioned many times in the literature. Based on previous work and evaluation of the relevant literature, this work describes the production of a chemically stabilized ceramic (CSC) via the glass-ceramic route based on surface and bulk crystallization of glasses with high SiO_2 concentrations. Furthermore, the mechanisms of stabilization depending on the crystallization conditions are presented and the resulting effects on the thermal and mechanical properties of the generated material are discussed. The ternary system $\text{SiO}_2 - \text{Al}_2\text{O}_3 - \text{CaO}$ was selected for screening experiments, where the effect of the dopant ratios, the raw material preparation and the aging temperature were investigated with respect to the crystallization behavior as well as the stabilization mechanism of the β -cristobalite phase. Thermal and mechanical properties were discussed based on dilatometry and X-ray diffraction (XRD). Furthermore, a technological route to produce materials with a strongly suppressed phase transition is presented. Material properties such as flexural strength, thermal shock resistance and deformation resistance are presented. In further work, investigations must be carried out to optimize the glass-ceramic manufacturing technology and the aging behavior. Synthesis conditions and compositions for the glass-ceramic route have to be identified, where a deformation-free (in the temperature range $\leq 1600^{\circ}\text{C}$) and compact material with high thermal shock resistance can be produced.

Effect of precursors properties and mixing on the development and final properties of dense boron carbide and B-rich boron carbide

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C5_2, Z4 Room (Level -3), septembre 15, 2025, 10:50 - 13:10

Ceramic based armor is generally used to protect a vehicle or person against the impact of a small caliber projectile. This protection consists of a ceramic layer on the front, attached to a metal or composite support, called "backing". The purpose of the ceramic layer is to erode the projectile and distribute the force on the backing. Among the three well-known ceramics (Al₂O₃, SiC and B₄C), boron carbide ceramic, known as B₄C, has the highest efficiency while being the lightest ($\rho = 2.52 \text{ g cm}^{-3}$) but its cost and loss of performance when subjected to large non-hydrostatic stresses (like the one caused by an impact of WC core threat), limits its use in the specific situations where the weight is the crucial parameter. However, in the B-C binary phase diagram, a solid solution of the boron carbide phases is defined from one side by the B₄,3C crystalline phase, the common phase in the literature called B₄C, and on the other side by the boron-rich B₁₀,4C crystalline phase [1]. These B-rich boron carbide ceramics are lighter than the conventional B₄C ceramic, with a density of 2.46 g/cm³ against 2.52 g/cm³ for the conventional B₄C [2] and an increase of the B/C ratio could reduce the brittleness and sensitivity of the ceramic as reported in the literature [3, 4]. These specificities make B-rich boron carbide ceramic a promising candidate for ceramic based armor thanks to the improved versatility and remarkable properties and lightness.

The objective of this work is to set up an approach to develop fully dense B₄,3C and B₁₀,4C ceramics starting from the same precursors and following the same protocol in order to compare their final microstructural and mechanical properties. The effects of elemental precursors properties and mixing method on the reactivity and Spark Plasma Sintering behavior is discussed. Complete microstructural and mechanical properties are presented and reveal that B-rich boron carbide ceramics can present Young's modulus and Knoop hardness very close to the values measured for B₄,3C while being lighter.

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Sol-gel derived SiOC(H) particles as inorganic components of hybrid bigels based on polyelectrolyte complexes for HIV prevention

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C5_3, Z4 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Hybrid gels and bigels containing inorganic drug carriers embedded into a polymeric matrix emerge as suitable option with promising features for the prevention of the sexual transmission of HIV. We report on the preparation of freeze-dried polyelectrolyte bigels containing sol-gel derived mesoporous SiOC(H) particles for vaginal administration of drugs. The antiretroviral drug Tenofovir (TFV) and the poorly soluble Dapivirine (DPV) have been introduced into the hybrid. The aim of this work is the development of freeze-dried polyelectrolyte bigels for vaginal administration of drugs. The selection of the temperature of the treatment for the consecution of the SiOC(H) particles allowed loading two drugs with different physicochemical characteristics which are subsequently released to the releasing media (simulated vaginal fluid) because of the presence of the polyelectrolytic complexes in the polymeric matrix. Impedance spectroscopy characterization allows identifying the different wettability of the vaginal films in the presence of the mesoporous SiOC(H) particles as well as the penetration of the fluid to allow the drugs to be released.

Novel multi-functional porous Si₃N₄-SiC composite for high-temperature applications

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C5_4, Z4 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Porous Si₃N₄-SiC composites are potentially very attractive in various applications such as chemical-gas industries, nuclear power plants, and automobile industries, and as heat-absorbing materials for solar thermal power plants and electromagnetic radiation shielding materials for commercial and military applications. The fabrication of these advanced composites generally requires expensive raw materials and very high temperatures necessitating advanced sintering techniques, thereby making these materials very expensive. In this work, a novel technique for fabricating these porous composites at a low temperature of 1200°C using phosphoric acid both as a binder and pore former has been proposed. Two different Si₃N₄-SiC composites with different SiC particle sizes and varying SiC content have been fabricated. The operating sintering mechanism in the work can be succinctly described as the reaction between H₃PO₄ and SiO₂ (present on the Si₃N₄ powders' surfaces), since H₃PO₄ does not react with Si₃N₄ and SiC. Two separate phenomena have been proposed to describe the sintering cycle. First, the volatilization of H₂O in H₃PO₄ producing pyro-phosphoric acid (H₄P₂O₇), and second, the reaction between H₃PO₄ and SiO₂ to form silicon pyro-phosphate (SiP₂O₇). SiP₂O₇ can form a strong, water-insoluble, acid-resistant phase::, that can bond well to Si₃N₄ and SiC particles and provide strength to the compact. A detailed study of the influence of the composites' composition on their microstructure and mechanical properties has been carried out. The results show that both the SiC particle size and its content strongly influence the strength, stiffness, and elastic anisotropy of the fabricated composites. Despite the significantly lower fabrication temperature, the mechanical properties of the porous composites are comparable to the best reported values in the literature.

Establishing a processability window for laser processing of regolith simulants: Ex-situ analysis and in-situ monitoring

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Laser Powder Bed Fusion (PBF-L) is one of the few additive manufacturing (AM) technologies with potential for constructing large structures on the Moon using only in-situ materials. Space agencies such as ESA and NASA have outlined roadmaps that include lunar landing pads, blast shields, and habitats built via AM. In-Situ Resource Utilization (ISRU) is critical to these efforts, as the cost of launching large amounts of material from Earth remains prohibitive.

This research builds on a preliminary study that successfully demonstrated 2.5D printing in the high-fidelity lunar regolith simulant (LRS) LHS-1, directly on a loose powder bed. An extensive experimental campaign will now investigate a viable process window for PBF-L of LHS-1 parts with the mechanical qualities required for the construction of large structures. The printed components will be evaluated for geometrical accuracy using a benchmark model developed in collaboration with SAGA Space Architects.

Extensive ex-situ characterization will provide a fundamental understanding for optimizing the process window alongside in-situ monitoring via high-speed imaging to analyze laser-substrate interaction in real time. Lunar regolith has highly irregular morphology, a wide particle size distribution, and variable chemical composition, making closed-loop process control, and consequently in-situ monitoring, likely necessary for large-scale construction without extensive pre-processing or site restrictions. While high-speed imaging has been used to optimize PBF-L for metallic materials, it has never been demonstrated for an LRS. In conclusion, this work aims to optimize PBF-L for lunar construction by addressing engineering constraints and setting the scene for a closed-loop control framework.

Thermo-Mechanical and Tribological Analysis of WC/Ti(C,N)-FeNi Ceramic-Metallic Compositions Obtained By Colloidal Processing

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C5_3, Z4 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Cutting tools are mostly based on the WC-Co system due to its exceptional abrasive properties, including high hardness, toughness and wear resistance; these qualities make them ideal for heavy-duty applications. However, the production of essential materials for cemented carbide manufacturing, such as tungsten and cobalt, presents significant challenges due to the toxicity of Co and the political strategic nature of both metals in the European Union, which makes them susceptible to significant fluctuations in price and availability. Furthermore, although Co is the preferred binding material for WC, as it forms a solid solution, its toxicity, price, relatively low melting point and oxidation resistance are prompting the need for the search of alternative composites for faster processing speeds.

Therefore, other binder and ceramic materials have been investigated aiming the substitution of Co. Researchers are particularly focused on developing more cost-effective and environmentally friendly manufacturing routes. One promising strategy is the use of Fe-based metal phases in combination with colloidal processing techniques. By employing colloidal processing, stable suspensions are created in which the particles are effectively dispersed within an aqueous medium. This dispersion prevents oxidation, a common issue when working with metal-based powders.

This study examines the performance of a new class of cutting materials produced by varying the binder composition of standard cemented carbide composites. By replacing the cobalt binder with FeNi, two economical and more sustainable composites result: Ti(C,N)-FeNi and WC-FeNi, since powder precursors were obtained via colloidal processing. Properties such as hardness, flexural strength, fracture toughness and wear resistance have been evaluated, from room temperature up to 800 °C, to simulate service environmental conditions. The results of these evaluations were then compared with those of Co-based commercial cemented carbide systems. The results show a slight advantage for the alternative Fe-Ni binder tools as evidenced by a 10 % and 25 % increase respectively in both flexural strength and fracture toughness at low temperatures with WC in the hard phase; however, the effects of using Ti(C,N) are inconclusive. The study demonstrated that these new Fe-based materials exhibit promising properties and could potentially replace traditional cemented carbide materials in industrial applications that demand high performance under harsh operating conditions.

From the properties of ceramic slurries to sintered elements - shaping through aqueous-based ceramic suspensions.

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C5_2, Z4 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The development of technology brings challenges to modern materials. They must not only have excellent mechanical and strength properties but also have complex geometries. In addition, waste emissions and pollutants accompanying production are being reduced. As a result, technologies that reduce machining, such as 3D printing and drop-casting, are being thrived. Both of the techniques above can be used to form specific shapes. 3D printing techniques allow easy modification of the complex geometry and the degree of filling of the parts. On the other hand, drop-casting makes it possible to obtain spherical elements. They can be both solid and porous. The porous effect is obtained by adding organic or inorganic compounds.

The ceramics industry is irreversibly linked to emissions of gases, such as carbon dioxide. This is related to the decomposition of carbonates and the removal of organic binders, among other things. Although complete zero-emission is impossible to achieve, it is necessary to minimize it. Replacing some organic binders with water is important in this regard. It is also crucial to control the selection of organic additives whose decomposition does not involve the emission of toxic compounds. For this reason, it is essential to perform thermal analysis coupled with a mass spectrometer to determine the products of thermal treatment. In addition, thermogravimetry will make it possible to determine whether the organics have been removed in their entirety, and differential thermal analysis will help select the debinding process parameters.

It is essential to take a comprehensive approach to shaping ceramics. The study considered the water-based Al_2O_3 and ZrO_2 ceramic slurries' rheological properties (dynamic viscosity and viscoelastic features). It also allowed the selection of organic components and their amounts, e.g. 2-carboxyethyl acrylate. The nature of the debinding process and its products were determined by STA/MS analysis. The shaping process, inter alia DIW, was carried out, and the basic mechanical properties (Vickers hardness, fracture toughness) of the sintered parts were studied, followed by their microstructure analysis.

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Shaping of ceramic beads via UV curing assisted drop-casting method

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

One of the key challenges in manufacturing ceramic materials is shaping beads with high sphericity and a uniform size distribution. Ceramic microbeads are typically formed by dropping a ceramic suspension containing alginates (as a gelling agent) into solutions with calcium ions. However, this approach often results in residual calcium ions in the sintered bodies, which can negatively impact their properties. This study aims to produce ceramic materials (alumina and zirconia) with spherical geometry using UV curing-assisted drop-casting [1]. This method exposes droplets of photocurable ceramic dispersions with hydrophilic properties to UV irradiation while falling through a hydrophobic non-solvent. Ceramic beads have diverse applications, such as in ultrafine grinding of non-metallic minerals, printing inks, pharmaceuticals, and food. However, producing these beads in a controlled, repeatable, and cost-effective manner, with perfect sphericity and uniform size distribution, remains a significant technological challenge. Additionally, the possibilities for final machining are often limited. The proposed method addresses these challenges effectively. Moreover, the process is easily automated, and the UV-curable dispersions use water as a solvent, making the approach more environmentally friendly.

In this study, the authors present results on optimizing the photocurable ceramic suspensions' composition. The influence of various dispersing agents, monomers, and photoinitiators on the rheological properties was evaluated. Extensive rheological measurements led to water-based ceramic suspensions with desirable properties, including a high water-to-monomer ratio, high solid content, shear-thickening behavior, and relatively low viscosity. Additionally, the study focused on determining the optimal shaping process parameters to produce ceramic microbeads with high circularity, uniform densification, and minimal microstructural defects.

[1] J. Eur. Ceram. Soc., 42 (2022), pp. 3957-3967

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Challenges and new solutions in manufacturing ceramic matrix composites

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Ceramic matrix composites (CMCs) can be fabricated by traditional ceramic manufacturing techniques, for example: hot pressing, extrusion, colloidal processing, or other methods, such as infiltration of preforms, centrifugal casting and additive manufacturing. Each shaping technique requires using specific processing agents which allow obtaining slurries or pastes of demanded rheological properties or provide other desirable features of the materials. These functional additives are as follows: dispersing agents, binders, monomers, (photo)initiators of polymerization, plasticizers, surfactants, pore-forming agents, precursors of reinforcing phase, etc. Possibilities of using different organic additives in the processing of CMCs will be presented (water-based monomers, sugar-based and polymeric deflocculants, polyacrylic binders, coordination complexes). The following issues will also be discussed: multifunctionality of selected compounds, thermal decomposition of additives during the sintering, fabrication of gradient composites, additive manufacturing of CMCs, ceramics reinforced by metallic nanoparticles.

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Colloidal processing of ceramic matrix composites

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Ceramic materials exhibit exceptional properties, including high corrosion, heat, and wear resistance, as well as remarkable hardness. Additionally, they can display n-type and p-type conductivity, piezoelectric and ferroelectric properties, and optical transparency, making them suitable for a wide range of applications in both bulk and coating forms.

To ensure high-quality, defect-free microstructures—especially in composite materials where one phase must be homogeneously distributed within the matrix—fabrication methods must be carefully chosen. For bulk ceramics, colloidal processing techniques effectively meet these requirements for both single-phase and composite materials.

In this research, colloidal methods were used to produce high-density ceramic materials incorporating metallic particles or reduced graphene oxide flakes. These additives significantly influence the mechanical and functional properties of the final material. For ceramic-metal composites, the metallic phase was introduced using precursors such as acetylacetonates or other metal salts. This approach enables the homogeneous distribution of even small quantities of additives throughout the suspension and, ultimately, the composite. Furthermore, the use of precursors facilitates the formation of metallic nanoparticles, which enhance the material's properties compared to ceramic matrix composites reinforced with microparticles obtained via conventional powder metallurgy techniques.

The wet forming method was also employed to fabricate ceramic-rGO (reduced graphene oxide) composites. However, due to graphene's nearly two-dimensional structure and strong tendency to agglomerate, achieving a homogeneous composite through this technique is challenging. To address this, our research utilized the chemical functionalization of graphene oxide to enhance its dispersion and solid loading in alumina and zirconia suspensions while simultaneously reducing viscosity.

This study analyzed the impact of sintering conditions, graphene oxide modification, and the use of metallic precursors on the microstructure and mechanical properties of ceramic-matrix composites.

3D printing of ceramic materials reinforced with metallic nanoparticles

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Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Ceramic-metal composites represent a particularly significant class of materials, as they integrate the beneficial properties of both ceramics and metals, resulting in enhanced properties of the final material. The presence of metallic particles in a ceramic matrix can act as a barrier to crack propagation, thereby improving the fracture toughness of the product. The effectiveness of this reinforcement depends on multiple factors, including the size, distribution, and morphology of the metallic phase. Micrometer-sized particles limit the ability to control the microstructure, as achieving uniform distribution of the metallic phase within the ceramic matrix is more difficult. This can lead to local inhomogeneities and a deterioration in the mechanical properties of the products. However, the use of metallic nanoparticles comes with certain technological challenges due to their strong tendency to agglomerate. Additionally, because of their high flammability, they require special storage conditions (in a cool, dry inert gas to prevent surface oxidation). A promising approach in the fabrication of ceramic-metal nanocomposites involves the use of metallic phase precursors. These precursors decompose and undergo reduction at elevated temperatures, facilitating the in-situ formation of finely dispersed metallic nanoparticles within the ceramic matrix.

The aim of the research was optimization of the ceramic pastes composition to obtain zirconia matrix composites, manufactured by Direct Ink Writing (DIW). Metallic phase was introduced to the pastes in the form of metallic powder or metallic precursor. Additionally, thermal analysis (TG/DTG/DTA/MS) was performed for the green bodies, metallic powders, and metallic precursors, which enabled the selection of appropriate sintering parameters. The important stage of the research was the characterization of the obtained samples, which included Vicker's hardness and fracture toughness tests, as well as SEM and XRD analysis.

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Effect of process parameters and feedstock composition on the functional properties of 3D-printed ceramic-based composites

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Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Additive manufacturing, commonly known as 3D printing, has emerged as a transformative technology for shaping ceramic and composite materials. Unlike conventional molding techniques, additive manufacturing methods, such as Direct Ink Writing or Fused Deposition Modelling, enable the precise fabrication of complex geometries without the necessity of casting molds. This not only enhances design flexibility but also significantly reduces production costs, particularly for customized or low-volume components. By eliminating the need for extensive tooling, 3D printing is highly suitable for both mass production and the creation of single, specialized elements tailored to specific requirements.

The present research aimed to develop and optimize colloidal systems for the fabrication of functional ceramic-based composite materials using additive manufacturing methods. The study focused on the formulation of stable dispersions with well-controlled rheological properties to ensure their suitability for 3D printing by material extrusion. A crucial aspect of the research was the selection and optimization of organic additives which play a crucial role in stabilizing the suspensions and enhancing their printability. To achieve this, rheological characterization of the prepared dispersions was performed to assess their proper viscosity, shear-thinning behavior, and flow stability. Then, printing parameters were systematically analyzed and adjusted to achieve optimal printing performance, ensuring consistent layer deposition and defect-free structures. The printed ceramic-based composite materials were subjected to detailed physicochemical properties evaluations and microstructure analysis to examine the effect of process parameters and feedstock composition on the functional properties of 3D-printed ceramic-based composites.

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Smart Ultraporous 0D-Nanocarbon Containing Ceramic Composites for Environmental Remediation

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C5_3, Z4 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

In a time of extreme and multiple crises, the synthesis and processing of advanced materials with multiple functionalities play a crucial role. Sustainable usage of our existing natural resources without further exploitation, combined with alternative technologies such as nanoremediation of the ecosystems, is one of the most significant worldwide challenges of our day.

The present era is represented by the use of “smart” and intelligent materials exhibiting tunable properties as function of different stimuli and their development is strongly needed in almost all spheres of life. As modern-age smart materials, 0D carbon-based ceramic composites show exceptional mechanical and optical properties, tunable surface structure, and ultrahigh specific surface area, just to mention few of their outstanding features which have attracted a lot of attention in the last years, these materials have found various applications in fields including sensing, optical computing, quantum computing, electrical energy storage, as well for wastewater treatment.

In this presentation, the development and processing of novel multifunctional quantum confined ultraporous 0D-nanocarbon-based polymer and ceramic composites with well-defined nanostructures, synthesized via sol-gel process and polymer derived ceramics route will be introduced, underlining the relationship between the processing / phase composition / nanostructure and the properties of the target ceramic nanocomposite materials consisting of 0D-nanocarbon-based phases (such as ultrasmall nanodiamond (UND), ultrasmall bucky nanodiamond (UBNDs) or ultrasmall onion-like carbon (UOLC)) finely dispersed or confined within a ceramic matrix (i.e., silica or Si₃N₄). Combining 0D-ultrasmall-nanocarbons with a ceramic material in a single functional nanostructure, it results in a novel smart approach to exploit the physicochemical properties of both materials concomitantly for applications in environmental remediation, more precisely here, for the dyes and heavy metals detection and adsorption from water.

Silicon-based ceramics: influence of sintering atmosphere

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Silicon-based ceramics, including silicon carbide (SiC) and silicon nitride (Si₃N₄), are advanced materials renowned for their exceptional mechanical, thermal, and chemical properties. These ceramics exhibit high hardness, excellent thermal conductivity, and remarkable resistance to thermal shock, oxidation, and wear. Due to these attributes, silicon-based ceramics are extensively utilized in high-temperature applications, such as components in gas turbines, heat exchangers, and advanced refractory materials.

The sintering atmosphere plays a crucial role in the densification and final properties of silicon-based ceramics. The choice of atmosphere can significantly influence the microstructure, mechanical properties, and thermal stability of the sintered ceramics.

In the present study, the influence of sintering variables without the application of pressure on the properties of silicon carbide and silicon nitride specimens has been investigated. The forming process employed was uniaxial pressing, and the firing was conducted in a graphite resistance furnace without the application of pressure. Thus, the influence of the environmental conditions of the samples, the firing cycle, and the firing atmosphere on the final properties of the obtained samples has been studied, analyzing their impact on the final properties.

The project “Cerámicas avanzadas para motores de propulsión - PROPULCER” is founded by Instituto Valenciano de Competitividad Empresarial (IVACE+i).

Sandwich Structured SiCf/Si₃N₄ Composite with Discontinuous Absorption Attenuating Layer for Temperature-Insensitive and Broadband Microwave Absorption

Mr. Yuchen Cao¹

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C5_4, Z4 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Achieving temperature-insensitive microwave absorption (MA) over a wide temperature range is an immensely challenging task due to the inherent variations in electromagnetic response and energy conversion characteristics. Herein, we present a novel silicon carbide fiber-reinforced ceramic matrix MA composite (CMC) with a structural-functional-integrated design based on the absorption attenuation layer concept. Through a comprehensive exploration utilizing complementary experimental and computational techniques, we systematically analyze the relationship between key structural parameters of the absorption attenuation layer and microwave absorption characteristics. The results demonstrate that the sandwich-structured SiCf/Si₃N₄ exhibits exceptional broadband radar wave absorbing properties. Notably, the introduction of a discontinuous periodic structure in the absorption attenuation layer significantly enhances the absorbing capabilities. The experimental findings demonstrate that the discontinuous sandwich-structured SiCf/Si₃N₄ achieves an effective absorption bandwidth (EAB) of 11.4 GHz (6.6-18 GHz) at a thickness of 3.9 mm, corresponding to a reflection loss of ≤ -10 dB. Furthermore, due to the unique scattering and interference cancellation effects of the metastructure, the DSS-SiCf/Si₃N₄ exhibits temperature-insensitive electromagnetic performance under elevated temperatures. Importantly, the EAB and average reflection loss of the composite remain essentially unchanged even when the temperature is elevated to 600 °C. This work provides a significant advancement in the design of "thinner, wider, stronger, and temperature-insensitive" microwave absorption components with practical applications.

Interfacial Mechanics and Polarization Behavior of Structural-Functional-Integrated SiC/Si₃N₄ Composites in Different Fiber Preform

Dr. Jie Liang¹, Pro. Fang Ye¹, Pro. Qiang Song¹

¹China, Xi'an, China

C5_4, Z4 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

The demand for structure-functionally integrated materials for applications in high-temperature environments has increased significantly. SiC/Si₃N₄ is the most suitable material candidate due to its excellent exceptional temperature resistance, high-temperature stability, toughness and dielectric tunability. Currently, the design of ceramic matrix composites (CMC) for electromagnetic wave (EMW) absorption is mainly centered around microstructural design and macrostructural design, thus the design of fibers at mesoscopic scale is neglected. In this work, three SiC/Si₃N₄ composites were prepared by CVI process using two-dimensional half (2.5D), three-dimensional four-direction (3D4X) or three-dimensional five-direction (3D5X) braided structures as preforms.

It is evident that altering the orientation of the fiber bundles will result in alterations to the mechanical and dielectric properties. Initially, it may be easily posited that elevated tensile strength and permittivity only come from elevated fiber content. However, it is imperative to acknowledge that the pore structure and matrix distribution of the composites are affected during matrix preparation due to the different fiber preform structure. According to our results, the 3D4X composites have the highest proportion of intra-bundle pores, indicating that the thermal residual stress at the interphase is relatively minimal (interphase zone is more effectively protected), so that the deviation between the tested and theoretically calculated values of its tensile strength is minimized. In addition, unexpectedly, following the destruction of the BN interphase of 2.5D and 3D5X composites, the formation of a SiC/Si₃N₄ interface occurs. This phenomenon leads to the enhancement of interfacial polarization and the high-temperature insensitivity of 3D5X composites. 3D5X composites exhibit effective absorbing properties within a broad temperature range of 25-900 °C.

Multiscale synergistic design of SiCf/SiBCN-based metamaterial for high-performance electromagnetic wave absorption in a wide temperature domain

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C5_4, Z4 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Electromagnetic wave (EMW) absorption materials effectively synergize room temperature (RT) and high-temperature absorption are essential for harsh environments applications such as stealth aircraft and aerodynamically heated components of aero-engines. Herein, an ingenious multiscale design strategy is proposed by combining the SiCf/SiBCN composite with metastructure to achieve synergy RT and high-temperature absorption. Firstly, as the skeleton material, the microstructure, electromagnetic parameters, and high-temperature EMW absorption performance of the SiCf/SiBCN composite have been systematically investigated. After optimizing the metastructure and corresponding geometric parameters, the SiCf/SiBCN composite with a frustum pyramid structure has exhibited exceptional broadband and temperature-insensitive absorption characteristics. The effective absorption bandwidth (EAB) of optimized SiCf/SiBCN-based metamaterial reaches 34.8 GHz (5.2~40 GHz, covering 96.7% within the tested frequency band) at RT, while the EAB remaining 12.5 GHz (5.5~18 GHz, covering 89% within the tested frequency band) even at 1100 °C. Notably, it maintains stable absorption against oblique incidence (within 40°) under transverse electric polarization. The broadband absorption mechanism of the wide temperature domain and the oblique incidence are ascribed to optimized gradient impedance matching and multiple attenuation resulting from multiscale design. This study pioneered the fabrication of high-performance EMW absorption metamaterial that synergizes broadband, wide temperatures domain as well as oblique incidence insensitivity.

Achieving High-Temperature Stable Structural Color through Nanostructuring in Polymer-Derived Ceramics

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C5_2, Z4 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Structural colors present many advantages over traditional pigment-based colors, which often contains scarce or toxic chemical compounds and are prone to UV degradation. To make use of these benefits in demanding environments, there's growing interest in creating structural colors out of ceramic materials. Polymer-derived ceramics (PDCs) are a great option because they combine ease of shaping in their polymeric form with excellent temperature resistance after being converted into ceramics. This study presents the fabrication development of non-iridescent structural colors by (nano)structuring a silicon oxycarbide (SiOC) PDC. The developed functionally graded material (FGM) with an inverse photonic glass 3D structure, takes advantage of SiOC's natural light-absorbing properties, producing a bright structural color that remains vivid even in white backgrounds with diffuse illumination conditions. The study explores the relationship between the process, structure, and properties of the resulting structural color by analyzing each layer of the functionally graded material (FGM) during the fabrication process. To show the flexibility of working with PDCs, the FGM design is also adapted to an additive manufacturing approach, where free-form structural colored shapes are printed by direct writing. Finally, the FGM-PhG structural colors were found to have an impressive thermal stability, maintaining their nano features, porous structure and properties at temperatures up to 1000 °C for 100 hours, enabling their use in demanding environments without degradation.

Processing, microstructure development and mechanical properties of reactively sintered SiC ceramic composites reinforced with various NbC fillers

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembere 15, 2025, 13:15 - 14:30

Our fast developing world has ever greater demands on the development of new progressive materials and technologies for a very wide range of applications across the aerospace, defence, energy, medical and transport sectors. The main reason for attracting attention to ceramics as is mainly due to its excellent properties such as high hardness, refractoriness, exceptional wear resistance and resistance in aggressive corrosive environments. However, ceramic inherent brittleness strongly limits its widespread, reliable technical application. Nowadays, we are increasingly faced with the inevitable need to design and develop new advanced ceramic composite materials with increased damage tolerance. The presented systematic study investigates the influence of the sintering parameters on microstructure development and basic mechanical properties of reactively sintered SiC ceramic composites reinforced with various NbC fillers. The main attention of the research is focused on the in-situ synthesis of SiC matrix during reactive sintering through the SPS technique, with the addition of reinforcing NbC phase in the form of globular particles and synthesised ceramic fibers in the range from 5 to 20 wt.%. The reactive sintering conditions were optimised, the temperature varied from 1800 to 2100 °C, and dwell time from 10 to 20 mins. Microstructural characterisation was performed by scanning electron and transmission electron microscopy with EDS, and phase composition by XRD. Basic mechanical properties, such as nano/micro/macro hardness, fracture toughness, bending strength, and elastic modulus were measured. The combination of in-situ reaction and SPS resulted in the prepared high damage tolerant ceramic composites. The relationship between microstructural development and basic mechanical properties has an important role in the further development of these perspective materials.

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UV-Curing-Assisted Drop-Casting as a novel approach in the production of ceramic beads

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

One of the primary challenges in the manufacturing of ceramic materials is achieving the shaping of microbeads with high sphericity and uniform size distribution.

This research aims to produce alumina materials with spherical geometry using UV-curing-assisted drop-casting, a novel shaping technique introduced by Falkowski and Zurowski [1]. In this approach, droplets of photocurable ceramic dispersions with hydrophilic properties are exposed to UV irradiation while falling through a hydrophobic non-solvent.

This study presents the results of optimizing the composition of photocurable ceramic suspensions. The effects of varying amounts and types of dispersing agents, monomers, and photoinitiators on the rheological properties were investigated. Extensive rheological measurements led to the development of a water-based ceramic suspension with desirable properties: a high water-to-monomer ratio, high solid content, shear-thickening behavior, and relatively low viscosity. Additionally, the authors focused on selecting process parameters to produce ceramic microbeads with high circularity, uniform densification, and no microstructural defects.

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SiOC-Based Strain Gauge with Ultrahigh Piezoresistivity at High Temperatures

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C5_3, Z4 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

The nonlinear response of strain gauges at high temperatures has restricted their applications despite their high-precision and real-time measurement capability. This work addresses this limitation by utilizing the easy preparative access and versatility of silicon oxycarbide-based (SiOC) thin films as strain gauges offering outstanding high-temperature robustness and giant piezoresistive response. The sensitivity of the strain gauge is assessed with continuous cyclic loads, tensile and compressive, resulting in gauge factors of ca. 2000–5000. The linearity of the response is preserved up to 700 °C with a shift in the electrical response occurring at temperatures beyond 500 °C, switching the SiOC film from semiconducting to conducting behavior. This change causes a drop in the gauge factor of the SiOC-based thin films; nevertheless, it is still significantly higher than that of metallic and Si-based commercial strain gauges. Notably, the studied thin films can regulate the effect of temperature enabling them to be a highly sensitive device with good reversibility and replicability in high-temperature environments. Furthermore, the electrical shift at 460 °C broadens the application of the SiOC film as a current-limiting device and temperature sensor.

Electron Paramagnetic Resonance Spectroscopy of Fast and Ultrafast Sintered 3YSZ Ceramics

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C5_4, Z4 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

The defect chemistry of 3 mol% Y_2O_3 -stabilized ZrO_2 (3YSZ) plays a crucial role in its optical and electronic properties, particularly in relation to oxygen vacancy formation and cation reduction processes. In this study, the impact of sintering and heating rates on the concentration and nature of defects in 3YSZ was investigated using Electron Paramagnetic Resonance (EPR) spectroscopy. To explore a wide range of heating rates, two advanced sintering techniques—Spark Plasma Sintering (SPS) and Ultrafast High-Temperature Sintering (UHS)—were employed to examine the formation of paramagnetic centers, such as Zr^{3+} ions, oxygen vacancies (F-centers), and defect clusters.

EPR analysis reveals a strong correlation between heating rate, defect concentration, and blackening, with distinct variations in defect populations as sintering conditions change. Beyond certain processing thresholds, a transition in defect behavior is observed, where shifts in EPR signal intensity and defect types suggest the emergence of alternative charge compensation mechanisms, defect clustering, or modified electronic states. Additionally, higher sintering rates influence both the onset temperature and intensity of these emerging defects, shifting their activation threshold and altering their relative concentrations. At higher sintering temperatures, an additional EPR-active defect species emerges, increasing in concentration up to a certain point, after which a reduction in primary defect concentration is observed, despite intensified optical blackening. This behavior suggests the formation of clustered defects, spin-pairing effects, or deep electronic states not detectable by EPR.

By elucidating the influence of sintering kinetics on defect structures, this study provides insights into the controlled engineering of oxygen vacancies, charge transport mechanisms, and optical properties, relevant to YSZ applications in solid oxide fuel cells (SOFCs), thermal barrier coatings, and electroceramics.

Modeling the Extrusion Process of PPS Solar Collectors

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The European Union has stated clear objectives regarding reduced carbon emissions and increasing energy self-sufficiency as part of its broader environmental and energy policies. Among various technologies, the utilization of solar collectors that absorb and convert sunlight into usable thermal energy, is particularly relevant to achieving these strategic goals. Flat-plate solar collectors made of polyphenylene sulfide (PPS) offer the advantage of lower weight compared to traditional collectors based on metals like aluminum or copper. Reduction in weight makes installation easier and reduces transportation costs, while ensuring robust thermal performance and maintaining resistance to high temperatures and corrosion.

Inaventa Solar, a manufacturer based in Norway, produces flat-plate solar collectors using high-performance polymers, designed to provide heat for low and medium-temperature applications. Within the extrusion process, high-pressure molten PPS is forced through a die with numerous narrow channels to create thin-walled, high-performance solar absorbers. While the height and width of the water channels is adjustable and approximately 6 mm x 15 mm, the total width of the plate produced by the extruder is 1830 mm.

Accurate control of the die outlet temperatures, especially aiming for uniformity across the width direction to ensure consistent temperature in the PPS, are crucial for producing absorber plates suitable for use in solar collectors. A detailed CFD model was developed to enhance process understanding and to predict how process-related factors such as screw speed (line speed), barrel temperature, and cooling rate affect the extrusion performance and product quality. The model accounts for the heaters and the solid components of the extruder. It captures the complex flow of molten PPS from its entry to the die, through multiple narrow horizontal channels, to the die exit, where the absorber sheet is shaped. Recordings from thermocouples integrated into the extruder validated the model's predictions successfully.

A digital representation of the extruder, combined with integrated sensors and cameras, was developed to enhance control, increase productivity, and minimize waste. However, executing a detailed 3D model is computationally intensive and time-consuming, making it unsuitable for real-time predictions. To address this limitation, a reduced order model (ROM) was developed based on the CFD model, enabling real-time predictions and thus control of the extrusion process. This work presents the detailed CFD model and its surrogate, its verification against temperatures recorded during production, and examines the impact of variations in production speed, PPS inlet temperature, and extruder heater power settings.

Advanced Finite Element Modeling of Reinforced PPS Extrusion for Solar Thermal Collectors: Integrating Crystallization Kinetics and Thermo-Mechanical Behaviour

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C6_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Energy efficiency and sustainability are critical considerations in modern manufacturing, driven by the need to reduce environmental impacts, lower costs and to apply to stringent quality standards. In manufacturing processes one can minimize energy consumption by reducing production defects and integrating advanced technologies - such as IoT and AI - for real-time energy management. Prediction of defects and their prevention are essential for reducing scrap rates in production, as they ensure higher resource efficiency, lower costs, and improved product quality. Simulations play a pivotal role in enhancing sustainability by enabling better decision-making and process design with reduced need for physical tests.

Inaventa Solar, located in Norway, specializes in the development and production of solar thermal collectors, which captures and absorbs solar radiation to convert it into usable energy. Their manufacturing process is a unique extrusion method that produces structured sheets of Polyphenylene sulphide (PPS) reinforced by 10% glass fibres. However, adding fibres leads to strongly anisotropic material properties, which poses challenges for numerical simulations of the process.

In this paper, we present a novel modelling methodology to represent glass fibres in PPS sheets with a Finite Element Model (FEM) capturing the material anisotropy. Further, we have modelled the PPS extrusion process using our in-house software (SiSim) to predict the thermo-mechanical behaviour of the material [1]. After exiting an extrusion die, the sheets are first cooled in a calibrator, where the thickness is controlled by an external pressure. Further downstream, the sheets enter an annealing oven, where a sufficient degree of crystallization is achieved through a heating cycle. The process simulations capture the crystallization phase of the PPS along with the thermal-induced stresses in the model while passing through the calibrator and the annealing oven. The modelling has been conducted in three steps starting with:

1. Developing a material model for FE simulations to represent reinforced PPS,
2. Defining the model behaviour in a unit-scale model to investigate the effects of geometry and temperature differences in the die,
3. Applying these learning outcomes to a global model of the PPS based thermal sheets.

The resulting global model is validated against physical data collected during the extrusion process and the crystallization model is validated against Differential Scanning Calorimetry test data. Finally, a surrogate model for the FE model is integrated with sensors to provide live predictions of defects in the manufacturing line.

Experimental quantification of the uncertainty in the mechanical properties of short fiber reinforced thermoplastics

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C6_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The injection molding process is one of the most important processing techniques for short fiber reinforced thermoplastics. This is mainly due to the fact that parts with complex geometries can be produced in large quantities at reasonable cost. However, the injection molding process influences the mechanical properties of the final part in a non-deterministic due to natural occurring uncertainties [1]. This makes reliable predictions using common simulations methods rather difficult. As the fibers dominate the mechanical behavior the influence of the injection molding process on typical fiber characteristics such as the fiber content, the aspect ratio and fiber orientation are the main cause for the occurring scatter. Additionally, the scatter in bulk material properties contributes to the resulting variability in part properties. This aspect is of particular importance for mechanically recycled polymers as the additional recycling step causes further fiber breakage [2].

Overall, it is not obvious if the scatter occurs due to slight variations of the fiber orientation or changes in fiber length during the process. Furthermore, it is also not clear to which extent the polymer matrix contributes to the scatter of the mechanical properties and whether it can be attributed to the elastic or viscous behavior of the polymer.

In order to investigate the mentioned effects experimentally, several test specimens are prepared by varying the process settings in the injection molding process. Tensile tests and dynamic mechanical analyses are conducted to analyze the scatter of the mechanical properties. Additionally, μ CT scans are carried out to verify how the injection molding process affected the fiber orientation and fiber length. To be able to quantify the material-induced uncertainties, two different batches of a post-consumer recycled material are investigated and compared to a virgin material.

Results have shown that the fiber length directly affects the fiber orientation. However, it was shown that the change of process settings in the injection molding process leads to a change in fiber length and fiber orientation as desired and the occurring scatter was successfully quantified.

[1] Wittemann, F., Krauß, C., Kärger, L.: Efficient Approximation of Varying Fiber Orientation States in Injection Molded Pars Under Consideration of Multiple Manufacturing Uncertainties in Applied Composite Materials 32, 149-172 (2025). <https://doi.org/10.1007/s10443-024-10268-3>.

[2] Bernasconi, A., Rossin, D., Armanni, C.: Analysis of the effect of mechanical recycling upon tensile strength of a short glass fibre reinforced polyamide 6,6 in Engineering Fracture Mechanics 74, 627-641 (2007). <https://doi.org/10.1016/j.engfracmech.2006.10.002>.

Revalorization of Ion Exchange Resins in elastomeric matrix

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C6_2, Seminario 7 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Ion exchange resins (IER) are widely used in several industrial fields, mainly in water purification systems. Recently, these resins are used as active media to store chemical elements to be used to dry-electropolish metals and composite materials. This process is an innovative technology capable of polishing complex geometries, maintaining tolerance by doing an homogenous post-processing average roughness reduction. This process uses sulfonated polymeric IER particles, capable of absorbing and retaining the electrolytic active liquid media under service-like working conditions. These particles lead to produce a layer-by-layer roughness reduction, from peaks to valley creating oxides during the oxidation/redaction process which is absorbed and attached to the active media decreasing the life-time under service-like working conditions. Several Key-factors control the IEP life-time, being the most important one: size, the electrical parameters, etc. of the object to be polished, and the number of specimens processed in the machine. However, the main problem of this technology is that the active media may be resubstituted every 100 hours to maintain the quality of the process. Currently, active polymeric media is incinerated generating CO₂ increasing greenhouse gases. Within the aforementioned information, there is a need to revalorize and/or find a reutilization route of all the IER used to achieve a zero waste in 2026.

In this work, a protocol to revalorize the IER used in the dry-electropolishing process are used as a reinforcement particle to develop a new composite polymeric material was developed trying to improve the mechanical strength for the composite developed material. Two different binders (Polylactic acid (PLA) and Thermoplastic polyurethane (TPU)) with four polymeric IER charges were investigated (0 “used as reference”, 10, 20, and 30 wt. %). After that prior to conduct the specimens though an injection process, the homogeneity of the different investigated mixtures was investigated by using thermogravimetrically and calorimetric analysis. Finally, the different mixtures were mechanically tested through tensile tests to be able to correlate the polymeric charges and the binder nature with their macroscopic properties (young’s modulus, maximum tensile strength, plasticity index, and ductility). Finally, the microstructure of the composite as well as the post-morten specimens will be microscopically investigated by using Focused Ion Beam and Scanning Electron Microscope.

Potential of pultrusion for the production of C/C composites

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C6_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Carbon fiber reinforced carbons (C/C) are lightweight and high-temperature materials with a density of less than 2 g/cm³ and operating temperatures exceeding 2000 °C. The carbon matrix can be produced either by gas-phase infiltration of a fiber preform (Chemical Vapor Infiltration, CVI) or by impregnating the fibers with suitable resins followed by pyrolysis (Polymer Infiltration and Pyrolysis, PIP). In the PIP process, the fibers are impregnated with a low-cost phenolic resin and formed into carbon fiber reinforced plastic (CFRP) composites using various shaping techniques, e.g. hand lay-up, winding, resin transfer molding, and hot pressing. During the subsequent pyrolysis process at temperatures up to 2500 °C, the plastic matrix transforms into glassy carbon. This results in mass loss and volume shrinkage, leading to a cracked C/C composite. To achieve dense C/C materials, multiple re-impregnation and pyrolysis cycles are usually required. According to the state of the art, the available technologies result in high production costs and geometrical constraints. Therefore, there have always been attempts to reduce the costs of C/C composites by using low-cost raw materials, modifying the matrix composition, or altering the CFRP forming process. In the current contribution, a new approach for the production of C/C composites by utilizing pultrusion as one of the most cost-effective manufacturing processes for fiber-reinforced plastics is introduced. Compared to the state of the art, this process can produce profiles of various cross-sections in large lengths with fiber volume fractions of up to 70%. Additionally, matrix additives can be integrated into the process to influence the properties of the final C/C composite. The main focus of the work will be on the influence of different process parameters such as pultrusion speed, fiber architecture, and the usage of additives such as graphite. The composites are mainly characterized by light and electron scanning microscopy, density and porosity measurements, and three-point bending tests. The parameter-dependent properties of the pultruded C/C composites are presented and discussed.

Enhancing Sustainability in Polymers: Gum Rosin as a Key Component for Green Solutions

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C6_2, Seminario 7 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The growing demand for eco-friendly solutions in the automotive and footwear sectors is driving innovation in material development through bio-based and sustainable raw materials. These industries, with significant environmental footprints, seek to integrate greener alternatives without compromising technical performance and quality. This work highlights advancements achieved by incorporating gum rosin resin derivatives into polymeric matrices, showcasing their potential as multifunctional natural raw materials for synthetic and biodegradable polymeric solutions.

The RN21 project intends to valorise natural resin extracted from pine trees and their derivatives as versatile bio-based raw materials, and pretends to enhance the resin sector's value chain, expanding its applications to packaging, textiles, automotive, and footwear industries. Experimental workflows include formulation, compounding, sample production, and performance evaluation, with a focus on maintaining or improving key technical properties.

In the automotive sector, gum rosin resin derivatives have been applied to interior components produced via injection moulding. Selected for their thermal stability and compatibility with conventional polymer processing techniques such as extrusion, these derivatives enable the development of bio-based polymeric matrixes with enhanced mechanical properties and processability. Research within a Portuguese consortium achieved incorporation levels of up to 30%, resulting in materials with bio-based content of up to 40%. These innovations align with industry sustainability goals while maintaining or exceeding the performance of conventional materials.

The footwear sector has similarly adopted gum rosin resin derivatives in the development of polymeric compositions for soles. By incorporating up to 20% of these derivatives into bio-based polymeric matrices via extrusion compounding, materials with a bio-based content of up to 55% were developed. These compositions exhibit mechanical robustness and processability, meeting the demands of industrial-scale production and the growing need for sustainable footwear solutions.

Results demonstrate the significant impact of gum rosin derivatives on the environmental footprint and functionality of polymer-based materials. By leveraging abundant and renewable resources, this work provides a pathway to sustainable innovation in materials science, addressing the pressing need for eco-friendly alternatives in high-impact industrial applications.

This work acknowledges the RN21 project, funded by the Environmental Fund through Component 12 – Promotion of Sustainable Bioeconomy (Investment TC-C12-i01 – Sustainable Bioeconomy No. 02/C12-i01/2022), of European funds allocated to Portugal by the Recovery and Resilience Plan (PRR), within the scope of the European Union (EU) Recovery and Resilience Mechanism, framed within the Next Generation EU, for the period 2021–2026.

Discrete Element Method Approach for Powder Flow Modelling in Rotational Moulding

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C6_2, Seminario 7 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Robomoulding is an innovative rotational moulding technique that offers lower power consumption, automation, and the ability to produce more complex products compared to traditional methods. It also comes with greater flexibility in motion and temperature control. In order to end up with well-shaped products with a uniform thickness, typically, trial-and-error approaches are used to set up and fine-tune the process settings, but this is inefficient and time-consuming. To reduce set-up time and improve process understanding, this research focuses on modeling the powder flow. A high-fidelity model based on the discrete element method (DEM) is developed to capture the complex behavior of powdered materials during moulding. Hereto, irregular particle shapes are introduced, as in previous research it was shown that small spheres do not allow for interlocking and as such are not capable of representing accurately the dynamic angle of repose (DAOR) of the powder. A design of experiments is conducted to generate a response surface model (RSM) that links powder particle settings with the DOAR. The high-density polyethylene (HDPE) powder is characterized using the DOAR in a GranuDrum™. The optimal set of model parameters is determined by combining the RSM together with measurements from the physical setup. These parameters are validated in the GranuDrum™ framework and further empirically validated in a full-process simulation to predict powder distribution. The simulation results show strong agreement with the powder distribution in the physical product, demonstrating the model's effectiveness in improving process insight and reducing reliance on trial-and-error methods.

Incorporation and Optimisation of Post-Consumer Recycled (PCR) Polyethylene for Advanced Rotomoulding Applications

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C6_2, Seminario 7 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Post consumer recycled materials (PCR), from domestic packaging waste, were assessed in order to understand the relationship between processing and properties in the rotational moulding (RM) process. Domestic PCR material was considered because RM recycled materials can be less abundant and stable in supply. The PCR materials from packaging streams allow the use of consistent feedstocks from sophisticated recycling systems. Despite this, it was established, since the material was not intended for use in RM, many factors such as, PCR polymer properties, zero-shear viscosity and thermal stability restrict the use of recycled materials in this polymer processing technique.

This work provides an overview of studies adopting strategies from the wider polymer processing literature on how to incorporate PCR, but applied to the RM process. In particular this work addresses the collection of baseline data which analysed processing behaviour and quantified mechanical properties for recycled high-density polyethylene (rHDPE) and linear-low-density-polyethylene (LLPDE) blends. Increases in porosity were recorded with an increase in rHDPE, due to an increase in zero-shear viscosity. Blends containing 30% PCR content recorded a greater than 50% reduction in impact performance. Such reduction in properties limits the number of useful applications. As a result, approaches to reduce viscosity, improve impact performance and restabilization were made.

Investigation regarding mechanochemical processing focused on reduce the viscosity of the rHDPE materials. In this work, increases in elongation at break of up to 230% were observed, however mechanochemical processing did not significantly change zero shear viscosity under such conditions. In addition, powder size and shape negatively effected the rotational moulding process.

Addition of copolymers and impact modifiers was reviewed via twin-screw extrusion. This study assessed addition of ethylene propylene diene monomer rubber (EDPM), styrene block copolymers (SBC), polyolefin elastomers and ethyl vinyl acetate (EVA). Improvements in impact strength over 100% were observed.

Another avenue for assessment regarding mechanical properties and performance is that related to 'restabilisation' as defined in the literature. The influence has been explored on rotational virgin materials, identifying changes in densification during processing. Increases of 33% peak impact strength were observed when using recycled material blends, however an extended processing time was required. Addition of antioxidants delayed the increase in density in line with previous virgin studies.

Overall, this is a summary of work aimed to improve the quantity of recycled content, and material performance for rotational moulding, an area of literature which remains broadly unexplored.

Engineering Lignin/Recycled Polymer Composites as Precursors for Sustainable Carbon Fibers

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C6_2, Seminario 7 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The global pursuit for environmentally friendly and cost-effective precursor materials for carbon fiber production has led to the exploration of lignin-derived products [1]. Lignin, an abundant plant component and a major byproduct of the paper industry, presents a sustainable alternative for several advanced applications. The aromatic nature of lignin makes it a potential source for graphite-based materials such as carbon fibres [2]. Most carbon fiber production methods require solution polymerization and fiber forming through wet spinning, with a heavy environmental burden. Melt spinning is an alternative technique for the production of cost-effective fibres that does not require the use of solvents, is environmentally friendly and an industry-ready process [3]. In the present work, lignin was melt mixed with polymers to create composite fibres. Three polymers were selected, namely glycol-modified polyethylene terephthalate (PET-G), a blend of polycarbonate with acrylonitrile-butadiene-styrene (PC/ABS), and polybutylene terephthalate (PBT), and softwood Kraft lignin obtained by the LignoForceTM process was used. The composites were produced with lignin contents of 50 and 60 wt.%. A prototype modular small-scale fully intermeshing co-rotating twin-screw extruder coupled to a prototype die for fiber spinning, performed melt mixing and fiber spinning in a single step. Composite fibers were thermally stabilized by heating in air at rate of approximately 0.5°C/min. The as-produced and thermally stabilized fibers were characterized by thermal analysis (thermogravimetry and differential scanning calorimetry), infrared and Raman spectroscopies, and mechanical testing. It was observed that, approximately above 250 °C, the chemical and physical characteristics of the lignin-rich composite fibres undergo changes, with an apparent increase of the aromatic content. Mechanical properties such as the storage modulus increased after thermal stabilization. In conclusion, the proposed strategy is interesting to produce high lignin content fibres with potential for thermal treatment and formation of carbon fibres. Further studies will focus on the carbonization process.

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Roll to Roll Manufacturing of Multifunctional High-Nanotube-Content Nanocomposite Fabrics

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C6_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Carbon nanotubes (CNTs) have long been considered promising for development of advanced composite materials, due to their outstanding properties along with low density. Particularly, composite materials with high nanotube content are often necessary in order to achieve mechanical, thermal or electrical conductivity requirements. Various applications of free-standing polymer nanocomposites have shown promise at the laboratory scale; however, scalable integration and fabrication methods are needed in order to meet the technology readiness level for commercialization. We have developed a solution method for the production of such nanocomposites in the form of nonwoven fabrics using a thermoplastic polyurethane (TPU) adhesive. Appropriate selection of the solvents and optimization of a TPU solvent/non-solvent volume ratio enhanced interactions between CNTs and polymer chains in solution, improved CNTs disentanglement, and significantly reduced the filtration time for a fast recovery of composite sheet of controlled composition. The method provides for controlled adsorption of TPU on the nanotubes surface for tailoring of the nanocomposite properties (e.g. conductivity, strength, toughness and adhesion). The resulting prepreg-like fabrics can be handled and employed analogously to other fabric and prepreg materials. CNT/TPU fabrics have been layered, laminated or infused to produce thick nanocomposites, or integrated with conventional composites, for a series of multifunctional composites demonstrations (e.g., electromagnetic shielding, heating, flame resistance, thermoelectric). We partnered with the Canadian company Integran Technologies through the Innovative Solutions Canada (ISC) Program to translate this batch filtration method to a roll-to-roll fabrication process. This new fabrication process not only supports larger-scale, continuous fabric production, crucial for industrial application, but also facilitates direct deposition onto other substrates and the production of other high-nanomaterial content nanocomposites.

Enhancement of UV Resistance and Water Repellency in Aramid Nonwoven Fabrics via TiO₂ and HDTMS Coating

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Aramid nonwoven fabrics are widely utilized in industrial applications that require durability in extreme environments, such as aerospace and military sectors, due to their excellent mechanical properties, chemical resistance, and thermal stability. However, exposure to UV radiation with sufficient energy to degrade amide bonds and aromatic rings can lead to significant chemical degradation. Furthermore, prolonged moisture exposure can disrupt the hydrogen bonding network, resulting in a deterioration of mechanical properties. To overcome these issues, research has focused on improving UV resistance through chemical modifications, multilayer structures, and UV-blocking coatings, as well as enhancing water resistance through grafting, coating, and lamination techniques. Among these approaches, coating technology is particularly advantageous as it preserves the intrinsic structure of the fiber while adding functional properties.

In this study, a dipping method using a titanium(III) chloride (TiCl₃) solution was employed to coat the surface of aramid nonwoven fabrics with TiO₂, which provides a UV-scattering effect to improve UV resistance. To further enhance water repellency, hexadecyltrimethoxysilane (HDTMS), a hydrophobic agent with a long alkyl chain, was coated onto the TiO₂ layer via a sol-gel process. This dual-layer coating aimed to maintain the fabric's performance under humid and UV conditions. The surface microstructure of the coated nonwoven fabric was analyzed using scanning electron microscopy (SEM), and the composition of the coated particles was examined through Fourier-transform infrared spectroscopy (FT-IR) and energy-dispersive spectroscopy (EDS). The functional performance of the TiO₂/HDTMS-coated aramid nonwoven fabric was evaluated in terms of thermal and mechanical properties, UV absorption capability, and contact angle measurements. This research demonstrates a promising dual-functional coating strategy that enhances both UV resistance and water repellency in aramid nonwoven fabrics, contributing to their long-term durability and applicability in extreme environments.

Acknowledgments

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Beeswax Content Effects on Mechanical Properties and Antioxidant Activity of Beekeeping Foundation Sheets

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To address the issue of waste generation from conventional disposable beekeeping foundation sheets, a reusable polypropylene (PP)-based beekeeping foundation was developed. However, when PP-based foundation sheets are exposed to outdoor environments for extended periods, ultraviolet (UV) radiation accelerates oxidative reactions, leading to physical and chemical degradation phenomena such as discoloration and deterioration of aroma. These issues can alter the structure of the foundation sheet and reduce bee-friendly. To mitigate these problems, beeswax was used as an additive, providing both improved bee-friendly and antioxidant effects. However, excessive addition of beeswax can deteriorate the overall physical properties of the foundation sheet; therefore, an appropriate formulation ratio that considers both mechanical properties and antioxidant performance must be established.

This study developed a PP composite material for beekeeping foundation sheets that balances mechanical properties and antioxidant performance. Homo polypropylene (homo PP) was compounded with beeswax, with beeswax content set as a variable to evaluate its antioxidant effects. In addition, to compensate for the reduction in mechanical properties caused by beeswax addition, inorganic fillers such as talc and wood flour, as well as organic compatibilizers, were added to enhance the performance of the composite material. These components were uniformly mixed through injection molding, then molded into foundation sheet shapes by injecting them into molds under high temperature and pressure.

To evaluate the changes in properties and antioxidant effects according to beeswax content, composites containing 2.5, 5, 7.5, and 10 phr of beeswax were manufactured. The thermal properties of the fabricated PP composites were analyzed using Differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA). Mechanical property changes were measured using a Universal testing machine (UTM). Surface analysis to confirm beeswax elution was performed using a Scanning electron microscope (SEM). In addition, to compare and evaluate the degree of photo-oxidation of the manufactured PP composites, Oxidative induction time (OIT) and fourier transform infrared spectroscopy (FT-IR) were utilized.

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Preparation and characterization of eco-friendly composites utilizing waste leather and water-dispersed polyurethane

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In 2019, the European Union (EU) set a goal of achieving carbon neutrality by 2050 through 'The European Green Deal'. To achieve this objective, the automotive industry has been actively promoting the utilization of recycled materials and the advancement of recycling technologies for leather derived from end-of-life vehicles (ELVs). While metals such as steel exhibit high recycling rates, natural leather and polyurethane (PU)-based artificial leather seats present significant challenges due to their bulkiness and limited recyclability, resulting in their predominant disposal through incineration or landfilling.

This study aims to mitigate the environmental impact of the automotive industry by developing an eco-friendly recycled composite material for automotive interior applications through the recycling of waste leather recovered from discarded automotive seats. To minimize VOCs emissions, water-dispersible PU was employed as a binder instead of organic solvent-based PU, and the material was processed into a wet-laid nonwoven.

The adhesive layer and the grain layer were removed from the natural leather seat recovered from the scrapped car through a shaving machine, and the removed leather was subjected to the fibrosis of the leather through a sieve to manufacture waste leather fibers. The resulting waste leather fibers were blended with water-dispersible PU to fabricate composite nonwovens, and the effects of varying fiber content on the composite properties were systematically analyzed. The morphology of the nonwovens were observed using a scanning electron microscope (SEM) to analyze changes according to the variables. The mechanical properties were assessed using a universal testing machine (UTM) to determine the reinforcing role of waste leather fibers in the composite structure. Additionally, the thermal properties of the composites were analyzed using differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA).

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HYBRID BALLISTIC HELMET MADE IN A ONE-STEP PRESSING PROCESS

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C6_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Ballistic head protection based on the composite technologies (hybrid or single-blade composite) should protect the user's head against bullets and fragments differing in the energy of the penetration. Ballistic resistance of above-mentioned protections depends on impact angle, type and velocity of the bullets and on the material system used for the processing of the helmet as well as its shape.

Developing technology of ballistic head protection is aimed at finding new high-strength materials, mainly based on ultra-high molecular weight polyethylene (UHMWPE) fibres, reducing the mass of the final product while increasing its ballistic protection. The idea of the study was based on the thesis that the stable connection of the two types of the fibrous materials differing in the structure, topography as well as in type of the polymer (para-aramid and polyethylene) will increase the ballistic resistance as well as allows to reduce the mass of the final products. Ballistic helmets were evaluated using ballistic impact attenuation test as well by estimation of the Head Injury Criterion (HIC).

The development of ballistic head protection technology is synergistic with the development of new composite high-strength materials, based mainly on UHMWPE fibers, reducing the mass of the product while increasing its ballistic protection.

The idea of the presented research was based on the thesis that a stable combination of two types of fibrous materials differing in structure, topography, as well as the type of polymer (elaborated composition of para-aramid and polyethylene fibres) will increase ballistic resistance and also reduce the weight of the final products.

The aim of the research was to develop a hybrid ballistic helmet with reducing of the risk of head injuries. The newly developed head protections' solution for special tasks was based on the extensive virtual model elaborated in software designed for modelling physical phenomena.

The designed helmet meets the parameters included in the PN-V-87001:2011, NIJ Standard 0106.01 and PN-EN 397+A1:2013-04 Standards, while reducing the probability of head injuries by designing the helmet structure in such a way that the HIC parameter, which is a measure of the probability of head injury resulting from an impact, reaches the level of ≤ 800 , assuming that the areal density of the helmet will be $\leq 8.8 \text{ kg/m}^2$.

The project "Hybrid combat helmet reducing the risk of head injuries" was implemented under the Smart Growth Operational Programme 2014-2020, contract number: POIR.01.01.01-00-1293/20-00 and supported by European Regional Development Fund.

Europium-based 3D structures fabricated via Multiphoton Lithography for increase of Photoluminescence in optical frequencies

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Recent advances in material science's field have revealed high potential in development of novel applications using high photoluminescent materials. One of this very interesting materials is Europium (Eu), which has shown interesting properties in the optical frequencies. Motivated by the high photoluminescence that Eu shows, here we present a fabrication method using Multiphoton Lithography (MPL) focusing on ultra-fast LEDs and nano lasers using all-dielectric devices.

MPL is a 3D fabrication process relying on direct laser writing using ultrafast laser sources and suitable photosensitive materials which offers a few tens of nm resolution for rapid 2D and 3D printing with a layer-by-layer approach. For the purposes of our research, Europium(III) acetate hydrate is processed in Europium methacrylate (EuMAA) diluting it in methacrylic acid to achieve Ligand exchange. Then, EuMAA is incorporated in our in-house hybrid material, SZ2080, well known for its chemical, mechanical and optical properties. This Zr-based material enables the fabrication of 3D structures with high resolution using MPL, and due to the chemical stability, it can host different luminescent ions. Different concentrations of EuMAA were tested to achieve the maximum increase of photoluminescence with the lowest fabrication defects.

The final hybrid materials are processed using MPL, to create 3D structures, with two different excitation sources. One using a fiber green laser (515 nm) and the other using a fiber IR laser (780 nm). The processed samples undergo through calcination process at different temperatures in order to remove the organic part and activate Eu to exhibit high photoluminescence in 3D structures with micro and nanoscale size. The samples then, are characterized using Micro- photoluminescence spectroscopy with different excitation wavelengths.

Using specific 2D and 3D geometries, known as metamaterials, photoluminescence can rise even more and potentially be used in photonic devices, such as in the development of all-dielectric LEDs, lasers, and single photon emitters.

Advancing Robot-Based Direct Laser Interference Patterning Through IR Process Monitoring and Neural Networks Evaluation

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C7_3, Machuca Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Direct Laser Interference Patterning (DLIP) is a well-established technique for fabricating micro- and nano-scaled structures, enabling surfaces with advanced properties such as reduced wear and friction. This single-step process offers high throughput and significant potential for automation. However, achieving full automation necessitates the integration of robust online process monitoring to ensure consistent quality of the produced structures.

In this study, we demonstrate an innovative approach combining in-line process monitoring with advanced machine learning methods for evaluating and predicting product quality. Specifically, the emission of radiation due to localized heating during DLIP was monitored using an infrared (IR) imaging system, while the captured signals were analyzed using a Convolutional Neural Network (CNN).

To validate this method, stainless steel substrates were patterned by modifying various laser parameters, including fluence, repetition rate, and process velocity. The IR monitoring system measured important thermal effects during the structuring process, including the average temperature and the size of the temperature field. The surface structures created were then examined using confocal microscopy. Relationships between the process settings, the IR data, and the surface structures were identified. This information was used to train the CNN to predict the quality of the surfaces.

The integration of IR monitoring within the DLIP process ensures real-time quality assurance by providing immediate feedback on the manufacturing parameters. Furthermore, the trained CNN demonstrated reliable predictions of the resulting surface topography, optimizing evaluation processes and eliminating the need for post-production analysis.

This approach represents a significant step toward fully automated and intelligent DLIP processes, combining precision monitoring with advanced predictive analytics to enhance manufacturing efficiency and product quality.

Direct Laser Writing of hybrid biocompatible 3D scaffolds for tissue engineering

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Developing an ability to fabricate high-resolution, 3D hybrid biocompatible structures at microscale is crucial to achieve novel scaffolds for tissue engineering. Generally, hydrogels have been widely employed as synthetic analogs of 3D extracellular matrices (ECMs), with their physical properties such as degradability and porosity playing a critical role in regulating the behavior of cells. In this study, we fabricated 3D scaffolds at microscale in order to use them as 3D ECMs mimicking the natural environment of cells. We present the design and development of a novel hydrogel-based photoresist tailored for fabricating 3D hybrid biocompatible scaffolds through multi-photon polymerization (MPP). The proposed photoresist consists of polyethylene (glycol) diacrylate (PEGDA) as a hydrogel incorporated with zinc-magnesium ions in varying concentrations. These ions play the role of photoinitiator absorbing the tightly focused laser beam resulting in MPP of PEGDA. This method is a versatile 3D-printing technique enabling us to design complex architected structures with high accuracy which is crucial to achieve the desirable properties of the ECMs (such as mechanical properties). Biodegradable metals such as zinc and magnesium, have been regarded as next-generation, biomedical implant materials to promote tissue repair and regeneration. These ions are naturally ambient in the human body playing a critical role in cell proliferation and differentiation. This photoinitiator-free approach (biodegradable metal ions instead of toxic chemical compounds) provide a new pathway for the development of 3D biocompatible scaffolds that are promising candidates for tissue engineering applications.

Laser-Based Directed Energy Deposition with Mullite: A Step Forward for Lunar Regolith Printing

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C7_1, Machuca Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

In-situ resource utilization (ISRU) is pivotal for sustainable space exploration, enabling the use of local materials to construct infrastructure on extraterrestrial bodies. Additive Manufacturing (AM) techniques, particularly Directed Energy Deposition (DED), hold immense promise for fabricating lunar structures using regolith. However, the scarcity of actual lunar regolith necessitates the use of simulants. Mullite, an aluminosilicate ceramic with thermal and chemical similarities to highland lunar regolith, was investigated in this study for its suitability in DED-based applications.

This research explored the high-temperature behavior of mullite within a laser-based DED process. Experiments included optimizing process parameters such as laser power, scanning speed, and substrate material while leveraging in-situ monitoring via short-wave infrared (SWIR) imaging and microstructural analysis. Deposition trials were performed on mullite-based and stainless steel substrates, focusing on single and multilayer tracks.

The study defined a feasible process window for mullite, identified challenges like porosity and thermal stresses, and evaluated the microstructural integrity of printed parts. Results demonstrated mullite's potential as a regolith simulant, providing critical insights into achieving defect-free fabrication and scalable ISRU solutions. These findings advance the application of AM technologies in extraterrestrial environments, contributing to the goal of establishing permanent lunar settlements.

Multi-Scale Hierarchical Patterns: A New Frontier in Surface Blackening

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C7_3, Machuca Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

The fabrication of durable and multifunctional blackened surfaces on engineering steel is critical for advancing optoelectronic applications, such as infrared sensing and solar absorbers. This study investigates the use of direct laser writing (DLW) and direct laser interference patterning (DLIP) to create hierarchical textures on AISI 304 stainless steel. The process combines DLW-generated honeycomb macrostructures with DLIP-fabricated microgrooves to produce single- and multi-scale patterns. The resulting textures were characterized in terms of topography, optical reflectance, wettability, and mechanical durability.

The hierarchical textures demonstrated significant improvements in optical performance, with enhanced light absorption due to the synergistic effects between macro- and microstructures. Spectral reflectance measurements confirmed a reduction in reflectance across the visible and infrared spectrum, showcasing the effectiveness of the multi-scale designs in creating highly absorptive surfaces. Furthermore, wettability tests revealed that these textures provide multifunctional properties, such as improved hydrophobicity, making them suitable for use in extreme environmental conditions.

Mechanical durability was evaluated through an abrasive wear test, which showed that the DLW-generated honeycomb structures provide critical protection to the finer DLIP patterns. This protective effect enhances the resistance of the textured surfaces to wear, ensuring the retention of their optical and functional properties under abrasive conditions. The surfaces were also subjected to acid etching in citric acid solutions, revealing that multi-scale structures exhibit superior resistance to acid-induced degradation compared to single-scale patterns. The hierarchical textures effectively slowed the penetration of acid into the oxide layer, preserving the surface functionality.

The demonstrated scalability, flexibility, and robustness of these laser-based processes make them promising candidates for industrial applications requiring high-contrast, antireflective, and wear-resistant surfaces. These findings pave the way for the broader adoption of laser-textured blackened surfaces in demanding optoelectronic and environmental applications.

Direct Laser Interference Patterning with High-Power Multimode Fiber Laser

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Direct Laser Interference Patterning (DLIP) has long been a preferred method for fabricating periodic micro- and nanostructures on large surface areas. Traditionally relying on single-mode lasers, DLIP has been limited by laser power, constraining its application for high-throughput industrial processing. This study introduces the integration of a high-power multimode fiber laser, capable of delivering power in the multi-kW range, with the specially designed Extended Laser Interference Patterning System (ELIPSYS®). This configuration successfully addresses the challenges of low spatial coherence and beam quality, enabling precise interference and unlocking the potential of multimode lasers for microfabrication.

The system demonstrated the ability to produce periodic line-like structures with spatial periods as small as 6.0 μm on stainless steel surfaces, providing versatility for various application needs. By optimizing laser parameters, such as pulse energy and pulse overlap, the process produced high-quality patterns with aspect ratios up to 0.8 while maintaining a high homogeneity across large areas.

Upscaling the high power of the multimode fiber laser enables unprecedented processing speeds, meeting industrial demands for scalable and high-throughput manufacturing. This work marks a significant advancement in DLIP technology, extending its applicability to large-scale, efficient surface microstructuring and opening new possibilities for advanced functional applications.

A Combined Experimental and Simulation Approach to Understand Thermal Signatures, Bead Geometry, and Microstructural Changes in Laser-DED of Hastelloy-X

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This study investigates how the cooling rate and the melt pool life influence the bead geometry, microstructure, and microhardness of laser-directed energy deposited (DED) Hastelloy-X. The cooling rate as well as the melt pool life data were extracted from the thermal signatures captured by an IR pyrometer during the deposition process at different laser input processing conditions. Additionally, a thermal model was developed using finite element modeling software, incorporating temperature-dependent material properties, a Gaussian heat distribution, and accounting for convective and radiative heat losses, as well as the latent heat of vaporization of the material. The results predicted by this simulation closely matched the captured online thermal signatures of the molten pool. The simulation also provided insights into the remelting of the previously deposited layer during the deposition of the subsequent layer, a phenomenon that is challenging to capture with an IR pyrometer. The microstructure and phases of the deposited Hastelloy-X were examined using a scanning electron microscope and an X-ray diffractometer, respectively. The microstructural analysis revealed that the evolution was closely linked with the molten pool life and the cooling rate, which in turn depends upon the input laser attributes. With an increase in cooling rate and decrease in molten pool life, a modest reduction in grain size was observed. In addition, an increasing trend in microhardness values was detected on account of higher cooling rate. Furthermore, an increase in the melt pool lifetime resulted in an increased bead width, hence compromising the aspect ratio of the bead.

Laser Beam Welding of IN625: optimization of process parameters

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Thanks to their good heat resistance, Ni-base superalloys are employed in the manufacturing of components for aeronautic, aerospace and energy fields. The repairing process of these components, when damaged, is of paramount importance due to the high costs related to their manufacturing. High-energy density techniques can be successfully employed to obtain reliable repaired parts, nevertheless a deep investigation on the effects of the welding parameters is crucial to optimize the process and improve the service life and reliability of the repaired parts.

In fact, welding process affect the microstructure of the Melted Zone (MZ) and Heat Affected Zone (HAZ) leading to several issues, such as a variation of mechanical properties and local chemical composition due to segregation of alloying elements; precipitation of secondary detrimental phases; solidification and liquation cracking.

In this work, Laser Beam Welding (LBW) has been employed to investigate the welded seams on 2.5 mm thick plates of IN625 superalloy. Seams have been obtained varying the laser power ($P_m = 1700/2000/2300$ W), laser speed ($v = 15/20/25$ mm/s) and power modulation ($R = P_{min}/P_{max} = 0,6/0,8/1$).

Microstructural observations of the welded plates through Optical Microscopy (OM) and Scanning Electron Microscopy (SEM), and Vickers micro-hardness tests along the seams, have been carried out to investigate the influence of process parameters variation, namely the input energy density, on MZ and HAZ.

The optimal process parameters, leading to seams without macro-defects, such as cracks and pores, have been identified in $P = 2000$ W, $v = 25$ mm/s, $R = 0,6$.

This work was supported by PRIN 2022 project, ELAPSE: Laser Welding and Repair of Superalloys (project 20225YNH4M). ELAPSE is financed by European Union through PNRR funds.

Porous ceramics from laser surface melting of eutectic mixtures: Mg-stabilized zirconia

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C7_1, Machuca Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

Porous ceramics with connected porosity are relevant in many applications including porous supporting electrodes in high-temperature electrochemical devices, filters, or membrane supports. To tune the pore size, its connectivity and tortuosity different technologies have been developed [1]. By etching a sacrificial phase, the final porosity structure is determined by control of the microstructure of the ceramic composite before etching. Eutectic materials solidified from a melt can give rise to especially homogeneous microstructures of micrometric and submicron size. In this communication we will present results on the porous ceramic resulting from laser surface melting of MgO-ZrO₂ mixtures. The as-solidified composite consists of Mg stabilized zirconia majority phase with around mainly fibrous 30 vol % MgO. The overall alignment of the phases is determined by the melt-pool shape, while the microstructural size and distribution depend also on the solidification rate and dominant cooling mechanisms, either in flat or cylindrical surfaces. Plates and cylinders of the composite with different microstructures have been surface laser melted. Appropriate homogeneous microstructures have been achieved on preheated plates. The achievement of a homogenous solidified layer with appropriate microstructure on the cylinder samples has proven more difficult. Next, the MgO has been etched out in selected ground plate samples. The gas permeability through the porous plates measured using N₂ or a CO₂-N₂ mixtures is in the range from 10⁶ to 3x10⁶ barrer (or 3·10⁻¹⁰ to 10⁻⁹ mol m⁻¹ s⁻¹ Pa⁻¹) with average pore diameters below 1 micron. These are moderate values as correspond to ceramics with 30 vol% porosity. They will be analyzed to the light of the detailed sample microstructure and solidification conditions.

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On synergy of theory and experiment in ultrashort laser irradiation of bandgap materials

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C7_2, Machuca Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

When powerful ultrashort laser pulses couple with the surface or bulk of a bandgap solid, they create a dense, relatively cold free-electron plasma, a forerunner of laser-induced structural modification of materials. Nowadays the techniques employing laser-induced structural modification of materials experience tremendous development with applications in various fields ranging from electronics, photonics, and information storage to microfluidics and biomedicine. Additionally, new types of lasers are under development with higher average power, higher repetition rate, higher energy in the pulse, with shorter pulse duration, in burst mode regimes, covering missing ranges of laser wavelengths. Experimental diagnostics for monitoring laser-induced phenomena with femtosecond temporal resolution and sub-micrometer spatial resolution are still under development and numerical modeling plays an important role in understanding the fundamental mechanisms in ultrafast processes.

This work has been focused on the synergy of theory and experiment in laser irradiation of bandgap materials using spatiotemporal shaping of laser beams and dual-wavelength excitation. Several theoretical predictions based on simulations with state-of-the-art models will be discussed and their experimental verifications will be presented. In particular, a strong enhancement of localized absorption of laser energy inside fused silica glass using a sequence of two laser pulses at different wavelengths will be considered with the analysis of the whole chain of the processes triggered by the laser pulse and continuing until the final imprinting of a modified structure into the material matrix. For multi-shot irradiation regimes, the simulations have revealed the paramount importance of the defect accumulation not only because of easier ionization of material by successive laser pulses but also due to the associated positive change of material refractive index. This enabled to uncover physical mechanisms behind the non-reciprocal writing of waveguide structures inside glasses. For the case of silicon ablation with dual-wavelength irradiation, sophisticated modeling has been shown to describe quantitatively the experimental data on material excitation depending on the sequence of IR and visible laser pulses. This study demonstrates the importance of adequate theoretical models, which enable understanding the processes in condensed matter at an ultrafast time scale.

Fabrication of Raman-Nath and Bragg diffraction gratings on ophthalmic polymers by ultrashort laser pulses

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The inscription of diffractive elements in ophthalmic polymers to induce refractive index changes is of great interest in the fields of Optics and Ophthalmology to be applied for refractive correction. In this work, fabrication of linear periodic patterns in hydroxyethyl methacrylate by means of high-repetition rate femtosecond laser pulses is reported. In particular, both Raman-Nath and Bragg gratings have been inscribed underneath the surface to study to what extent the dimensions of the gratings are involved in the final refractive index change.

As the laser source, high-repetition-rate Ti:sapphire laser with a pulsewidth of 120 fs working at 80 MHz has been used. Compositional and structural modification was studied by means of micro-Raman spectroscopy. Finally, periodic patterns were characterized by diffractive techniques to ascertain the diffractive properties of the periodic patterns.

Ultrashort pulsed laser-assisted biomineral coating on an additive manufactured Ti64 implant for enhancing osseointegration

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C7_3, Machuca Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Surface treatment of bioimplants is essential to control the interaction between implant surface and host environment for successful acceptance of bioimplant by the patient's body. The present study deals with ultrashort pulsed laser-assisted cerium co-doped hydroxyapatite (Ce:HAP) coating onto 3D-printed Ti6Al4V titanium alloy. The flat titanium discs of 15 mm diameter and 1 mm thickness were designed in CAD software and fabricated using selective laser melting (SLM) technique. The fabricated Ti6Al4V discs were spin-coated (5500 rpm, 60 s) with a slurry containing 5 ml of chitosan and 2 mg of Ce:HAP. Further, the coated surface was irradiated using Chromacity Laser (1040 nm, 200 fs, 200 MHz) at the optimized laser processing condition using a CNC-controlled XYZ-table (100 nm resolution). Surface morphology, microstructural properties, chemical composition and interfacial properties of the irradiated biomineral layer were analysed using SEM, XRD and EDX. The results indicate that ultrashort pulsed laser-assisted biomineral coating is a promising method for the production of ceramic coating on 3D-printed titanium which can be aligned with the implant manufacturing process.

Effect of doping on the formation and coherent propagation of LIPSS in zinc oxide films induced by fs-laser irradiation

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C7_2, Machuca Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Transparent Conductive Oxides (TCOs) are materials with low resistivity and optical absorption in the visible spectrum, which makes them of vital importance for numerous applications (displays, photovoltaics, transparent heaters...) [1]. In spite of its large-bandgap, un-doped ZnO shows a relatively large n-type conductivity at room temperature due to the donor character of oxygen vacancies. In addition, it can be easily doped with different elements to improve its conductivity and turn it into a proper TCO [2] while preserving most of its interesting properties, such as biocompatibility, piezoelectric response or antibacterial activity [3].

The presence of dopants can also be used to facilitate its modification via processing with ultrafast lasers. As in the case of other TCOs [4,5], LIPSS formation [6] upon fs-laser irradiation could potentially be used for generating topographic, optical and electrical anisotropies. However, inducing large scale, homogeneous and controllable anisotropies based on LIPSS requires their formation and coherent propagation over macroscopic regions.

In this work, we have analysed the formation and coherent propagation of LIPSS by fs-laser processing ($\lambda = 1030$ nm, $\tau = 350$ fs) in ZnO films doped with different trivalent oxides (X_2O_3 , X being Al, Ga, In, Yb...). Depending on the dopant and doping level both the formation of LIPSS and their coherent propagation can be successfully triggered, evidencing the importance of generating a small amount of linear absorption at the laser wavelength (1030 nm) upon doping. We will analyse the role of the film composition and its evolution upon laser processing in the resulting structures in order to maximize the induced anisotropies while preserving good electrical and optical behaviour.

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Ultrafast structural transformations of Fe under sub-ps pulsed laser annealing

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C7_2, Machuca Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

The phase transitions in iron, encompassing their nature, pathways, and driving forces, have long been a topic of debate. Gaining a deeper understanding of this process is crucial to addressing fundamental questions in condensed matter physics and potentially enhancing technological applications. To this end, we investigated the atomic structure of a thin Fe layer following sub-picosecond pulsed laser annealing using ultrafast time-resolved X-ray diffraction (see [1] for method). Due to the strong electron-phonon coupling in iron, the laser pulse energy was transferred to the lattice on a time scale of 1 ps. This rapid heating led to ultrafast melting. Under conditions below complete melting, this was followed by a solid-solid transition in the remaining crystalline phase. Given the extremely high rate of heating (on the order of 10^{15} K/s), the observed transformations do not align with the phase diagram known for slow (equilibrium) heating. The formation of the fcc-Fe phase is kinetically hindered, and the bct-Fe phase appears at the melting temperature. This behavior aligns with static ab initio theoretical simulations, which predict phonon softening at high temperatures and consequent tetragonal lattice distortion. The experimental results presented here provide new insights into the dynamics of martensitic phase transitions.

[1] Acta Mater. 276 (2024) 120043

Laser surface alloying of 316L stainless steel with 316L+20wt% Cu alloy

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C7_1, Machuca Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

In the present study, 316L stainless steel was surface alloyed with 316L+20wt% Cu using laser-based powder bed fusion (PBF-LB) additive manufacturing technique. Alloying of Cu in 316L can enhance the antibacterial activity. The influence of the process parameters, such as laser power and rescanning strategy, on the microstructure, chemical gradient, and homogeneity was investigated. 316L + 20 wt% Cu powder-mix was used as feedstock. The size and morphology of the feedstock powders were characterized with a scanning electron microscope (SEM). Surface alloying of 316L + 20wt% Cu powders was carried out at a range of process parameters: laser power: 175 W to 235 W, and number of laser scans: single scan, double scan, and triple scan, respectively. The layer thickness of the powder and hatch spacing were kept constant at 50 μm and 90 μm , respectively. The surface roughness of the samples was analysed under optical profilometry. Defects like porosity, cracks, and segregation were characterized by using optical microscopy, scanning electron microscopy, and Energy-dispersive X-ray spectroscopy. Chemical homogeneity in the bulk sample improves with higher laser power and remelting. Cu was found to segregate at grain boundaries, which increases the solidification cracking susceptibility. Adopting a triple laser scanning strategy has resulted in a dense and defect-free surface. Hardness distribution was measured and correlated with the homogeneity in the chemistry and the resultant microstructure of the modified surface.

Keywords: 316L+20 wt% Cu; Powder mix; Chemical homogeneity; Defects; Microhardness.

Femtosecond Laser 3D Printing of Nanocrystals via Two-Photon Absorption for Enhanced Biomedical Chiral Sensing

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C7_2, Machuca Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Chiral-molecule detection and sensing are critical in various fields such as life sciences, chiral drug development and micro-nano optical devices. The ability to detect and differentiate chiral enantiomers is essential for a range of applications, yet current technologies for chiral detection, particularly for trace-level signals, still face significant limitations. In this context, the chiral construction and optical properties of inorganic nanocrystals have emerged as a key research focus for the development of advanced chiral-enhanced sensing platforms.

In this abstract, we propose a novel approach that leverages nanocrystals as chiral building blocks, integrating them through 3D laser printing technology based on two-photon absorption. We employ photosensitive small molecules as molecular "glue" in the printing process to enable the formation of highly ordered 3D chiral structures composed of functional nanocrystals with high purity. These structures aim to exploit the unique chiral optical properties of the nanocrystals to amplify the sensitivity and selectivity of biomedical chiral sensing.

Our research investigates the formation mechanisms of the printed chiral nanostructures, focusing on the molecular-level interactions between lasers and nanocrystals. We optimize key printing parameters such as light intensity, exposure time, and molecular composition to enhance the resolution and homogeneity of the printed structures. Additionally, we explore the relationship between the intrinsic optical properties of the nanomaterials and the optical chirality of the printed 3D structures, aiming to clarify the mechanisms that lead to enhanced chiral signal detection.

To demonstrate the potential of our approach, we conduct in-situ laser processing of various nanocrystal types, achieving regional selectivity and interference-free integration. This will enable the construction of chiral nanophotonic platforms that offer enhanced chiral sensing capabilities, as well as new possibilities for polarization-based sensing and biomedical imaging applications.

Our findings will not only provide valuable scientific insights into the relationship between laser processing and nanomaterials, but also offer a theoretical framework for the future development of biomedical detection technologies. This research has the potential to revolutionize biomedical chiral sensing applications in a wide array of fields, including pharmaceuticals, diagnostics, and environmental monitoring.

The influence of laser surface treatment on the microstructure and friction-wear properties of Ti

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C7_1, Machuca Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The work concerns changes in the microstructure and tribological and wear properties of Ti grade 1 as a result of laser surface treatment. To shape the microstructure of the Ti grade 1 surface layer, a pulsed ytterbium fiber laser operating with a power of 6-60W, pulse length of 100 and 200 ns and frequencies of 10, 20 and 48 kHz was used. The analysis of the microstructure changes included examination of the chemical composition (EDS) and phase composition (XRD) as well as the microstructure of the surface layers using a confocal microscope and scanning electron microscope. It was shown that, depending on the laser surface treatment parameters used, the surface layers clearly differ in their chemical and phase composition and surface roughness. Laser surface treatment allowed for an increase in the friction-wear properties of Ti grade 1, which was tested in the ball-on-disc test in dry contact with a corundum ball as a counter-part material (3.2 mm in diameter, load 1 N). The value of the wear index Wv for laser-processed samples was 10 times lower than for unprocessed samples. The increased wear resistance of laser-processed Ti grade 1 was caused by the partial phase transformation of alpha-Ti into beta-Ti and the grain refinement that occurred as a result of the rapid heating and cooling induced by laser processing in the area of the near-surface layer. As heating and cooling conditions significantly affect the oxidation reactions of the titanium and resulting type of titanium oxide, their presence and amount also influenced on resistance to wear and CoF. Overall, compared to untreated Ti grade 1, the friction coefficient values for the laser-processed samples were two times lower.

Numerical simulation of weld heat input effect on microstructure and hydrogen diffusion in thick-walled S690 submerged arc welded joints

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

High-strength, low-alloy (HLSA) steels such as S690 are an attractive option for heavy industries such as offshore wind turbines and peripheral equipment due to their combination of excellent mechanical properties and weldability. The construction of these thick-walled structures requires highly efficient welding processes such as submerged arc welding (SAW). However, SAW presents challenges related to delayed hydrogen assisted cold cracking (HACC). Despite its importance, the effect of different diffusion coefficients on the cold cracking susceptibility of different microstructures within SAW-welded S690 steels is not fully understood. For this reason, the present study focuses on comparing the cold cracking susceptibility of thermomechanically rolled (TM) or quenched and tempered (QL) variants of S690 steel. SAW was performed on specimens of both steel grades to produce weldments consisting of weld metal, heat-affected zone (HAZ), and base metal. Electrochemical hydrogen permeation tests (ISO 17081) were performed to determine the microstructure specific coefficients. Using the obtained coefficients, a numerical model was developed to identify the time- and microstructure-dependent local hydrogen diffusion and its influence on the distribution within the welds. The results showed that the TM grade exhibited slightly accelerated hydrogen diffusion compared to the QL grade, which is beneficial for hydrogen reduction and increases the HACC resistance. However, the further simulations with different ply sequences showed that the welding heat input (i.e. welding ply sequence) had a significantly higher effect on hydrogen accumulation. Specifically, increased welding heat input and increased thicknesses decrease hydrogen diffusivity. For this reason, microstructure-specific hydrogen diffusion played a minor role in thick-layer SAW joints compared to the need to control the welding parameters (layer sequence, individual layer thickness, welding heat input).

HIP effect on superalloy casting weld repair

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C8_2, Seminario 6 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Hot Isostatic Pressing (HIP) is a process that involves simultaneous application of a high pressure and elevated temperature in a specially built vessel. HIP is a process used to densify powders and sintered parts, but it is also a standard ancillary operation in superalloys to reduce porosity in casting and health microcracks in welding process, and more recently, in additive manufacturing (AM). Thus, HIP improves mechanical properties of final component. This work is carried out within a welding process and microcracks related to this process in a nickel base superalloy.

Traditionally, there are two ways to measure HIP effectiveness for evaluation of microcrack healing in welding operation:

- 1) Metallurgical cut ups.
- 2) Mechanical testing.

In both cases, a sample with a certain number of specimens is manufactured with the same welding process for all the specimens. Then half of the population is HIPed and the other half is left as it is. Finally, specimens are evaluated for any or both methods mentioned above.

This procedure shows an evident weakness which is that in no case, HIP effect is checked over the same volume of material. Besides, in the case of metallurgical cut ups it is well known that a random number of cut ups is not representative of microcracks population unless, cut up sample size will be big, which is not the case in most of the studies.

The proposal to overcome these issues is to use Computed Tomography System (CT-scan), which is a non-destructive technique (NDT), and evaluate the same volume of material before and after HIP operation. Thus, the evolution with HIP of a set of microcracks can be studied and results analysed depending on their particular characteristics of each microcrack in terms of location, size, width or others.

An Easytom XL equipment from RX Solutions will be used for this study with micro and nano capabilities. The equipment has a potential voxel resolution up to 400nanometes which leads to a defect resolution around 1,2microns. However, measurement parameters and sample size will be optimized for expected crack size seen during previous screening through metallurgical cut ups.

In summary, this work shows an effective new way to evaluate HIP effect in those processes, such as welding, where HIP operation is used for improving metallurgical condition.

Chemical and microstructural evolution of the interface during simulated HIP diffusion welding of 316L and Inconel 625 alloys

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C8_2, Seminario 6 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Diffusion welding is a solid-state joining process by which two or more surfaces are welded using high pressure and temperature. This process allows welding of entire surfaces to fabricate large-scale components for fission or fusion power plants. During the process, the interface formed by surfaces evolves: densification and voids closure occur by diffusion and visco-plastic deformation mechanisms. Bounding joint migration is also observed thanks to grains coarsening and triple junctions movement. In most cases, the interface disappears after welding diffusion bonding plateau and the mechanical properties of the final component are sufficient to meet the required specification.

However, joining materials in which stable oxides or carbides form easily is not straightforward. This is the case of nickel rich stainless steels as alloy 800 or nickel based alloys as Inconel 625. These materials contain a low amount of aluminium and titanium, which diffuse and segregate at the welded interface into stable oxides and carbides. These reduce grain boundaries mobility across the interface, reducing its final mechanical strength. Despite this drawback, these materials are of a great interest due to their excellent high temperature mechanical properties and their high corrosion resistance compared to conventional 316L austenitic stainless steels.

The goal of this work is to study the evolution of the surface chemistry of the two investigated alloys (laminated sheets) by interrupting several heat treatments, simulating the HIP cycles envisaged. For this purpose, a full study of chemical surfaces evolution with temperature (up to 1100 °C) is done on a 316L stainless steel and on an Inconel 625 nickel-based alloy. Heat treatments are realized under vacuum in order to have a diffusion welding representative atmosphere during the heat treatment of each sample. Surface characterisation techniques as scanning electron microscope (SEM) coupled by energy dispersive X-ray spectroscopy (EDX), X-ray photoelectron spectroscopy (XPS) and glow discharge optical emission spectroscopy (GDOES) are used to observe from surface to the bulk the variation of the alloy's chemistry after each heat treatments.

This study aims to better understand the chemical evolution of the joining interface during the diffusion welding cycle in order to optimize the process for materials containing carbides or oxides forming elements.

Deformations in large aluminium automotive subframes

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C8_2, Seminario 6 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

In the automotive industry there is a market trend toward producing larger cast structures, as this reduces the need for mechanically joining numerous metallic pieces and decreases weight by minimizing the use of joining materials. At the same time the demand for lightweight automotive parts is increasing together with the market for electric cars. Lighter cars are necessary in order to compensate for the heavy weight of batteries and to enable longer range by smaller batteries. Aluminium components in cars last longer than steel, reduce wear on road infrastructure due to lighter weight, and are more energy-efficient to recycle than steel or composites, supporting sustainability. The larger parts that are made with only one material type will be easier to recycle, which promotes sustainable production patterns. However, to produce the larger one-piece cast structures in aluminium, deformations must be controlled. Aludyne Norway is the largest producer of safety critical aluminium automotive subframes in Europe, and is developing new tools and technologies together with customers to reach this goal. In addition to defects like porosity and cracking it is especially the distortions that have to be controlled in order to increase the size of single piece products. The casting process includes the solidification in a mould, cooling after ejection from the mould, sand core knock-out and removal of the feed gates followed by the heat treatment process including quenching and artificial ageing. Generally, we will then have a deviation from the detailed CAD geometry. Remark that the deviations do not only appear from thermal gradients and internal stresses developed during solidification, cooling and degating, but also from the mould distortions. The mould will be hot and thereby thermally expanded when the liquid metal solidifies against the mould walls. The mould distortions are typically the main cause of the as-cast deformation. After solidification the heat treatment with creep at high temperatures will add to the distortions, and large thermal gradients can lead to deflections and warping during water quenching. Industrial data shows very large variations in quench distortions dependent on the position in a rack with automotive parts. The whole process chain is modelled with a finite element model, developed in-house by the authors, and results are compared with industrial data from several different products, both regarding as cast deformations and regarding movement during quenching with respect to positions in the heat treatment rack.

Experimental Study of Dissimilar Yb: YAG Laser Beam Welded Inconel 718 to Ti-6Al-4V

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The present study investigates the microstructural evolution and characterization of dissimilar metal lap welds between copper-plated Inconel 718 and Ti-6Al-4V alloys, focusing on the influence of varying copper plating thickness and laser power density on the resultant joints' microstructure. Each weld involved copper-plating one of the two base metal (BM) plates employing an acid bath, varying the plating duration to control the final copper thickness. Dissimilar welding was performed on 2 mm plates using a Yb: YAG laser at two distinct power densities, namely 1.3 and 1.5 kW, allowing an assessment of heat input variations on weld integrity. The microstructural analysis of the fusion zone (FZ) and heat-affected zones (HAZs) was performed using visible light microscopy (VLM) and scanning electron microscopy (SEM) coupled with energy dispersive spectroscopy (EDS), while the joints' crystallographic structure was examined via X-ray diffraction (XRD). Mechanical performance estimation was carried out through Vickers microhardness testing. The metallographic examination revealed defects such as keyhole porosity and cracking, particularly at the BM interface, as well as lack of penetration in specimens welded at 1.3 kW power. Moreover, macrosegregation was observed, especially in welds where the Ti-6Al-4V BM formed the upper section of the lap joint, a phenomenon attributed to the different solubilities and diffusivities of Al and V. Additionally, Marangoni convection further influenced the non-uniform distribution of these elements due to cooling rate variations and directional solidification, which contributed to crack initiation. Microstructural examination indicated that the joints were primarily characterized by the precipitation of ternary intermetallic compounds (IMCs) consisting of Ni, Cu, and Ti, findings that also correlated with the Vickers microhardness results. In conclusion, a higher laser power density was observed to improve weld penetration while reducing the occurrence of crack formation.

Keywords: electroplated copper interlayer, dissimilar metal welding, Yb: YAG laser beam welding, Inconel 718, Ti-6Al-4V, microstructure, Vickers microhardness.

Analysis of Austempered Ductile Iron Castings Reinforced with Titanium Carbides

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C8_2, Seminario 6 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The aim of the presented research was to produce a new cast composite material based on the attractive engineering material ie. ADI (Austempered Ductile Iron). The transformation of ADI cast iron into a composite material was based on SHSB (Self-Propagating High-Temperature Synthesis in Bath) reaction. This was a “solid Ti” – “solid C”, which ensures that TiC particles are obtained in the microstructure of the alloy. The titanium carbides are thermodynamically stable as a result of their covalent bonding nature, so they do not undergo transformation during the heat treatment process. In the present work castings with different wall thicknesses ranging from thin-walled, i.e. 3 mm, up to 25 mm were attained. The study showed that it is possible to produce a ADI using the SHSB reaction in which titanium carbides of up to 5µm in size are evenly distributed in metallic matrix. Heat treatment was carried out to attain upper and lower ausferrite, reinforced with titanium carbides. The characterization of novel ADI material in terms of mechanical and performance properties was carried out using XRD (synchrotron radiation), light microscopy, scanning microscopy and mechanical properties. Finally, it was shown that ADI strengthened with TiC using SHSB synthesis makes it possible to obtain an attractive material that can be used in demanding areas such as defence, railroad or automotive.

Key words: ADI, heat treatment, “in situ” composites, MMCs composites, SHSB reaction, titanium carbides.

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Solidification and structure of thin-walled austenitic ductile iron castings

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C8_2, Seminario 6 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Austenitic ductile iron, with a nickel content of 20% to 36%, is characterized by nodular graphite that is relatively uniformly distributed within a face-centered cubic matrix. This unique microstructure gives the material relatively high strength, ranging from 380 to 550 MPa, along with exceptional ductility, often achieving elongation exceeding 45%. In addition to its excellent mechanical properties, Ni-Resist ductile iron offers high resistance to creep, corrosion, and wear. It also boasts outstanding castability and machinability, making it a versatile material for various industrial applications. Capable of performing reliably across a broad temperature range from -200°C to 850°C, it is widely used in demanding environments. Typical applications include gas turbine housings, gas compressors, motor components, and other critical engineering parts that require both structural integrity and durability under harsh conditions.

This study presents research findings on the primary structure and graphite eutectic formation in castings with wall thicknesses characteristic of thin-walled components (≤ 5 mm), compared to thicker castings (25 mm). The investigation explored the use of Ti, Zr, Nb, and CeO₂ as potential grain refiners. Metallographic analyses, including electron backscatter diffraction (EBSD), were conducted to examine the macro- and microstructural characteristics during the primary and eutectic solidification of austenitic ductile iron. Additionally, novel quantitative assessments were performed to evaluate the morphology and distribution of graphite nodules. The results demonstrated that in thin-walled castings, the primary structure can be effectively refined using Ti and CeO₂, promoting a transition from columnar to equiaxed grains. This transformation is strongly influenced by metallurgical process parameters and the cooling rate at the onset of solidification.

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Investigation of medieval arquebuses made from malleable iron

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

In the 15th and 16th century, arquebuses played a decisive role for military operations.

Several arquebuses were provided for non-destructive testing, such as ultrasonic testing, hardness testing and borescope measurements in order to investigate the forge welding processes in this medieval age. In addition, one piece of an arquebus was investigated by light optical microscopy and wet chemic analysis and was compared to wall closure parts from the same age.

Pig iron was produced by a wolf furnace where roasted iron ore and charcoal was fed. The iron was reduced in the solid state and further beaten out.

It was found that the carbon content of the pieces is very low, and the slag amount and composition differ in dependence of the application. The production of the arquebuses under investigation was done by mandrel forging. The initial material was beaten out to a rectangular blank, which was twisted on a mandrel and further forge welded. Apparently, different blank geometries have been used, i.e. stepwise and beveled, which, together with the pre-material and forging conditions has a strong influence on the final geometry and quality of the forging welds.

The Pögl family was a famous family at that time in Styria/Austria with several hammer mills. They developed an advanced forge welding procedure which resulted in outmatching material and product quality.

Additively Manufactured short carbon fibre reinforced Polymer and Aluminium alloy Multi-Material joints using Friction Stir Welding (FSW) for light and thermal management applications in the transport sector.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The EU aims to be climate-neutral by 2050 – an economy with net-zero greenhouse gas emissions. In this sense, lightening the weight of components used in the transport sector has become a strategic point for reducing CO₂ emissions. In this context, the gradual replacement of actual 100% aluminium components with hybrid aluminium-polymer solutions can become a strategic line for the transport sector. These innovative approaches aim to reduce weight while ensuring properties such as heat dissipation; a capability that polymers alone often lack. Friction Stir Welding (FSW) emerges as a crucial advanced technology for joining aluminium and polyamide (PA6) reinforced with short carbon fibres, both additively manufactured.

Friction Stir Welding offers several advantages, including the ability to create strong, defect-free joints at relatively low temperatures, minimizing thermal distortion and preserving the mechanical properties of the materials involved, but definitely, the most important advantage of FSW is that the material does not melt. As industries seek to improve efficiency and sustainability, the development of these hybrid materials reflects a promising trend towards innovative engineering solutions that leverage the unique properties of each constituent material, ultimately leading to enhanced product performance and longevity.

This study employed a heavy-duty robot equipped with a Friction Stir Welding (FSW) head to create joints between multi-materials fabricated through additive manufacturing. The polymer matrix, polyamide 6 reinforced with short carbon fibres, was produced using Material Extrusion (MEX), while the aluminium alloy AlSi10Mg was manufactured via Laser Powder Bed Fusion (L-PBF). To ensure the integrity of the polymer and prevent degradation due to elevated temperatures, optimal processing parameters were meticulously determined. Furthermore, to enhance the mechanical strength of the joints, various interlocking strategies were developed and strategically implemented by the research team. Comprehensive visual inspections of the joints were conducted alongside mechanical testing to assess the viability and effectiveness of this innovative approach. The results aim to contribute significantly to advancements in multi-material welding technologies within the context of additive manufacturing.

In this international research study facilitated by the European Multhem project under the Horizon Europe program, the successful integration of polymeric materials with aluminium alloys was achieved through the FSW technique. Innovative interlocking strategies between the two materials enhanced the mechanical strength of the joints. This solution applies to two actual industry use cases in the transportation sector, including one for an aerospace component belonging to the multinational THALES.

Optimization of A-TIG welding for X5CrNi18-10 stainless steel

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The paper presents the influence of the activation flux type on activated flux tungsten inert gas welding (A-TIG) of the X5CrNi18-10 stainless steel. In introduction part properties and application in energy production sector of X5CrNi18-10 stainless steel was investigated. The A-TIG process was explained and the possibility of welding stainless steels using the A-TIG process to maximize productivity by applying reduced or completely without edge preparation was presented. In the experimental part 3 mm thick X5CrNi18-10 stainless steel sheets have been welded in butt joint configuration using TIG and A-TIG welding methods. Three substances were examined as single component fluxes in this experiment: calcium oxide (CaO), silicon dioxide (SiO₂) and ferric oxide (Fe₂O₃). The welding process was performed by automatic guiding system driving a TIG welding torch. With selected A-TIG welding technology machining preparation of plates and consumption of filler material have been avoided. Specimens sectioned from the produced welds have been subjected to bend testing according to the standard ISO 5173:2023, macrostructure analysis and corrosion resistance analysis. The results have confirmed that this type of stainless steel can be welded without edge preparation and addition of filler material when silicon dioxide (SiO₂) as single component flux is used.

Influence of brazing parameters on the microstructure and mechanical properties of nickel-based superalloys joints

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C8_2, Seminario 6 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Furnace brazing is a well-established process in the aerospace industry, especially for the assembly of turbine components. The joint is created thanks to the diffusion of elements between the base metal (the parts to be assembled) and a liquid filler metal of similar composition. This complex process leads to the formation of numerous phases in the joint and a modification of the base metal in its vicinity. The present work, a collaboration between Safran Aircraft Engines and the Institut des Matériaux de Nantes Jean Rouxel, aims to study the impact of brazing parameters, such as the brazing duration and temperature, on the microstructure of the joints and its mechanical performances. To gain a better understanding of the role of grain boundaries on the diffusion process, two base metals are being compared: a polycrystalline nickel-based superalloy and a single crystal. This study also examines how boron and silicon, used to lower the melting point of filler metals, affect the joint microstructure and properties. As reported in previous studies, they tend to form hard and brittle phases, particularly detrimental to the mechanical properties. Therefore, two filler metals with different melting point depressant elements are compared.

The microstructures were characterised using Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS) and Wavelength-Dispersive Spectroscopy (WDS). Electron BackScatter Diffraction (EBSD) was also performed to identify the different phases encountered within the joint. The mechanical properties were assessed thanks to microhardness testing.

Influence of weld-related thermal cycles on the sensitization of AA5XXX

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Aluminum alloys, particularly AA5XXX, find widespread application in critical sectors like maritime and automotive industries. However, their susceptibility to stress corrosion cracking (SCC) following welding processes poses a significant risk of premature failure. This phenomenon is attributed to the formation of a brittle beta phase during post-weld cooling, a process known as sensitization. This study employs advanced computational tools to investigate the influence of welding-induced thermal cycles on the kinetics of beta phase formation in AA5XXX alloys. By simulating the evolution of microstructural phases and predicting the extent of sensitization, this work aims to provide valuable insights for optimizing welding parameters and developing robust post-weld heat treatment strategies to mitigate SCC risk and enhance the long-term reliability of these critical components.

Microstructure comparison of welded Nitinol thin foils with linear, oscillating and pulsed laser beam

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Nitinol is meanwhile a well-known smart material with its superelastic and shape-memory behaviour. It is a good choice for demanding applications from medical, aerospace, robotics and other important technological fields. One significant stumbling block is through its poor workability. Welding may be a good solution for producing complex shapes. Especially if very tiny parts are needed, laser welding of thin foils of Nitinol may open the way for new challenging applications like antennas and other innovative products. In previous work of the authors it was shown that oscillation of the laser beam was favourable for welding Nitinol components with regard to the mechanical properties, microstructure and alteration of transformation behaviour of the weld. As for the welding of thin foils pulsed laser beam has also have been advantageous for the resulting microstructure, the goal of the presented study was the investigation of the microstructure development and the properties of Nitinol thin foils welded with pulsed in comparison to continuous laser beam. The combination of laser beam oscillation and pulsed operation has not yet been investigated for welding thin Nitinol foils.

Experimental evaluation of TIG lap welds made from 316L sheets for use in liquid hydrogen storage tanks.

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C8_1, Seminario 7 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The shipbuilding industry is currently facing challenges in the development and construction of onboard liquid hydrogen (LH₂) storage tanks. Austenitic stainless steels (e.g., 316L) are among the materials considered suitable candidates for use as the inner part of the tank in direct contact with LH₂.

In the context of the current work, AISI 316L TIG welds carried out on thin sheets, which were previously subjected to certain levels of uniaxial pre-strain (10%, 20%, 30%, and 40%), were evaluated in terms of their microstructure and hydrogen uptake. The investigation covers a range of selected heat input rates in relation to the welding conditions. Cathodic charging was used to introduce hydrogen into the weld metal and the heat-affected zone.

The effect of hydrogen was evaluated in two aspects: the amount of hydrogen absorbed and its impact on the mechanical properties of the weld. In this regard, Thermal Desorption Spectroscopy (TDS) analysis and hardness tests were performed for selected combinations of the experimental conditions employed.

The results obtained so far allow for the correlation of microstructural features and hydrogen absorption with the welding conditions used for the welds. It is anticipated that the experimental findings will shed light on the mechanism of hydrogen uptake and its interaction with the weld metal (WM) and the heat-affected zone (HAZ) exposed to liquid hydrogen (LH₂). This is expected to contribute to the development of structures with tailored properties for LH₂ storage and marine transportation applications.

Identification of the dissipative micro-mechanisms during mixed-mode fracture of pressureless silver sintered joints in power packages

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Lead-based solders remain in use for high-power semiconductor devices due to a lack of alternatives. Pressureless silver sinter is the most promising replacement, offering a high melting point, excellent electrical and thermal conductivity, low elastic modulus, and low processing temperature. This study investigates the microscopic failure mechanisms affecting interface fracture toughness in two pressureless sintered silver interconnects under mixed-mode delamination. One material contains nanoparticles (NP) between 100–800nm, while the other consists of microflakes (μF) between 1–10 μm . Both were sintered between silver-electroplated copper plates at 250°C and 280°C, forming $\sim 45\mu m$ porous silver layers.

The mixed-mode fracture behaviour was measured with a custom miniature mixed-mode bending setup achieving steady-state delamination at a controlled mode-mixity between mode-I and -II loading, with in situ optical microscopy and digital image correlation to monitor the crack-tip strain field evolution [1,2]. Each test was complemented with post-mortem Scanning Electron Microscopy (SEM) fractography analysis.

The two interconnect materials show pronounced differences in failure behaviour, either interface delamination or bulk fracture, and mixed-mode interface fracture toughness. The NP-interconnects exhibit an expected (nearly linear) increase in interface fracture toughness with increasing mode angle. However, the μF -interconnect exhibits a never-reported minimum in the fracture toughness at $\sim 15^\circ$ mode angle, constituting a 3-fold decrease compared to mode-I delamination. Careful investigation of the cracked samples, by combining side-view SEM imaging, optical profilometry of the fracture surface, and x-ray CT scanning, revealed the intricate details of this unexpected behaviour, showing, e.g., that the fracture morphology switches from bulk to interface fracture between a mode angle of 0° and 30° . This study offers valuable insights into the complex interplay between the microstructures of the interconnect, its failure micro-mechanisms, and the resulting mixed-mode interface fracture toughness [3].

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High-temperature interactions of amorphous alloys TiCuZrPd with a Kovar substrate

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Modern industrial applications require joining of heterogeneous materials without increasing weight, particularly in the sectors of transportation, aerospace, and automotive industry where enhanced mechanical and thermal properties are essential. In particular, the rapidly developing space sector imposes specific requirements and exhibits significant interest in joining dissimilar materials, especially in applications where monolithic structural components are replaced by chemically and structurally complex materials. The most promising method for achieving durable joints is high-temperature brazing, which enables bonding without melting the base metal, thereby preserving its initial structure and properties, provided that a properly selected brazing filler and optimized temperature-time parameters are used in the joining process.

Consequently, the research on the welding of dissimilar materials was conducted, focusing on the analysis of physicochemical phenomena occurring at the solder/substrate interface. High-temperature joining of FeNiCo alloy was investigated using amorphous TiCuZrPd solder with varying palladium and tin content. The commercial Kovar alloy (4J29) was used as the substrate. Wettability tests showed that for the solder alloys indicated as Pd-10 and Pd-14, the wetting angle was about 47°, while for Pd-20 and Sn-2, it was around 87°. Despite the limited wettability, durable and homogeneous joints were obtained without defects such as separation, cracking, or discontinuities in the intermetallic layer. At the substrate-solder interface, a reaction zone was formed, consisting of two intermetallic layers: Fe₂Ti (IMC1) and Ti₂Cu/CuTi (IMC2), resulting from the diffusion of elements between the filler metal and the substrate. The least favorable properties were observed for joints with Pd-14 solder. DSC analysis revealed that the solder material retains its glassy properties under rapid heating during the high-temperature joining process, passing through a supercooled liquid phase with high deformability typical of metallic glasses, enabling precise adaptation to the joint geometry. TMA analysis indicated a linear volume change of the system during heating, up to the point of the increased plastic deformation under the stress. Structural cross-sectional studies confirmed the formation of a reaction IMC zone on both edges of the solder-substrate interface. The results demonstrated that brazing of the system Kovar/Pd-X/Kovar is feasible at 880°C without the need for interlayer or fluxes. The results demonstrated that brazing of the system Kovar/Pd-X/Kovar is feasible at temperature 880°C.

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Component-test for determination of welding residual stresses and their effect on stress relief cracking in thick-walled welds

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Controlling the residual stress level during welding of creep-resistant Cr-Mo-V steels is crucial to avoid so called stress relief cracking (SRC) during post weld heat treatment (PWHT) of large-scale components. In the present study, a laboratory scale test specimen (slotted sample with 400 mm width, 400 mm length and 25 mm thickness) was used to simulate thick-walled component welds made of 13CrMoV9-10. The aim was to identify the level and distribution of residual stresses to evaluate the suitability of the specimen for laboratory based SRC testing. High restraint was ensured by the specimen geometry with a narrow welding gap in the center. This gap was filled by multi-layer submerged arc welding. Two specimens were welded with identical parameters and compared in the as-welded state and after PWHT (705 °C for 10 h). Neutron diffraction was used to determine the residual stresses in the weld metal, the heat-affected zone (HAZ) and the base material at different depths longitudinal, transverse, and normal to the welding direction. The experiments were performed on the former instrument E3 of the research reactor BER II of Helmholtz-Zentrum Berlin (HZB), Germany. Complementarily, laboratory X-ray diffraction was applied to characterize the surface residual stresses. In the welded condition, especially in the weld metal and the adjacent HAZ, the longitudinal residual stresses reached values of up to 1,000 MPa to 1,200 MPa due to the increasing strength and hardness of the CrMoV-material during welding. The conducted welding experiments revealed that way higher residual stresses in the welded joint have to anticipated before the PWHT is performed than it was expected in advance. This demonstrated the necessity of suitable component-like welding tests as they must ensure realistic mechanical stiffness (hindered shrinkage of welding joint by slotted self-restraint sample) and heat dissipation conditions (definition of minimum welding joint thickness vs. welding process-specific heat input).

Microstructural and Mechanical Properties Study of Friction Stir Welded 316L Stainless Steel

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C9_3, U1 Room (Level 0), settembre 18, 2025, 17:00 - 19:00

Bead on plate Friction Stir Welding (FSW) was used in the current study to simulate butt welding of 316L stainless steel, which requires a WC welding tool and high welding parameters. Once the optimal welding parameters had been determined, the cross section of the plate was metallographically inspected to ensure that the weld had penetrated through the entire thickness and that the FSW'ed material had no defects or WC particles originating from the welding tool. Optical and Scanning Electron Microscopy (SEM) metallographic characterization, along with microhardness tests, were performed on each of the different zones of the welded joint, namely, the parent material, the heat affected zone (HAZ), the thermomechanically affected zone (TMAZ), and the stir zone. Both the parent material and the FSW'ed material were subjected to tensile tests and fractography studies. As for the parent material, there were minor differences between specimens whose longitudinal axis was parallel to the rolling direction of the plates and specimens whose longitudinal axis was normal to the rolling direction. FSW'ed specimens showed higher microhardness and yield strength, but fracture always occurred within the stir zone. An Electron Back Scatter Diffraction (EBSD) and Transmission Electron Microscopy (TEM) study were performed to investigate the microstructural changes during welding. The occurrence of microstructural changes during welding as well as their influence on the mechanical properties will be referred and discussed.

Recrystallization mechanisms activated during multi-pass forging of austenitic stainless steels

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C9_3, U1 Room (Level 0), septembre 18, 2025, 17:00 - 19:00

Multi-pass forging is widely used to produce large components in austenitic stainless steels for Generation III and III+ nuclear reactors. A better understanding of the multi-pass forging process is essential for optimizing the final microstructure and mechanical properties of the materials. This study aims to investigate and model the microstructural evolution during multi-pass thermomechanical processing, with particular emphasis on the mechanisms of dynamic and post-dynamic recrystallisation. To achieve this, uniaxial hot compression tests were performed as an experimental simulation of multi-pass hot forging, exploring different thermomechanical conditions and focusing on small strain increments. The resulting microstructures were characterised using SEM-EBSD. The EBSD data were then used to develop a mean-field model integrating dynamic and post-dynamic recrystallisation phenomena. In addition, the effects of successive deformations on the microstructure were analysed to better understand the role of elastic stored energy in recrystallisation mechanisms and its effect on the final grain size distribution.

Textural evolutions in aluminum alloys building by multi-layer friction surfacing (MLFS) deposition

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C9_3, U1 Room (Level 0), septembre 18, 2025, 17:00 - 19:00

The texture of aluminum alloys in additive manufacturing (AM) using multi-layer friction surfacing (MLFS) was analyzed through electron backscatter diffraction (EBSD) characterization. This study focused on three different aluminum alloys: AA5083, AA6061, and AA7075. After conducting MLFS deposition in the solid state and optimizing the corresponding processing parameters, various sections of the consolidated aluminum alloy structures were characterized using EBSD to reveal their microstructural details and dominant orientations. The textural assessments indicated a significant contribution of shear-based components induced by the friction stirring process, particularly in the direction normal to the building orientation (BD). Comparing the three alloys, it was found that as the fraction of secondary phase precipitates increased from AA5083 to AA7075, the predominant shear-based texture was notably influenced by the role of micro- and nano-scale precipitates. Microscopic observations suggest that these precipitates can affect the dynamics of recrystallization (DRX) through particulate-stimulated nucleation (PSN) and Zener-pinning mechanisms. Consequently, the preferred orientation shifts from the ideal shear texture to a greater prevalence of other texture components.

Microalloyed steel wires reinforced with a titanium core

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C9_1, Picasso Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

To achieve the desired combination of strength and ductility, metal-to-metal composite systems are increasingly being used. The primary advantage of such structural materials lies in two aspects: first, the ability to combine the properties of the individual components within the composite, and second, a thorough understanding of their mechanical and physical properties, which facilitates their use under specific operating conditions. This latter aspect means that new metal-to-metal composite materials require fewer tests and preliminary studies before their potential application, particularly for structural components that are critical from a safety perspective.

The presented research results concern a multilayered material produced through multi-stage wire drawing. The resulting heterostructural material is based on microalloyed steel and reinforced with Ti particles formed by fragmentation of the internal layers of the steel-Ti multilayer systems. The wire drawing process was studied for initial diameters of 6.5 mm, 1 mm, and 0.3 mm. Two basic configurations were used for the studies: tube-tube-rod and tube-rod, made of microalloyed steel and Ti. The evaluation of rheological properties, both of the individual components and the final multilayered systems, enabled a discussion of the relationships between the parameters of the wire drawing process and the development of the microstructure and the accompanying strengthening mechanisms, particularly grain refinement.

At a relatively early stage of the experimental studies, variations in the occurrence of severe plastic deformation (SPD) effects, such as continuous recrystallization, were observed in the Ti layers and the steel matrix. Mechanical property studies of wires with diameters of 1 mm and 0.3 mm, supported by microstructural analysis using optical and scanning microscopy, revealed the complexity of the interaction of various strengthening mechanisms on the rheology of the examined multilayered systems. Particular attention was given to the development of strain hardening in the heterogeneous systems under study. Comparing wires drawn without inter-stage annealing to those subjected to heat treatment revealed different impacts of the multi-stage wire drawing history on both the effects of continuous recrystallization and the interactions between neighboring steel and Ti layers.

Based on the obtained results, conclusions were formulated to guide further research on heterostructural systems produced through plastic deformation.

Acknowledgment

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Application of the stochastic model of thermomechanical processing to simulation of the evolution of heterogenous microstructures and evaluation of the uncertainty of the product properties

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C9_2, U1 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

Two aspects of the thermomechanical processing of steels are considered in the paper. The first is problem of the heterogeneity of the modern steels' microstructure, which has been intensively studied during last few decades. It was shown that complex phase steels with heterogeneous microstructure show excellent mechanical properties. The second aspect is connected with uncertainty of the properties of products. Many researchers have pointed out recently that the knowledge of the possible spread of parameters, such as a grain size, is needed for a reliable design of the production processes. In the industrial conditions the variations of final product properties are caused by uncertainties in the boundary conditions during the manufacturing and by the stochastic character of some metallurgical phenomena. We assumed that the stochastic model of multi-step hot deformation and controlled cooling after deformation can deal with both these aspects. In the stochastic hot deformation model a random character of the recrystallization was introduced. The model was extended by including phase transformations during cooling after hot forming. Nucleation of the new phase was considered as random process. In consequence, prediction of the heterogeneity of the microstructure in the room temperature became possible. Reliability of the model depends, to a large extend, on the proper identification of the coefficients in this model. Identification of the hot forming model was based on the inverse analysis for the hot compression tests. Identification of the stochastic model of phase transformation was based on the continuous cooling dilatometric tests. The complete model calculates histograms of the grain size during thermomechanical processing, as well as histograms of microstructural parameters of the final products after cooling. Relations between microstructure and mechanical properties allow to evaluate the uncertainty of the latter. In the present work the model was applied to simulations of industrial processes of rolling and controlled cooling of eutectic steel rails and bainitic steel rods. Histograms of the microstructural parameters were calculated for various cooling strategies. Advanced features of the microstructure, which decide about products properties, such as interlamellar spacing in the pearlite or thickness of ferrite plates in the bainite, were calculated. The variations of final product properties, which include hardness of rails and strength of rods, were evaluated.

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Enhancing mechanical properties of NbTi alloys by thermomechanical processing

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C9_3, U1 Room (Level 0), septiembre 18, 2025, 17:00 - 19:00

Ductile NbTi alloys are prominent superconducting materials that exhibit superconductivity under high magnetic fields, making them suitable for particle accelerators, fusion reactors and magnetic resonance imaging (MRI) systems. For example, Nb-47wt.%Ti alloy is utilised in the superconducting magnets of the Large Hadron Collider (LHC) at CERN and in the poloidal field and corrector coils of the ITER magnet system, while Nb-55wt.%Ti alloy is employed in components of the superconducting radiofrequency crab cavities for the High Luminosity LHC (HL-LHC) upgrade. Compared to other high-performance superconductors, NbTi alloys are more cost-effective, have more suitable mechanical properties, in particular ductility, and are easier to fabricate, making them the practical choice for most applications. Metallurgically, both Nb-47wt.%Ti and Nb-55wt.%Ti are full β -phase alloys, due to their high niobium content. However, compared to α -phase or $\alpha+\beta$ -phase titanium alloys, these bcc β -phase alloys exhibit lower mechanical strength and Young's modulus.

This study focuses on enhancing the mechanical properties of β -NbTi alloys through thermomechanical processing, specifically cold working (CW), heat treatment (HT), and their combination (CW+HT). The goal was to refine the grain structure, minimize contamination, and achieve a hardness exceeding 170 HV1. Nb-47wt.%Ti and Nb-55wt.%Ti alloys were subjected to compressive deformation to 40% strain and rolling reductions of 35%, 65%, 82%, and 94%, respectively. Subsequent HT was performed at various temperatures to analyse the combined effects of CW and HT. As-received and processed samples were analysed using computed tomography (CT) to verify the absence of flaws or imperfections induced by CW. Further characterization of the materials was conducted using light microscopy (LM), scanning electron microscopy with energy-dispersive spectroscopy (SEM+EDS), X-ray diffraction (XRD), microhardness testing, and nanoindentation to evaluate phase composition, microstructure, and mechanical properties as functions of HT temperature and applied strain.

The findings demonstrated that cold working followed by heat treatment significantly enhanced the mechanical properties of both alloys. For the Nb-55wt.%Ti alloy, different levels of CW followed by HT at 400°C resulted in a 50% increase in hardness. Similarly, for the Nb-47wt.%Ti, a rolling reduction of 65% combined with HT at 375°C led to a 20% increase in hardness. These improvements were attributed to the synergistic effects of second-phase precipitation and cold work-induced strengthening mechanisms.

Cooling Effect of Remaining Water Layer on Various Steel Surfaces

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C9_1, Picasso Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

Accurate prediction and control of the cooling process during hot rolling are crucial for producing high-quality steel with the desired mechanical properties. In many steel companies, hot-rolled steel plates or strips are commonly cooled on a run-out table or in a continuous annealing line using laminar jets or spray cooling, which involves a large amount of water impinging on the steel surface. This process forms a water layer on the top surface, which changes the cooling intensity significantly. The water layer is often removed by water wipers or using air knives; however, thin water layer remains on the surface in most cases. Due to surface tension, this thin water layer forms on both the top and bottom surfaces. The remaining water layer is also formed when using light sprays and can significantly affect the final temperature of the steel strip, especially if the target temperature is below 500 °C, as confirmed by steel producers. This study experimentally investigates the influence of the remaining water layer on heat transfer during cooling after hot rolling. Cooling experiments were conducted using a full-cone spray nozzle and moving steel samples with two different surface finishes: a grinded surface ($R_a = 0.9 \mu\text{m}$) and an oxidized surface ($R_a = 3.1 \mu\text{m}$, oxide thickness $27 \mu\text{m}$). The cooling effect of the remaining water on both surfaces was compared to determine the impact of surface quality.

HPT processing of Cu-Mo composites with tailored properties for thermal management

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C9_1, Picasso Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The growing power density of modern electrical devices requires advanced materials with high thermal conductivity and controlled thermal expansion to ensure efficient heat dissipation and long-term reliability. Copper-molybdenum (Cu-Mo) composites are attractive candidates for thermal management applications due to their unique combination of thermal properties. However, conventional processing techniques, such as powder metallurgy, often result in porosity and limited microstructural control, which can negatively impact their thermal performance. An alternative way would be severe plastic deformation which enables to obtain fully dense materials with significant grain size refinement and improved material homogeneity.

The purpose of this study is to fabricate Cu-Mo nanocomposite from an array of individual disks using high pressure torsion (HPT), determine number of turns required to obtain homogenous microstructure, determine mechanism of its formation and characterize the obtained microstructures and resulting thermal properties. Nanocomposite was fabricated from a system of 3 layered Cu-Mo-Cu disks with thickness 0.4, 0.2 and 0.4 mm. The samples underwent HPT processing with varying numbers of revolutions (from 10 to 200). The results indicate that a fully homogeneous nanostructure, with equiaxed Cu grains (~30 nm in diameter) and dispersed Mo particles (~20 nm in diameter) is obtained after 200 revolutions. The grain size reduction of copper matrix is larger by an order of magnitude comparing to pure Cu, whose grain size after HPT is usually about 250 nm. Additionally, thermal conductivity measurements conducted using the laser flash analysis (LFA) method revealed that the processed Cu-Mo composites demonstrated only a slight reduction in thermal conductivity compared to bulk Cu, making them viable candidates for heat spreaders. The absence of porosity and the uniform dispersion of Mo ensured improved thermal stability, which is crucial for applications in high-power electronic devices.

This study highlights the potential of HPT as an effective method for producing Cu-Mo nanocomposites with tailored microstructures and optimized thermal properties. The results suggest that HPT-processed Cu-Mo composites could serve as a promising alternative to conventionally manufactured thermal management materials, offering improved performance and processing flexibility.

Keywords: Cu-Mo composites, nanostructured materials, thermal management, high-pressure torsion, thermal conductivity, microstructural refinement.

Effect of Stacking Fault Energy Regulation on the Microstructure and Mechanical Properties of Cu-Al-Zn-Sn Alloys

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Recent research has led to the development of new coloration methods for metallic materials. Among these, surface treatments have been widely used and optimized for different metals. However, a major drawback is that the colored layer is easily damaged by external influences and chemical reactions. To address this issue, we developed color alloys by selecting intermetallic compounds or solid solutions that naturally exhibit specific colors. In solid-solution alloys, these unique colors result from optical transition energies reflected within the visible light spectrum, which can be controlled through careful compositional design. Most transition energy-controlled color alloys are based on Cu alloys, but their weak mechanical properties make them difficult to apply in various fields. To improve this, we modified the microstructure of Cu-Al-Zn-Sn alloys through cold rolling, hot rolling, and annealing processes. We focused on defects formed in Cu-based alloys with low stacking fault energy during plastic deformation and heat treatment, intentionally inducing these defects to enhance mechanical properties. Additionally, by adjusting the Al content, we controlled the stacking fault energy to regulate defect density and analyzed how these changes affected mechanical performance. Our findings provide insights into the development of color alloys with both enhanced mechanical strength and tunable optical properties.

Carbon Nanomaterials Reinforcements in Inconel 718: Enhanced Strength, Thermal Stability, and Tribological Characteristics

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C9_1, Picasso Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The increasing demand for extended component lifespan and reduced energy consumption requires the development of novel materials. Metal matrix composites (MMCs) reinforced with various carbon nanomaterials have the potential to achieve high strength, superior thermal stability, and enhanced self-lubrication characteristics [1-3]. Carbon nanomaterials might serve as effective solid lubricants at elevated temperatures due to their higher thermal decomposition resistance compared to conventional liquid lubricants. Typically, these materials are applied as coatings to achieve self-lubrication [4]. This study investigates an alternative approach by incorporating carbon nanomaterials into a nickel-based superalloy matrix (Inconel 718) to develop particle-reinforced self-lubricating MMCs for potential application in extreme environments.

Bulk composites were fabricated from powders via severe plastic deformation using high-pressure torsion (HPT) of Inconel 718 with different quantities of graphite, graphene, and carbon nanotubes (CNTs). The objective is to find optimal processing parameters and solid lubricant concentrations to achieve optimum tribological and mechanical properties.

Despite differences in chemical bonding, a homogeneous distribution of the solid lubricant phase was achieved through a combination of colloidal mixing and HPT deformation. Microhardness measurements were conducted to analyze the evolution of hardness as a function of graphite content, applied strain, and processing temperature, resulting in ~1.6 GPa hardness differences compared to the Inconel 718 reference material. Micro-tensile tests revealed exceptionally high tensile strength values exceeding 2.1 GPa for MMCs reinforced with up to 1wt% graphite, while maintaining ductile deformation behavior. In-situ high-temperature nanoindentation and X-ray diffraction confirmed superior thermal stability of graphite-reinforced composites. Stable self-lubrication and mild wear behavior, with a sixfold reduction in the coefficient of friction for 5wt% graphene- and CNT-reinforced composites as confirmed by micro-tribological testing.

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The influence of thermal interference fit value on the stress and strain distribution in the area of divided tools used in the dynamic hot hammer forging process

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C9_2, U1 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

One of the methods for generating cost savings in the die forging process of heavy products on a hammer is the use of split dies. The selection of appropriate models for predicting die wear allows for the identification of areas with the most intense wear, which can be incorporated as a replaceable die insert. The nature of the hammer forging process requires the use of uniform tools, as any additional elements used to connect the insert with the die fail to function effectively during dynamic forging. Therefore, the only feasible way to incorporate a replaceable insert is by joining it using thermal interference fit. This phenomenon not only enables the connection of tool components but also introduces additional modifications to the stress and strain state before and during the forging process which has a significant impact on the tool load level and its durability.

This study presents research on the modification of stress and strain states in the tool area through the application of varying thermal interference fit values between the main part of the forging die and the replaceable insert. To achieve this, a research methodology was proposed, utilizing the analysis of strain field changes on the tool surface using a Digital Image Correlation system (DIC). The analysis covered both the tool during the interference fitting process and the simultaneous temperature gradient equalization, as well as during the forging process under laboratory conditions with full control of process parameters (such as tool movement speed, pressing force, and instantaneous tool positions). The research results were compared with numerical simulations (FEM) of the test. Additionally, an industrial forging process was analyzed, with particular attention to tool wear mechanisms and the distribution of stress and strain in tools joined using thermal interference fit.

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Severe Plastic Deformation for Processing of Additive-Manufactured Alloys

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C9_1, Picasso Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The constant need for high performance engineering components supports the efforts for expanding the design envelopes through the realization of complex shapes and geometries by additive manufacturing. Although additive manufacturing (AM) can accurately account for the geometrical features, mechanical behavior is inherently limited by the material properties and how the part is built. Therefore, improvement of additive-manufactured components from a mechanical property perspective has several technological implications. Since severe plastic deformation (SPD) has long been utilized to achieve extraordinary physical and mechanical properties in a variety of material systems, its utilization following AM deserves further investigation.

In this work, multiple cases on the utilization of SPD technologies as post-AM processing tools for mechanical response enhancement are provided by highlighting the recent efforts in various alloys. As such, this study demonstrates the potential of SPD assisted thermo-mechanical processing (TMP) for obtaining unprecedented properties in additive-manufactured alloys with evidence from different materials, whereby optimum selection of post-AM processing parameters and part geometry are crucial.

Grain boundary engineering in nanostructured metals

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C9_1, Picasso Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The high strength of nanocrystalline and ultrafine-grained materials is commonly compromised by early crack initiation at and easy propagation along grain boundaries. Thus, to increase the damage tolerance of such materials requires strategies to subdue crack nucleation along grain boundaries. We will present two different strategies to increase the damage tolerance of grain boundaries in ultrafine-grained iron and nickel. First, low-angle boundaries with a spacing of hundreds of nanometer can be engineered by cyclic high-pressure torsion. Such dislocation boundaries have a low misorientation, inherently reducing the energy of the boundary and raising its cohesion. Moreover, due to the limited misorientation, slip transfer across the boundary is facilitated. A main advantage of the concept is that low-angle boundaries can be synthesized independent of the crystal structure, in contrast to the prominent concept of nanotwins. The boundary misorientation and grain spacing can thereby easily be tuned via the applied torsion angle and the number of cycles. Second, segregation of specific elements to grain boundaries can either reduce (e.g. S, P) or raise (e.g. C, B) their cohesive strength, as demonstrated for coarse grained materials. We transferred this idea to the nanoscale by synthesizing B and B-C doped ultrafine-grained iron samples via high-pressure torsion. Although strain-induced segregation to the boundaries is already accessible at room temperature, we will show by APT measurements how the interfacial excess can be optimized via high-temperature HPT or annealing. Lastly, we will present first mechanical tests to verify the success of each concept with respect to grain boundary strengthening.

Microstructural aspects of plastic deformed martensite decomposition in the Ti-6Al-4V alloy

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C9_2, U1 Room (Level 0), septiembre 18, 2025, 14:30 - 16:30

The formation and decomposition of martensite in titanium alloys is usually associated with their heat treatment to achieve high mechanical properties. The presence of α' and α'' martensitic phases in these alloys also determines the effects of thermomechanical processing or additive manufacturing. Analysis of the results of previous studies indicates that the decomposition mechanism of plastically deformed α' martensite differs from that of undeformed, occurring during conventional tempering. This paper presents the results of TEM and SEM microscopic investigations of Ti-6Al-4V alloy plastically deformed in the quenched state and tempered statically – i.e. conventionally - and dynamically - by a high-temperature plastic deformation process. The change in grain morphology during the martensite decomposition process has been assessed, including the change in grain orientation (EBSD), as well as the reorganisation of structure defects.

Mechanical and electrochemical analysis of AA5083- AA7075 dissimilar alloy joints fabricated by friction stir welding

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C9_3, U1 Room (Level 0), septiembre 18, 2025, 17:00 - 19:00

This present study aims to produce high-strength (AA7075), high-corrosion resistant (AA5083) dissimilar joints of Al alloys through friction stir welding (FSW) technique for marine applications. The dissimilar joints of Al alloys were fabricated with standardized FSW process parameters (i.e., 1100 rpm of tool rotational speed, 50 mm/min of welding speed, and 2° tilt angle). Detailed analysis of weld characteristics, mechanical properties, and corrosion behaviour are carried out to establish the effectiveness of the FSW technique for dissimilar welding. The hardness profiles across the weld regions revealed a significant increase in hardness within the stir zone compared to the base metals, attributed to the fine-grained microstructure generated during the FSW process. The ultimate tensile strength of the optimized FSW joint is found to be 80% of the AA7075 base metal, indicating good joint efficiency. Microstructural analysis through optical microscopy and SEM provides insights into the grain structure and phase distribution within the weld zone. The stirred zone exhibits a refined equiaxed grain structure as a result of dynamic recrystallization during FSW. Corrosion behavior was assessed using Tafel plots and Electrochemical impedance spectroscopy (EIS). The Tafel plots illustrated that the welded joint exhibited a corrosion potential and current density the same as base metals, suggesting that the FSW process did not lower the corrosion resistance of the materials. EIS results provided further evidence of the weld's stability in corrosive environments, with impedance spectra indicating better corrosion resistance.

Evidence for a new work hardening stage at colossal strains

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C9_2, U1 Room (Level 0), september 18, 2025, 14:30 - 16:30

Traditional work hardening stages have been investigated for decades and the underlying mechanisms are widely accepted. Because of dynamic recovery mechanisms, work hardening quickly diminishes and ceases already at relatively small equivalent strains ($\epsilon_{VM} > 10$). At this stage, commonly referred to as the steady state or saturation regime, a dynamic equilibrium between grain refinement and dynamic recovery (i.e., by mechanically driven grain boundary migration) is established. A vast number of studies using severe plastic deformation techniques support the existence of this saturation regime. Meanwhile, few reports question such steady state, but suggest another strain hardening regime might be entered for strains >1000 . Nevertheless, so far, neither an in-depth analysis nor a general theory for such ultra-SPD strain hardening has been established.

In the present work we subject pure metals to HPT at room temperature up to exceptionally high strains ($\epsilon_{VM} > 10000$). The results confirm the existence of a saturation stage, but provide solid evidence for the reinitiation of strain hardening at colossal strains ($\epsilon_{VM} > 1000$). This behavior can be observed independent of the crystal structure. Detailed microstructural investigations confirm that the new work hardening stage manifests in noticeable additional grain refinement and hardness increase. Although at this stage the strain hardening rate is weak, a distinct hardness gain ($\sim 30\%$ compared to the classic steady stage condition) can be measured. Texture, and the existence of subgrains still support dislocation-based plasticity. Unexpectedly, the specimens subjected to such colossal strains possess – despite their reduced grain size – an improved thermal stability, which according to atom probe tomography, cannot be related to a continuous impurity take up during HPT deformation. Other mechanisms, thus need to explain the reinitiation of work hardening as well as the intriguing thermal stability, which will be the center of discussion.

Effects of Severe Plastic Deformation under the particular conditions of the KoBo Extrusion Process of Various Metallic Materials

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C9_3, U1 Room (Level 0), septiembre 18, 2025, 17:00 - 19:00

The KOBO extrusion process is an unconventional method of extrusion based on the phenomenon of superplasticity as an effect of a special state caused by the oscillatory motion of the die. It allows to perform the process at low temperature with severe plastic deformation (SPD) under cyclic change of deformation path conditions and to significantly reduce the force of the press. It is possible to extrude lightweight metals and alloys (e.g. aluminum and magnesium alloys) in cold extrusion with high extrusion ratios compared to conventional hot extrusion. The work presents mechanical behaviour of various metallic materials under different conditions resulting from localized plastic flow in shear bands and intensive generation of point defects (self interstitials) This phenomenon is the result of the oscillatory movement of the die by a certain angle and frequency The influence of the die geometry on process realization, parameters and the properties of the extrudate. were performed using dies with different face portion geometry. The extrudate obtained from billets of various internal structure was examined for mechanical properties and macro/microstructure, showing that, with adequate modifications to the tool face part geometry, it is possible to reduce the extrusion force and obtain extrudate with desired properties. Basing on analysis of microstructure and mechanical features of the product obtained in Kobo extrusion it was shown effect of superplasticity represented e.g. by high elongation.(about 800% of aluminum alloy 7075) but in this case microstructure does not require nanometric sizes of the grains and metal can undergo extremely large, uniform deformations without breaking. In case of deformation in KoBo extrusion the superplastic flow of metals requires verification especially in relation to the traditionally accepted conditions of superplasticity: fine grain size, high temperature, low strain rate, low stress. The specific conditions of the plastic deformation in the low-temperature KOBO process, with particular emphasis on the original plastic flow mechanism and the role of point defects and concentration of atoms, excessive concentration of interstitial atoms preserved in extruded products (nanoclusters) as well as taking into account the demonstrated significant impact of the die geometry on the mechanical behavior of the deformed metal, show the possibility of use KoBo extrusion as SPD process.

Evaluating Techniques for Identifying Isotopically Spiked Non-Metallic Inclusions in Steel

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D1_3, Andalucía III Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Non-Metallic Inclusions (NMIs) are primarily microscopic particles, typically in the size range of a few micrometers, present in steel. These NMIs are inevitably formed during the steelmaking process and significantly influence both the chemical and physical properties of steel. Given their impact, it is crucial to study their formation and modification. By understanding the origin and behavior of NMIs during production, targeted countermeasures can be implemented to reduce the number of detrimental NMIs in specific steel grades. As a result, downtimes in the steelmaking process can be minimized and the product quality can be enhanced. The implementation of tracing techniques allows the identification of the origin of NMIs. One novel promising approach lies in stable isotope labelling. Due to the modification of the isotopic ratio of, for example, one component in the slag, it is possible to study the steel/slag/refractory system in more detail. In the present study, the MgO used in the slag was spiked using an enriched stable ²⁶Mg isotope. By measuring the isotopic ratio of slag, refractory and NMIs, it was possible to identify whether NMIs were modified or originated by slag or crucible. Sensitive measurement techniques are required to determine the isotopic composition of slag and refractory as well as to evaluate the origin of NMIs.

Within this study, three analytical approaches were compared in terms of their applicability to measure the isotopic ratio in NMIs. The first analytical method was Laser Ablation - Inductively Coupled Plasma-Mass Spectrometry (LA-ICP-MS), a fast analyzing technique with limited spatial resolution (1 – 50 µm). As the second technique, Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) was applied. This method has a minimum spatial resolution of 35 nm and, hence, enables an investigation of the entire spectrum in single atomic layers. Due to the coupling of ToF-SIMS to Scanning Electron Microscopy with Energy-Dispersive X-ray Spectroscopy (SEM/EDS), it is possible to obtain elemental and isotopic information about the investigated NMI. The third method is atom probe tomography, which has the highest spatial resolution and allows measurements on the atomic level. Here, only small parts of an NMI can be investigated since the analyzable sample size is only a few hundred nanometers in size. All three techniques successfully detected the ²⁶Mg spike in the isotopically modified slag. Within this work, advantages as well as challenges of the applied analyzing methods are discussed.

Accurate nanoscale temperature determination in in-situ TEM heating using PEET

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D1_2, Andalucía III Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

In-situ scanning/transmission electron microscopy (S/TEM) heating experiments are critical for understand thermally induced microstructure phenomena and dynamics in materials, such as phase transformations in alloys. Thereby accurate in-situ temperature measurements of the TEM specimen on the nanometer scale is essential to correlate the findings from in-situ heating experiments with other microstructure information, e.g. with predictions from phase-temperature and phase-time diagrams.

In this study, we utilized plasmon energy expansion thermometry (PEET) and use the dependence of the bulk plasmon peak in an energy electron loss spectrum (EELS) with temperature. Using COMSOL multiphysics modelling and in-situ STEM-EELS experiments, we tested PEET's validity and accuracy using a tungsten (W) test TEM sample. Tungsten serves as an ideal model material with its high melting temperature (above 3000 °C) and sharp plasmon resonance in EELS, which benefit PEET with a wide implementation temperature range and precise determination of the energy of the bulk plasmon peak. We evaluated the accuracy of PEET for mapping local temperatures in a tungsten TEM sample from room temperature to 700 °C. Linear regression of the shift in plasmon energy and corresponding temperature values yielded an achievable temperature resolution of ± 30 °C. Additionally, we investigated the impact of a varying, inhomogeneous sample thickness on PEET accuracy and found that uncertainties in temperature increased from 41 °C to 49 °C due to local stress effects during TEM sample preparation and a larger surface-to-volume ratio when the thickness varied between 30–40 nm and 60–70 nm. In case of tungsten, we have calibrated this thickness-dependent effect below a thickness of 60 nm and propose a method to correct for this deviation by taking into account the broadening of the bulk plasmon peak.

Our findings demonstrate that PEET can provide quantitative temperature measurements on the nanometer scale when considering TEM sample thickness, thus improving the reliability of structure-property correlations in in-situ S/TEM heating experiments.

THICKNESS-DEPENDENT INTERFACE AND SURFACE POLARITY IN INFINITE-LAYER NICKELATE FILMS AND SUPERLATTICES

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D1_1, Andalucía III Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

The interplay between polarity, atomic structure, and electronic properties at oxide heterointerfaces and surfaces is a fundamental factor governing emergent quantum phenomena in correlated oxides. In infinite-layer nickelates, polarity-driven reconstructions are hypothesized to play a pivotal role in shaping their unique electronic behavior, particularly in superconducting thin films. Here, we investigate the thickness-dependent interface polarity, oxygen distribution, and atomic-scale distortions in NdNiO₂/SrTiO₃ superlattices and Pr_{0.8}Sr_{0.2}NiO_{2+x} thin films through a comprehensive multi-modal characterization approach, combining four-dimensional scanning transmission electron microscopy (4D-STEM) and electron energy-loss spectroscopy (EELS).

In NdNiO₂/SrTiO₃ superlattices epitaxially grown on SrTiO₃ (001) substrates, we uncover a progressive modulation of the oxygen content across the nickelate layers, indicative of a polar-driven interfacial reconstruction. The extent of this reconstruction is found to be thickness-dependent, with cation displacements reaching ~0.025 nm in 8NdNiO₂/4SrTiO₃ superlattices—twice as large as those observed in their 4NdNiO₂/2SrTiO₃ counterparts. These pronounced structural distortions suggest a strong orbital polarization emerging post-reduction, corroborating theoretical predictions of two-dimensional electron gas formation at pristine NdNiO₂/SrTiO₃ interfaces. Such observations highlight the critical influence of interfacial polarity in dictating electronic properties within reduced nickelates.

Concurrently, in Pr_{0.8}Sr_{0.2}NiO_{2+x} thin films, we directly visualize a strong surface reconstruction characterized by polar distortions and octahedral rotations. Atomic-resolution EELS measurements reveal spatially varying Ni valence states, closely correlated with local atomic electric field mapping. These variations are attributed to oxygen vacancy formation induced by topochemical reduction, leading to significant electrostatic effects at the surface. The spatial extent of these surface distortions is confined to approximately three unit cells, underscoring the intrinsic role of polarity-driven structural modifications in tuning the electronic phase landscape of nickelates.

Our findings provide direct evidence of polarity-mediated structural reconstructions at both interfaces and surfaces in infinite-layer nickelate systems. By elucidating the correlation between oxygen content modulation, atomic-scale distortions, and electronic reconstructions, we offer critical insights into the fundamental mechanisms underpinning quantum phenomena in reduced nickelates. These results have profound implications for the design and optimization of nickelate-based quantum materials, particularly in the context of high-temperature superconductivity, where interfacial and surface polarity effects may serve as key tuning parameters for emergent electronic states.

In-situ insights into interfacial processes at reactive liquid-solid interface during magnesium corrosion using cryo-atom probe tomography

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D1_3, Andalucía III Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Interfacial reactions at liquid-solid interfaces especially corrosion has a critically impact on the infrastructure degradation and sustainability (1), failure of functional materials such as battery systems (2) and in medicine for biodegradable implants (3).

For the application of biodegradable metals, Magnesium (Mg) has a great potential however, Mg alloys corrode rapidly and uncontrollably, through mechanisms not fully understood. Consequently, there are still open questions regarding the influence of different alloying elements, their distribution and different electrolytes on the corrosion processes. Understanding the interfacial processes at the reactive liquid-solid interface that are responsible for the degradation mechanism requires analytical methods with high local and chemical analysis capability and ideally to measure these reactions in-situ, on an atomic length scale, which is currently lacking. Atom probe tomography (APT) provides analytical imaging in 3D with equal chemical sensitivity across the periodic table even for light elements such as nitrogen, carbon and hydrogen and with comparable spatial resolution and can therefore close the gap.

By correlating cryo-APT and transmission-electron microscopy, we observed outward growth of Mg hydroxide and inward growth of an intermediate corrosion layer of hydr/-oxides with different compositions during the corrosion of a MgCa alloy using deionized water. The high chemical sensitivity of APT revealed that instead of a MgO layer between the hydroxide and the surface of a Ca-containing Mg alloy, a Mg(OH) layer was formed, into which Ca partitions (4). The observation of a metastable defect phases at the reactive interface was possible, yet these early reaction products are highly reactive and must play a critical role in accelerating the corrosion.

We demonstrated a new approach where it is possible to quasi-"in-situ" analyse the reactive interfacial processes at the liquid-solid interface by APT and investigate the early corrosion mechanisms of a Mg alloy. However, a better understanding of these early stages of corrosion and their products is necessary to advance the understanding of corrosion processes and their modelling, and consequently for higher level of control over the biodegradation rate of future implant material.

This method could be applied to a wide range of systems to provide new insights into the interfacial processes responsible for the degradation of, for e.g., catalysts or battery materials.

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Multi-modal in-situ electron microscopy and spectroscopy of high-temperature structural evolution in phase-change and nanostructured materials

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Elevated temperature increases atomic mobility and promotes structural re-ordering kinetics, driving phase evolution, chemical reactions, atomic diffusion, and surface degradation processes. On-chip thin-film heating and temperature sensing technology for in-situ transmission electron microscopy (TEM) holder systems has enabled highly localized specimen heating, greatly improving heating time and sample stability during in-situ heating experiments investigating temperature-induced transformations. This has enabled rapid heating experiments up to over 1000°C with stable imaging and spectroscopic signal collection over timescales greater than 150 hours. Improvements to double-tilting mechanisms have allowed for minimized backlash and increased stability and orientation accuracy for imaging and diffraction of temperature-induced structural evolution.

In-situ heating experiments under TEM are presented for various nanoscale systems. Au nanoparticle surface rearrangement and sublimation at high temperature [1], Mo-W-Se 2D superlattice, heterostructure, and alloy evolution at high temperature [2], and Ge-Sb phase-change memory nanowire restructuring at intermediate temperature [3] are presented. This work highlights the use of in-situ ultrafast heating under TEM to gain crucial mechanistic insights into structural transformations in nanoscale and 2D materials.

Heating and biasing in both scanning electron microscope (SEM) and X-ray synchrotron systems using MEMS chips cross-compatible across all three platforms is now possible. The new multi-modal compatibilities allow correlation of microscopic and spectroscopic results across techniques and length scales, supporting investigations into mechanistic relationships between microstructure, chemistry, and temperature.

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4DSTEM-in-SEM in event driven mode to characterize metallic materials

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D1_3, Andalucía III Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Over a past decade, 4DSTEM has emerged as a powerful tool in TEM, enabling simultaneous acquisition of spatial and diffraction information [1]. Recent advancements in direct electron detector technology now allow the integration of 4DSTEM even into SEM, opening up new possibilities for in situ studies in a controlled environment [2]. So far characterization of 2D materials such as MoS₂ and graphene have been demonstrated [3-5]. Enabling this novel technique for bulk materials can offer valuable insights into real-world performances. This integration could also have potential for in situ studies because of the large chamber of SEM than in TEM. However, the slow data acquisition rate poses a challenge. In this talk, we highlight the integration of 4DSTEM in SEM focusing on a novel event-driven mode to accelerate data acquisition rate and its application to metallic materials. Also, we address the challenges posed by sample thickness and SEM parameters optimizations. Our experimental setup includes an in-house configuration utilizing the MiniPIX TPX3 camera from ADVACAM. The event-driven mode significantly reduces the data storage requirements compared to conventional frame-based method, which is a key challenge in high-throughput 4DSTEM. The acquired data is processed using python scripts and stored as 4D data set. Utilizing open-source platforms like LiberTEM and py4DSTEM, virtual bright and dark-field (BF and DF) images were generated. As an example we present a nanograin Pt thin film was deposited by DC magnetron sputtering directly on TEM grid. Using the MiniPIX detector, the 4D data set with 250 x 250 pixel in real space was acquired. A virtual DF images (using LiberTEM) and in-plane orientation map (derived from radial Fourier analysis) were developed revealing the nano grain size of thin film as one of its key characteristics. The in-plane orientation maps can be exemplified to determine the misorientations between phases providing valuable insights into materials structure. In conclusion, the successful integration of 4DSTEM-in-SEM offers significant advances in understanding material performance and establishing a foundation for ongoing breakthroughs in this field.

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Enhancing the photocatalytic performance of carbon nitrides through controlled local structure modification

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D1_2, Andalucía III Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Carbon nitrides are the most efficient and intensively studied earth-abundant photocatalysts. Their direct application in industry is prevented by several factors, including high recombination rate, deficient charge transport, and the lack of absorption above 460 nm. Here we investigate how the photocatalytic performance of layered carbon nitrides can be enhanced through: (1) fine tuning of the local crystal structure, using poly(heptazine imides) (PHI) with various cations ($M = H^+$, Na^+ , K^+ , Mg^{2+}) as a model system; (2) creating a heterojunction between PHI and e.g. poly(triazine imide) (PTI). We combined X-ray powder diffraction, low-dose HR-TEM and ADF-STEM imaging, energy filtered electron radial distribution function (EF-eRDF) analysis obtained from rotational electron diffraction data, valence electron energy loss spectroscopy, ELNES and EXELFS analysis in order to obtain a detailed understanding of the local structure, chemistry and electronic properties of modified PHIs and correlate it with photocatalytic performance.

For M-PHIs with various cations ($M = H^+$, Na^+ , K^+ , Mg^{2+}) we showed that both the short-range order (due to the sizes and charges of the solvated metal cations) and the medium-range order (due to the formation of twist domains between carbon nitride layers) considerably influence the photocatalytic hydrogen evolution rate. Na-PHI displays the best performance among other PHIs with metal cations in oxidation state +1, as the size of the solvated Na^+ cation, together with the presence of the rotational defects, enables cations to occupy positions in the channels equidistantly from nitrogen in polyheptazine layers. The combination of twist defects and the even higher charge of Mg^{2+} promotes a faster interlayer charge transfer and a more efficient polarization of the heptazine backbone in Mg-PHI, leading to an unprecedented quantum efficiency of 7.14%.

The formation of a PHI/K-PHI heterojunction was realized for the first time and showed an improved photocatalytic O_2 reduction performance compared to pure phases. We explain the latter by the specific structural alignment of the polymeric phases along the c-axis, which enabled an improved charge transfer between PTI and PHI. Based on an analysis of SE- and ADF-STEM images, ELNES and EXELF, and the general thermochemical behavior of precursors we proposed a possible mechanism for the heterojunction formation. We believe that at the early stages a thin PTI layer is formed; K-PHI starts to crystallize at the defect sites of PTI inside the gas pockets formed in the salt melt.

We gratefully acknowledge financial support by the Max Planck Society.

Towards Single-Pattern Absolute HR-EBSD without using Simulated Patterns as Reference

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D1_3, Andalucía III Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Over the years, High Angular Resolution Electron Backscatter Diffraction (HR-EBSD) has become a reliable tool for measuring misorientations and relative stresses (elastic strains) in crystalline materials with high sensitivity. However, in the absence of stress-free intragranular reference points, absolute stress measurements are not yet routinely performed, despite their potential to provide new insights into the nano- and micromechanics of a wide range of (poly)crystalline materials. The extension from relative to absolute cross-correlation-based HR-EBSD, using a simulated EBSD pattern as a reference, remains an area of ongoing development. However, this approach is limited by factors such as inaccuracies in EBSD pattern simulations and uncertainties in the experimental EBSD geometry. Consequently, an absolute HR-EBSD approach that does not rely on simulated reference patterns or any experimentally obtained stress-free reference pattern would be of significant interest to the community.

Recently, global correlation frameworks have been proposed, demonstrating the potential for non-simulation-based absolute HR-EBSD by leveraging crystal symmetry, simultaneous correlation between multiple (intergranular) patterns, and co-correlation of the pattern center. However, experimental validation on polycrystalline samples has been challenging, and excess-deficiency features (band asymmetry) in the patterns are expected to introduce complications.

To address these challenges, we have further developed this framework to reduce complexity and to enable absolute, non-simulation-based HR-EBSD correlation using only a single EBSD pattern. Specifically, we correlate different regions within the same pattern using crystal symmetry operators. By applying all available symmetry operators, we perform multiple parallel correlations within a single pattern, treating absolute in-plane stress components, absolute orientation, and pattern center parameters as degrees of freedom.

In this presentation, we will first demonstrate how the framework operates and performs on idealized simulated patterns. Further validation on single experimental stress-free patterns, acquired using a direct electron EBSD camera, will highlight the impact of excess-deficiency features on experimental accuracy, as confirmed through comparisons with dynamically simulated patterns. To mitigate these effects, we introduce an integrated excess-deficiency correction approach, demonstrating that non-simulation-based absolute HR-EBSD is within reach.

Resolving Overlapping EBSD Patterns Using Iterative Dynamic Template Matching

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D1_3, Andalucía III Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Overlapping Kikuchi diffraction patterns often hinder accurate phase identification in Electron Backscatter Diffraction (EBSD). We present an iterative approach using dynamic template matching in AztecCrystal MapSweeper [1] of dynamically simulated patterns [2] and Gaussian-blurred pattern subtraction to resolve overlapping diffraction signals. Our method first identifies the best-fit simulated Kikuchi pattern using dynamic template matching. This pattern is then blurred to match the experimental image optimally and subsequently subtracted, revealing the underlying weaker signal. Reapplying dynamic template matching to the residual pattern ensures accurate detection of minor phases that would otherwise remain omitted. This method significantly improves phase discrimination in complex materials, addressing a key limitation of conventional EBSD analysis. This method doesn't require a known orientation relationship between two patterns [3] or close neighbor experimental patterns like previously published approaches [4]. During the talk several examples will be shown.

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Development of a High-Throughput method for Microstructure Analysis of Aluminum HPDC components

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D1_3, Andalucía III Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

As the automotive industry transitions towards electrification, the demand for lightweight, high-performance materials grows rapidly. High-pressure die-casting (HPDC) aluminum (Al) alloys are widely used in electric vehicle (EV) applications due to their excellent strength-to-weight ratio, mass production capability, and cost-effectiveness. However, optimizing these alloys and processing parameters for improved mechanical properties and corrosion resistance of the casting components requires a detailed understanding of their microstructure and chemical composition. In traditional characterization methods for Al alloys in the scanning electron microscope (SEM), a single sample piece is often mounted, polished, and analyzed individually. The process is often time-consuming and labor-intensive, limiting the speed of product development in industrial settings.

This study presents a high-throughput method to analyze HPDC Al components by using SEM, in addition to the standard optical microscopic analysis, incorporating automated imaging, energy-dispersive X-ray spectroscopy (EDS) analysis, and advanced data processing techniques. With the help of 3D printing, polymer-based sample holders were designed and produced to hold multiple samples, enabling efficient sample preparation and SEM analysis. Automatic SEM imaging, EDS mapping and data analysis enable comprehensive microstructure and chemical analysis for identification of key alloying elements, secondary phases such as intermetallic compounds, and defects such as porosity and oxide inclusions.

The proposed high-throughput SEM methodology has significant implications for the automobile industry. By accelerating the sample preparation and microstructure characterization process, this approach facilitates rapid iteration in alloy and casting parameter design, ultimately supporting the development of next-generation lightweight materials and optimizing manufacture for EV applications. It can be integrated into industrial quality control workflows, enhancing process monitoring and defect mitigation strategies. Finally, this method can be readily adapted to general materials research.

New insights into luminance quantification via correlated photoluminescence and confocal Raman microscopy

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D1_2, Andalucía III Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Spectroscopic techniques are fast, non-destructive and easy to apply, providing valuable structural and functional information for material analysis across different applications. However, a typical limitation is the difficulty of quantifying intensity (usually given in arbitrary units), as it depends on different factors like equipment, optical paths, illumination power and detector efficiency. These variations make it challenging to compare optical responses across different instruments. This work presents a novel methodology for correlating the arbitrary intensity units from a photoluminescence (PL) spectrometer and a high-resolution confocal Raman microscopy, with luminance values ($\mu\text{cd}/\text{mm}^2$), facilitating the quantitative analysis of luminescent materials.

To develop this methodology, reference composite samples were prepared by dispersing Eu_2O_3 particles (0.1–10 wt%) in an epoxy matrix to achieve a homogeneous distribution. These samples were characterized using photoluminescence spectroscopy, and their luminance was measured with a luminancemeter. The results demonstrated a clear correlation between the PL intensity (in arbitrary units) and the emitted luminance at a given excitation wavelength. Furthermore, since Eu_2O_3 exhibits photoluminescence emissions under certain excitation conditions, we extended this approach to confocal Raman microscopy.

The results demonstrate that the photoluminescence intensity (in arbitrary units) measured with a PL spectrometer and with a confocal Raman microscopy can be quantitatively related to luminance ($\mu\text{cd}/\text{mm}^2$) obtained from a luminancemeter. It was also found that the optical response of these Eu_2O_3 -epoxy composites does not follow a strictly linear relationship with concentration, highlighting the necessity of developing reference samples across a defined concentration range for accurate calibration. Therefore, constructing reliable calibration curves is essential for precise luminance quantification.

The proposed methodology was validated, demonstrating its applicability in anti-counterfeiting applications, specifically in the quantification of luminescence in cotton-type paper doped with Eu_2O_3 , similar to that used in security documents. Thus, it has been observed that this methodology allows the quantification of luminance at both macro and microscopic scales by confocal Raman microscopy, offering a simple and versatile tool to detect security markers in forensic applications.

Ultimately, this study enables luminance quantification in both photoluminescence and Raman spectrometers, with potential industrial and scientific applications. It also introduces a new approach to analyzing luminance at the microscopic scale, offering unprecedented luminescence correlation for various emerging applications.

Detection of magnetic circular dichroism from individual atomic planes in a scanning transmission electron microscope

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D1_2, Andalucía III Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

In an analogy to XMCD[1], the discovery of electron magnetic circular dichroism (EMCD) in transmission electron microscope (TEM) in 2006 [2] opened the possibility of mapping the orbital and spin moments in magnetic materials with atomic resolution. In EMCD experiments, electron energy loss (EELS) spectra at specific conjugate scattering angles in the reciprocal space contain magnetic information and their difference, called EMCD signal, can be used to determine orbital to spin moments ratio by applying theoretical sum rules.

When conducting EMCD experiments in scanning TEM mode, the resolution of analysis is determined by the size of electron probe which, in modern probe-corrected STEMs, can easily reach atomic resolution. Yet, the detection of quantitative EMCD signals at atomic scales remains elusive due to challenges associated with convergent beam setups. The strength of EMCD signal generally goes down with increasing convergence angles. Most importantly, EMCD experiments need the acquisition of two or more momentum-resolved EELS spectra, which would require to scan the same region of the specimen multiple times in STEM-EMCD experiments. This poses additional challenges to ensure spatial registration with atomic precision among multiple datasets. In our previous works[3], we addressed this issue by performing single scan EMCD experiments using customized hardware apertures. Building on this approach, we now demonstrate quantitative EMCD detection at atomic-plane resolution in STEM-EMCD experiments for (110) atomic planes of an iron (Fe) crystal. We not only quantify EMCD signals extracted from individual atomic planes, but we also reveal variations in the orbital to spin moments ratio between adjacent atomic planes. This enables unprecedented sub-atomic resolution in STEM-EMCD experiments.

The atomic plane resolved STEM-EMCD experiments were conducted using a a Thermofisher Titan G3 50-300 PICO fourth generation transmission electron microscope at Ernst-Ruska Center for Microscopy and Spectroscopy using Electrons (ERC), Forschungszentrum Jülich, Germany. This microscope is equipped with a Schottky-type high-brightness electron gun (FEI X-FEG), a monochromator, a CS probe corrector (CEOS DCOR), a CS-CC achro-aplanat image corrector (CEOS CCOR+), a post-column imaging energy filter (Gatan Quantum 966 ERS) and a Gatan K3 direct electron detector.

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High sensitivity electron holography combined with in situ biasing for studying dielectric and ferroelectric nanocapacitors.

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D1_1, Andalucía III Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Dielectric and ferroelectric materials are ubiquitous in microelectronic devices because of their ability to polarize in response to an applied electric field. They spur much fundamental and applied research over the years: the ability to measure polarisation locally and charge trapping is essential to furthering understanding and to develop a new generation of devices. Whilst ferroelectric and dielectric properties can be readily measured macroscopically using electrical methods, the task is difficult at the nanoscale and for thin-film materials.

In this presentation, we will show how the internal electric fields can be quantitatively mapped at the nanoscale within different dielectric and ferroelectric nanodevices using in situ electrical biasing and off-axis electron holography. For this purpose, we have implemented the dynamic microscope automation associated to a dedicated instrumental chain. Using a real-time measurements of sample drifts and interference fringes, followed by feedback control of the microscope to compensate for instrumental instabilities, this automation allows holograms to be acquired with unlimited exposure times and the implementation of sophisticated phase reconstruction techniques. The signal-to-noise ratio has thus increased by more than an order of magnitude and it is now possible to measure phase variations of a few mrad with a spatial resolution of 1 nm (for an electrostatic potential, this corresponds to variations of a few mV). The instrumental chain ranges from source-meter control software to the various protection systems against electrostatic discharges on electrically connected nanostructures. For example, the capacity of a nanocapacitor prepared for electron transparency does not exceed 1 fF (10⁻¹⁵ F).

We studied twin trilayer nanocapacitors, HfO₂/Al₂O₃/HfO₂ and Al₂O₃/HfO₂/Al₂O₃ and also a ferroelectric Hf_{0.5}Zr_{0.5}O₂ (HZO) tunnel junction. Our results highlight the presence of trapped charges at the different dielectric/dielectric and ferroelectric/dielectric interfaces with a strong effect on the distribution of the internal electric field. The trapped charge densities depend on the stacking sequence (leading to different interfacial layers in terms of defects due to different processing) and the sign of the bias. In addition, we succeeded to map the polarisation switching of the HZO film as the voltage gradually increases to the coercive voltage, observing that switching occurs via the nucleation and lateral growth of domains.

This ability to determine the internal electric field in a large field of view and to quantify the trapped charge densities at each of the interfaces in the stack open avenues to engineering and optimize nanodevice performances.

Correlation of feldspar crystalline phases with measurement artifacts in confocal Raman microscopy

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D1_2, Andalucía III Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Raman spectroscopy is nowadays increasingly being used in industry beyond the academic space. There are several reasons, including the use of portable Raman spectrometers which allows to perform analyses outside labs, the capacity of doing microscale/in-situ studies and also non-destructively analyses without special preparation of the samples. Among some applications, these advantages are particularly relevant in the study of mineral samples. One of the important point in Raman spectroscopy is the selection of the measurement laser wavelength. The use of 785 nm wavelength laser, practical for the study of highly fluorescence materials, is often avoided within this field due to the anomalous response usually observed in natural and synthetic minerals and in glass-ceramic specimens, that mask the structural Raman signal. To date, the cause of the phenomenology that gives rise to this type of response is not precisely known. The family of silica-based glass-ceramic materials exhibits an enhanced Raman signal in the region of 1000-2500 cm⁻¹ for this wavelength. The intensity and shape of the Raman signal seems to depend on the interaction between the glassy and crystalline parts of the microstructure and are usually associated with photoluminescence [1-5]. Therefore, the main objective of this work is to establish a correlation between the structural Raman response measured with a 532 nm laser with the artifact Raman response observed when using the 785 nm laser in feldspar crystalline phases such as anorthite and albite. For this purpose, different glass-ceramic materials were synthesized. The microstructures analyzed by confocal micro-Raman microscopy combines the use of two excitation wavelengths (532 and 785 nm) at selected regions, thus allowing to explain the role of each glassy and crystalline phase in the enhanced Raman response of the designed materials. In addition, different techniques such as X-ray diffraction (XRD) and scanning electron microscopy (SEM) were used to complement the microstructural characterization of the different glass-ceramic materials studied in this work.

Atomic resolution DPC-STEM imaging of magnetic signal in antiferromagnets

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D1_1, Andalucía III Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Efficient manipulation of antiferromagnetic (AF) domains and domain walls has opened up new avenues of research towards ultrafast, high-density spintronic devices [1,2]. AF domain structures are known to be sensitive to magnetoelastic effects, but the microscopic interplay of crystalline defects, strain and magnetic ordering remained largely unknown. We have explored antiferromagnetic CuMnAs thin films in which imaging by X-ray photoemission electron microscopy (XPEEM) revealed that its AF domain structure is dominated by nanoscale crystalline defects [3]. The results emphasized the crucial role of these defects in determining the AF domains and domain walls, and provided a route to optimizing device performance in term of scaling limits for the data density in the bulk of the antiferromagnet. However, even smaller magnetic objects were indirectly observed in the material, but they remained below the detection limit of the established XPEEM methods.

Here, we achieved atomic resolution imaging of abrupt AF magnetic domain walls in CuMnAs epilayers by utilizing scanning transmission electron microscopy (STEM), differential phase contrast (DPC) and 4D-STEM techniques [4]. Identification of the magnetic domain DPC signal was based on the specific symmetry of the CuMnAs crystal, where the opposite magnetic Mn sublattices occupy crystallographically distinct noncentrosymmetric sites. With a focus on small field-of-view high-resolution imaging, we could associate the DPC-STEM signals with two types of abrupt Néel vector reversals: The first type occurs at a crystallographic antiphase boundary defect, while the second type forms in a part of the epilayer with no crystallographic perturbation detectable by STEM.

The DPC-STEM magnetic signal was reconstructed by calculating the shifts of the center of mass (COM) of Ronchigrams recorded by a pixelated detector. The signal intensities were plotted as a function of integrated [001] component of COM shifts corresponding to the direction of the Lorentz force due to sublattice magnetic Mn moments pointing in the (001) easy plane of antiferromagnetic CuMnAs. This qualitative assessment of the magnetic order in Mn sublattices was paradoxically possible in substantially thick TEM lamellae, above 50 nm, and with small collection angles, below 10 mrad, since dynamical diffraction effects can be of advantage for magnetic imaging, which was revealed by Pauli multislice STEM-DPC simulations [4].

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EDS and EELS of Lithium in a 0.5 to 30 keV Electron Microscope

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D1_2, Andalucía III Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

This paper will present quantitative EDS and EELS maps of Lithium-based materials acquired from 0.5 to 30 KeV with a cryogenic specimen holder. State-of-the-art results acquired with the Hitachi SU-9000 dedicated STEM will be shown. This microscope has EELS capabilities that allow Li detection [1]. It is also equipped with the Extreme EDS system from Oxford Scientific that can detect the $K\alpha$ line of Lithium. Results on several Li compounds used in battery materials as well as Li-based minerals will be presented.

Advanced Microstructure Characterization to Decode Solidification and Phase Transformation Induced in Additively Manufactured Tool Steel

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 15, 2025, 13:15 - 14:30

This investigation demonstrates the power of integrating cutting-edge characterization methodologies for comprehensive understanding of microstructure genesis in additively manufactured 33CrMoV12 tool steel [1]. Microstructure, microtexture, and chemical microsegregation of the as-built steel are explored through a multi-scale approach integrating X-ray diffraction (XRD), electron backscatter diffraction (EBSD) including parent austenite reconstruction [2], secondary ion mass spectrometry (nano-SIMS) [3], and a novel chemical analysis technique coupling backscattered electrons and X-rays within a scanning microscope (SEM-BEX) [4].

As expected, the as-built microstructure consists predominantly of a fine martensitic matrix; however, a surprisingly high fraction of retained austenite also remains (approximately 25%). A secondary structure is detected—superimposed on the primary matrix—comprising colonies of roughly cylindrical cells marked by strong intercellular segregation of C, Cr, Mo, and Mn. Characteristic of cellular solidification under high cooling rates, this microstructure has been frequently reported for metallic alloys with austenite matrix produced by AM (stainless steels, Ni-based alloys), but occurs much more rarely in steels undergoing subsequent solid-state transformations, and has never been observed in this grade.

EBSD analysis enables investigation of relationships between key microstructural features resulting from solidification: the parent austenitic structure, growth directions of segregated cellular colonies, and retained austenite preferentially localized between cells. Notably, the principal axes of solidification cells align with <100> directions of parent austenite grains reconstructed from final martensite orientation maps. This alignment suggests that steel solidification occurs entirely within the austenitic phase, contrary to the ferrite-then-austenite sequence predicted under equilibrium conditions. Non-equilibrium solidification calculations using the Gulliver-Scheil model enable quantitative correlation between the exceptionally high retained austenite content and chemical segregations that depress the Ms temperature in intercellular regions.

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Development of an Integrated UTM and PIXE System with Proton Beam Irradiation for Real-time Material Testing

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The integration of real-time mechanical testing and non-destructive elemental analysis under radiation exposure is an important step forward in understanding material behavior in extreme environments. The present work focuses on the development of integrated universal testing machine (UTM) and particle-induced X-ray emission (PIXE) systems utilizing the MC50 cyclotron beamline. The aim is to provide a comprehensive insight into material performance by enabling simultaneous evaluation of mechanical properties and elemental analysis during proton beam irradiation. Currently, this setup includes a proton and neutron beam irradiation system, a beamline configuration, and a vacuum sample holder. Next steps include integrating UTM with real-time stress-strain monitoring capabilities and optimizing PIXE detector alignment for high-resolution elemental analysis. This integrated system will allow simultaneous observation of mechanical deformation and elemental redistribution under combined thermal and irradiation stresses, simulating high-radiation and high-temperature environments. Expected results include the ability to relate changes in mechanical properties to changes in elemental composition, which provides a new approach to material characterization. This bifunctional platform is expected to significantly improve the understanding of material behavior in nuclear, aerospace, and other high-intensity applications. By combining UTM and PIXE features, the system will establish a new standard for advanced material testing and provide critical data for the development of resilient materials tailored to extreme conditions.

Development of a PIXE Analysis System Using the MC50 Cyclotron Beamline

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Particle Induced X-ray Emission (PIXE) is a non-destructive analytical technique widely used for the precise identification of elemental compositions in materials. This project aims to develop a PIXE system utilizing the MC50 cyclotron beamline, designed to enhance analytical precision and versatility across a broad range of applications. The current infrastructure includes proton and neutron beam irradiation systems, a well-configured beamline, and a vacuum sample holder. A key focus of the development process is the precise control of proton beam energy to optimize elemental excitation and improve analysis accuracy. By tuning the proton energy, the system will provide enhanced detection capabilities for various elements while ensuring minimal interference from background signals. The integration of advanced detector alignment and beamline optimization is expected to enable efficient and reproducible elemental mapping. Once completed, the PIXE system will offer a robust platform for material analysis in areas such as environmental studies, cultural heritage preservation, and advanced material research. This project aims to establish a high-performance PIXE analysis system, advancing the potential of non-destructive elemental characterization for both academic and industrial applications.

Resolving the limits of the J-integral in a nanocrystalline Cantor alloy using multi-method stress-strain mapping

Dr. Michael Meindlhumer¹, Dr. Juraj Todt¹, Noel Sheshi², Dr. Anton Hohenwarter¹, Dr. Manfred Burghammer³, Dr. Martin Rosenthal^{3,4}, Prof. Enrico Salvati², Prof. Daniel Kiener¹, Prof. Jozef Keckes¹, Dr. Markus Alfreider¹

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

In order to interpret irreversible microstructural processes occurring during elastic-plastic fracture of nanocrystalline materials, it is vital to elucidate multiaxial stress and strain fields in the vicinity of a progressing crack. Here, we present a multi-method nanoscale strain- and stress-mapping surrounding a growing crack tip in two identical miniaturized fracture specimens fabricated from a nanocrystalline FeCrMnNiCo high-entropy alloy. by focused ion beam (FIB) milling. The first cantilever was deformed in situ in a scanning electron microscope using the sequential loading-unloading approach to evaluate the incremental J-integral. Additionally, a point pattern was added on the surface of one cantilever using the FIB feature milling system, allowing for the detailed analysis of the complete 2D surface strain components during the experiment. Cross-sectional X-ray nanodiffraction (CSnanoXRD) at the ID13 beamline of the European Synchrotron (ESRF) with a spatial resolution of down to 200 nm was coupled with an in situ indentation device to uncover the multi-axial stress fields associated with crack growth in the second HEA cantilever. Loads of 22, 45 and 34 mN with consecutively increasing displacement were applied, which correspond to conditions of elastic loading, crack tip blunting and general yielding, respectively. At every loadstep, the CSnanoXRD data were gathered in a region of $30 \times 35 \mu\text{m}^2$ centered around the crack tip. In addition to the evaluation of the 3D stress tensor around the crack tip, small-angle X-ray scattering and full width at half microscopy techniques allowed for quantitative analysis of crack growth and to assess the defect accumulation in front of the crack tip qualitatively, respectively. Additionally, the experimental stress data were corroborated by an elastic-plastic finite element model. Furthermore, the stress and strain data were used to evaluate the J-integral around the crack tip and cross-validate it with the sequential unloading approach and the J- and/or K-values computed from the stress data. It could be shown that the sequential unloading approach overestimates the crack growth and the quantitative J-integral, the latter by a factor of ≈ 10 , due to significant amounts of plastic deformation buildup without crack extension. The quantitative experimental strain and stress results suggest a limit to the path-independence of the J-integral concept, which has significant implications in the development and assessment of modern damage-tolerant materials and microstructures.

Advancing 3D/4D Diffraction Imaging: ESRF's New ID03 DFXM Beamline

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D2_3, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The ESRF's Dark Field X-ray Microscopy (DFXM) beamline at ID03 represents a major leap forward in 3D and 4D mapping of crystalline orientation and strain, significantly enhancing multi-scale imaging of embedded microstructures. As part of the ESRF's EBSL2 Upgrade Project, ID03 introduces new possibilities for high-resolution, non-destructive characterization of bulk materials. Relocated and upgraded from ID06-HXM, the beamline is now equipped with state-of-the-art X-ray optics capable of delivering both pink and monochromatic beams, a newly developed high-precision goniometer, and an advanced detection system optimized for capturing subtle microstructural features with a spatial resolution on the order of 100 nm. This capability allows for detailed investigations of thick crystalline samples, providing new insights into their microstructural features.

DFXM is a diffraction-based imaging technique that maps the magnified diffraction signal from a crystalline element using an objective lens. This enables the direct visualization of 3D orientation and strain fields at the submicron scale, offering unique capabilities for studying complex microstructural phenomena. A key strength of ID03 lies in its integration of DFXM with complementary techniques, including 3DXRD, diffraction contrast tomography (DCT), and classical tomography, on the same experimental platform without the need to dismount the sample. This multi-modal approach allows researchers to study hierarchically ordered systems across multiple length scales, providing a more holistic understanding of microstructural behavior.

Since opening to users in April 2024, ID03 has supported a wide range of studies, from strain mapping in metals to functional material analysis in semiconductors, biominerals, and energy systems. We present examples from diverse material systems, including deformation and annealing structures in metals, which highlight the beamline's ability to resolve 3D grain structures and strain distributions with high precision. By enabling comprehensive, in-situ investigations, ID03 facilitates a deeper understanding of intricate structural, orientation, and strain-related phenomena, positioning itself as a powerful tool for advancing research in structure-property relationships across materials science disciplines.

Nanoscale examination of degradation in copper metallization layers using lab-based nanoTXM and DFXM

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

During application, high-power semiconductor devices undergo cyclic thermal loading caused by short circuit events. While the Cu metallization provides rapid cooling to the underlying semiconductor material, it is prone to thermo-mechanical fatigue caused by high thermal stresses due to the different thermal expansion coefficients. Determining the conditions for the onset of Cu metallization degradation, especially of void formation and crack growth, is therefore essential to further improve the reliability of high-power semiconductor devices in the future.

To understand the fatigue behavior Cu metallization layers were thermal cycled at heating rates of about 10^6 K/sec. At different degradation stages, the intragranular microstructure and strain evolution of singular Cu grains was observed, especially at high angle grain boundaries (HAGBs). Dark field X-ray microscopy (DFXM) measurements performed at the ID03 beamline at ESRF is used to study the crystal orientation across grains and their evolution during degradation, providing experimental evidence that mosaicity of Cu grains and residual elastic strain concentrations increase simultaneously in the vicinity of HAGBs. While this technique provides great access to the crystallographic information of the Cu structure, it is limited to a few grains and grain boundaries, lacking the big-picture approach to correlate the onset of crack and void formation with stress-strain distributions.

Lab-based transmission X-ray microscopy (TXM) with spatial resolutions of 50 nm allows precise examinations of microelectronic materials with significantly lower access barriers than synchrotron-based X-ray studies. The microscope can provide detailed nano X-ray tomographies (nanoXCT) and 2D radiographies of sufficiently thinned samples. However, this method can solely function in transmission geometry, thereby lacking the crystallographic information that would be needed for a conclusive approach to failure mechanisms.

Using lab-based nanoTXM and DFXM as complementary techniques achieves a comprehensive understanding of failure and deformation mechanism in the Cu metallization structures. Strain distributions in local grains can be correlated with small voids and cracks identified using nanoXCT, painting a comprehensive picture of intragranular microstructure refinement and condensation of structural defects near grain boundaries that perpetuate void formation and degradation in copper metallizations under fast-cycling thermal loads.

Dual Synchrotron X ray diffraction approach to strain imaging: application to quantum devices.

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Accurately imaging and quantifying strain fields at multiple scales is critical for enhancing the performance and reliability of functional devices. In this work, we present a novel approach that combines two advanced synchrotron X-ray diffraction techniques with high strain resolution (10^{-5}). The combination of Laue microdiffraction (μ Laue) and Dark Field X-ray Microscopy (DFXM) provides access to multiscale strain mapping in semiconductor materials. μ Laue, performed at ESRF's BM32 beamline, offers rapid access to the deviatoric strain tensor, mapping with ~ 300 nm spatial resolution. DFXM, conducted at ESRF's ID03 beamline, provides full-field strain maps with angular and spatial resolutions of 0.001° and 150 nm, respectively.

Here we introduce these two synchrotron techniques, illustrating them with an example of strain mapping of the Si layer from a quantum device (Josephson's Junction). Using μ Laue, we identified regions of interest (ROIs) within the device, separated the signal of the substrate, and extracted the deviatoric strain tensor components of the crystalline layers. This information guided the subsequent DFXM measurements, enabling precise strain analysis. Through DFXM, we obtained focused strain maps of the 400 reflection of Si in the region of interest, with measured strains on the Si layer of the device on the order of 10^{-4} .

This double technique approach provides a particularly useful strategy for imaging and quantifying all strain components in embedded layers, provided they exhibit sufficient crystal quality.

In situ study of precipitation kinetics in friction extrusion and consolidation of Al alloys using FlexiStir

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D2_2, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Abstract

Understanding precipitation kinetics is essential for modifying the microstructure and properties of aluminum alloys during thermo-mechanical processes such as friction extrusion (FE) and friction consolidation (FC), where both severe plastic deformation (SPD) and frictional heating contribute to phase evolution and precipitate behavior [1,2]. This study utilizes a specialized in-situ setup, FlexiStir, adapted for FE and FC, along with Small-Angle X-ray Scattering (SAXS) and Wide-Angle X-ray Scattering (WAXS), to investigate precipitation behavior in AA7075 and Al-Cu-Li alloys at the high-energy material science beamline P07 at PETRA III (DESY, Hamburg). The combined SAXS/WAXS technique enables real-time tracking and detailed analysis of the evolution of the precipitate size, distribution, and phase fraction throughout the thermo-mechanical process. Additionally, process temperatures were determined using lattice expansion of aluminum measured from WAXS signals.

The study highlights the influence of deformation and temperature in precipitation evolution. Initial results reveal that SPD accelerates precipitation kinetics, with grain size increasing during the process. However, the precipitate volume fraction decreases as the temperature rises. After cooling, an increase in precipitate volume is observed, which significantly affects the mechanical properties of these alloys. The insights gained from this study aim at optimizing FE and FC processes for high-performance aluminum alloys, advancing their applications in aerospace and other industries requiring superior mechanical and thermal properties.

Acknowledgement

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Operando Neutron and X-ray Diffraction: A Window into Microstructure Evolution in Laser Powder Bed Fusion

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D2_2, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Additive manufacturing (AM) has become an integral part of modern materials processing, enabling the production of geometrically complex components with high efficiency. Among various AM techniques, laser powder bed fusion (LPBF) is widely used for fabricating metallic parts with intricate microstructures. The process involves localized melting and rapid solidification of fine metal powders using a high-energy laser. However, the complex thermal cycles and dynamic phase transformations inherent to LPBF introduce challenges in controlling microstructure evolution, residual stresses, and defect formation. A thorough understanding of these transient phenomena is essential for optimizing process parameters and improving material performance.

Over the past decade, operando neutron and synchrotron X-ray diffraction have emerged as key techniques for investigating the real-time evolution of microstructures within and around the melt pool during laser-based AM processes. These advanced characterization methods provide insights into phase transformations, thermal gradients, and stress development—critical factors influencing the final material properties.

Conducting such experiments requires specialized sample environments that can replicate industrial AM conditions while remaining compatible with synchrotron and neutron beamlines. This presentation describes the approach developed at the Paul Scherrer Institute (PSI) to address this challenge. Several miniaturized experimental setups have been designed and integrated into beamlines at both synchrotron and neutron facilities, allowing operando studies on LPBF systems.

The capabilities of these setups are demonstrated through examples where operando X-ray diffraction is used to track phase transformations and thermal history in different alloys and multi-material systems, while neutron diffraction and Bragg edge imaging provides insights into residual stress evolution in bulk specimens.

By capturing transient phenomena in real time, these techniques contribute to a deeper understanding of AM process dynamics and generate valuable datasets for validating computational models and simulations. The findings help refine AM processing strategies, improve material performance, and enhance the reliability of additively manufactured components.

Structure-Property Relationships across Gradient Thin Films on Non-Planar Substrate Geometries

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

While functional properties of thin films have been extensively optimized for planar substrates, their behaviour on curved surfaces remains less understood due to characterization challenges. In this contribution, the complex relationship between nanoscale gradients in residual stresses and microstructure in both lateral and depth directions is elucidated for non-planar substrate geometries. Focusing on nanocrystalline protective thin films deposited on cutting tools, our findings reveal a significant impact of the substrate geometry on structure-property relationships in thin films.

Microstructural properties and residual stress gradients across the cutting edge area of an AlTiN thin film, deposited by magnetron sputtering on a cemented WC-Co insert, were characterized by cross-sectional synchrotron X-ray nanodiffraction (CSnanoXRD) at the ID13 beamline of the ESRF in Grenoble. The film-substrate interface was precisely aligned parallel to an X-ray beam, which was collimated to a cross-section of $75 \times 75 \text{ nm}^2$ using multilayer Laue lenses. Two-dimensional diffractograms were collected from approximately $40 \text{ }\mu\text{m}$ thick cross-sectional lamellae using an Eiger 4M detector. The data acquisition involved a field-of-view of $20 \times 20 \text{ }\mu\text{m}^2$, scanned with a step of 50 nm . The collected Debye-Scherrer rings were analysed using the pyFAI software package and revealed compressive residual stresses up to -5 GPa at the cutting edge, marking a 100% increase compared to adjacent areas. This difference can be explained by insights gained from microstructural characterization. Transmission electron microscopy revealed irregularities in grain size, grain orientation and elemental distributions that were correlated to the non-uniform plasma conditions at the curved substrate during the deposition process. Further, the strain across the cutting edge was evaluated using selective area electron diffraction, which allowed a correlation of the evaluated strain heterogeneities in the modulated grain size regions to the residual stress gradients from CSnanoXRD. To successfully unveil the convoluted process structure property interactions at non-planar substrate regions, nanoindentation and bending tests on microcantilevers fabricated using FIB were conducted at the edge region. A fracture stress of $\sim 8.5 \text{ GPa}$ was revealed at the cutting edge and marks an increase of $>10 \%$ compared to planar substrate regions.

Our findings demonstrate that the substrate curvature significantly affects mechanical properties through its influence on microstructure and residual stress gradients. Successfully unveiling the convoluted process-structure-property interactions opens new pathways for the optimization of thin films at geometrically complex and performance-critical regions. Beyond cutting tools, these insights hold promise for microelectronics and other advanced technologies, where thin film functionality is critical.

Local Lattice Distortion Analysis of TiVZrNb Lightweight High Entropy Alloys Using Pair Distribution Function (PDF)

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

High entropy alloys (HEAs) are a novel class of metallic materials consisting of multiple principal elements in near-equiatomic ratios, offering unique properties such as high strength, thermal stability, and exceptional performance in extreme environments. Among HEAs, body-centered cubic (BCC) alloys are particularly notable for their high-temperature performance, but challenges such as high density and limited ductility have restricted their broader applications. This study focuses on designing lightweight BCC TiVZrNb HEAs by optimizing atomic size misfit to enhance lattice distortion and solid-solution strengthening.

The alloys were fabricated using vacuum arc melting and homogenized at 1373 K for 1 hour to achieve chemical uniformity and eliminate segregation. Synchrotron-based Pair Distribution Function (PDF) analysis quantified local lattice distortion induced by atomic size misfit. The analysis revealed significant local lattice strain within the first and third coordination shells of the BCC structure, as evidenced by the full-width at half-maximum (FWHM) of the peaks. These results confirmed a strong correlation between lattice distortion and solid-solution strengthening, driven by atomic size misfit. This research underscores the critical role of lattice distortion and atomic size misfit in enhancing the mechanical properties of lightweight TiVZrNb alloys. The findings establish the potential of these alloys as high-performance materials for structural applications in extreme environments, including aerospace and energy systems.

3D Mapping of Intragranular Strain and Microstructure in Recrystallized Iron Using Dark-Field X-ray Microscopy

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Assessing residual strains in metals is crucial for understanding their thermomechanical behavior, but probing them in 3D remains challenging due to the limitations of traditional techniques, which are often destructive or lack sufficient spatial resolution.

In this study, we performed a correlative investigation of intragranular local residual strain and orientation distributions in a fully recrystallized pure iron sample using Dark-Field X-ray Microscopy (DFXM) and Diffraction Contrast Tomography (DCT). Despite the fully recrystallized state, DFXM revealed significant heterogeneities in residual strain, indicating that strain fields persist even in the absence of a well-defined dislocation network. By analyzing multiple grains, we extracted their strain distribution, misorientation, and dislocation density, which was found to be on the order of ~ 0.0005 , 0.1° and 10^{10} m^{-2} , respectively. To complement DFXM results on local strain and orientation measurements at a 100 nm resolution, we probed the same sample using DCT to obtain the 3D grain structure, mapping the shape, size, and orientation of individual grains over a large volume of approximately $300 \times 200 \times 200 \text{ }\mu\text{m}^3$. The combination of the two datasets allowed us to resolve individual dislocations within specific 3D grains and determine their Burgers vectors. This identification was achieved by combining the grain orientation data from DCT with machine learning-based analysis of the strain and misorientation data extracted from DFXM. Additionally, the full 3D grain structure provided by DCT enabled further discussion on the origins of local residual strains, particularly in relation to interactions with neighboring grains during grain growth.

This correlative approach enabled high-resolution strain mapping across a representative volume, linking bulk characterization with local defect analysis. Our findings demonstrate the potential of integrating these two techniques, DFXM and DCT, highlighting the advantages of a multiscale approach for advanced characterization of strain heterogeneities and grain-level interactions in metallic systems.

X-ray diffraction mapping at the DanMAX beamline - Large areas, texture, and tomography

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D2_3, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Narwhal tusks, mice bones, lizard skin, unfolded batteries, additively manufactured piezoceramics, catalyst nanoparticles on alumina support, and biochar from pyrolyzed sewage sludge are just some of the many materials that have been measured with X-ray mapping techniques at the DanMAX beamline. Common for the previously mentioned materials is their hierarchical nature. “Conventional” powder diffraction provides information on the average atomic structure of the probed powder, but to properly study hierarchical materials we require spatial resolution. The low emittance MAX IV (Lund, Sweden), the world’s first 4th generation synchrotron, allows us to easily and fast focus the X-ray beam on the micron scale. Combined with fast linear scanning stages and optimized scanning strategies it is possible to raster scan macroscopic samples of thousands of square millimeters with micrometer resolution. The large area coverage has made it possible to map battery degradation in aged pouch cell batteries, without having to cut or slice the components.

An upstream fluorescence detector and a photon-counting CdTe area detector provides not only contrast from the elemental composition, but also diffraction contrast of the crystalline species as well as texture contrast from the azimuthal variation of the diffraction rings. In biological samples this can be used to map element deposition during growth, hierarchical crystallization, and crystallite orientations, as seen in e.g. bones, shells, and teeth. With texture mapping we can follow template-induced preferred crystallite orientations in additively manufactured ceramics, aiding in the understanding and production of highly specialized piezoelectric components.

Adding rotations to the raster scan gives the opportunity to do X-ray diffraction computed tomography (xrd-CT), giving 3D reconstructed images, where each voxel contains a full diffraction pattern. The diffraction provides contrast between different crystalline phases, even when those phases have the same nominal composition and density. An example includes the aging of MoS₂ catalyst particles deposited on nano porous alumina support pellets, where the depth-profile of the pellets are of interest.

Both 2D and 3D diffraction mapping techniques produce large amounts of data, not uncommonly hundreds of thousands or millions of diffraction patterns. The efficient data structure at DanMAX allows live integration of the collected area detector images and data analysis or tomographic reconstruction immediately following the data collection. A wide range of python-based jupyter notebooks makes it easy and quick to perform qualitative analysis of the large mapping datasets.

Using Small-Angle Scattering to Investigate the Structure of Mesoporous Silica and the Spatial Arrangement of Ionic Liquid Films at the Pore Surface

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The use of mesoporous materials, e.g., ordered mesoporous silica (OMS), for molecular heterogeneous catalysis is of great interest for industrial applications [1]. By embedding an organometallic catalyst inside the mesopores, high surface areas and high catalyst loadings can be realized. The use of an ionic liquid (IL), which contains the catalyst and adsorbs in a thin film on the surface of the OMS (Supported Ionic Liquid Phase, SILP), thus represents a pragmatic approach to significantly increase the selectivity of reactions [3]. To clarify the role of confinement, scattering methods such as small-angle X-ray scattering (SAXS) and small-angle neutron scattering (SANS) are powerful techniques to investigate the structure of nanoscale objects and complement the results of other analytical methods.

Based on SAXS data recorded of pristine OMS materials, we developed a universal multiscale model to analyze the structure at different, independent structural levels, describing the pore-to-pore distance, pore diameter, microporous corona thickness and the micropore length scale. By extending the model with the scattering contribution of the IL, we show that as the filling degree of the pore volume increases, the IL first fills the corona of the micropores and then forms a shell, whose thickness is believed to play an important role in the performance of the confined catalyst. Utilizing scheduled complementary SANS measurements to adjust the scattering contrast via the pressure-dependent filling of the OMS materials with deuterated methane will not only provide more information about the accessibility of micro- and mesopores, but also about the ILs spatial arrangement in the OMS material [4], i.e., whether it penetrates both micro- and mesopores, whether it uniformly wets all pore surfaces or whether the IL even blocks parts of the pores.

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Synergetic use of powder diffraction and electron backscatter diffraction

Prof. Andreas Leineweber¹, Dr. Stefan Martin¹

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D2_2, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Powder X-ray diffraction (PXRD) and electron backscatter diffraction (EBSD) are common techniques to analyse the global phase content and phase distribution locally of solid-state materials. However, particularly in the case of EBSD, little attention is often paid to the use of appropriate structure models employed for indexing, especially when dealing with phases of non-trivial crystal structure. This contribution will give some examples of EBSD analysis of intermetallic phases where X-ray diffraction of the same materials has been able to provide complementary information, e.g., on lattice parameters or to distinguish between different structural variants (ordering variants" or polytypes).

In this talk different alloy systems containing different forms of CoSn₃ (ordered and disordered stacking variants) will be dealt with, as well as Cu₆Sn₅ comprising different superstructures or varying long-range ordering. It is also shown how one can derive simplified crystal structure models allowing for robust indexing. Thus, one gets rid of ambiguities of the determined crystal orientation (which may not be of interest anyway) due to pseudosymmetry, however, at the cost of possibly extractable physical information.

3D Intragranular Orientation Mapping in Cold-Rolled Ferrite at Industrially Relevant Deformation Levels

Dr. Aditya Shukla¹, Dr Mads Carlsen², Dr Nikolas Mavrikakis³, Ms Virginia Sanna¹, Dr Yaozhu Li¹, Ms Marilyn Sarkis¹, Dr Carsten Detlefs¹, Dr Can Yildirim¹

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Thermomechanical processing of metals introduces high dislocation densities, altering material properties through mechanisms such as work hardening. Non-destructive 3D mapping of deformation microstructures remains a challenge due to limitations in characterization tools. This study combines Dark-Field X-ray Microscopy (DFXM) and texture tomography (TT) to investigate and compare deformation structures in 50% and 65% cold-rolled ferrite. DFXM enables non-destructive 3D mapping of intragranular deformation structures, resolving dislocation cells with elevated densities and misorientation values up to 5°, at a resolution of 100 nm. TT complements this by providing 3D grain orientation data, aligning grains relative to the rolling direction and bridging the effects of neighboring grains on deformation. These data are also validated with complementary Electron backscatter diffraction (EBSD) measurements. The combined approach reveals the evolution of intragranular deformation structures, cell size distributions, and strain hotspots as a function of deformation, advancing our understanding of plasticity and the interplay between local and global deformation behaviors. This framework offers critical insights into deformation mechanisms and recrystallization in metals.

In Situ Deformation Experiment at the Swedish Materials Science Beamline at PETRA III

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D2_3, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Deformation induced microstructural changes are frequently investigated in the literature using a large variety of different techniques. Observing these changes and the evolution of the microstructure in situ is much less common, due to the limited number of techniques providing insights non-destructively into metallic materials. The Swedish Materials Science beamline at PETRA III utilizes high-energy synchrotron radiation to obtain diffraction and/or imaging information. For several applications high energy synchrotron radiation hits the balance between penetration power and temporal resolution providing information from volumes of engineering relevance with a speed suitable to investigate real word conditions. In this talk, the combination of different techniques will be shown through examples of deformed microstructure characterization.

Analytical characterisation of nuclear material by multiscale approach

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D2_2, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Nuclear materials may have several morphologies and speciation in the solid state divided with different oxides or fluorides of uranium for fuel manufacture and reprocessing in the solid state, in ceramic forms (oxides or carbides), such as fuel pellets packaged in sheaths or inserted into glass matrices for waste packaging.

Depending on the generation of the nuclear reactor, different fuel/jacket systems can be envisaged with assemblies consisting of heavy elements and light elements such as: (UO₂/Zircaloy), (UO₂, PuO₂/Zircaloy), ((U,Pu)C, SiC/SiC), (UO₂, SiC/SiC).

Optimisation of the behaviour of materials in service or in an accident situation for reactor life, safety and security purposes is based on studies and test infrastructures related to operating conditions as well as scenario studies serious accident that could result in the fuel melting at 2000°C with the components reactor (B4C control bar, steel cooling tank, concrete reactor enclosure)

In this last theme, the multi-phase material at various spatial scales obtained by simulating a core fusion is called corium. It is the subject of numerous studies, in particular to supply basic data for reactor behaviour simulation codes in terms of design and safety in service, as well as to guide dismantling operations.

These behaviour studies require knowledge of the elemental composition and speciation of the materials tested. This allows for the optimization of manufacturing quality as well as the prediction of the physicochemical behaviour of materials over their lifetime under nominal or accidental conditions. This knowledge is enabled by the elementary and structural characterization means of SEM/EDS/STEM/EBSD, EPMA, Laue diffraction and x-ray and neutron diffraction. This talk presents the analytical developments and techniques adapted to these materials, particularly for the quantitative analysis of light elements in heavy matrices, the identification of multi-scale phases by diffraction methods, the elemental quantification on the solids and the powders as well as the consideration of the behaviour of these materials during preparation phases.

Ultrafast melting of polycrystalline Palladium: bridging experiment and simulation with X-ray free-electron laser probing

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D2_2, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Due to its extremely short timescale, the non-equilibrium melting of metals is exceptionally difficult to probe experimentally. The knowledge of melting mechanisms is thus, to a large extent, based on the results of theoretical predictions and computer modeling. This work reports on the ultrafast melting of thin polycrystalline palladium films studied by an optical laser pump – X-ray free-electron laser probe technique and two-temperature molecular dynamics simulations. By acquiring, with a sub-picosecond resolution, the X-ray diffraction snapshots, we capture the transient atomic structures of the sample during its transition from the crystalline to the liquid state. The diffraction data are correlated with large-scale molecular dynamics simulations. Bridging the timescales of the experiment and the simulation allows us to formulate a consistent atomistic picture of the melting transition [1]. We find that with increasing density of deposited energy, the melting process accelerates, and its mechanism progressively varies from heterogeneous, initiated inside structurally disordered grain boundaries, to homogenous, proceeding catastrophically in the crystal volume on a picosecond time scale, close to that of the electron-phonon coupling.

Reference:

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Advanced operando X-ray diffraction to explore power electronics in space and time

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D2_3, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

In the semiconductor industry, the rising demands for higher performance and reliability require the deployment of novel in-situ test concepts to uncover dynamic processes that govern the device functionality. In addition, to current established methods, for the static investigation of power semiconductors, operando characterization techniques will provide a comprehensive understanding that is essential for the advancement of future technologies. Power electronic devices are complex embedded heterostructures, consisting of different materials with different material properties. Consequently, nondestructive techniques are required to investigate fully functional systems. Due to structural features in the size of few nanometers as well as processes in the nanosecond range, most techniques are meeting their physical limits. In contrast, X-ray diffraction (XRD) based techniques fulfill most requirements to explore various dynamic processes occurring in power semiconductor applications. In particular, in-situ stress testing of functional chips was utilized to study (i) the fatigue of Cu metallization layers as well as (ii) the electric fields in high electron mobility transistors (HEMT). Power electronics undergo cyclic thermal loading caused by short circuit events. Due to mismatches of the thermal expansion coefficient, large thermo-mechanical stresses arise within the individual layers. Such stresses can lead to plastic deformation within the metallization and cause material fatigue. Dedicated test structures were developed to enable thermal-mechanical cycling with application relevant heating rates up to 10^6 K/s. Subsequently, in-situ 20 kHz X-ray diffraction was utilized at the MS-Powder beamline of the Paul Scherrer Institute in Switzerland to reveal biaxial stresses rising within the Cu metallization during a single heating pulse. Subsequently, the microstructural evolution causing Cu fatigue was investigated using in-situ dark field X-ray microscopy (DFXM) at the beamlines ID03/ID06 of the European Synchrotron Radiation Facility (ESRF) in France. Here, several hundred heat pulses were applied to visualize the changes of the intragranular strain and misorientation of a single Cu grain through the course of thermo-mechanical cycling.

HEMTs are based on wide-bandgap semiconductors such as heteroepitaxial (Al)GaN layers grown on Si substrates. Due to the piezoelectric nature of GaN wurtzite, the change of the electric field during hard switching generates significant lattice strain within few nanoseconds. This effect can be utilized for real time visualization of the local electric field within the active device area. Operando DFXM measurements at the beamline ID01 of the ESRF were used to map the piezoelectric strain field during device switching down to 1 ns temporal and ~ 150 nm spatial resolution.

Influence of trace and tramp elements on the phase transformation behavior of low-carbon steel analyzed by in-situ high-energy X-ray diffraction

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D2_2, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

In the effort to decarbonize the steel industry, a shift toward more sustainable processing routes has gained momentum. One such approach involves the use of scrap metal in combination with electric arc furnace (EAF) production route. This method however, introduces higher levels of trace and tramp elements, which can impact the phase composition, microstructure, and mechanical properties of the final steel products.

In this study, the phase transformation behavior of low-carbon steel with varying concentrations of trace and tramp elements was investigated. A reference alloy produced via the conventional BF route was compared to two trial alloys processed through the EAF route, with intentionally increased trace and tramp concentration.

To assess phase transformation temperatures and phase evolution during heat treatment, dilatometry experiments were conducted in conjunction with in-situ high-energy X-ray diffraction (HE-XRD) measurements. Rietveld refinement was utilized to quantify the volume fractions of ferrite, cementite, and austenite, providing insights into phase stability and transformation kinetics. Additionally, detailed microstructural characterization was performed using light optical microscopy (LOM) and scanning electron microscopy (SEM). Electron backscatter diffraction (EBSD) analysis was employed to qualitatively assess the presence and distribution of martensite.

The results indicate that the presence of trace and tramp elements leads to an expansion of the critical transformation temperature range, directly influencing phase formation during cooling. The increased presence of these elements facilitates the evolution of displacive phases, such as martensite and bainite, accompanied by retained austenite. These microstructural changes have important implications for the mechanical properties of steel, particularly in applications requiring controlled phase distributions to achieve specific strength and toughness characteristics.

Advancing Laboratory-Based 3D X-ray micro-beam Diffraction for Multiscale Materials Characterization

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D2_3, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

X-ray diffraction-based three-dimensional, non-destructive characterization has become a cornerstone for investigating the internal microstructure, crystallographic orientation, and defect distributions in polycrystalline materials. These techniques provide critical insights into materials' mechanical and functional properties, playing a pivotal role in materials science, engineering, and manufacturing. However, most advanced 3D diffraction methods are available only at large-scale synchrotron facilities, where access is limited due to restricted beamtime availability, logistical challenges, and high operational costs. These constraints hinder routine investigations and broader adoption in academic and industrial research.

To overcome these limitations, the development of laboratory-based 3D X-ray diffraction instruments is crucial. These systems would enable researchers to conduct 3D characterization routinely, significantly increasing accessibility to these powerful techniques. Laboratory diffraction contrast tomography (LabDCT) represents a major step forward, allowing the 3D reconstruction of fully recrystallized materials with grain size larger than 15 μm at a spatial resolution of 5 μm , using conventional laboratory-based X-ray CT systems. However, despite its success, LabDCT remains limited to relatively coarse-grained microstructures, requiring further advancements to extend its capabilities to finer microstructures and more complex materials.

To enhance the capabilities of laboratory-based diffraction techniques, we have developed a new 3D X-ray micro-beam Laue diffraction (Lab-3D μ XRD) technique. By integrating a conventional X-ray micro-CT system and newly developed Pt-coated twin paraboloidal capillary X-ray focusing optics, we have successfully demonstrated its feasibility. Additionally, incorporating a state-of-the-art photon counting detector has enabled the characterization of small grains ($\sim 5 \mu\text{m}$) and additively manufactured materials, the latter being particularly challenging due to their high defect content. By combining Lab-3D μ XRD with LabDCT and micro-CT, we establish a multiscale and multimodal 4D (x, y, z, time) characterization framework for studying microstructural evolution. This approach expands the capabilities of 3D X-ray diffraction beyond synchrotron facilities, offering an accessible and versatile solution for advanced materials characterization.

High-energy synchrotron X-ray diffraction and its applicability for depth-resolved residual stress analysis

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Residual stresses (RS) play an important role in many industrial materials and processes. They are of utmost importance as they strongly influence strength, corrosion resistance, and fatigue properties of metallic materials under service conditions. They also lead to excessive waste of material as they are often unknown or only estimated. High-energy synchrotron X-ray diffraction is a suitable tool to explore nondestructively depth-resolved RS in the bulk of materials.

A monochromatic high-energy X-ray beam in combination with a conical slit cell (CSC) enables the determination of the strain components over the whole sample thickness with sufficient spatial resolution. The CSC has several concentric ring slits that are focused on a spot within the sample by their conical shape. The analysis of full diffraction rings enables de simultaneous determination of all strain components in the plane orthogonal to the beam by taking advantage of the 2D detector. This setup allows resolutions that can be customized depending on the beam energy and on the beam size. Despite the advantages of this technique, it is not widely spread.

A white high-energy X-ray beam is well known for RS determination. It can be used either in near surface stress gradient measurements (reflection geometry) or in transmission condition for bulk measurements. Diffraction data are usually collected using energy-resolved HPGe detectors positioned at independent diffraction planes and the gauge volume can be controlled using incident and scattered beam slits. This technique usually requires performing and analysing data with the $\sin^2\psi$ approach.

Helmholtz-Zentrum Hereon operates two beamlines at DESY (Hamburg, Germany): P07-High Energy Materials Science beamline and P61A White Beam Engineering Materials Science beamline, which offer the above-mentioned techniques. In this work we present the characterization of RS in a variety of samples and geometries to observe the synchrotron capabilities for RS determination of normal and shear stresses in the bulk of materials, sub-surface RS analysis, a cross-comparison between both techniques, and the influence of individual diffraction peak or full pattern analysis for coarse-grained materials. The analysed materials are an additively manufactured austenitic steel 316L part in as-built and heat-treated conditions, a Grade S355 hot-rolled structural steel solely elastically loaded or with stresses generated by significant plasticity, a nickel-based alloy plate with a 3-pass slot weld, and a refill friction stir spot welded aluminium sample.

Welding at the Beamline, the Beamline P61A and its use for Materials Manufacturing Research

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D2_3, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The development of new metallic materials as well as their manufacturing and processing techniques has consistently benefited from synchrotron X-ray characterization. X-ray diffraction can characterize phase transformations, stresses and texture, while X-ray imaging allow for observation of phase boundaries, defect formation, etc. Particularly, the high intensity provided by synchrotrons allows for in-situ characterization of transient phenomena such as welding. The use of synchrotron X-ray scattering techniques for materials manufacturing applications does have some requirements. On one side, experiments typically cannot be downsized leading to mm to cm thick samples, requiring high X-ray energies. On the other, materials manufacturing techniques typically introduce high spatial heterogeneity, requiring spatial resolution within the material's bulk. The beamline P61A, operated by Helmholtz-Zentrum Hereon at the PETRA III synchrotron in Hamburg is uniquely equipped for performing metallic materials manufacturing experiments. The beamline uses a high flux white beam with usable energies from 20 to 200 keV, and can be used both for imaging or energy dispersive diffraction, which enables the definition of a gauge volume within the sample, allowing for the characterization of samples with through thickness heterogeneity. P61A has been in operation for 4 years, and over its short history, has seen consistent demand for ex and in situ characterization of welding processes. This talk will present the beamline, its instrumentation and key performance numbers. A selection of user science cases will be presented, with focus on how different welding experiments have been performed. Finally, the talk will show future developments and how these can be applied to materials manufacturing studies.

X-Ray Stress Tensor Tomography

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D2_1, Seminario 4 + 5 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The material properties of poly-crystalline engineering materials, such as fatigue strength and corrosion resistance, are closely linked to local strain and residual stress distributions. Consequently, precise strain measurements on micrometer scales are critical for validating model-based predictions regarding failure and lifespan—particularly for safety in automotive and aerospace applications. Currently, two primary categories of non-destructive techniques exist for depth-resolved strain measurement in poly-crystalline materials, both of which involve complex setups.

An alternative approach utilizes a pencil beam and X-ray powder diffraction for tomographic reconstruction of local strain and stress tensor components. In 2015, Lionheart and Withers mathematically demonstrated that information from six points on a single diffraction ring, combined with six appropriately chosen sample rotations, suffices to reconstruct all six strain tensor components. However, this method presents significant experimental challenges, and they noted the potential for a reconstruction method using fewer rotational axes.

In this presentation, we will illustrate that employing a single rotation with eight segments derived from two diffraction rings provides a robust foundation for the tomographic reconstruction of the six planar strain and stress tensor components. Scans conducted on shot-peened and control martensitic steel samples at the ID11 beamline of the ESRF in Grenoble, France, yielded reconstructed stress tensor components that align with expectations and corroborate laboratory surface results. Integrating data from two different diffraction rings requires the incorporation of X-ray elastic constants into the forward model. We treated these constants as additional free parameters in the minimization process and will showcase the potential of this approach for directly measuring them.

This innovative method for measuring depth-resolved strain and stress tensor components features a simplified setup, making it adaptable to a variety of existing beamlines. Consequently, strain and stress tensor tomography holds significant promise for transforming the field of strain and stress measurement.

xrd_simulator: Towards a PyTorch-based framework for FEM simulation of crystalline materials and diffraction experiments

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

X-ray powder diffraction, particularly synchrotron-based techniques, is a powerful tool for characterizing crystalline materials. However, conventional diffraction analysis often relies on collapsing diffraction signals into one-dimensional profiles for fitting, which eliminates critical information related to crystallographic texture and local strain fields. This limitation hinders the extraction of spatially resolved microstructural details essential for advanced materials characterization [1].

To address this challenge, the open-source Python package `xrd_simulator` enables the simulation of monochromatic X-ray diffraction experiments directly from finite element method (FEM)-based meshes [2]. By incorporating crystal deformation and polarization effects, `xrd_simulator` facilitates realistic diffraction simulations of deformed microstructures obtained from prior FEM calculations. Figure 1 presents a schematic representation of the primary reference systems used in an `xrd_simulator` experiment.

This work focuses on an ongoing effort to accelerate diffraction simulations by reimplementing `xrd_simulator` in PyTorch with GPU acceleration. This transition significantly enhances computational efficiency, enabling simulations of FEM meshes containing up to one million tetrahedral elements within seconds, compared to the tens of hours required by CPU-based methods. Figure 2 illustrates the results of an `xrd_simulator` experiment and a potential application of the tool in testing 3D reconstruction techniques such as XRD-CT [3].

Beyond simulation, the framework is intended to be extended into a direct analysis tool by leveraging the PyTorch forward model for inverse problem-solving. By minimizing the difference between experimental and simulated diffraction patterns, this approach aims to refine microstructural parameters such as crystal orientations and phase distributions within the sample, providing a pathway toward automated, high-throughput diffraction data analysis [4].

Influence of the interfacial strength on wear resistance in Ni-SiC composite

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D3_7, Albéniz Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Wear resistance is one of the most important properties for materials. Increasing its value is of interest for both scientists and industry. One of the typical approaches is to apply anti-wear coatings on mechanically poor materials instead of the use of high-end materials, usually expensive, in bulk.

Anti-wear coatings can be prepared by means of electrodeposition. However, the tribo-mechanical performance of deposited metal may not be reliable enough. To increase anti-wear properties even further, one can use co-electrodeposition in order to produce metal-matrix composite coating, such as Ni-matrix with SiC particles as reinforcement.

Properties of composites are derivatives of not only matrix and reinforcement, but also their interface. If the connection is weak, it may lead to premature fracture and poor performance. Macroscopically conventional methods to measure interfacial strength are tensile and bending tests. However, one have to take into account geometry of the interface. Especially for micro-sized samples, where interface cannot be considered flat anymore. In this work, we combined experimental and numerical methods to study interfacial strength in Ni-SiC composites and its influence on wear resistance.

New experimental procedure includes FIB-milling of micro-beams with matrix-reinforcement interface, beam bending with nanoindenter until fracture and AFM scanning of fracture surface. Then, numerical approach was employed. FEM model was built based on experimental geometry of each studied micro-beam. Interfacial strength was computed.

Also, macroscopic wear was measured in typical ball-on-flat geometry. The results were analyzed based on interfacial strength results.

Both interfacial strength and wear resistance depend on fabrication process and method was proved useful for small-scale testing of experimental interfaces.

Defects in glass to metal bonds of electric terminals for hermetic seals

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Electric connectors are of fundamental importance for the long-term impermeability of hermetic seals. These connectors, made from glass and metal, function as electric terminals, guaranteeing power supply to the vessel's interior while ensuring a gas-tight enclosure. However, glass to metal bonding presents challenges because of dissimilar material characteristics, such as different melting temperatures, thermal expansion, and ductility. Time consuming, non-destructive tests (He-leak tests) in the manufacturing line expose a certain batch-dependent failure rate in a late stage of production. This study aims to investigate the root cause of the defects in the joint area of hermetic seals to optimize the production process and minimize waste. Separately, we inspected the quality of the incoming hermetic seal and its alteration during production. Micro-computed tomography tests reveal spherical cavities in the glass body and cracks along the glass-metal interface. During installation and subsequent assembly, significant temperature differences caused by the welding processes lead to thermal strain in the geometry close to the seal, causing crack initiation or growth in the glass body. Temperature measurements during the welding process quantify the acting thermal gradient. These data are used to validate a FEM model (Simufact Welding) which can subsequently aid in the welding procedure to minimize the load on the glass-metal interface. Based on the gained knowledge process optimizations preventing defects in the electrical terminals of hermetic seals ensure high quality and long-lasting products.

Elastic Microstructures in Bulk Metallic Glasses — Are They Real?

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Abstract

Amorphous metallic alloys, known as metallic glasses (MGs), are distinct from conventional crystalline alloys due to their unique disordered structure. Unlike crystalline alloys with an ordered, periodic atomic arrangement, MGs appear homogeneous and monolithic when studied at meso- and macroscopic length scales. Compatible with atomistic simulations and not unsurprisingly, they exhibit structural heterogeneity at the lower nanometer scale, as observed experimentally with AFM techniques. However, elastic property mapping by nanoindentation revealed elastic fluctuations at length scales about an order of magnitude larger (~ 100 nm) - their origin is still under debate.

Our previous work identified an elastic correlation length of around 150-200 nm in a Zr-based alloy (Materials & Design 229 (2023) 111929). It ruled out chemical fluctuations as the underlying origin, suggesting that cooling constraints during solidification may be a contributing factor. This hypothesis can be seen as the local microstructural manifestation of cooling-induced internal residual stresses known to exist in MG rods and revealed by focused ion beam–digital image correlation ring-core milling (Materials & Design 104 (2016) 235-241).

Here, we further investigate this idea by examining various casting geometries and thermal histories, tracking how elastic decorrelation lengths change with sample size and position within the MG samples. We find that thermal annealing reduces decorrelation length-scale gradients and reduces the position-dependence of the elastic fluctuations (Scripta Materialia 255 (2025) 116380). As a new step in our nano-elastic property assessment, we leverage spatially-resolved scanning nanobeam diffraction to narrow down the possible structural origin of these elastic signatures.

Nanoindentation and Defect Dynamics in Irradiated Fcc NixFe1-x Alloys: Insights from Experiments and Atomistic Modeling

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D3_3, Albéniz Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Fcc NixFe1-x single-crystal alloys are key model systems for studying defect evolution under self-ion irradiation at room temperature, with fluences ranging from 4×10^{13} to 2×10^{15} ions/cm² [1,2]. This study investigates the effects of irradiation-induced defects on the nanomechanical response of NiFe alloys through a combination of experimentally guided nanoindentation and atomistic simulations. Defects in the irradiated materials were characterized using transmission electron microscopy (TEM), providing essential input for molecular dynamics simulations of overlapping collision cascades to prepare irradiated samples at various doses [3].

The simulations revealed mechanisms of defect formation and evolution, including the emergence of an A15 Frank-Kasper phase within the {111} plane in pure Ni, Ni_{0.88}Fe_{0.12}, and Ni_{0.77}Fe_{0.23} at fluences up to 2×10^{14} ions/cm², serving as a precursor to Frank loop nucleation. The findings also highlight the critical role of Fe atoms in influencing dislocation nucleation and evolution. In Ni_{0.77}Fe_{0.23}, compact 3D precipitates heavily decorated with Fe atoms were observed. However, these precipitates remained too small to evolve into Frank loops, even at elevated fluences.

Nanoindentation experiments and simulations demonstrated a notable increase in hardness in irradiated alloys compared to their pristine counterparts [4,5]. From the atomistic modeling, we provide detailed analyses of the irradiated samples revealed surface morphologies, dislocation densities, and strain mappings to discuss the mechanisms of dislocation pinning during mechanical loading due to irradiation-induced defects. These defects were found to obstruct dislocation motion, contributing to the enhanced hardness of the material.

Overall, this study provides critical insights into the interplay between composition, irradiation-induced defect structures, and their mechanical consequences in NixFe1-x alloys. These findings enhance our understanding of the mechanisms underpinning radiation resistance in these materials, supporting their potential applications in radiation-intensive environments.

[1] E. Wyszowska et al. *Nanoscale* 15, 4870 (2023).

[2] A. Ustrzycka et al. *Int. J. Plasticity* 182, 104118 (2024)

[3] K. Mulewska et al. *J. Nucl. Materials* 586, 154690 (2023)

[4] L. Kurpaska et al. *Materials & Design* 217, 110639 (2022).

[5] F. Dominguez-Gutierrez et al. *J. Appl. Phys.* 135, 185101 (2024)

Residual stress and machining path optimization based on artificial intelligence

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The residual stress in manufacturing of material itself and post-processing to manufacture the aerostructure component has been a crucial issue for the dimensional accuracy of the manufactured aerostructure component. In this research, the application of artificial intelligence has been introduced for the prediction of residual stress and machining path optimization for the 2xxx series aluminium alloy which is outlined in Figs. 1 and 2, respectively. The Bulk Residual Stress (BRS) which is induced by quenching after extrusion was predicted by the ANN model with respect to geometry of material and quenching parameters. The Machining-Induced Residual Stress (MIRS) was predicted by the simple regression model with respect to machining parameters. The data set for each residual stress prediction was prepared by using finite element simulation and experimental results where contour and X-Ray Diffraction (XRD) methods were used for the experiment of the residual stress. Both BRS and MIRS were applied into finite element simulation for the distortion prediction of machining without any fracture model to describe element deletion in machining. In the simulation, the BRS was initially mapped into the extruded material with its geometry and quenching condition. Based on the machining parameters such as tool, feed rate, width of cut, and RPM, the MIRS come to be inserted into the integration points of the element which is located machined surface. Then, through the additional simulation time step to satisfy the force equilibrium which is violated by the BRS and MIRS, the machining-induced distortion could be predicted only by the BRS and MIRS whereby it is possible to perform numerically efficient finite element simulation for the prediction of machining-induced distortion. As far as machining path optimization is concerned, since MIRS includes the machining process parameters, XGBoost regression model was adopted because of its feature which combines several decision tree models to give the best prediction and shows excellent prediction for small datasets.

High Strain Rate Mechanical Behavior of Structurally Graded Materials Processed by Surface Mechanical Attrition Treatment (SMAT)

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D3_5, Albéniz Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

The service lifetime of structural components is often limited by surface-initiated failure. Surface hardening treatments aim at preventing crack initiation while preserving the properties of the bulk material. The so-called Surface Mechanical Attrition Treatment (SMAT) induces severe plastic deformation through repeated multidirectional impacts of ultrasonically accelerated spherical shots. This creates a gradient microstructure that transitions from nanocrystalline just beneath the treated surface to coarse-grained deeper within the sample. While significant hardening has been evidenced at conventional testing velocities, the behavior of this microstructurally graded layer at high strain rates - typical in collision scenarios and a common cause of component failures - remains less understood.

Nanoindentation tests at medium to high strain rates (0.1/s, 1/s, 10/s, 100/s) were conducted on cross sections of SMAT processed austenitic 316L steel, pure copper, and Inconel 718 to investigate their hardness and strain rate sensitivity. The hardness was evaluated using the Merle-Higgins-Pharr method for high strain rate nanoindentation testing. The measurements reveal a distinct hardness gradient within the SMAT layer, and show that the overall strain rate sensitivity of the SMAT treated material increases at high strain rates.

Acknowledgement

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Enhanced mechanical and tribological properties of nitrogen-doped PVD MoS₂ coatings in rolling-sliding contact

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D3_7, Albéniz Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Friction causes energy dissipation and wear in mechanical parts. The exorbitant cost that this could incur across the world is usually mitigated by the use of lubricants. Liquid lubricants are most common due to their ease of handling. However, under certain extreme environments, their use may not be feasible. That holds particularly for vacuum applications, for which molybdenum disulfide (MoS₂) is a very sought-after dry lubricant alternative. MoS₂ exhibits low friction values and high chemical stability across a broad range of temperatures and pressures.

Nitrogen doping has recently gained traction as a possible pathway toward further improving the mechanical properties and the tribological performance of transition metal dichalcogenides coatings, such as WS₂ [1]. To assess the impact of nitrogen-doping to PVD MoS₂ coatings, specimens were deposited by magnetron sputtering in a reactive nitrogen environment, using different gas flows. The resulting MoS₂ coatings were characterized for surface morphology and roughness, coating thickness and density, chemical composition, as well as mechanical properties. To evaluate the influence of nitrogen incorporation on wear and tribological behavior, all characterizations were performed both before and after rolling-sliding tests. Results demonstrate a beneficial effect of nitrogen doping on wear behavior without altering the friction coefficient under higher loads.

[1] T. W. Scharf, A. Rajendran, R. Banerjee, F. Sequeda, Thin Solid Films 2009, 517, 5666.

Orientation dependence of serrated flow: insights from microcompressed Mg-Gd single crystals

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D3_11, Albéniz Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Important aspects of serrated flow, such as the influence of plastic anisotropy and twinning are yet to be fully understood. These aspects are particularly important in alloys systems of the HCP family, including Mg alloys which exhibit strong anisotropy and twinning. Moreover, efforts to identify the dominant slip systems in the serrated flow regime in polycrystalline materials have been challenging, as such investigations are complicated by the presence of grain boundaries and the interaction between grains. To address these challenges, single crystals of a Mg-Gd alloy were tested using a combination of microcompression and microstructural characterization tools, including EBSD and TEM based EDS/STEM measurements. The study also benchmarks the temperature and strain rate dependencies of the alloy against pure Mg crystals in similar orientations. The results reveal that serrated flow in Mg alloys is markedly anisotropic. This anisotropy arises from differences between the Burgers vector for slip/twinning, and variations impurity diffusivity parallel and perpendicular to the basal plane. The work also provides compelling evidence that the solute drag mechanism, rather than the widely accepted dynamic strain aging mechanism, underlie serrated flow in the alloy.

In-situ SEM micro-shear experiments to evaluate the failure modes of metallization interfaces in electronics

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

In the rapidly evolving field of microelectronics, the reliability of metallization stack interfaces is critical for the performance and longevity of devices. This study focuses on the measurement of shear strength of an interface between a copper (Cu) metallization and a thin (<50nm) dielectric cap, meant to prevent metal oxidation. Depositing a thicker, service dielectric (Silicon nitride, SiN, 500nm) and milling prismatic test structures with an in-plane footprint visible at an optical microscope (10x10μm) enabled relocation and successful shear interface tests using a bi-directional nanoindentation device, which served as a preliminary step to rank the strength of two cap recipes under comparison. While testing on standalone nanoindentation platforms is convenient in terms of throughput and has the potential to be partially automated, the assessment of failure modes relies on ex-situ observation methods, lacking deep insights into the origins of different kind of failures. But these insights are necessary to understand the root-cause of the failures and, potentially increase the system robustness as well as formulate life-time models, which is essential for designing more reliable microelectronic devices. Therefore, this research aims to deepen our understanding of these interface fracture phenomena through in-situ micro-shear experiments conducted within a Scanning Electron Microscope (SEM), allowing for a quantitative real-time observation of the shear behavior and interface failures.

Utilizing nanoindentation techniques within the SEM, we examined the cross-section of the Cu/cap interface upon shear, enabling the observation of failure modes as they occur under applied stress.

We distinguished between ductile and brittle failure modes, providing a comprehensive analysis of the conditions that led to each type of failure. Through meticulous observation and analysis, we aim to establish a clearer correspondence between the observed failure behavior and the signatures of failure in the load/displacement signal, being the latter the only link between insightful in-situ experiments and higher throughput standalone shear experiments.

To further enhance our understanding, a thorough root cause analysis of both ductile and brittle failure modes was conducted. By identifying the underlying causes of these failures, we hope to provide valuable insights that can improve material selection and interface engineering in microelectronics.

In conclusion, by combining standalone nanomechanical testing with validation by in-situ SEM experimentation, this research contributes to the ongoing efforts to improve the reliability of metallization interfaces in microelectronics. The findings from this study will enhance our understanding of interface behavior and pave the way for more robust microelectronic devices.

High-Temperature Nanoindentation Behavior of Single-Crystalline Titanium: A Molecular Dynamics Study

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The mechanical responses of the single-crystalline hexagonal close-packed (HCP) metals, such as titanium (Ti), make them highly valuable for applications requiring excellent strength-to-weight ratios and high-temperature stability. Titanium's ability to maintain mechanical performance at elevated temperatures (600–1300 K) has been observed through nanoindentation experiments. Obtained results of the local hardness and elastic modulus values, i.e. nanoindentation behaviour at elevated temperature, reveal the connection of dislocation mechanisms and defect nucleation. The main focus of this work is a computational study of the high temperature effects on the mechanical deformation properties of a single-crystalline Ti during a nanoindentation test. Molecular dynamics (MD) simulations of a spherical nanoindentation are carried out at two indenter tip diameters and crystalline sample orientations [001], [10-10], and [11-20], for a temperature range of 10–1000 K. The study examines how the temperature increament affects the nanoindentation process, altering dislocation densities, slip mechanisms, atomic displacements, and the local hardness, as well as its agreement with experimental findings.

Investigating humidity-driven variations in fracture toughness of alumina using microcantilever testing and Gaussian regression approach

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D3_4, Albéniz Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Slow crack growth (SCG) is a critical phenomenon in ceramics, caused by stress-dependent cleavage at the crack tip and enhanced by the interaction of environmental humidity with atomic bonds at the fracture site. This causes cracks to propagate slowly over time, even under stress levels below the material's nominal strength, often resulting in catastrophic failure. Understanding SCG is essential for ensuring the long-term reliability of ceramic materials.

Although extensively studied in macroscopic specimens, this phenomenon has only recently been investigated at the microscopic scale. While recent microscale studies have provided some insights, they remain limited in the range of environmental conditions tested.

This study aims to investigate the fracture toughness of monocrystalline and polycrystalline alumina under varying environmental humidity conditions and to develop a comprehensive model of its performance across these conditions.

Stress intensity factors (K) are measured in laser-ablated and focused ion beam (FIB)-milled bridge-notched microcantilevers and micropillars using a nanoindenter that provides precise control over a broad range of humidity levels. Finite Element Method (FEM) simulations are conducted to explore the mechanisms of SCG in microcantilevers. A Gaussian regression process (GRP) is employed to optimize the experimental design and quantitatively modeling the relationship between stress intensity factors and environmental humidity.

The combination of laser ablation and FIB milling has proven to be an effective method for rapidly and precisely producing a large number of samples, enabling extensive testing and enhancing statistical robustness. Preliminary results obtained applying the GRP on previously reported data ($K=3.5$ MPa $m^{1/2}$ in vacuum, $K=1.5$ MPa $m^{1/2}$ in air, $K=0.9$ MPa $m^{1/2}$ in water) reveal a non-linear decrease in fracture toughness with increasing humidity. While earlier studies assumed a linear trend, GRP indicates a steeper decline at lower humidity levels, stabilizing around 75% of relative humidity. This behavior is likely due to the saturation of water molecules interacting with atomic bonds at the crack tip, where K is reduced by moisture-assisted SCG.

This study presents a novel integrated approach for analyzing fracture toughness at the microscale under varying environmental conditions. The method enhances accuracy in characterizing fracture behavior across a broader range of humidity levels than previously studied and significantly accelerates the testing process compared to conventional techniques. This approach offers a new framework for future investigations into the environmental effects on fracture mechanics and SCG across a wide range of materials.

Multiscale Modeling of Creep Deformation in 30CrMoNiV11-5 Steel: Integrating Mean-Field Theory, Dislocation Dynamics, and Experimental Validation

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D3_2, Albéniz Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

30CrMoNiV11-5 is a high-strength, low-alloy steel recognized for its excellent mechanical properties, including high tensile strength, toughness, and good fatigue resistance. This material is widely used in demanding applications, such as aerospace components, where durability and reliability are essential. Its composition—comprising chromium, molybdenum, nickel, and vanadium—enhances its performance under extreme conditions, making it a preferred choice for industries requiring materials capable of withstanding high stress and harsh environments. However, prolonged exposure to high temperatures and stresses results in creep deformation, that accumulates over time. Accurately predicting the creep behavior of 30CrMoNiV11-5 is therefore of paramount importance.

The existing literature on the creep behavior of 30CrMoNiV11-5 includes studies utilizing machine learning techniques to predict creep rupture time, tensile mechanical properties, and microstructural evolution. These studies rely on reliable datasets derived from experimental measurements or numerical simulations. However, experimental creep tests are inherently time-consuming, often requiring several years to complete. While numerical simulations provide an efficient means of creep deformation and rupture predictions, they present significant challenges due to the complex microstructural evolution of the material under high stress and temperature conditions. To address these challenges, we applied a Mean-Field Creep (MFC) model for creep analysis. Based on Ghoniem's modeling framework and further developed by F. Riedlsperger, it integrates dislocation dynamics with a mean-field methodology to describe creep phenomenon. The MFC model simplifies the complexity of dislocation interactions by averaging their collective behavior and tracking the evolution of dislocation density over time. Central to this approach is the modified Orowan equation, which relates the creep strain rate to dislocation density, Burgers vector, and dislocation velocity. This framework links microscale dislocation behavior to macroscale material performance. To enhance the accuracy of predictions in the tertiary stage of creep, we incorporated the damage evolution equation from the phenomenological elasto-visco-plastic creep law developed by Morch (ULiege PhD 2022).

Given the limited availability of experimental data for parameter identification of the MFC model and its validation, we conducted a series of standard creep tests (SCT) to extract creep curves at various stress and temperature levels. The microstructure states at different material stages, is a key feature for the MFC model too and it was characterized. This experimental campaign validates the MFC model, enabling more reliable predictions of the long-term creep behavior of 30CrMoNiV11-5 under operational conditions.

Atomic scale simulations of plasticity in Cu/Ag nanolamellar systems

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D3_2, Albéniz Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Combining several materials to improve the mechanical properties of the assembly is a longstanding approach, used for example in lamellar composites systems. In the last decades, modern synthesis methods, such as severe plastic deformation, were developed and applied to metallic lamellar composites, allowing for a reduction of their layers width to less than 100 nm. The remarkable mechanical properties that these nanolamellar systems show are mainly imparted by the increasing role played by the interfaces in their plastic behavior. In that context, the nanolamellar bi-metallic Cu/Ag composite is particularly interesting. Indeed, experimental observations reveal in this system the coexistence of two different kinds of interface, whose interaction with extended defects such as dislocations and mechanical twins is very different. On the one hand, the "heterotwin" interface is a strong obstacle to the transmission of dislocations or twins. On the other hand, these defects are easily transmitted across the "cube on cube" interface. Because of the high lattice mismatch between copper and silver (around 12%), both interfaces are semicoherent and characterized by a network of misfit dislocations, which interact in a specific way with extended defects coming from the layers. The interfaces can also be sources for extended defects.

We thus performed molecular dynamics simulations of the deformation of Cu/Ag nanolamellar systems. These atomistic simulations are particularly well suited to the nanometric scale and to the study of the plasticity mechanisms at play in such nano-systems. We considered different stress fields applied to the systems and analyzed in particular the nucleation of dislocations or twins from the interfaces. The role of defects at the interface, such as atomic steps, observed experimentally, was also investigated by introducing them in a controlled way into the simulated systems.

Keywords: Cu/Ag nanolayers, interface, plasticity, molecular dynamics

Atomistic Mechanisms of Dislocation Motion and Reaction in Laves phases

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D3_1, Albéniz Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

Recent studies have revealed new slip mechanisms in Laves phases [1] and highlighted the thermally activated nature of synchro-shear partial dislocation glide [2-3]. However, the atomistic mechanisms underlying dislocation reactions, twinning, and phase transformations remain unclear. In this study, we investigated dislocation motion and reactions in C15 NbCr₂ Laves phases through high-angle annular dark field scanning transmission electron microscopy and atomistic simulations.

Experimental observations enabled the reconstruction of dislocation core and lock structures, while simulations provided insights into underlying mechanisms of dislocation motion and reaction. Using nudged elastic band calculations, we characterized the mechanisms of individual partial dislocations forming intrinsic stacking faults, coupled partial dislocations forming extrinsic stacking faults, and their reactions forming Lomer-Cottrell and Hirth locks.

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[2] Xie, Z., Chauraud, D., Atila, A., Bitzek, E., Korte-Kerzel, S., & Guénolé, J. (2023). Unveiling the mechanisms of motion of synchro-Shockley dislocations in Laves phases. *Physical Review Materials*, 7(5), 053605.

[3] Xie, Z., Chauraud, D., Atila, A., Bitzek, E., Korte-Kerzel, S., & Guénolé, J. (2023). Thermally activated nature of synchro-Shockley dislocations in Laves phases. *Scripta Materialia*, 235, 115588.

Molecular dynamics study of nanotwinned gold thin films deformation

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septembre 15, 2025, 13:15 - 14:30

Crystal defects may play an important role in improving the properties of materials. This is the case for twin boundaries, which impart to nanotwinned materials a remarkable combination of high mechanical strength and good ductility, without loss of electrical properties, their resistivity being identical to that of coarse-grained materials. Indeed, the twin boundaries, that divide the matrix into two symmetric orientations, can hinder the motion of dislocations, making it more difficult for plastic deformation, leading to the desired mechanical strength. However, because of the high symmetry of the associated microstructure, the scattering of conducting electrons at a coherent twin boundary is reduced, preserving the electrical conductivity of the metal, conversely to what happens for other grain boundaries.

In that context, we performed tensile tests on gold thin films with nanotwins, in-situ under X-ray diffraction and we observed, for some loading axes, the growth of twins in the crystal. To better understand the deformation mechanisms occurring in these materials, we conducted atomic scale simulations for systems as close as possible to the experimental ones. Such simulations are tools particularly well suited to this type of study, making it possible to accurately describe the configurations of defects such as dislocations, grain boundaries, twins, etc. They naturally reproduce key material properties such as elasticity coefficients, stacking fault or twin boundary energies. Moreover, atomic scale simulations and experiments tend to converge to similar size scales. However, special care must be given to the selection of the interatomic potential used in molecular statics and molecular dynamics simulations. For this study, we selected two interatomic potentials on the basis of the correspondence of their gamma curves to the ones obtained with ab initio calculations.

Then, we first investigated the stability of a nanotwin in a gold thin film, before submitting it to applied stress in a direction similar to the experimental one. The preliminary results on the thin film deformation show the glide of partial dislocations along the coherent twin boundary and the detachment of partial or extended dislocations from the junction between coherent and incoherent twin boundaries.

Keywords: nanotwins, twin boundary, atomic scale simulations, deformation

In-Situ TKD Tensile Testing Reveals Complex Nanoscale Deformation Twinning in Rhenium

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Deformation twinning (DT) plays a central role in the plastic deformation of hexagonal close-packed (HCP) metals, due to their insufficient amount of slip systems. DT can enable plasticity along the c-axis when pyramidal slip is not possible. However, DT has also been associated with reduced ductility, high residual stresses, and the promotion of fracture. As a result, DT complicates the broader adoption of HCP metals in industry. While DT has been extensively studied, fundamental questions persist regarding twin nucleation, growth mechanisms, and the interaction of twins with surrounding microstructural features, such as grain boundaries and other twins.

This study employs a novel in-situ transmission Kikuchi diffraction (TKD) methodology developed in-house at EMPA Thun, which is capable of sub-10 nm resolution orientation mapping during micro tensile testing [1]. Applied to single-crystal Rhenium under c-axis tension, we reveal previously unobserved mechanisms relating to the commonly observed $\{11\bar{2}1\}\{11\bar{2}6\}$ extension twin (ET), specifically the formation of secondary ETs within primary ETs. Together with interactions between intersecting primary twin variants, the secondary ETs lead to the formation an apparent nanograined microstructure. Based on the insights gained into the fundamental deformation mechanisms of Rhenium, implications for its accommodation of plastic strain are discussed. This includes the effect of secondary ETs on twin thickening mechanisms and fracture behavior, particularly considering the expected intense shear localization at the interfaces of matrix and secondary ET.

[1] T. Vermeij, A. Sharma, D. Steinbach, J. Lou, J. Michler, and X. Maeder, “In-situ Transmission Kikuchi Diffraction Nano-tensile Testing,” Oct. 29, 2024, arXiv: arXiv:2410.22107. doi: 10.48550/arXiv.2410.22107.

Tensile Twinning in Magnesium: A Correlative Nanomechanical and Atomistic Study

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D3_10, Albéniz Room (Level -2), septembre 17, 2025, 17:00 - 19:00

Grain boundaries (GBs) and their migration play a significant role in the deformation and texture modification of magnesium (Mg) alloys. A comprehensive understanding of their mechanical behavior during deformation can facilitate the design of Mg alloys with tailored properties. This work investigates tensile twinning, one of the most critical mechanisms in Mg. Micropillar compression tests, combined with atomistic simulations, were conducted on a-axis oriented Mg single crystals and bi-crystals with a pre-existing tensile twin boundary. The results indicate that tensile twinning is the primary deformation mode during compression along the a-axis, leading to a substantial stress drop in the stress-strain curve. The critical stress for twinning is primarily governed by twin nucleation and propagation. In bi-crystal samples, twinning occurred either sequentially or simultaneously in each grain, with the pre-existing twin boundary acting as a barrier to twin propagation. The findings from this study provide deeper insights into tensile twinning behavior in Mg.

References:

[1] Hirsch J, Al-Samman T. *Acta Materialia*, 2013, 61(3): 818-843.

[2] Wang H, et al. *Computational Materials Science*, 2024, 240: 113025.

Effect of polishing on near-surface residual stresses in commercially pure titanium

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D3_11, Albéniz Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Polishing is a mechanical process conducted on metallic materials to obtain a smooth, mirror-like surface, exempt from defects. It is usually conducted prior to metallographic observations, as a step in surface treatments or simply as a finishing process. As any mechanical processing method, polishing induces residual stress, which can be beneficial or detrimental to the structural integrity of materials. It is therefore of interest to evaluate the magnitude of residual stresses induced by this process. Studying the polishing process is complex due to its multi-parametric nature as well as the small length scale of occurring mechanisms. While it has been theorized in the past that an amorphous layer is created on top of a polished sample, it was demonstrated with modern tools that chips were removed over time, therefore making the polishing process more analogous to a cutting process. In this study, commercially pure titanium was polished to evaluate the weight of different polishing parameters on the induced residual stresses in the chosen material. These parameters include abrasive particle size, polishing load and polishing time. The samples were first stress-relieved through heat-treatment and electropolished to obtain a fully stress-relieved surface. The samples were then mechanically polished with a semi-automatic polisher using different parameters. Analysis of residual stress was conducted via ring-core FIB-DIC (Focused Ion Beam-Digital Image Correlation). This method enables depth-resolved residual stress analysis of the polished samples with submicron depth resolution. The results show that polishing induces significant compressive stresses in the first few micrometers of the surface. The effect of different polishing parameters is shown through a design of experiments.

Strain rate dependence of slip vs. twinning in c-axis compression of α -titanium

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D3_5, Albéniz Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Deformation twinning plays a crucial role in governing the plastic behavior of hexagonal close-packed (HCP) metals, primarily due to the limited availability of easily activated slip systems. Twinning is often associated with reduced ductility and the generation of high residual stresses, which can contribute to material failure through cracking. Understanding the nucleation and propagation of twinning in HCP metals is essential for optimizing their mechanical properties and enhancing their performance in various engineering applications. In this study, we explore the strain rate sensitivity of deformation twinning and non-basal slip systems.

In-situ uniaxial compression tests of micro-pillars in single crystal pure alpha-titanium at different strain rates ($\dot{\epsilon}$), ranging from 10^{-3} to 45^3 s^{-1} . All experiments were conducted with the [0001] crystal orientation aligned with the loading axis. The crystallographic orientation, active slip systems as well as the distribution of the geometrically necessary dislocation (GND) within the deformed volume of the material were analyzed using post-mortem cross-sectional transmission Kikuchi diffraction (TKD) of the deformed pillars. Additionally, post-mortem transmission electron microscopy (TEM) is used to characterize the activated dislocations and twin plane features under different deformation conditions.

A transition from slip-dominated to twin-dominated deformation is observed as the strain rate increased. At low strain rates ($\dot{\epsilon} < 10^2 \text{ s}^{-1}$), plasticity was primarily governed by dislocation slip, with twinning remaining inactive. In contrast, at high strain rates ($\dot{\epsilon} > 10^2 \text{ s}^{-1}$), plasticity was predominantly accommodated by $\{11\bar{2}2\}$ $\langle 11\bar{2}3 \rangle$ deformation twinning.

By combination of post mortem TKD and TEM techniques, our work adds new pieces towards the fundamental comprehension of deformation twinning in HCP metals at the micron scale and at high strain rates.

Plasticity beyond Fundamental Building Blocks: A Case Study of Sm-Co Intermetallics

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D3_3, Albéniz Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Intermetallic materials often consist of structurally related phases, as complex crystal structures contain repetitions of fundamental building blocks. In this study, SmCo₂ and SmCo₅ are investigated as the building blocks of SmCo₃ and Sm₂Co₁₇. The activated slip systems in these phases were examined using slip trace analysis, micropillar compression and Density Functional Theory (DFT). It was initially hypothesized that SmCo₃ would follow the lowest-energy slip pathway observed in SmCo₂ and SmCo₅. However, our results suggest that the stacking of the SmCo₂ and SmCo₅ units alters the electronic bonding between interatomic layers, thereby modifying the most favorable slip system. Additionally, the activation of non-basal slip systems is significantly restricted in SmCo₃ and Sm₂Co₁₇, limiting their contribution to plastic deformation. Further analysis using DFT revealed deviations from simple shearing in non-basal slip pathways. Bonding analyses were performed to elucidate the underlying factors influencing slip behavior. Ultimately, our work builds a connection between complex intermetallic phases and their structurally related building blocks by characterizing their slip mechanisms and correlative bonding properties.

Publications:

T. Stollenwerk, N. Z. Z. Ulumuddin, P.-L. Sun, S.-H. Lee, M. Seehaus, K. Skokov, O. Gutfleisch, Z. Xie, S. Korte-Kerzel, *Acta Materialia* 2024, 266, 119669.

T. Stollenwerk, P. C. Huckfeldt, N. Z. Z. Ulumuddin, M. Schneider, Z. Xie, S. Korte-Kerzel, *Advanced Materials* 2024, DOI 10.1002/adma.202414376.

Multiscale Modelling of Superplasticity of Ti-6242

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D3_2, Albéniz Room (Level -2), septembre 15, 2025, 10:50 - 13:10

The superplastic forming (SPF) process enables the manufacturing of complex-shaped aerospace components in a single operation (e.g., air inlets, engine pylons). However, its implementation requires high temperatures, around 900°C for titanium alloys, and very slow forming cycles, making the process highly costly. Optimizing SPF involves reducing forming temperatures, which in turn requires the development of alloy microstructures that enhance ductility at lower temperatures. To achieve this optimization, numerical simulation appears to be an effective approach, as it provides a detailed understanding of mechanical behavior at different scales. This work presents the results of a multiscale (micro and macro) numerical analysis conducted on the polycrystalline dual-phase alloy Ti-6Al-2Sn-5Cr-2Mo (Ti-6242) to improve its superplastic properties. The microstructural mechanical properties of the different phases were characterized through in-situ thermomechanical experiments performed at various temperatures using High Energy X-ray Diffraction (HEXRD). This technique enabled real-time monitoring of microstructural evolution in addition to macroscopic mechanical behavior. The local heterogeneity of the material, in terms of microstructural length scale, is discussed. A crystal plasticity model coupled with various homogenization techniques was implemented to account for local grain rotation and deformation. This work highlights the contribution of microstructural characterization on the accuracy of numerical models and as well the capacity of the constitutive model to predict superplasticity in Ti-6242 alloy.

Micro-texture dependent variation of microscale residual stresses in Ti-6Al-4V

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D3_11, Albéniz Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Residual stresses can be detrimental to the mechanical performance of titanium alloys. Research on residual stresses in titanium alloys post-deformation generally focuses on macroscale stress distribution. Nevertheless, microscale residual stresses can vary significantly from the macroscopic behavior in a material like titanium, which has considerable elastoplastic anisotropy. Understanding the influence of local crystallographic texture on microscale residual stresses requires further research. Localized textured regions, also called macrozones or micro-textured regions (MTR's), are prevalent in titanium alloys. These develop during the material's manufacturing process. The anisotropic deformation behavior of MTR's can significantly affect the development of residual stresses in the material.

In this study, the macroscale and microscale residual stress distribution in Ti-6Al-4V bars was evaluated experimentally on sections along the rolling and transverse direction after four-point bending. The macroscopic and microscopic residual stresses were characterized across the bar thickness using synchrotron X-ray diffraction (sXRD) at DESY beamline P07 and the Focused Ion Beam – Digital Image Correlation (FIB-DIC) ring-core milling technique, respectively. The sXRD measurements were used to probe a gauge volume containing several clusters of grains, revealing a typical post-bending macroscale residual stress profile. In contrast, the FIB-DIC measurements were used to probe smaller gauge volumes of 5 μm , enabling the possibility of exploring the residual stress state within individual grains in specific MTR's. The residual stress profiles obtained across the bar thickness using sXRD were observed to be shifted significantly from the neutral axis of the bar, indicating tension-compression asymmetry. The microscale residual stress data obtained via FIB-DIC measurements were shown to have several outliers compared to the macroscopic residual stress values measured at similar locations via sXRD. Localized crystallographic texture analysis was used at locations where such outliers were observed, in order to demonstrate the relationship between grain (or MTR) orientation and microscale residual stress variation in a plastically deformed Ti-6Al-4V bar.

Keywords: Titanium alloy, residual stresses, FIB-DIC, Synchrotron XRD.

Lattice strain distribution in BCC polycrystals - How does the local grain neighbourhood influence microstructural strain level

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D3_6, Albéniz Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Strain and stress heterogeneities determine the lifetime and failure of structural materials. Understanding the relationship between macroscopic and microscopic strains is essential for a quantitative assessment of the micromechanical behaviour of polycrystalline materials. In this work, we combine Diffraction Contrast Tomography (DCT), Far-field 3DXRD (FF-3DXRD), and Phase Contrast Tomography (PCT) measurements at beamline ID11 of the European Synchrotron Radiation Facility (ESRF) to capture the shape, arrangement, orientation, and average elastic strain tensor of a representative ensemble of grains during mechanical loading. The finalized dataset encompasses the relevant information for each grain within the investigated volume throughout the entire loading sequence.

Our analysis follows two distinct approaches: (1) a statistical analysis of strain tensor distribution evolution during loading across all grains, correlating mechanical grain behaviour with microstructural properties such as size, orientation and neighbourhood; and (2) a focused investigation of individual grains and their local neighbourhood and how the local properties affect the strain level in individual grains. By investigating grains with higher strain levels, we reveal microstructural factors relevant for strain localization and subsequent damage initiation.

In the talk, our latest findings on strain heterogeneities in bcc-iron as a model material are presented. We investigated more than 5000 grains representing the gauge section of a micro tensile samples during tensile deformation. Different annealing protocols have been utilized prior to the experiments to vary the eigenstrains of our samples in order to investigate how different initial eigenstrains affect the evolution of the strain distributions during loading. The deformation sequence predominantly focused on the elastic regime, with only the final two steps exceeding the yield strength. This experimental design allowed us to follow the transition from elastic to plastic deformation on the microstructural level for a large number of grains, providing relevant insights into micromechanical deformation behaviour.

Our approach presents a significant step forward in understanding the evolution of strain heterogeneities and microplasticity in polycrystalline materials during tensile deformation, with the potential to be also applied to multiphase materials and offering valuable insights for optimizing material design and processing strategies for more damage tolerant materials in structural applications and metal forming.

Accelerated discovery of novel materials: The need for high-throughput analysis of crystal structure, chemical composition, mechanical and functional properties integrated into a single instrument combined with machine learning

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D3_3, Albéniz Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Combinatorial synthesis methods such as co-deposition of thin-film material libraries enables high-throughput and cost-effective discovery of novel materials. While synthesis is done typically in hours, a comprehensive chemical and microstructure characterization of the library can take several months in a typical lab environment. In this work we've developed the long missing companion technique for rapid materials screening: A high-throughput characterization instrument that combines automated mapping of chemical composition, phase analysis, as well as mechanical, optical and electric property mapping. The novel instrument integrates X-ray diffraction (XRD), X-ray fluorescence (XRF), nanoindentation (NI), optical (LM), and electrical 4-point probing (4P) into a single stand-alone, automated system with a total footprint of 2m².

Typical screening experiments consist of 500 measurement positions covering an entire 4" wafer; with a typical duration of 15 hours for XRD, XRF, NI, 4P and LM measurements that result in a comprehensive database on each of these 500 points. We will present an overview and detailed analysis of this database exploiting smart evaluation algorithms. These include correlation to open-access database of materials properties such as the "Materials Project" based on calculations using Density Functional Theory (DFT) as well as advanced machine learning algorithms to improve predictive models for material properties.

As a first case study we investigated the mechanical properties of thin film combinatorial material libraries of the CuAgZr metallic glass system. Our findings indicate that the presence of high oxygen levels in Cu-rich areas, resulting from post-deposition oxidation in regions of less dense packing, markedly influences the mechanical performance of these alloys. Additionally, our research uncovers that nanoscale structural nuances play a significant role in determining the plastic yield and flow behavior of the alloys. Among various machine learning models evaluated, the multi-layer perceptron algorithm excelled, delivering accurate predictions of hardness for alloys not previously tested, thereby offering insightful directions for ongoing material research.

Modeling of single crystals and polycrystals of NiAl using the Deformable Discrete Element Method

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Many important materials are polycrystals with a cubic crystal structure. Examples are aluminum and copper with the face-centered cubic (FCC) structure, iron and chromium with the body-centered cubic (BCC) structure, as well the BCC intermetallic NiAl which is the main focus of this study. A widespread way of modeling such materials at the microscale is by using the Finite Element Method (FEM). In the present work, an alternative approach based on the Discrete Element Method (DEM) is employed instead. Both methods have advantages and disadvantages, with FEM being potentially less computationally intensive and more accurate in some applications, while DEM being better adapted to handling discontinuous phenomena like fracture.

A DEM model is created by filling a given volume with spherical particles of the same or different sizes and bonding adjacent ones together by cohesion. The effective properties of the ensemble are calibrated by adjusting stiffness parameters of the inter-particle bonds. A single crystal of cubic symmetry can be modeled by using either a random-dense packing of DEM particles or a cubic-symmetric periodic one, both having a cubic-symmetric distribution of bond stiffness coefficients. The second approach is followed in this work, since the first one faces difficulties reproducing properties of highly anisotropic crystals like NiAl. The simple cubic (SC) arrangement of particles is adopted, with deformable DEM (DDEM) particles used instead of standard ones [1] – a change which increases the range of values of effective parameters that can be obtained. In particular, it allows easy representation of the elastic properties of NiAl crystals.

The transition to the polycrystal is made by subdividing a representative volume into grain sub-volumes and filling them with SC patterns of DDEM particles at different orientations, corresponding to EBSD test results. It is ensured that proper attachment conditions at the grain boundaries are created, where SC patterns of different orientations meet. The results of simulations for NiAl in the linear-elastic regime are presented and discussed in connection with future tests of larger deformations leading to grain-boundary fracture.

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Mechanical properties of RE-Ni₂ Laves phases and effect of vacancy on partial dislocation motions

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D3_10, Albéniz Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Laves phases, one of the largest intermetallic groups, are promising candidates for hydrogen storage alloys and economically viable superalloys. However, their inherent brittleness has limited widespread industrial application.

A deeper understanding of their deformation mechanisms could help overcome this limitation. Recent advancements have elucidated the role of antisite substitution and alloying as crucial factors in enhancing the ductility of Laves phases. However, the influence of vacancy defects remains unclear due to their rarity owing higher formation energy compared to antisite defects, despite predictions that vacancies strongly influence dislocation mobility.

To this end, the mechanical properties of rare-earth Laves (RNi₂) phases were investigated to understand the effect of vacancy-type defects on dislocation motion, with both experimental and computational approaches. The hardness and reduced modulus of RNi₂-Laves phases (R=Er, Y, Sm, and La) were evaluated by the correlative nanoindentation technique, which provides orientation-dependent mechanical properties. Additionally, the mechanisms of partial dislocation motion under influence of vacancies were explored with atomistic simulations using machine learning interatomic potentials.

The origin of interface stress transition in Cu/W nanomultilayers

Dr. Yang Hu¹, Dr. Giacomo Lorenzin¹, Dr. Jeyun Yeom¹, Dr. Manura Liyanage², Prof. Dr. William Curtin², Dr. Lars Jeurgens¹, Dr. Jolanta Janczak-Rusch¹, Dr. Claudia Cancellieri¹, Dr. Vladyslav Turlo¹

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D3_2, Albéniz Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Controlling intrinsic stresses in nanomultilayers (NMLs) is essential for reliable mechanical performance and multifunctional properties. In Cu/W NMLs, a shift from positive to negative interface stresses arises under varying deposition conditions, yet the underlying atomic-scale mechanisms remain insufficiently understood. Here, we employ a neural network potential with ab initio-level accuracy to elucidate how intermixing at Cu/W interfaces drives this stress transition. Follow-up simulations further reveal that although interfacial intermixing is thermodynamically unstable, it enhances resistance to interface sliding and fracture. By directly linking interface chemistry to intrinsic stress, our approach bridges the gap between atomic-scale interface phenomena and the macroscale mechanical behavior of NMLs. These insights enable the design of NML coatings with tunable stress states and improved mechanical performance, opening new avenues for applications ranging from flexible electronics to protective coatings.

DVC-Driven Analysis of Mechanical Deformation in SLM WE43 Scaffolds with In Situ X-ray Characterization

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Porous magnesium scaffolds produced via laser powder bed fusion (LPBF) show great potential for bone regeneration due to their ability to support tissue ingrowth and enable fluid transport. Magnesium implants also possess mechanical properties closely matching those of bone, thereby minimizing stress shielding effects. Understanding the load-bearing capacity and mechanical behavior of these scaffolds is crucial for optimizing their performance and ensuring a uniform stress distribution that promotes a controlled failure mode.

Cubic scaffolds ($10 \times 10 \times 10 \text{ mm}^3$) of WE43 magnesium alloy with open porous structures, designed with different lattice geometries (BCC, FCC, TPMS) and an average strut diameter of $500 \text{ }\mu\text{m}$, were fabricated using LPBF. Their mechanical properties and failure mechanisms were investigated through in situ synchrotron X-ray microtomography compression tests under varying mechanical loading conditions.

This study explores the application of Digital Volume Correlation (DVC) to analyze the mechanical behavior of magnesium scaffolds. DVC provides a detailed assessment of localized deformations and strain fields across the scaffold structure under mechanical loading. By examining the evolution of these parameters, this work aims to enhance the understanding of the mechanical response and failure mechanisms in magnesium scaffolds.

We will address the complete DVC workflow, encompassing uncertainty analysis, residual examination, and the evaluation of displacements and strain fields. This comprehensive approach provides valuable insights into the mechanical behavior of Mg scaffolds for bone regeneration applications.

Finite element modeling of effective mechanical properties of multiphase metal matrix composites with various interphase zone

Dr. Szymon Nosewicz¹, Dr. Grzegorz Jurczak¹

¹Institute of Fundamental Technological Research of the Polish Academy of Sciences, Warsaw, Poland
 POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
 Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Metal–matrix composites (MMCs) are an important class of materials in which the microstructure can be tailored to have superior properties by comparison with non-reinforced alloys. Depending on the manufacturing process, MMC can be more complicated than just a two-phase material combination. Due to solubility and temperature-driven diffusion, another phase is formed between two phases of the composite, which exhibit properties quite different from those of its surroundings. Such interphase plays a critical role in the composite. It may not only modify the physical properties of the composite but also change the quantitative global behavior of the composite material [1].

The proposed research investigates how variations in the plasticity and damage parameters of the interphase influence the effective mechanical properties of a representative volume element (RVE) representing a metal matrix composite (MMC). This study is driven by the understanding that the mechanical properties of the interphase, often not well characterized, can significantly affect the overall behavior of the composite. To explore this, a finite element (FE) model was employed to simulate the composite's effective response, with interphase properties ranging from highly brittle with low ductility and toughness to highly ductile, resembling the matrix material. The numerical simulations were performed on the example of sintered nickel-silicon carbide composite, where the interphase characteristics depend on the manufacturing process. The modeling approach utilized several advanced frameworks:

- The Gurson-Tvergaard-Needleman model for the matrix
- An elastoplastic model with damage for the interphase/particle
- A cohesive zone model for the interface

It shows the significant influence of interphase properties on stress-strain evolution, fracture modes, and effective composite properties - ultimate tensile strength, fracture strain, and toughness. Each composite component's deformation and damage behavior (matrix, interphase, particle, interfaces) has been studied. As the yield stress, hardening curve, and fracture strain of interphase together with interface strength and its fracture energy evolved, more than six fracture modes have been observed, which is the key to the mechanical performance of a complex three-phase system.

Separation of humidity, strain rate and temperature effect on the orientation dependent micromechanical properties of cortical ovine bone

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D3_6, Albéniz Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Metabolic bone diseases such as osteoporosis have a significant impact on the bone quality and its properties. One out of three women and one out of five men at above the age of 50 are affected by osteoporosis [1]. However, only about 75% of the age-related increase in fracture risk can be attributed to a decrease in bone mass, bone density or changes in skeletal architecture [2]. To better understand the age- and disease-related increase in fracture risk, a closer look at the hierarchical structure of bone and its most important building blocks is required. The basic building blocks are type I collagen, hydroxyapatite and water. Water has a major influence on load transfer by facilitating interface sliding. The water content of healthy cortical bone is in the range of 10-20 vol.% but can drop to around 5 vol.% by the age of 60 [2].

In total 419 micropillars were tested in the axial and transverse fibril orientation under 56 different experimental conditions to study the effects of water content, temperature, and strain rate on the properties of ovine cortical bone. Quasi-physiological conditions and fracture relevant conditions were mimicked by varying the bone water content (3.1 wt.% - 8.3 wt.%), the temperature (25°C -60°C), and the strain rate (0.1-100 s⁻¹).

Micropillars were fabricated by femto-second laser ablation. Additional finite-element simulations were carried out to correct for the taper of the ablated micropillars. Polarized Raman spectroscopy was applied to determine the mineral-to-matrix ratio, the collagen quality and the orientation of the mineralized collagen fibrils. The analysis of the data with the paired t-test did not indicate any significant change in the amide I sub-band ratio, which suggests that the temperature and humidity applied did not degrade the collagen in the tested samples. The effect of temperature and water on the mechanical properties could finally be separated by applying a linear modeling approach. This results in a temperature related softening of 1.2 MPa/K and 33-111 MPa/wt.% water. Moreover, the activation parameters provide an indication about the rehydration process of bone. The results highlight the effect of hydration on the mechanical behavior of bone and are valuable for future multiscale simulations of fracture risk in patients, as the age- and disease-related decrease in the moisture content of bone can be taken into account.

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Ab initio simulations of small nanoparticles mechanical properties

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septembre 17, 2025, 13:10 - 14:30

Because of their small size and high surface-to-volume ratio, nanoparticles often show specific properties making them interesting systems for many applications in various fields such as biomedicine, biochemistry, catalysis, electronics, etc. They are also largely used as reinforcement components in many materials because their mechanical properties are often better than their bulk counterparts. Indeed, nanoparticles can be synthesized with few or even no internal defects. These latter are potential sources of dislocations or cracks, thus limiting the strength and toughness of bulk materials. In contrast in nanoparticles, dislocations have to be formed at surfaces or homogeneously, which implies much higher stress levels. Nanoparticles are thus often much stronger than the corresponding bulk materials.

It is now well established experimentally and by means of numerical simulations that the strength of materials tends to increase when the size of the considered system decreases, up to characteristic dimensions of about ten nanometers. What remains unsolved is if that increase persists at the lower scales, when the dimensions are further reduced down to a few nanometers.

In that context, we performed ab initio molecular dynamics simulations to investigate the mechanical properties of nanoparticles with sizes of 1 to 2 nanometers. The use of first-principles calculations offers the required accuracy for such a study and complements advantageously experimental studies, giving direct access to the deformation mechanisms. The nanoparticles were compressed along several directions, various shapes were studied and materials with different crystallographic structures were considered: silicon, silicon carbide, aluminum and tungsten. The obtained results show that the strength depends on the nanoparticles shape in all cases, whereas its variation with size depends on the material. The famous "smaller is stronger" rule seems to break down for some systems, though the theoretical bulk strength can be reached or even exceeded depending on the nanoparticles shapes and the compression orientations. Amorphization occurs in most of the nanoparticles, but different and original plasticity mechanisms are also observed in some cases.

Keywords: nanoparticles, compression test, first-principles calculation, molecular dynamics

Mechanistic Insights into Strengthening via Precipitate Assemblies Using In Situ Micropillar Compression of Ni-Cr-Al-Nb Alloys

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Ni-base superalloys, such as Inconel 718 or 625, achieve precipitate hardening primarily through the metastable, ordered γ'' phase, unlike most superalloys that rely on $L1_2$ -ordered γ' phase [1]. The addition of Nb with traces of Ti, promotes γ'' formation (stable variant: δ -phase), which can precipitate on pre-existing γ' phase within the γ -matrix, creating γ - γ' - γ'' composite precipitate assemblies [2]. Such microstructures are proven effective in enhancing strength, for instance, a Ni-Cr-Al-Nb alloy shows a strength increment of $\sim 15\%$ compared to Rene88 at 700 °C [3-4]. However, the underlying strengthening mechanisms and the quantitative role of composite precipitate assembly to the overall strength remain unexplored. In this study, we aim to enhance the mechanistic understanding of induced strengthening due to composite precipitate assemblies by examining the dislocation interactions with such assemblies. To achieve this, variations in the γ - γ' - γ'' microstructure are induced by heat-treating Ni-16Cr-4Al-6Nb(at%) alloy. Micropillars of diameter 1 μm were fabricated using FIB and yield strength at room temperature was measured through in situ SEM micropillar compression test using diamond flat punch under displacement control mode at a strain rate of $1/10^3$. The measured yield strength (2% offset) after 700 °C for 1000 h was approximately 1146 ± 41 MPa, consistent with literature [4]. At 800°C for 100 hours, there was a 1.4-fold improvement, while a short-duration annealing at 700°C for 100 hours followed by 800°C for 100 hours resulted in a strength enhancement of 1.5-fold. The critical resolved shear stress (CRSS) was then calculated from the yield strength by considering the highest Schmid factor. A cumulative distribution function (CDF) of CRSS from different heat treated samples was analyzed to elucidate the impact of microstructure post heat treatment. The 3D-APT analysis of γ' - γ'' -precipitates in Ni-Cr-Al-Nb alloy post heat treatment revealed the presence of δ -phase in addition to γ - γ' - γ'' microstructure after heat treatment at 800°C for 100 hours. Given that the pillars were fabricated within the similar grain orientation, two potential strengthening mechanisms are postulated: solid-solution strengthening and precipitate strengthening. TEM investigations of deformed pillars were conducted in aberration-corrected TEM to comprehend the deformation behavior. This talk will show and discuss the factors contributing to the strength in Ni-Cr-Al-Nb alloys post heat-treatment.

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Micromechanical Assessment of Electrodeposited Zinc Coatings: A Comparative Study of Spherical Nanoindentation and Micropillar Compression

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D3_5, Albéniz Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Zinc and its alloys have gained significant attention in biomedical applications due to their biocompatibility and controlled biodegradation properties. However, their widespread adoption for implants is limited by relatively low strength and brittleness in as-cast form. Due to Zn's low melting temperature (419.5°C, 0.43T_m), it exhibits unusual mechanical behavior at room temperature, including dynamic recovery, recrystallization, and enhanced grain boundary mobility. These thermally-activated processes, combined with limited work hardening and inverse Hall-Petch behavior below 25 µm grain size, make conventional strengthening strategies ineffective while making Zn an intriguing material for fundamental mechanical studies.

This research investigates the correlation between microstructure and mechanical behavior in electrodeposited (ED) Zn coatings, focusing on validating spherical nanoindentation (NI) methodology against established micropillar compression techniques for evaluating local plastic deformation in anisotropic HCP materials. Four distinct pure Zn coatings were synthesized under varying ED parameters, resulting in different grain sizes, morphology and crystallographic textures. EBSD analysis revealed that in all coatings, the c-axis <0001> direction was oriented perpendicular to the deposition direction and parallel to the surface, with a predominant {10-10} texture component whose {11-20} contribution increased with grain refinement and transition from columnar to equiaxed grains. The mechanical properties were evaluated using both spherical NI and micropillar compression techniques. Spherical NI was performed on both top surfaces and cross-sections to assess the influence of grain orientation on mechanical properties. The micropillar compression tests revealed yield strengths ranging from 100 to 800 MPa, with spherical NI showing similar trends but consistently lower values. Hardness and Young's modulus extracted from spherical NI tests in continuous stiffness mode were comparable to conventional Berkovich NI measurements. Detailed microstructural characterization and post-mortem analysis revealed that the discrepancy between NI and micropillar compression results was more pronounced in columnar microstructures but became negligible in ultrafine-grained equiaxed microstructures. This difference can be attributed to uniaxial loading in micropillar compression versus complex stress states in spherical NI, particularly significant in highly textured materials.

This study demonstrates that spherical NI can serve as a reliable alternative to micropillar compression for mechanical characterization of HCP materials, especially for ultrafine-grained microstructures. Moreover, unlike micropillar testing, spherical NI does not require FIB preparation, thus avoiding potential artifacts from ion damage. The comprehensive approach involved in this work provided valuable insights into the relationship between ED processing parameters, microstructure, and mechanical properties of Zn coatings.

Evaluation of Strain Rate Sensitivity in a Superplastic Zn-1Cu Alloy: A Comparative Study of Nanoindentation Instrumental Effect

Ph.D. Wiktor Bednarczyk¹, Ph.D. Maria Wątroba², Ph.D. Jakub Kawałko¹, Priv.-Doz. Verena Maier-Kiener³, Prof. Piotr Bała¹

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D3_7, Albéniz Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Strain rate sensitivity (SRS) measurements are widely employed to assess creep-related deformation at high temperatures or to determine the strain rate sensitivity parameter and activation volume of ultrafine-grained metallic materials at room temperature. The recently developed nanoindentation strain rate jump (SRJ) test has significantly accelerated SRS parameter evaluation in small samples and thin films. The introduction of constant strain rate loading has enhanced the reliability of this technique by minimizing depth-related effects. However, the repeatability of SRJ measurements across different testing devices and bulk samples remains largely unexplored.

In this study, the SRS of a room-temperature superplastic Zn-1Cu alloy processed via equal channel angular pressing (ECAP) and cold rolling was investigated. This material was chosen to exaggerate the SRS effect while minimizing challenges associated with high-temperature measurements. Bulk compression ($\varnothing 3 \times 4.5$ mm) and tension ($1 \times 2 \times 5$ mm) samples were fabricated using wire electro-discharge machining, while nanoindentation measurements were performed on polished surfaces perpendicular to the deformation direction. SRJ tests were conducted at three constant strain rates using KLA G200, Alemnis ASA, and Femtotools FT-NMT04 nanoindenters, as well as an Instron 5966 universal testing machine.

The results reveal significant discrepancies between different testing devices. Hardness SRJ curves from displacement-controlled nanoindenters exhibit abrupt changes in hardness values upon strain rate transitions, whereas the load-controlled KLA G200 shows a more gradual response with smaller variations between strain rate steps. Despite a relatively good correlation between nanoindentation and bulk behavior, notable discrepancies were observed. These findings underscore the need for further standardization and cross-validation of nanoindentation-based SRS measurements to ensure reliable comparisons across different testing platforms.

Stress-strain Relationship of Metals by Indentation Tests

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D3_7, Albéniz Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

The relationship between stress and strain in materials characterizes their deformation behavior, ranging from elastic loading at low stresses to yielding, work hardening, and eventual failure at higher stresses and strains. This relationship is typically determined through tensile tests using macroscopic samples.

In the realm of 3D interconnects, the small volumes of material make traditional tensile tests impractical. Copper (Cu) interconnect structures can be evaluated using nanoindentation hardness and reduced modulus measurements, spherical indentation tests, and compression experiments on pillar structures.

This paper explores the transition from elastic to plastic deformation in spherical indentation and highlights the significance of the constraint factor, which plays a crucial role in the relationship between hardness and yield strength and is material dependent. A comparison between the spherical nanoindentation stress-strain method and microscale pillar compression tests will be presented for Cu and Fe-Si. The indentation and compression experiments are performed on a new TI990 TriboIndenter platform with improved noise levels and sensitivity.

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Insights into the Origins of Friction in Hard Materials from Two-Axis Nanoindentation

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D3_5, Albéniz Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Friction is commonly thought to be controlled by processes in small asperities between two sliding surfaces. The asperities hold a large fraction of the mating surfaces apart and thereby dramatically increase the local contact stresses. In this study, a special two-axis nanoindentation system was used to examine the mechanics of deformation of micron-scale asperity contacts by sliding a spherical diamond indenter with a radius of $\sim 2\text{ }\mu\text{m}$ over a flat plate of fused silica under a combination of normal and transverse loading. The nanoindentation system is comprised of two independently controlled nanoindentation actuators oriented transverse to each other in such a way that the forces and displacements of each can be independently controlled and monitored. The two actuators can also be operated in continuous stiffness mode (CSM) to measure both the normal and transverse contact stiffnesses and the degree of energy dissipation during sliding through the phase shift of the CSM load and displacement oscillations. Tests were conducted by holding the normal force on the spherical indenter constant and ramping the lateral force at a constant rate. The extent of plasticity during sliding was varied by controlling the magnitude of the normal load so as to produce either a perfectly elastic contact or a combination of elastic and plastic deformation. Atomic force microscopy (AFM) was used to image the scratch tracks, and finite element simulations were used to confirm and explain some of the observations from the nanoindentation data. Results are presented and discussed in terms of prevailing ideas on the mechanistic processes that control friction in single asperity contacts, with special emphasis on differences between purely elastic contact and contact that involves both elastic and plastic deformation.

Toward High Strain Rate Nanoindentation Testing

Dr. Mohammed Tahir Abba¹, Prof. Benoit Merle¹

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D3_5, Albéniz Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

Knowledge about the local mechanical behavior at high deformation rates is crucial to increase the safety of components that involve impact loadings such as bird impacts in the aviation industry, automobile crashes and many others. In the past few years, the scope of nanoindentation has increasingly expanded toward high strain rates. However, the new developments are hindered by the equipment electronics, test methodologies and inertial effects at very high strain rates.

This talk will focus on both the technical implementation of high constant strain rate nanoindentation and the development of custom methods to analyze the high-speed data [1]. It will showcase a displacement-controlled instrument, which was designed around piezoelectric transducers and fast signal processing electronics allowing sampling rates of up to 1 MHz. Experimental measurements at strain rates of up to 10^5 s^{-1} will be demonstrated, along with a discussion of the current bottlenecks in high constant strain rate indentation.

Acknowledgement

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In situ Transmission Kikuchi Diffraction (TKD) Tensile Testing

Dr. Tijmen Vermeij¹, Mr. Philipp Kroeker¹, Dr. Amit Sharma^{1,2}, Douglas Steinbach³, Dr. Jun Lou³, Dr. Xavier Maeder¹, Dr. Johann Michler¹

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D3_9, Albéniz Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

We present a novel methodology for in situ Transmission Kikuchi Diffraction (TKD) tensile testing that enables nanoscale characterization of the evolution of complex plasticity mechanisms. By integrating a modified in situ Scanning Electron Microscope (SEM) nanoindenter with a microscale push-to-pull device and a conventional Electron Backscatter Diffraction (EBSD) detector, we achieved TKD measurements at high spatial resolution during mechanical deformation. A dedicated focused ion beam procedure was developed for site-specific specimen fabrication, including lift-out, thinning, and shaping into a dog-bone geometry. The methodology was demonstrated on several case studies: (i) a metastable β -Ti single crystal, on which we quantified the initiation and evolution of nanoscale twinning and stress-induced martensitic transformation, (ii) an HCP Re single crystal loaded along the c-axis showing complex nanoscale twinning and twin-to-twin interactions, and (iii) a CuAl/Al₂O₃ nanolaminate, which exhibited nanoscale plasticity and twinning/detwinning in a complex microstructure. Furthermore, we explore the possibilities for performing elastic and plastic strain measurements using HR-TKD and SEM-DIC, respectively, alongside regular TKD mapping. Overall, this approach provides a robust alternative to in situ EBSD and transmission electron microscopy testing, with the potential of providing local stress-strain data, facilitating detailed analysis of deformation mechanisms at the nanoscale.

High-strength and non-brittle crystalline-amorphous PVD-ALD nanolaminates of amorphous alumina and AlCoCrFeNi high-entropy alloy

Mr. Samuel Bojarski^{1,2}, Dr. Simon Tsianikas^{1,3}, Dr. Amit Sharma^{1,4}, Dr. Chunhua Tian^{1,5}, Dr. Tijmen Vermeij¹, Dr. Johann Michler¹, Dr. Xavier Maeder¹

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D3_9, Albéniz Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Over the past few decades, there has been extensive research interest in reducing characteristic length-scales in materials in order to achieve high strengths without compromising ductility. One popular strategy has been the refinement of grain size through "nanolaminate" architectures: alternating layers of two different materials with sub-micrometre thicknesses. For most material pairings deposited by physical vapour deposition (PVD), the alternating layers disrupt columnar grain growth, retaining sub-micrometre in-plane grain size through the thickness of sample. In parallel, a new approach to metallurgy emerged: the idea that near-equiatomic mixes of five or more elements should be stabilised in a single phase by their high entropy of mixing, rather than decomposing into intermetallic phases. This field of "high-entropy alloys" (HEAs) has produced some of the strongest metals ever reported, without compromising on ductility or toughness. We have combined these two strategies to create nanolaminate films using the AlCoCrFeNi HEA: both metal-metal fcc/bcc multilayers (exploiting the dependence of phase on Al content in this alloy); as well as metal-ceramic nanolaminates with 2 nm atomic layer deposition (ALD) amorphous alumina interlayers. Microstructural analysis confirms that the ALD layers effectively disrupt out-of-plane grain growth and retain small in-plane grain size. Micropillar compression experiments show that this system is exceptionally strong for a metal, and still plastic in its deformation. Through post-deformation TEM imaging, we show that the amorphous alumina interlayers deform in a ductile manner co-operatively with the metal layers, remaining continuous even under significant local strains. We discuss possible mechanisms capable of explaining the co-operative non-local deformation of the amorphous layer, and how these layers contribute to the nanolaminate's high strength.

How experimental micromechanics can help in the design of High Temperature Superconducting magnets

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D3_6, Albéniz Room (Level -2), septembre 16, 2025, 14:30 - 16:30

The need for strong steady magnetic fields, above 40 T, raises several new challenges in the design of superconducting magnets. As a start, the field requested exceeds the limitations of the consolidated LTS technologies, leading us to the use of HTS technology. Besides the difficulty of making HTS magnets, the challenges at ultra-high field are found in the structural mechanics, driven by electromagnetic forces, and quench protection, due to the high stored energy density. ReBCO, the leading candidate for ultra-high field magnets, is produced in the form of thin tapes, consisting of multiple layers of different materials with very diverse nature and properties. Understanding the elastic and plastic behavior of these materials is crucial for both the magnet design process and advancing technological development to meet end-product requirements. However, the small size of HTS makes it impractical to employ macroscopic mechanical tests for characterizing the required mechanical properties at the right scale. In this paper we show how nanomechanical testing can help to address this issue. More specifically, elasticity, plasticity and toughness of REBCO materials are measured at the scale of the tape's constituents at room temperature and at cryogenic temperature (120 K). The paper concludes by highlighting the main results of our initial test and the forthcoming developments in the field of nanomechanical testing to aid in the design of HTS superconductors.

Metal-Ceramic Nanolaminate Design for Enhanced Mechanical Properties

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D3_9, Albéniz Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Metal-ceramic multilayer composites exhibit improved strength, ductility, and toughness due to the synergistic effects of their differing properties and characteristics. In such composites, interface strengthening and microstructural control through grain size and layer refinement play a crucial role in determining mechanical properties. In this study, we present experimental data on the fabrication and mechanical behavior of nanolaminates composed of metallic alloy layers with thicknesses ranging from 30 to 120 nm, alternating with thin amorphous Al₂O₃ interfaces measuring 2 to 5 nm. The metal and oxide are deposited using physical vapor deposition (PVD) and atomic layer deposition (ALD), respectively, in a hybrid deposition chamber without breaking the vacuum.

The incorporation of these thin amorphous oxide interfaces between the metal layers serves several purposes: a) it disrupts the columnar growth of the metal alloy film, allowing for a smaller and more controlled grain size, b) it regulates diffusion, c) it inhibits the propagation of dislocations and twins, and d) it controls grain boundary migration and recrystallization during annealing.

As a model system, we fabricated Cu_{1-x} – Al_x (where X represents 0, 5, and 12 at.%) multilayers and subjected them to micropillar compression, micro-tensile mechanical testing, nanoindentation, in situ tensile transmission Kikuchi diffraction (TKD), and 4D-STEM experiments. By varying the aluminum content, we can precisely control the stacking fault energy within the interlayer, thereby influencing the formation and size of nano-twins. The roles of various small-scale mechanisms, such as Hall-Petch strengthening, solid solution effects, and interface strengthening, will also be discussed.

High-Speed nanoindentation mapping for a deeper understanding of microstructures

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D3_7, Albéniz Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

High-speed nanoindentation mapping (HSNM) has evolved into a scanning-probe-like technique, enabling large-area, high-resolution characterization of microstructures. By directly imaging variations in mechanical properties, phase boundaries, and deformation mechanisms, it provides critical insights into heterogeneous materials. However, key challenges remain, primarily in extracting phase-specific mechanical properties from large datasets, a task that requires statistical, machine learning and deep learning approaches allowing also to retrieve second-order information such as pop-ins, phase transformations, and strain localization events. Integrating HSNM with electron backscatter diffraction (EBSD) and energy-dispersive X-ray spectroscopy (EDX) further demands precise dataset alignment and registration algorithms to ensure accurate phase-property correlations.

In this work, phase identification in HSNM datasets is demonstrated using statistical machine learning techniques such as k-means++, k-medoids, Gaussian mixture models (GMM), and skew-normal deconvolution. Correlation with EBSD is performed through map registration and consensus algorithms, ensuring robust phase differentiation. A case study on advanced high-strength steels (AHSS) demonstrates the effectiveness of this approach in resolving mechanically distinct phases that are otherwise challenging to differentiate due to crystallographic similarities.

Pile-up effects pose an additional challenge in nanoindentation, leading to overestimation of hardness and modulus, particularly in compliant phases. Traditional correction methods rely on atomic force microscopy (AFM), limiting throughput and applicability to HSNM. Here, a high-throughput correction framework is introduced, leveraging HSNM-induced surface roughness changes quantified via optical profilometry and calibrated through machine learning. By selectively applying correction only to piling-up phases, universal calibration functions are derived, validated through finite element modeling, and demonstrated on WC-based hard metals, effectively eliminating AFM dependency.

Extracting phase-specific stress-strain behavior is another advancement. The interaction volume of spherical indenters is not only material-dependent but also poorly constrained, limiting phase resolution. Axisymmetric indenters provide a confined interaction volume, and when combined with HSNM-driven phase deconvolution, enable accurate phase-specific property extraction. Indenters of varying geometries introduce controlled stress states, distinguishing elasto-plastic responses at the nano-scale.

The impact of grain boundary states on mechanical failure in nanocrystalline materials

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Nanocrystalline materials exhibit increased strength due to the structural constraint on dislocation mobility. However, severely inhibiting dislocation mobility can lead to high local stress concentrations and subsequently localized early failure, i.e. low toughness and ductility. In the case of nanocrystalline systems processed by severe plastic deformation the grains get fragmented by formation of new boundaries through dislocation entanglements, leading to high contents of extrinsic grain boundary dislocations as opposed to conventional materials. These materials even exhibit a counterintuitive 'hardening-by-annealing' phenomenon, opposed to the 'softening-by-annealing' through recovery processes in coarse grained materials. This change in behavior originates from the fact that, at such small grain sizes, dislocation sources in the grain interior are considerably rare and necessitate a high activation stress due to geometric constraint, leaving the dislocation source structure/density at grain boundaries as the governing factor for plasticity.

The present work showcases a single phase equiatomic Fe-Cr alloy processed by high pressure torsion to obtain a system with sub-100 nm grain size, which was deliberately altered using sequential heat treatments to modify the local grain boundary state at constant grain size (300°C), as well as to investigate the grain size influence via moderate grain growth to approximately 300 nm (500°C). Due to the limited specimen size during high pressure torsion (<0.5 mm) the material was investigated using in situ micromechanical testing techniques, ranging from tensile testing with additional point feature tracking to obtain detailed information on strain localization to continuous J-integral measurement to determine elastic-plastic fracture characteristics.

Furthermore, the correlative (non-)equilibrium nature of grain boundaries was elucidated by damping measurements using micromechanical spectroscopy as well as correlative Synchrotron X-Ray investigations.

This multitude of data allows us to fully capture the changes in strength, ductility, strain localization, fracture toughness and anelasticity within one material system, with only the grain boundary structure/area as the main factor of change. The obtained correlations between these parameters will be discussed in detail to elaborate a pathway for structural grain boundary engineering without the necessity of chemical modifications.

A novel approach to determine the brittle-to-ductile transition temperature via dynamic nanoindentation

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D3_4, Albéniz Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

Traditional methods for determining the brittle-to-ductile transition temperature (BDTT), such as Charpy impact testing, require multiple samples and involve costly preparation. To overcome these challenges, we developed an innovative approach using nanoindentation with continuous stiffness measurement (CSM). This technique allows for the evaluation of the stiffness ratio, i.e. the ratio between the loading slope and the unloading stiffness, during a single indentation test. Since loading involves both elastic and plastic deformation while unloading is purely elastic, this ratio provides valuable insights into the relative fractions of plastic and elastic deformation. Previous studies have used similar methods to assess constraint factors and derive flow curves via spherical indentation.

In this study, we extended the approach by conducting nanoindentation experiments across the temperature range from $-150\text{ }^{\circ}\text{C}$ to $25\text{ }^{\circ}\text{C}$. Our results show that the stiffness ratio of an austenitic alloy remains nearly constant across this temperature range, whereas a ferritic alloy exhibits a pronounced increase at lower temperatures. This trend indicates a shift toward more elastic deformation, consistent with the expected brittle-to-ductile transition. A key advantage of our method is its robustness against thermal drift, a common challenge in non-ambient nanoindentation testing. As a result, it ensures highly reliable measurements with minimal stabilization time.

In summary, our approach provides a cost-effective and efficient alternative to conventional BDTT testing. Future work will focus on refining the transition temperature estimation by applying this method to a broader range of materials.

In situ TEM tensile testing of small-scale model systems to study the effect of ordering and interfaces

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

Size effects decisively influence the properties of materials at small length scales. In the context of mechanical properties, the trend of ‘smaller is stronger’ has been well established. However, to this day it remains challenging to find suitable testing geometries and setups to test mechanical properties on small scales while avoiding pitfalls such as preparation or testing artefacts. Therefore, certain aspects of small-scale mechanics have barely been explored.

Here we use in situ TEM tensile testing to study the effect of interfaces and atomic-scale ordering on mechanical properties. We use a flexible copper nanowire platform as a small-scale model system which allows us to test different aspects of materials on the nanoscale. The nanowires are alloyed with gold and the ordering is tuned using different heat treatments. Tensile testing of wires with different degrees of ordering (as inferred from 4D-STEM) reveals a transition from twin to slip-based plasticity and a change in yield strength. Besides studying ordering we test ALD based Aluminum oxide films coated onto our nanowire platform. This gives us the possibility to test the mechanical properties of ultrathin coatings and understand the role interfaces play in the deformation process.

A novel 3-electrode-based backside H-charging setup for in-situ micromechanical study: Development and demonstration

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D3_10, Albéniz Room (Level -2), septembre 17, 2025, 17:00 - 19:00

Hydrogen (H) is leading the global campaign in search of sustainable energy materials to replace conventional fossil fuels. However, due to hydrogen embrittlement (HE), materials can experience a significant shift in their mechanical properties and undergo brittle failure in the presence of hydrogen. Conventional ex-situ testing methods suffer from hydrogen outgassing and concentration gradients during the testing. Furthermore, large specimens require longer charging cycles, making sample preparation a time-consuming process. In pursuit of deconvoluting the specific interactions between hydrogen and individual microstructural features, novel in-situ electrochemical deformation techniques involving simultaneous H-charging and micromechanical testing, have been recently developed at our laboratory. To integrate the three key aspects of HE studies (H-charging, micromechanics, and microstructural investigation) into one single platform, an in-situ 3-electrode-based back-side H-charging cell will be presented, that is designed to be compatible with scanning electron microscope-based analytics. Continuous H-charging is therefore performed on thin samples subjected to external loading (nanoindentation and micropillar compression) to study the stress-strain behaviour of a low alloy cast steel (G20Mn5, A. Yaktiti et al. Corrosion Science 199 (2022) 110208) and a Ni bicrystal at various deformation rates ($10^{-4} \text{ /s} < \dot{\epsilon} < 10 \text{ /s}$).

Dynamic Nanoindentation – A Key to Advanced Materials Understanding Under Extreme Conditions

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D3_5, Albéniz Room (Level -2), septiembre 16, 2025, 10:30 - 13:10

The demand for materials capable of withstanding extreme environments—such as high and cryogenic temperatures, aggressive electrochemical conditions, and high strain rates—has driven the evolution of nanoindentation techniques. Dynamic nanoindentation, particularly continuous stiffness measurement (CSM), has emerged as a powerful tool for characterizing mechanical properties beyond conventional quasi-static methods. By enabling real-time analysis of hardness, modulus, and time-dependent deformation behavior, dynamic nanoindentation provides critical insights into material performance under application-relevant conditions.

Recent advancements have extended these methods to extreme testing environments, including in-situ electrochemical charging, high-temperature oxidation-resistant coatings, and cryogenic material studies down to liquid helium temperatures. A further enticing proposition for materials scientists is to characterize the flow behavior of materials with minimal experimental effort while ensuring highly reliable results. Although it is established as a standard method for extracting hardness and Young's modulus, the technique has not been fully exploited for determining localized flow curves. This gap exists due to the inherent challenges in understanding the correlations between mechanical properties obtained from spherical indentation experiments and uniaxial data.

To address this issue and accurately account for tip imperfections, a calibration procedure based on fundamental geometrical considerations is applied. This procedure lays the groundwork for strain-rate-controlled experiments, enabling the depth, thus strain dependent evaluation of the constraint factor while considering mechanical properties and induced strain.

These protocols are applicable under both ambient and non-ambient conditions, including electrochemical scenarios, by employing a novel in-situ electrochemical charging approach known as the side-charging cell. It is evident that electrochemical charging not only increases hardness and flow stress but also results in a reduced constraint factor. This reduction provides further insights, indicating a significant influence on the deformation behavior under electrochemical charging.

This contribution highlights the latest developments in dynamic nanoindentation and demonstrates its crucial role in accelerating high-throughput materials design for next-generation engineering applications. By bridging the gap between laboratory precision and real-world conditions, dynamic nanoindentation paves the way for a deeper understanding of materials under extreme conditions.

Creep Dominated High Cycle Fatigue of Freestanding Gold Thin Films: Microstructure and Temperature Dependent Deformation Mechanisms

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D3_9, Albéniz Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

Freestanding metallic thin films experience cyclic loading conditions when they are used in flexible electronic devices, e.g. as interconnects. While supported thin films have been extensively studied, comparatively little is known about the fatigue behavior of freestanding films, largely due to experimental challenges. In addition to sharing unique PVD microstructures, freestanding films stand out due to the ubiquitous presence of a free surface, which likely further alters the classical fatigue mechanisms known from their bulk counterparts.

Using bulge testing, we investigated the widespread columnar ultra-fine grained and nanocrystalline microstructures by conducting a comprehensive investigation of the high cycle fatigue behavior of gold thin films over a temperature range of 20 to 100°C, closely reflecting operational conditions in microelectronic devices. Interrupted testing, coupled with transmission electron microscopy, was used to monitor the microstructural evolution. Through analysis of activation parameters and comparisons to reference creep bulge tests, we demonstrated that the cyclic behavior is dominated by creep mechanisms. Cyclic creep was evidenced for all microstructural conditions and temperatures. At 100°C, nanocrystalline films exhibited an unexpected fatigue limit. The distinct behaviors of columnar ultrafine-grained and nanocrystalline samples will be discussed in detail during the presentation.

[1] A. Krapf, D.D. Gebhart, C. Gammer, M.J. Cordill, B. Merle. *Materials Science and Engineering: A*, 887 (2023). <https://doi.org/10.1016/j.msea.2023.145759>

[2] A. Krapf, B. Merle, D.D. Gebhart, M. Reiter, A. Lassnig, M. Göken, M.J. Cordill, C. Gammer. *Advanced Engineering Materials*, 26 (2024). <https://doi.org/10.1002/adem.202400216>

MecaNano COST Action - European Network for the Mechanics of Matter at the Nano-Scale

Prof. Benoit Merle¹, Dr. Marie-Stéphane Colla², Dr. Marc Legros³, Dr. Aleksija Djuric⁴, Prof. Diletta Giuntini⁵, Dr. Verena Maier-Kiener⁶, Prof. Ulrich Kerzel⁷, Prof. Edoardo Rossi⁸, Prof. Tamara Aleksandrov Fabijanic⁹, Prof. Dan Mordehai¹⁰, Prof. Daniel Kiener⁶, Dr. Julien Guénolé¹¹, Dr. Wiktor Bednarczyk¹², Dr. Volker Hofmann¹³, Prof. Stefan Sandfeld¹³, Dr. Peter Dusan Ispanovity¹⁴, Prof. Flavio Abreu Araujo², Dr. Gabrielle Tiphéne², Dr. Solène Dassonneville¹⁵, Dr. Megan Cordill¹⁶

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D3_1, Albéniz Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

The European Network for the Mechanics of Matter at the Nano-Scale (MecaNano) is a European Cooperation in Science & Technology (COST) Action (CA21121). The network has successfully connected over 400 researchers from diverse fields, including experimentalists, simulation and machine learning experts, and data scientists, fostering knowledge exchange and collaboration. MecaNano aims to advance the multiscale understanding of the mechanical behavior of materials, unlocking new possibilities for the development of novel materials with enhanced performance and durability.

This presentation will provide an overview of MecaNano's past achievements and upcoming events. Beyond bringing together researchers from different scientific backgrounds, the Action has placed emphasis on promoting inclusivity, with strong representation from Young Researchers and Innovators in the network and leadership. The establishment of lasting transnational collaborations through Short-Term Scientific Missions, general meetings, and workshops has further strengthened the European Research Area. These efforts position MecaNano to continue advancing micro- and nanomechanics research, addressing emerging challenges through interdisciplinary approaches that integrate machine learning and data science.

References

Further information can be found at: <https://www.mecanano.com>

A combined experimental-computational study of the compression of hemispherical nanoporous gold nanoparticles

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D3_1, Albéniz Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

Nanoporous gold (NPG) exhibits unique mechanical properties due to its high surface-to-volume ratio and intricate ligament network. In this talk, we present an integrated experimental and computational approach to investigate the inhomogeneous deformation of sub-micrometer scale hemispherical NPG nanoparticles (NPG-NPs) under compression. Using a combination of the dewetting method and dealloying of Ag-Au alloys, we fabricated NPG-NPs with an average ligament diameter of 13 nm and overall diameters ranging from 200 to 800 nm. Structural characterization revealed a limited number of grain boundaries, predominantly twin boundaries. Compression experiments using a flat punch showed an initial linear load-displacement response, followed by a significant slope increase beyond a critical depth. To elucidate the underlying mechanisms, molecular dynamics (MD) simulations were performed on NPG-NPs with varying sizes, porosities, and ligament diameters. The simulated load-displacement curves closely matched experimental results, confirming the validity of our computational approach. A key finding of this study is the inhomogeneous densification of NPG-NPs, which is localized beneath the compressing punch. By analyzing the dislocation density profiles, we correlated the densification region with the mean-free path of dislocations and their depletion due to the nanoporous structure. The observed increase in slope in the load-displacement curves is attributed to interactions between the densified region and the substrate. Based on these insights, we propose a model for inhomogeneous deformation that enables the evaluation of contact stresses in experiments. Furthermore, we discuss the broader implications of this model for understanding the mechanical behavior of NPG structures under nanoindentation. This work provides a deeper understanding of the mechanical response of nanoporous materials at the nanoscale, offering valuable insights how to analyze indentation of NPG structures.

Impurities Affecting Grain Boundary Cohesion in Nanostructured Tungsten: A Micromechanical Study

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D3_4, Albéniz Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

The exceptional properties of tungsten, including its high melting point, low vapor pressure, and outstanding high-temperature strength, make it a prime candidate for plasma-facing components in fusion reactors. However, its application is limited by inherent brittleness and sensitivity to impurities, particularly at grain boundaries. While grain refinement to ultrafine- and nanocrystalline regimes substantially increases strength and improves helium swelling behavior, these fine microstructures exhibit predominantly intercrystalline fracture, indicating that grain boundaries are the weakest microstructural link. Consequently, modifications to grain boundary cohesion significantly impact material strength. This study investigates the influence of a DFT (density functional theory) informed element selection at grain boundaries on the mechanical properties of ultrafine-grained tungsten. Ultrafine-grained and nanocrystalline tungsten was synthesized containing elements predicted to strongly segregate at grain boundaries and affect grain boundary cohesion. Specimens were manufactured through multiple processing routes, including spark-plasma sintering, high-pressure torsion (HPT), and thin film sputter deposition. Due to the fine microstructure and limited material volume, mechanical properties were characterized using small-scale testing techniques. In-situ microcantilever bending experiments were conducted, enabling straightforward specimen preparation via focused ion beam, while allowing tensile loading of the material to probe grain boundary cohesion. Results demonstrate a correlation between the content of doping elements and the mechanical response, revealing the profound impact of impurities at tungsten grain boundaries. This study advances the understanding of structure-property relationships critical for developing more damage-tolerant tungsten components for the extreme conditions in future fusion reactors.

Multi scale micromechanical testing for new Polymer Core Solder Ball (PCSB) interconnections reliability in operating conditions

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D3_3, Albéniz Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Microelectronics manufacturers are in constant research of optimization of their processes and materials in order to miniaturize further, increase reliability and comply to European directives.

New solders balls are proposed for BGA (Ball Grid Array) interconnections [1,2]. These Polymer Core Solder Balls (PCSB) are made of polymers coated by several metallic layers obtained by electroless plating. They are brazed on circuit boards with a lead-free alloy to attach microelectronics components. The ball/braze system is studied to assess its reliability and gather accurate input for numerical modelling. A multi-scale analysis is performed on the PCSB to understand their mechanical behaviour at the ball/braze system level and characterize the materials at the layer level.

Indeed, the metallic layers exhibit different microstructures and mechanical properties than their bulk macro-scale counterparts. Micromechanical tests (micro pillar compression and nanoindentation) are made on Cu and Ni coatings. This micro-scale characterization of mechanical properties such as Young's modulus and yielding stress enables the numerical simulation of the PCSB and clearly shows the difference with results obtained with bulk material properties [3]. The study is now focused on the lead free brazing alloy (SAC of Sn, Ag, Cu). Nanoindentation mapping is used to monitor the homogeneity of its mechanical properties.

Then, the ball and its braze make a complex system which is studied as a whole at mesoscopic level. Simple compression of PCSB validated the initial approach in [3] but the system undergoes vibrations and repeated stress in operating conditions. Cycling compression tests are thus carried out on soldered balls with a flat punch on a nanoindentation apparatus. They help understand the ball/braze system answer to fatigue and hopefully forecast potential failures. Subsequent numerical simulation of these tests should provide insight on mechanical phenomenon at stake.

Finally, the operating conditions exhibit temperatures from -40°C to 100°C. Hence, the results of aforementioned tests should be checked at different temperatures to provide accurate input to numerical models.

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- [2] Shih T. and al; IMC integrity for Sn96.7-Ag3.7 polymer core solder ball in BGA package. Proceedings of Technical Papers - International Microsystems, Packaging, Assembly, and Circuits Technology Conference, IMPACT, 2011.
- [3] Malkorra I. and al; Multi-scale in-situ micro-mechanical characterization of Polymer Core Solder Ball (PCSB) coatings for BGA interconnections. Microelectronics Reliability 148 (2023) 115135

Identification of material parameters by analyzing indentation test data using neural networks

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D3_3, Albéniz Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

The determination of the stress-strain curves of materials as well as the corresponding material parameters Young's modulus, yield strength, tensile strength and strain hardening exponents is an essential part during the design and calculation of components under applied loads. However, the accuracy is significantly limited by the applied material model, the accuracy of the associated material parameters and the used measurement method. If more detailed metallic properties are to be represented, such as isotropic and kinematic hardening as well as creep, more complex material models are required. This is even more difficult if the measurements have to be non-destructive and therefore no standard specimens made from existing components are available.

Therefore, as part of the "SEEKI" research project involving the partners ASMEC, ICAMS, IKTS and SENGICON, indentation tests with spherical indenters are used to generate the measurement data. In order to ensure the sensitivity of the material parameters with regard to the experiments, not only force-displacement curves but also time-dependent curves and indentation profiles are obtained and used for identification. Furthermore, the data is normalized according to the sphere diameter. In this way, the application of the method is independent from the indenter size after possible size effects are ruled out.

In order to avoid the high computational cost of the necessary, time-consuming FE simulations for the numerical parameter identification, these were replaced by a machine learning algorithm, specifically a neural network. This is realized by training such a neural network using FE simulations of indentation tests as training data. It is then possible to predict the required force-displacement curves and indentation profiles in way less time during the identification process itself. Consequently, the restriction on gradient methods for minimizing the function value determinations is no longer necessary, and other robust methods, such as genetic algorithms, can now be used effectively.

It is shown that with the appropriate optimization of the hyperparameters within the neural network, the accuracy of reproducing the FE simulation results is remarkably high and therefore suitable for practical use. The reduction of the time required for a complete parameter identification process from several hours or even days to just a few minutes also makes the approach attractive for mobile applications. Therefore, a mobile measurement head is developed within the project, which, in combination with the new identification approach, allows the direct identification of the material parameters in field use.

Hot-Working Characteristics and Microstructural Evolution of INCONEL 625 Multiphase Superalloy

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D3_10, Albéniz Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Nickel-based superalloys, such as INCONEL 625, are widely used in various industrial sectors, including chemical, petrochemical, energy, and aerospace, where they operate under demanding conditions requiring exceptional mechanical strength and corrosion resistance at high temperatures. The combination of Ni and Cr gives these superalloys exceptional properties in severe operating environments, such as remarkable oxidation resistance, superior to stainless steels, especially at temperatures above 650°C, as well as high resistance to stress corrosion cracking and localized corrosion, including pitting and crevice corrosion, in aqueous environments, even those containing sulphides and chlorides. Optimal mechanical properties at high temperatures are achieved by controlling all parameters of thermomechanical processing, especially during hot-working, a control that is often difficult to achieve. This study examines the hot-working behaviour of INCONEL 625 superalloy by evaluating its deformability and microstructural evolution within the 1050 – 1200°C temperature range. The microstructural changes were analysed using X-ray Diffraction (XRD) and Scanning Electron Microscopy with Electron Backscatter Diffraction (SEM-EBSD), while deformability was assessed through the upsetting method with a gravity-drop hammer. The following structural characteristics were analysed: constituent phases, lattice strain, crystallite size, phase morphology. Experimental data on deformation resistance, specific mechanical work, and plasticity were collected and analysed based on deformation temperature and impact energy. The findings indicate that increasing the deformation temperature improves plasticity, and a detailed analysis of plasticity's growth rate as a function of impact energy revealed that higher impact energy results in a more pronounced increase in plasticity. Additionally, deformation resistance was found to decrease with rising temperature across all impact energies. Likewise, specific mechanical work followed a decreasing trend with increasing deformation temperature, irrespective of impact energy.

Keywords: deformability; microstructural evolution; deformation resistance; plasticity; nickel-based superalloys.

Acknowledgments

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Micro scale fracture and fatigue of electrolytes for solid state lithium ion batteries

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D3_4, Albéniz Room (Level -2), septiembre 15, 2025, 17:00 - 19:00

An all-solid-state battery would revolutionise the electric vehicles of the future. The successful implementation of an alkali metal negative electrode and the replacement of the flammable organic liquid electrolytes, currently used in Li-ion batteries, with a solid would increase the range of the battery, reduce recharging time and address the safety concerns. Current efforts to commercialise such batteries worldwide are failing and will continue to fail until we understand the fundamental failure processes taking place in these devices, which are inherently driven by mechanical failure on the nano- and micro- scale. In this talk I will show our development of both testing methodologies and understanding of materials behavior in key materials for solid state batteries. This will focus on micro scale fracture testing of oxide and halide ceramics for use as solid state electrolytes. We will show indentation fracture toughness measurements and in situ microcantilever fracture testing. This is performed on LLZO, Li₆PS₅Cl and Li₆PS₅Cl based composite solid electrolytes under a range of processing conditions to show the often understated (in the battery community) effect of processing on battery performance. Micro cantilever fatigue testing results will then be shown showing the S-N curve behaviour of the same materials out to thousands of cycles. The implications of these results for future battery design will be discussed.

Unsupervised learning of nanoindentation data of complex materials

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D3_3, Albéniz Room (Level -2), septiembre 15, 2025, 14:30 - 16:30

Nanoindentation is a key technique for characterizing the mechanical properties of materials at small length scales, providing high-resolution measurements of hardness and elastic modulus. While traditional approaches average results over a limited number of tests, statistical nanoindentation captures property distributions, revealing microstructural heterogeneity. Recent advancements in machine learning have further improved the analysis of large nanoindentation datasets.

In this study, Cu-Cr composites with controlled heterogeneity were used to assess the effectiveness of statistical nanoindentation in detecting mechanical property variations. Hundreds of nanoindentation measurements were performed across large sample areas to evaluate Young's modulus and hardness at varying indentation depths. To analyze the data, we applied the Gaussian mixture model (GMM), an unsupervised learning technique, to deconvolute mechanical property distributions and identify distinct mechanical phases within the composite.

A major challenge in statistical nanoindentation is determining the minimum dataset size needed for reliable predictions. To address this, we used a cross-validation approach to systematically assess how dataset size affects statistical reliability. By monitoring the convergence of mechanical property distributions, we identified the required number of indentations for meaningful results.

Our findings demonstrate the importance of data quantity and advanced analysis techniques in nanoindentation studies. The use of GMM enhances the interpretation of mechanical property distributions, offering a robust framework for characterizing multiphase materials. This work underscores the potential of machine learning in nanoindentation and provides insights into data sufficiency for reliable materials characterization.

Deformation twinning induced mechanical properties of layered twin-matrix FCC metallic materials

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D3_7, Albéniz Room (Level -2), septiembre 16, 2025, 17:00 - 19:00

Deformation twinning effect on the properties of slip and twin systems of face-centered cubic structure and the critical resolved shear stresses will be shown. The plastic shear modes of the deformed matrix structure – single glide oriented Cu-8at.%Al alloy crystals deformed by room temperature tension up to the onset of deformation twinning - and the plastic shear modes of bimodal twin/matrix layered structure – subsequently twinned Cu-8at.%Al crystals – were examined. It was found that all twin and slip systems of the matrix structure may operate independently and their critical resolved shear stresses are dispersed by about fifteen percent around the mean value. However, not all of the accessible slip and twin systems of the twin/matrix structure may operate independently and their critical stresses may differ by a factor of well over four. Also, inverse temperature dependences of the detwinning stress of face-centered cubic deformation twins will be shown studying the effect of temperature on plastic deformation properties of the FCC twin/matrix structure. The critical resolved shear stress of detwinning was found to increase with temperature when plastic deformation occurred by the π detwinning mode. However, when the alternative $\pi/3$ mode of detwinning was activated, a decrease of the shear stress with an increase of temperature was observed. Thus, the twin/matrix structure behaved in two opposite ways, showing anneal hardening (the π mode) or anneal softening (the $\pi/3$ mode) with increasing temperature.

Statistics of micro-deformation mechanisms of HCP zinc coatings quantified by SSLIP analysis of in-situ EBSD-SEM-DIC testing

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D3_10, Albéniz Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

HCP plasticity is complex due to the high anisotropy, apparent brittleness, and the alternative plasticity mechanisms that often activate, such as twinning, grain boundary sliding, and/or grain boundary migration, alongside plasticity of multiple active HCP crystallographic slip families. Detailed understanding of HCP plasticity is important for many applications, such as zinc corrosion coatings for steel. In this study, a range of novel methodologies for high-resolution and robust measurement and identification of micromechanical deformation mechanisms are applied to identify all the different plastic mechanisms. The methodologies are based on in-situ EBSD-SEM-DIC testing [1,2], capable of obtaining strain fields with a ~40nm spatial resolution aligned to EBSD microstructure maps [3], with recently developed advanced EBSD-SEM-DIC analysis routines to quantify all HCP slip system activity maps as well as the activity maps of twinning, grain boundary sliding, and grain boundary migration [4,5]. A detailed statistical analysis has been conducted of these different plasticity mechanisms and their mutual interactions in zinc coatings, including >300 grains, corresponding to a total grain boundary length of ~2.9 mm. This huge statistical analysis resulted in a detailed hypothesis that tries to explain the activation of the 4 active zinc slip families, the occurrence of twinning, and the statistical analysis between the various identified GB properties of each GB segment, including the identified in-plane sliding and/or apparent opening kinematics, its angle with the loading direction, the crystallographic misorientation angle. Additionally, the interaction between these plasticity mechanisms has been studied, as will be presented at EUROMAT 2025.

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Indentation stress relaxation tests for studying transient plasticity in metals

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D3_6, Albéniz Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Nanomechanical tests are moving beyond regular hardness and modulus measurements to encompass host of different mechanical properties like strain rate sensitivity, creep, and fracture toughness. Developing the capability to measure stress relaxation behavior of materials will be useful to not only extend the gamut of properties studied at the micro/nanoscale, but also to study fundamental time-dependent deformation behavior of materials.

This talk will discuss the development of a novel indentation-based stress relaxation test that can reliably extract the activation parameters for deformation at micrometer length scales. The developed testing methodology, data analysis framework and the validation results will be presented. Nanocrystalline metals were selected for validation tests because they do not show size effects in indentation since hundreds of nanometer sized grains are interrogated in the indentation zone. Therefore, the micromechanical response can be considered to be “bulk” even in case of these small-scale tests. The indentation results were systematically compared with compression tests on micrometer sized pillars which have previously been shown to exhibit “bulk” scale behavior. A good match was found between both indentation and micropillar compression tests validating the developed testing methodology. Further, stress relaxation results on single crystal metals will be presented to study the operative deformation mechanisms. This opens the possibility to perform transient stress-relaxation tests on thin films and individual grains in future to systematically study the deformation mechanism(s) in a wide range of materials.

In situ TEM investigation of fracture growth in novel nanolaminate thin films

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D3_9, Albéniz Room (Level -2), septiembre 17, 2025, 14:30 - 16:30

In-situ transmission electron microscopy (TEM) provides unprecedented opportunities to directly observe and understand deformation mechanisms in advanced materials, making it an invaluable tool for developing tougher nanostructured systems. This study presents atomically resolved insights into the fracture behaviour of Cu-Al multilayer thin films incorporating ultrathin amorphous Al_2O_3 interlayers. Through in-situ TEM tensile testing, we directly observed the dynamic interplay between crack propagation and microstructural evolution. The multilayer system, consisting of 30-120 nm thick Cu-10% Al layers separated by 2 nm Al_2O_3 interlayers deposited via atomic layer deposition (ALD), demonstrated remarkable toughness through multiple mechanisms. Our real-time observations revealed that void nucleation preferentially occurred at interfaces between the ALD layer and high-angle grain boundaries, forcing cracks to follow tortuous paths and thereby enhancing the material's overall toughness. The investigation uncovered several concurrent deformation mechanisms operating ahead of the crack tip, including dislocation glide, grain boundary sliding, detwinning, and grain rotation. Notably, we observed a significant reduction in twin fraction from 30% to 20% during crack growth, indicating that plasticity at the crack tip is partially accommodated through detwinning. Perhaps most remarkably, the amorphous Al_2O_3 interlayers exhibited unprecedented ductility, thinning from 2 nm to approximately 500 pm before failure. This exceptional behaviour in an otherwise brittle ceramic material, combined with the complex crack propagation pathways and multiple operative deformation mechanisms, contributes to the enhanced mechanical performance of these multilayer systems. These findings provide crucial insights for the design of damage-tolerant metallic thin films and demonstrate the potential of engineered interfaces in achieving superior mechanical properties in multilayer materials.

Plasticity of olivine at high strain rates: an experimental micromechanics study on meteorite impact dynamics

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D3_6, Albéniz Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Olivine plasticity at ambient temperature governs the strength of a terrestrial planet's lithosphere during crustal divergence, convergence, and subduction. It also plays a crucial role in planetary collisions, influencing the formation of microstructures that accommodate impact-induced deformation. Such naturally occurring deformation processes bridge over a large strain rate regime, that is typically difficult to achieve under laboratory conditions using a single test piece. Small scale mechanical investigations allow us to focus on a few microstructural features in a well-controlled manner, using a scanning electron microscope.

Plastic deformation of olivine samples could be accommodated by dislocation generation and motion, but local stress-induced amorphisation and cracking can also happen during external loading. This work focuses on single crystal olivine pillars machined by FIB, that were compressed at various strain rates (from 0.001/s up to 1000/s). The micromechanical setup was coupled with acoustic emission detection to monitor the elastic waves emitted during the compression testing. High (angular) resolution EBSD is applied to study the dislocation structure before and after deformation. Differences in the deformation processes observed on the pillar surface morphologies and also in the collected data will be presented.

Effect of temperature, strain rate and grain size on the strain partitioning in the Alloy 718 up to 650 °C: A HR-DIC investigation

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D3_8, Albéniz Room (Level -2), septiembre 17, 2025, 10:30 - 13:10

The Ni-based superalloy Alloy 718 (Inconel 718) is an excellent alloy candidate for structural components operating at intermediate temperatures. In the past decades, its mechanical behavior and damage behavior has been intensively investigated at high temperature to establish a relationship between its strain-rate sensitivity and its oxidation-assisted intergranular cracking (OAIC). The present study focuses on the effect of the temperature, the strain rate and the grain size effects on strain localization partitioning at grain boundaries (GBs), twin boundaries (TBs) and intergranular from room temperature up to 650 °C, in the Portevin-Le-Chatelier (PLC) and non-PLC domains. HR-DIC analysis and out-of-plane measurements were performed to quantify plasticity distribution and preferential cracking site at the microstructure scale depending on the strain rate. Changes in strain localization with the grain size and strain rate demonstrated the concomitant action of strain localization and environmental degradation on the OAIC.

INNOBIO Project – Predicting the behavior of casted bioceramics

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Ceramic raw materials are used as biomaterials due to their inert behavior within the human body, their ability to be shaped into various forms and porosities, their high compressive strength, and their excellent wear resistance properties. These ceramics are used in components of the musculoskeletal system, hip and knee prostheses, bone grafts, dental and orthopedic implants, and heart valves. Despite the limitations imposed by their brittleness and low tensile strength, phosphate bioceramics, hydroxyapatites, alumina, zirconia, and zirconia-toughened alumina (ZTA) are widely used in the manufacture of biomaterials due to their high biocompatibility, tribological properties, and bone integration.

The advantages and disadvantages of biocompatible materials are closely linked to the manufacturing processes of the final products. Therefore, scientific advancement focuses not only on the development of new materials but also on the improvement and optimization of manufacturing techniques. One of the most commonly used shaping techniques is casting, due to its versatility and ability to reproduce complex shapes. This manufacturing process involves pouring a liquid material, such as molten metal or melted plastic, into a mold to create a solid piece with the desired shape.

Although research in the development of medical materials using casting techniques began years ago, as it is an economically accessible and sustainable technique, it remains of great interest due to the refinement of the technique and the derived methodologies. The INNOBIO project focuses on detailed research of casting techniques, integrating numerical simulation to predict the behavior of materials after shaping, which will reduce development times, minimize associated costs, and improve the quality and reliability of the final products. This will facilitate the understanding and prevention of possible defects in manufactured parts by means of virtual prototyping, saving time and resources during the manufacturing process.

The project “Investigación para la Innovación en Nuevas Aplicaciones de Materiales Biocompatibles – INNOBIO” is founded by Instituto Valenciano de Competitividad Empresarial (IVACE+i) and the European FEDER Funds.

Crystallinity and mechanical properties in glass-ceramic glazes by Raman Spectroscopy

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The amount of crystalline phases in glass-ceramic glazes is a key factor in achieving their mechanical and technical properties, apart from the aesthetic modifications they entail (opacity, or gloss, among others). Considering the possibility of correlation of the amount of crystals in the glaze with the rest of the properties, in this work we have designed glaze formulations to adjust the amount of crystalline phases generated in the glaze during the sintering cycle.

The glazes have been evaluated by Raman spectroscopy paying attention to the differences in intensity of the crystalline phase spectra according to their quantity. From a calibration line and the use of chemometrics, the present quantity of crystallizations was predicted. The study has been compared with results obtained by XRD of the same samples, reaching similar results for both methodologies. In addition, the mechanical properties of the glazes have been compared with the results of crystallinity, finding a direct relationship between them.

The possibility of knowing the amount of crystalline phases by means of a simple Raman spectroscopy study and predicting the mechanical properties of the sample has been confirmed.

Delineating thin-film microstructure contributions during ultrafast laser irradiation using atomistic simulations

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D3_2, Albéniz Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Atomic and close-to-atomic scale manufacturing demand progress underpinned by enhanced precision and optimization of laser-controlled nanostructuring. Depositing a high-energy laser beam on metallic film results in microstructure changes that invalidate the laser process parameters and influence how the laser beam interacts with the target material, costing numerous energy and time-consuming trial and error experiments. To this end, capturing thin films' crystallographic orientations and microstructure effects becomes crucial for optimizing the laser-metallic thin film interactions; however, these effects remain largely unexplored at the atomic scale. We combined two temperature model and molecular dynamics to simulate ultrafast laser-metal interactions for gold thin films with varying crystallographic orientations and microstructure configurations. Additionally, the effects of underlying silica substrate and chromium adhesion layers were also investigated using experimentally validated material and laser parameters to include the effects of interfaces. Our simulations revealed that microstructure features, namely grain size, grain topology, and local crystallographic orientation, controlled the rate and extent of lattice disorder evolution and phase transformation, particularly at lower applied fluences. We obtained comprehensive insights encompassing both the nanomechanical and thermodynamic aspects of ultrafast laser-metal interactions at atomic resolution. These insights reveal that microstructure-aware/informed thin film fabrication and targeted defect engineering could improve the precision of nanoscale laser processing and potentially emerge as an energy-efficient optimization strategy.

Influence of material properties on the mechanical behavior of architected structures

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D3_9, Albéniz Room (Level -2), septembre 17, 2025, 14:30 - 16:30

Metamaterials enable the achievement of exceptional mechanical properties that are unattainable with conventional materials, primarily through the tailored geometry of their unit cells. In particular, combining high stiffness with significant elastic recovery—two typically conflicting properties—can be realized by leveraging structural instabilities such as elastic buckling and snap-through effects. While it is well established that unit cell's geometry plays a dominant role in determining metamaterial effective properties [1], the influence of the constitutive material remains less explored. This study aims to quantify and rank the impact of the constitutive material on the mechanical response of metamaterials, with a focus on rigidity and elastic recovery.

A combined experimental and numerical approach was used to investigate this influence. Additive manufacturing via the Laser Powder Bed Fusion (LPBF) process was employed to produce metamaterial structures incorporating instability-based deformation mechanisms. Compression tests were conducted with in situ Digital Image Correlation (DIC) [2] to capture local constitutive material behavior. Experimental results were compared with finite element simulations incorporating material laws that account for non-uniform plastic deformations. Additionally, the influence of different constitutive materials was analyzed on an identical unit cell geometry to validate the findings.

The study provides new insights into the role of the base material in metamaterial performance, offering valuable guidelines for optimizing material-geometry interactions in the design of high-performance structures.

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Exploring Mechanical Properties of Soft Materials at the Nanoscale Using Indentation Methods

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D3_11, Albéniz Room (Level -2), septiembre 18, 2025, 14:30 - 16:30

Soft materials, characterized by elastic moduli typically below 1 MPa, such as biopolymers, gels, and biological tissues, exhibit distinct mechanical properties compared to hard materials. Investigating these properties at the nanoscale offers new possibilities in fields like biomedical engineering, materials science, and nanotechnology.

Nanoindentation techniques, including Atomic Force Microscopy (AFM) and nanoindenters, were employed to assess the mechanical properties of soft samples. These techniques were applied to samples such as defined phospholipid bilayers, biomolecules (proteins, DNA), hydrogels, single cells, and tissue cultures. Additionally, correlative approaches using fluorescence and Raman microscopy were demonstrated. The presentation concludes with a discussion on the challenges of standardizing these measurements.

The goal is to develop more efficient methods for characterizing the mechanical properties of complex soft materials and understanding their properties at the nanometer scale. This also involves exploring their relationship to the molecular nature of certain processes, with implications for biological and biochemical sciences. Such characterization can enhance our understanding of the connections between physiological or disease states and changes in mechanical properties at the molecular, cellular, or tissue levels.

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A High-Throughput Framework For Pile-Up Correction In High-Speed Nanoindentation Maps

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D3_6, Albéniz Room (Level -2), septiembre 16, 2025, 14:30 - 16:30

Pile-up is a common issue in nanoindentation that occurs when material plastically deforms and accumulates around the indent, leading to an overestimation of mechanical properties such as hardness and elastic modulus. While the traditional method involves the use of AFM, which is accurate but time-consuming, this work presents a high-throughput approach leveraging optical profilometry to assess roughness variations induced by nanoindentation and correlate them with pile-up height, providing a fast and scalable correction method [1-2].

The framework was validated on bulk metals (Cu, Ti, Al, BMG) and thin coatings of 1 μ m thickness (Au, Cu, Ti). All materials were characterized using four high-speed nanoindentation maps at depths of 300 nm, 500 nm, 600 nm, and 1000 nm. A systematic methodology was developed to establish a linear correlation between surface roughness changes (S_a) measured by optical profilometry and pile-up height obtained via AFM. Finite Element Modeling (FEM) was employed to support the experimental findings and validate the calibration functions derived. The method was further applied to a cobalt-based alloy (Stellite 6B), a heterogeneous material with distinct mechanical phases, where machine learning-based clustering was utilized to selectively correct pile-up in the softer cobalt matrix while preserving the mechanical integrity of harder carbide phases. The implementation of this correction significantly reduced errors in hardness and modulus estimation, achieving an improvement of up to 7% in accuracy.

The results demonstrate that the developed method provides a reliable and efficient alternative to traditional pile-up correction techniques, making high-speed nanoindentation mapping more accurate and applicable to a wider range of materials. The identification of two distinct linear calibration functions, one for bulk materials and another for coatings, enables the framework's broad applicability. By integrating machine learning and high-throughput optical profilometry, this approach advances the precision of phase-specific mechanical property mapping, bridging a crucial gap in nanoindentation methodologies.

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Layered nanostructured magnesium alloys for hydrogen storage synthesized by accumulative fold-forging (AFF)

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D4_3, Z4 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

Accumulative fold-forging (AFF) is an innovative severe plastic deformation (SPD) technique used to consolidate magnesium foils, both with and without the incorporation of niobium particles. Advanced microscopy techniques were employed to study the formation of nano-grains and the bonding at the interfaces between the nano-layers. Following this, the hydrogen storage performance of the resulting layered nanostructures of magnesium alloys was evaluated in relation to the microstructural characteristics observed after the AFF processing of Mg and Mg/Nb materials. Hydrogenation and dehydrogenation tests were conducted at various temperatures, revealing that the interfaces formed by SPD, such as grain boundaries and nano-layers, significantly contributed to the results. Ultimately, the maximum hydrogen storage capacity of magnesium was achieved, although the kinetics of storage and release varied based on the testing temperature, the presence of niobium particles at the layer interfaces, and the extent of microstructural refinements induced by the AFF process.

Component test for the assessment of in-service welding on/onto pressurized hydrogen pipelines

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D4_2, Z4 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Hydrogen is the energy carrier of tomorrow and requires a reliable large-scale transport infrastructure. In addition to new pipelines, the conversion of existing natural gas (NG) pipeline grids is an essential part. The transport of hydrogen is fundamentally different from that of NG, as hydrogen can be absorbed into the pipeline material. Given the effects of hydrogen embrittlement, the material compatibility (low alloy steels in a wide range of strengths and thicknesses) must be investigated. However, pipelines e.g. require maintenance or the need for installation of additional outlets with the necessity of welding on/onto the pipelines while they are still in service, i.e. with gas flow under high pressure, such as the well-known "hot tapping". This in-service welding poses challenges for hydrogen operations. The challenge can be roughly divided into the possible austenitization of the inner pipe material exposed to hydrogen, the welding itself, which causes an increased temperature range. Both lead to a significant increase in hydrogen solubility and diffusivity compared to room temperature. In addition, possible surface reactions of the present iron oxides (e.g. magnetite or hematite) with the hot hydrogen should be considered. In this context, the knowledge of hydrogen pipelines is scarce due to the lack of operational experience. Fundamental experimental investigations are required to investigate the transferability from NG to hydrogen pipeline grids. For this reason, the present study presents a specially designed mock-up / demonstrator concept for the realistic assessment of the welding process conditions. The mock-up was designed to allow in-situ temperature measurement during the welding process as well as ex-post sample extraction for quantification of the absorbed hydrogen concentration. For safety reasons, the required volume of pressurized hydrogen was limited by inserting a solid cylinder to ensure a 1 cm thick layer of hydrogen gas. Welding experiments on the DN60 and DN200 pressurized mock-ups showed the possibility of safe welding on or onto pressurized hydrogen pipelines. Indeed, the austenitizing temperature was reached on the inner surface of the pipeline, especially on thinner-walled pipelines, using current welding parameter recommendations. This corresponded to an increased hydrogen uptake in the welded area of several ppm. From this point of view, the suggested component concept is a viable strategy for the screening of several materials and welding parameter combinations under realistic operational conditions.

Tracking hydrogen in metals: permeation and thermal desorption study using a deuterium tracer

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D4_2, Z4 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

It is known that hydrogen can enter the alloy material during service or manufacturing process and significantly deteriorate the mechanical properties of steel. Information on hydrogen permeation and desorption is crucial for better understanding the susceptibility to pitting corrosion and hydrogen embrittlement phenomena in order to obtain improved resistance to hydrogen-induced degradation in future materials development. Stainless steels commonly used in the nuclear industry and modified RAFM steels are preferred as structural materials for fusion reactors due to their good mechanical properties and corrosion resistance under the realistic conditions of the ITER and DEMO reactors. In this work, electrolytic deuterium uptake and desorption behavior in RAFM steels (with increased W and Si content) and 304 stainless steel was studied using thermal desorption spectroscopy (TDS) and electrochemical permeation (Devanathan-Stachursky method), supported by corrosion test before and after charging to evaluate the changes in surface condition during the charging process. A set of electrolytes were prepared from 99.98% heavy water (D₂O) to distinguish between naturally occurred hydrogen and deuterium introduced to the material by electrochemical charging. The overall conclusions are: the current densities as low as 1mA/cm² and time between 70-90 minutes is sufficient to permeate 0.4 mm thick steel in 0.1 M sodium arsenate solution and pure D₂O (pH 8). In these conditions, the best reproducibility of TDS results and the lower damage to the surface were observed. The deuterium (mass 4) and HD (mass 3) spectra of three steels displayed an asymmetric desorption peak at ~385–395 K (probably overlapping two maxima) and HD maxima at ~385–395, ~480-510 K. For all materials and charging conditions tested, the intensity of the mass 3 was higher than that of mass 4, and the deuterium uptake was greater when the electrolyte was stirred, the obtained values were 0.76 x 10¹⁵ at/cm²(stagnant) 2.36 x 10¹⁵ at/cm² (stirred). The Tafel plots for as received and after electrochemical charging samples showed a shift in the corrosion potential towards more noble values by approx. 0.02-0.1 V. The corrosion current density decreased 10 times, which indicates that an oxide layer was formed on the surface. Time intervals ranging from 8 hours to 7 days between the charging process and TDS measurements reduced the amount of retained deuterium for all analyzed steels when stored in air, however the mass 3 retention was not significantly affected. No such difference was observed for samples left in water of a normal hydrogen concentration.

Hydride-Driven Formation of Zirconium Islands in Irradiated Fuel Claddings: Alloying Element Segregation and Implications for Structural Nuclear Materials

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D4_1, Z4 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

High-burnup Zr-based nuclear fuel claddings develop c-component dislocation loops under irradiation, which correlate with accelerated degradation mechanisms such as hydrogen pickup and irradiation growth. Recent atom probe tomography (APT) studies by Mayweg et al. (JNM597(2024)155116) reveal that these loops host nearly pure zirconium (Zr) islands, accompanied by segregation of Fe, Ni, and Sn to loop peripheries and depletion of Sn/O within the loops. While these observations suggest a de-alloying behavior in c-loop, the origin of the Zr islands remains unresolved. Building on density functional theory (DFT) studies by Christensen et al. (JNM 445.1-3(2014)241-250), which demonstrated that alloying elements exhibit low solubility in Zr hydrides, we propose that the Zr islands are hydride phases stabilized by hydrogen accumulation in the faulted regions of c-loops.

The intrinsic strain associated with the c-loop structure—a 5-layer FCC-like stacking fault embedded in the HCP Zr matrix—creates an energetically favorable site for hydrogen segregation. Hydrogen migration into these regions relieves lattice strain, promoting hydride formation. This aligns with the pseudo-FCC sublattice of zirconium hydrides (ZrH), mirroring the distorted FCC geometry of the faulted loop. To validate this hypothesis, we perform DFT simulations of Zr-hcp/ZrH-fcc interfaces, systematically evaluating the stability of alloying elements (Sn, Fe, Cr, Ni, Nb) at interstitial and substitutional sites across pure Zr, hydride, and interfacial regions.

Our results reveal distinct destabilization hierarchies for hydrides: interstitial elements follow $\text{Nb} > \text{Sn} > \text{Fe} > \text{Cr} > \text{Ni}$, while substitutional elements follow $\text{Sn} > \text{Ni} > \text{Fe} > \text{Cr} > \text{Nb}$. This complements the trend in bulk hydride ($\text{Sn} > \text{Fe} > \text{Cr} > \text{Ni} > \text{Nb}$) by Christensen et al. (JNM 445.1-3(2014)241-250), highlighting the critical role of interfacial effects. Notably, Sn—depleted in loops experimentally—exhibits the strongest destabilizing effect substitutionally, aligning with its absence in Zr islands. Simulations of hydrogen-free Zr-hcp/Zr-fcc interfaces further confirm that c-loop instability arises from hydrogen accumulation, not intrinsic stacking faults.

These findings establish a mechanistic link between hydrogen trapping in c-loops, hydride formation, and alloying element redistribution. Hydrogen-induced hydrides create Zr-rich zones by expelling solutes to loop boundaries, consistent with APT observations. This work advances the understanding of irradiation-hydrogen synergy in Zr cladding degradation and provides a framework to predict solute behavior in hydride microstructures. By quantifying interfacial energetics and solute-hydrogen interactions, the methodology also serves as a foundation for extending this analysis to Ni- and Fe-based structural alloys, where hydrogen embrittlement and irradiation defects similarly govern performance.

Multi-Scale Computational Study of Hydrogen Adsorption and Phase Transitions in Metal-Hydrides for Energy Storage

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D4_1, Z4 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

The adsorption of hydrogen on the surfaces, sub-surfaces, and interfaces of metals and alloys is critical for developing solid-state hydrogen storage technologies. A fundamental understanding of these interactions is essential for optimizing hydrogen storage capacity and stability in metal-hydride systems. In this study, we integrate density functional theory (DFT) calculations with a variational framework to systematically analyze the energetics of hydrogen adsorption on various metal and alloy surfaces. Our approach identifies preferred adsorption sites, structural configurations, and phase stability as a function of hydrogen coverage.

The variational framework developed in this work provides new insights into the impact of adsorbed hydrogen on the structural and chemical stability of polycrystalline materials. By capturing phase transitions at surfaces and interfaces, our model explains how different material configurations can facilitate enhanced hydrogen storage. Specifically, we determine the critical hydrogen concentration necessary for phase separation within bulk systems, allowing co-existing surfaces to accommodate higher hydrogen uptake efficiently.

Additionally, we examine the kinetics of hydrogen adsorption and desorption, both at surfaces and in bulk metallic systems, to assess their influence on storage performance. A key aspect of our analysis is the evaluation of chemical strain induced by lattice expansion during hydrogen absorption and its subsequent desorption. This strain significantly affects the mechanical integrity of metal-hydride systems, influencing both storage efficiency and long-term durability. Our findings provide essential guidelines for designing hydrogen storage materials with improved mechanical resilience and optimal adsorption characteristics.

Beyond storage applications, metal hydrides derived from these materials also hold significant potential for energy technologies, including battery systems. Understanding the interplay between hydrogen adsorption, phase transitions, and mechanical stability will be crucial for the development of next-generation energy storage solutions. This study lays the groundwork for future experimental and computational research aimed at optimizing hydrogen storage in metallic systems, bridging the gap between fundamental materials science and practical energy applications.

Characterizing hydrogen in amorphous alumina thin films through integration of modeling, theory, and experiment

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D4_1, Z4 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

This talk discloses the effect of hydrogen impurities on the local chemical bonding states and structure of amorphous alumina films by predicting measured Auger parameter shifts using a combination of atomistic and electrostatic modeling. Different amorphous alumina polymorphs with variable H-content and density, as grown by atomic layer deposition, were successfully modeled using a universal machine learning interatomic potential. The annealing of highly defective crystalline hydroxide structures with experimental H-contents at the corresponding atomic layer deposition temperatures led to excellent agreement between theory and experiment in the density and structure of the resulting amorphous alumina polymorphs. The measured Auger parameter shifts of Al cations in such polymorphs were accurately predicted with respect to the H content by assuming that all H atoms are present in the form of hydroxyl ligands in the randomly interconnected 4-fold, 5-fold, and 6-fold nearest-coordination spheres of Al. As revealed by a combination of atomistic and electrostatic modeling, the measured Auger shifts with an increase in the H content and an accompanying decrease in the oxide density depend on the complex correlations between local coordination, bond lengths, bond angles, and ligand type(s) around the core-ionized atoms. These findings and fundamental knowledge contribute to advancing the design of e.g. hydrogen oxide barrier films, oxide membranes for H separation, H storage materials, and fuel cells for a hydrogen-based economy.

OPTIMIZATION OF ALPHA AND GAMMA ALUMINA CATALYSTS VIA ADDITIVE MANUFACTURING

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Additive Manufacturing (AM) has emerged as a transformative technology for fabricating advanced ceramic catalysts, enabling precise control over structural features while reducing processing time and material waste. This study focuses on optimizing alpha (α) and gamma (γ) alumina (Al_2O_3) catalysts produced via Direct Ink Writing (DIW), evaluating their structural, thermal and catalytic properties. γ - Al_2O_3 is widely used in ethanol-to-ethylene dehydration due to its high surface area, thermal stability and porosity, whereas α - Al_2O_3 offers superior mechanical strength, making it an ideal as a support material. This research examines the effects of the ceramic charge (CC) and sintering temperature on the microstructure and catalytic performance of DIW-printed Al_2O_3 scaffolds. The CC varied from 20 to 35 wt.% and sintering temperatures ranged from 400 to 600°C. Characterization of the scaffolds included phase composition, porosity, shrinkage and catalytic activity. The results demonstrate that these processing parameters critically influence key physicochemical properties. Shrinkage values ranged from 10 to 12%, directly impacting porosity and surface area. Notably, scaffolds with a CC of 32.5% sintered at 600°C exhibited an optimized microstructure, achieving an ethanol conversion efficiency of 99.7%, compared to 94.6% for samples sintered at lower temperatures. These findings underscore the importance of surface engineering via DIW-AM in developing high-performance catalysts, contributing to more sustainable and energy-efficient industrial processes.

Effect of gaseous hydrogen on polyethylene pipe materials

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D4_3, Z4 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

The shift to renewable energy systems necessitates efficient methods for storing surplus energy, such as converting it into hydrogen (H₂) through electrolysis. One potential solution for storing and transporting hydrogen is injecting it into existing polyethylene (PE) gas networks. However, the impact of hydrogen exposure on the mechanical properties and longevity of PE pipes, particularly in relation to slow crack growth (SCG), is scarcely investigated. While some studies suggest little effect on polymeric pipes, recent research indicates that high-pressure hydrogen may influence SCG behavior. This study explores the effects of prolonged exposure to gaseous H₂ at operational pressures (~10 bar) on PE pipes using fracture mechanics techniques, specifically cyclic Cracked Round Bar (CRB) tests. Two sets of PE100 pipes were examined: one exposed to gaseous H₂ for two years and the other subjected to water pressurization for over 1000 hours. The findings showed comparable SCG behavior between the pipes exposed to hydrogen and those exposed to water, suggesting that pressure, rather than hydrogen itself, may be the key factor affecting SCG performance.

In parallel, the question regarding the interaction of permeation rates and inner structure of the polymer is an intriguing one. Therefore, a study on the influence of processing conditions on the inner structure and subsequent permeation rates at operational pressure was performed. The study examined the impact of seven different cooling and pressure conditions, as well as degree of crystallinity on the permeation rate of gaseous H₂ through PE. While some differences could be found, the maximum change of permeation rate was found to be roughly 10%. This indicates, that regardless of the processing conditions of PE, the amorphous regions in between crystalline domains are the determining factor with regards to permeation and processing conditions alone cannot introduce big differences in permeation rate.

Digital material design guidelines for mitigation of hydrogen embrittlement

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D4_2, Z4 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

The global shift towards the widespread use of renewable energy sources, including hydrogen and hydrogen-based fuels, necessitates new safety standards and innovative material solutions for both emerging and established energy sectors. Modern multiscale computational methods offer a promising pathway to accelerate material development and address potential safety risks associated with materials early in their development cycle.

In this review, we highlight computational techniques that have been effectively utilized to propose various strategies for mitigating hydrogen embrittlement in high-strength steels and nickel-based alloys. Furthermore, we introduce novel methods developed at our center to study this phenomenon under diverse conditions. Our approach encompasses multiple length and time scales, ranging from atomic-scale quantum mechanical density functional theory calculations to continuum meso and macro scales represented by phenomenological thermodynamic and kinetic models, as well as the finite element method. These techniques enable us to analyze and predict the evolution of hydrogen-material interactions based on material composition, microstructure, time, temperature, and mechanical stress.

Hydrogen embrittlement of precipitation hardened austenitic alloys at liquid helium temperature – The role of hydrogen diffusivity and serrated flow

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D4_2, Z4 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

The influence of temperature on hydrogen embrittlement of the precipitation hardened Ni-based alloy N07718 has been previously studied down to cryogenic temperatures of 77 K, showing a reduction of the hydrogen induced ductility loss with decreasing temperature. It has been suggested that hydrogen diffusion is mandatory to cause the embrittling effect. However, operating temperatures of cryogenic tanks and valves for liquid hydrogen storage can go down to 20 K, where the effect of hydrogen on tensile properties remains poorly investigated for precipitation hardened fcc alloys.

In this study we conduct tensile tests with an initial strain rate of $3 \times 10^{-5} \text{ s}^{-1}$ at liquid helium temperature (4.2 K) and room temperature on two precipitation hardened alloys, namely Ni-based alloy N07718 and austenitic steel S66286, in an uncharged and a pressurised hydrogen charged state. Results show that virtually no hydrogen embrittlement has been determined at liquid helium temperature. This behaviour is discussed regarding the influence of serrated flow and the effect of cryogenic temperatures on hydrogen diffusivity. In addition, a diffusion model is applied to simulate hydrogen distribution within the two alloys at the investigated temperatures considering potential hydrogen trapping sites.

Characterization of the H₂-rich fuel combustion process - model and experimental approach

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Materials used in the aerospace industry must exhibit high resistance to extreme temperatures and aggressive combustion environments. In addition to assessing the impact of flame and high temperature on such materials, it is also crucial to gain a detailed understanding of the combustion process itself, its mechanisms, and the factors that govern its progression. Therefore, the aim of this study was to conduct computational simulations of combustion processes and perform experimental investigations of methane and methane-hydrogen mixture combustion under various conditions. A comparative analysis of the obtained results against numerical models was then carried out to assess their accuracy and identify key parameters influencing combustion processes. The experiments were conducted using a specialized research furnace, designed and manufactured by Proximo Aero, located in the Hydrogen Laboratory of Rzeszów University of Technology.

The impact of hydrogen on mechanical properties of nickel: a hybrid grand canonical Monte-Carlo/molecular dynamics study

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D4_1, Z4 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Despite decades of research, the dominance and co-occurrence of hydrogen embrittlement mechanisms in metals are still under debate. The complexity of such problem is further increased due to the interplay between atomic and microstructural aspects and the interaction with atomic hydrogen that are relevant for both, but not restricted to, the hydrogen enhanced local plasticity (HELP) and hydrogen enhanced decohesion (HEDE) mechanisms. Computer simulations allow the study of these mechanism under desired conditions and provide a detailed atomistic description of hydrogen interactions in the material and its effect of mechanical and microstructural properties. These simulation approaches are, however, under idealized controlled conditions that might not resemble realistic environments in which load-bearing alloys are used.

In this work is presented recent advances on a large-scale fully 3D atomistic simulations of various microstructural domains coupled with a hybrid grand canonical Monte Carlo/molecular dynamics (GCMC/MD) methodology to realistically study heterogeneous microstructures of nickel. This approach shed light on which mechanism, or which combination of those, is dominant and what is the effect of hydrogen in materials properties of Ni-based superalloys. The construction of defect phase diagrams using the chemical potential of hydrogen as the underlying variable is put forward on the interpretation of defect phases associated with H-embrittlement mechanisms in crack systems, type and orientation of grain boundaries, and the interaction of hydrogen with stacking faults and line defects.

Multi-species diffusion model for hydrogen within actual steel microstructure

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Properties and integrity of structural materials in service are strongly linked to their microstructure. The microstructure plays a key role in various embrittlement mechanisms, including hydrogen embrittlement (HE), which has drawn much attention in recent years due to a gradual transition to sustainable energy sources. The most common HE mechanisms include hydrogen enhanced decohesion (HEDE) and hydrogen enhanced localized plasticity (HELP), which can be strongly affected by diffusion behavior of H in the presence of other solutes. For instance, HEDE mechanism can be influenced by the reduction of hydrogen concentration at grain boundaries due to the presence of other interstitial elements. Similarly, the HELP mechanism can be affected by the redistribution of hydrogen near crack tips and the occupation of dislocation sites by competing interstitial species. In this work we investigate the diffusion and trapping behavior of a steel that contains multiple alloying elements that can affect H trapping within the microstructure using a multi-physics finite element method (FEM) approach. Diffusion inside of the bulk of the grains is described by a thermodynamically based model considering the trapping of each species/trapping site pair as well as a stress state. Conversely, the diffusion via interfaces is modelled using a semi-atomistic approach that incorporates atomistic input on the interface properties from density functional theory (DFT) calculations.

The influence of copper on the distribution and trapping of hydrogen in steels

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Copper (Cu) plays a dual role in steel production: it is a tramp element that poses challenges during processing due to its difficulty in removal, yet it is also intentionally added to certain steel grades, particularly in shipbuilding and offshore industries, to enhance corrosion resistance and hardening through Cu precipitation. The shift towards electric arc furnace (EAF) steelmaking and increased recycling rates are expected to raise the levels of tramp elements in future steel products. Cu precipitates, which transition through various phases and interface types with the iron matrix, not only contribute to hardening but also show potential in mitigating hydrogen embrittlement, although isolating their specific effects remains challenging.

In this study, we investigate the role of Cu segregation and Cu precipitates, in particular the influence of their morphology (bcc, 9R, fcc) on the hydrogen trapping strength of Cu interfaces with bcc iron (Fe) at the atomistic level with the aid of density functional theory (DFT) calculations. Furthermore, we subsequently use the calculated hydrogen trapping energies as an input to a thermodynamic hydrogen trapping model based on the Oriani equation in order to investigate the hydrogen distribution in a model steel microstructure. A model investigation of hydrogen uptake at Cu precipitates as a function of their shape and volume fraction provides a conclusion about their role in hydrogen embrittlement.

Hydrogen embrittlement mechanism in additively manufactured stainless steel

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D4_3, Z4 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

Laser Powder Bed Fusion (LPBF) is a promising manufacturing technique for advanced engineering components potentially offering improved mechanical properties. However, the performance of LPBFed components in hydrogen-rich environments remains largely unknown, raising concerns about long-term reliability for applications in hydrogen storage and energy conversion. This study investigates the hydrogen embrittlement (HE) mechanisms of LPBFed 316L SS, including experimental testing, microstructural characterisation, and computational modelling to establish a deeper understanding of hydrogen interactions with LPBFed manufactured materials.

Isothermal desorption spectroscopy (ITDS) demonstrates that LPBFed 316L exhibits higher hydrogen diffusivity compared to its wrought counterpart, suggesting an altered hydrogen transport mechanism within its melting pool boundaries and subgrain microstructure. Slow strain rate tensile tests (SSRT) with in situ neutron diffraction confirm that LPBFed 316L maintains a stable austenitic phase under mechanical loading, with no observable strain-induced martensitic transformation, even in hydrogen-charged conditions. It is also found with EBSD that hydrogen activates dislocation multiplication in the early stage of deformation, and the LPBFed microstructure can suppress this trend, reducing embrittlement susceptibility.

Further investigations using digital image correlation (DIC), reveal earlier initiation but slower propagation of cracks in all hydrogen charged specimens and macroscopic hydrogen-induced localised strain in wrought specimens, providing evidence on enhanced localised plasticity in hydrogen-charged samples. SEM also observe typical quasi-cleavage fracture surface in hydrogen charged samples. Mitigation of this phenomenon was found in LPBF specimens.

To bridge experimental findings with theoretical understanding, a dislocation-assisted hydrogen migration model was developed, providing quantitative insights into the hydrogen-trapping behaviour at subgrain boundaries. Simulations reveal that the fine subgrain structures in LPBFed 316L limit hydrogen accumulation at grain boundaries, reducing embrittlement susceptibility compared to wrought 316L. This novel mechanistic understanding supports the superior hydrogen embrittlement resistance of L-PBF 316L, positioning it as a promising material for hydrogen storage and energy applications.

This work provides compelling evidence that LPBF processing enhances hydrogen embrittlement resistance while providing higher mechanical strength, paving the way for the broader adoption of additively manufactured stainless steels in hydrogen-related applications. By integrating experimental findings with multiscale modelling, this study offers new perspectives into hydrogen-material interactions in advanced manufacturing technologies.

Numerical simulation of pressurized microtubular reversible solid oxide cells for hydrogen production

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Solid oxide cells (SOCs) are devices capable of separating hydrogen molecules from water vapor for storage and later use. Additionally, they can operate in reverse mode as fuel cells, converting the chemical energy of a fuel into electrical energy. In particular, microtubular solid oxide cell configurations have garnered significant interest in the scientific community due to their high efficiency under high-temperature operating conditions and the ability to withstand rapid thermal cycling during high-temperature operation, distributing heat more homogeneously across the structure and enhancing structural robustness. Additionally, in microtubular geometry, reducing the diameter increases power density per unit volume, as it provides a larger active area for the electrochemical reaction.

This study focuses on the performance of high-temperature microtubular solid oxide cell in fuel cell and electrolyzer modes between 600 and 800 °C, analyzing the effects of electrode gas pressurization (ranging from 1 to 10 bar) on polarization, the chemical reaction, temperature distribution, and thermal gradients under reversible operation conditions for hydrogen production and energy generation. A multiphysics model will be implemented using the computational tool Ansys for simulation and results analysis. This is an ongoing work which provide simulation results that are compared and validated with experimental data. The simulated models will contribute to a better understanding of the impact of gas pressurization on micro tubular solid oxide cell performance and serve as a design tool for high-temperature microtubular solid oxide cell systems.

Influence of ceramic additive in thermoplastic polymers for liners in Type IV hydrogen tanks

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Hydrogen tanks for mobility applications require a low weight to storage volume ratio. To achieve this, pressurized hydrogen storage vessels have evolved from fully metallic Type I vessels to the Type IV vessels. This lightweight design consists of an external load-bearing fibre epoxy composite structure wound onto a gas barrier liner that prevents hydrogen loss by permeation. The liner of Type IV vessels consists of a thermoplastic polymer, mainly HDPE or PA due to their low permeation rate and low material cost. This type of vessels faces challenges in terms of permeation requirements because hydrogen vessel regulations specify a maximum leakage rate per storage volume, while a further weight reduction is sought. The development of low permeability materials for these internal liners is of paramount importance.

Hydrogen diffusion can be influenced by the addition of impermeable fillers such as fibres or nanoparticles into the thermoplastic matrix. The rationale is to reduce the surface area to be permeated and create tortuous routes that increase the length of the diffusion path, reducing the material's hydrogen permeation.

The aim of the present study is to assess the effect of ceramic additives in PA6,6 for hydrogen storage applications, these compounds represent attractive materials for Type IV hydrogen containers in mobility applications. For this, ceramic platelets have been added to PA6,6 and small plates have been produced via injection moulding. The hydrogen permeation properties of the unreinforced and ceramic-filled PA6,6 have been evaluated using the differential pressure method, following the standard ISO 2782-1. This technique applies a constant pressure differential to evaluate hydrogen permeability, solubility and diffusion coefficients. The obtained results have been correlated with the resulting microstructure.

Investigating Hydrogen Embrittlement in Superalloys: The Role of Intermetallic Phases

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D4_2, Z4 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

The most widely used Ni-based superalloy, Alloy 718, shows significant hydrogen embrittlement. The strengthening precipitates γ' and γ'' as well as the grain boundary pinning δ phase play a significant role in the embrittlement of this polycrystalline alloy. In order to investigate whether superalloys with other grain boundary pinning phases show similar hydrogen embrittlement, two different γ' strengthened CoNiCr-based superalloys with additional intermetallic B2-structured β or D85-structured μ phase particles were investigated. NanoSIMS mapping revealed the highest hydrogen concentration localized within the grain boundary pinning μ precipitates, a finding corroborated by synchrotron diffraction measurements showing significant lattice expansion of the μ phase after hydrogen charging. Neutron diffraction experiments further indicate that the γ' phase absorbs more hydrogen than the γ phase, resulting in greater expansion and an increased lattice misfit between the γ and γ' phases. Tensile tests demonstrate a pronounced influence of hydrogen on the mechanical properties of samples charged with high-pressure hydrogen. The enrichment of hydrogen within the intermetallic grain boundary particles and strengthening precipitates promotes considerable crack initiation and facilitates crack propagation along weakened γ/γ' interfaces. These findings deepen the understanding of hydrogen embrittlement in superalloys and help to develop more hydrogen-resistant alloys.

Ab initio and atomistic simulations of defect induced hydride formation

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D4_1, Z4 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Climate change motivates the search for non-carbon-emitting energy generation and storage solutions. Metal hydrides show promising characteristics for this purpose. Using systematic ab initio and atomistic simulations, we explore the potential of the abundant defects in the materials such as grain boundaries, dislocations, and microcracks for enhancing the thermodynamics and kinetics of Al-based hydride formation.

Firstly, we consider tailoring and employing the negative pressure of microstructural and structural defects to enhance H solubility and thus hydride formation as a novel concept. Using the ab initio thermodynamics method, we created the negative pressure-dependent phase diagram of Alane hydride AlH_3 in the gas pressure and temperature domain. We demonstrate that such an enhancement at the negatively pressurized crack tip region is feasible by increasing the mechanical tensile load on the specimen. The theoretical predictions have been used to reassess and interpret atom probe tomography experiments for a high-strength 7XXX-aluminium alloy that shows a substantial enhancement of hydrogen concentration at structural defects near a stress-corrosion crack tip.

Secondly, using the ab initio simulations we studied the effect of grain boundaries on the stability and kinetics of hydride formation in TiFe and Al-based alloys. We calculate the concentration-dependent segregation energies of H to various grain boundaries such as $\Sigma 3$, $\Sigma 9$, $\Sigma 5$, and $\Sigma 11$ that are proven to have elevated H concentration. We explore the potential of these grain boundaries for enhancing the formation of hydrides by acting as nucleation sites through the results of these calculations. Based on these insights we derive strategies for exploiting metals as H-storage materials.

Multiscale Modelling of Hydrogen Diffusion in Polycrystalline Metals

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D4_1, Z4 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Hydrogen impurities in metals can severely degrade mechanical properties, a phenomenon known as hydrogen embrittlement. While numerous mechanisms have been proposed to explain this effect, their relevance under specific material conditions remains a topic of debate. Nevertheless, a key factor in all hydrogen-assisted damage mechanisms is the role of hydrogen diffusion and trapping, as the accumulation of critical concentrations at failure points occurs rapidly.

Modelling and simulation are essential tools for understanding hydrogen diffusion, but capturing these processes is challenging due to interactions across multiple length and time scales.

In this work, we present a multiscale modelling workflow—from the electronic to the continuum scale—to study hydrogen diffusion in polycrystalline nickel. We begin with an electronic-level analysis of hydrogen migration and trapping at selected nickel grain boundaries. These results inform a kinetic Monte Carlo model to determine effective diffusivities under various conditions, which are then used as input parameters for continuum-scale simulations of hydrogen concentration evolution in polycrystalline materials.

This multiscale approach accounts for key complexities, including grain boundary character and diffusion anisotropy. While demonstrated here for polycrystalline nickel, the framework is broadly applicable to other materials and microstructures, offering a versatile and predictive tool for assessing the effects of hydrogen exposure on metallic materials.

LOW TEMPERATURE CATALYTIC SUPERCRITICAL WATER GASIFICATION FOR CONTINUOUS HYDROGEN GENERATION FROM BIOMASS WASTEWATER

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D4_3, Z4 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

A continuous hydrothermal process is demonstrated, for the first time, that can operate at low gasification temperature (430 °C) and residence time (20 s) by combining supercritical water gasification (SCWG) and partial oxidation with in situ synthesis of virgin metal oxide nano-catalyst. This process addresses the challenges associated with catalyst deactivation of a fixed bed, tedious homogenous catalyst separation after the process and/or the need for high operating temperatures. Industrial biomass wastewater was used as the feedstock for generating hydrogen and methane-rich syngas, with a metal oxide nano-catalyst as a valuable co-product and cleaner water, lower in chemical oxygen demand (COD) and total organic carbon (TOC), as a liquid product.

Using olive wastewater as the feedstock, this gasification study experimentally investigated the impact of multiple variables: (1) COD feed concentration, (2) the in situ synthesis of different metal oxide nano-catalysts, (3) the partial oxidation coefficient (η) and (4) the nano-catalyst precursor solution concentration. The optimum conditions for the generation of hydrogen and methane from olive wastewater were a feed COD of 38.6 g/L, $\eta = 0.8$, and 60 mM precursor concentration for the in situ synthesis of Fe₂O₃ nano-catalyst. These optimised conditions were further investigated using spent lees and stillage. The efficiency of hydrogen and methane yields and COD reduction were in the order of stillage > spent lees > olive wastewater. The highest hydrogen molar selectivity, hydrogen and methane yields at 18.8 %, 17 and 11.4 mol/(kg biomass) respectively were obtained with stillage feedstock. Gasification, COD and TOC reduction efficiencies were 68.8–71.7 %, 72.6–76.5 % and 53.9–55.7 % respectively, with this process.

Importantly, this process was further validated by showing stable, steady-state gasification performance in terms of gas yields with olive wastewater, stillage and spent lees as the feedstocks during continuous operation for 40 min without any significant drop in performance. This study exemplifies that the co-generation of catalyst during SCWG is a promising and economically feasible direction for large-scale continuous generation of hydrogen and methane from different types of biomass wastewater at < 450 °C, whilst lowering its COD and TOC.

Hydrogen risk mitigation using high-porosity autocatalytic materials

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D4_3, Z4 Room (Level -3), septembre 18, 2025, 17:00 - 19:00

Hydrogen Risk Mitigation Using High-Porosity Autocatalytic Materials

Hydrogen is garnering significant interest as an energy vector pivotal to the ecological transition. While the majority of hydrogen is mainly produced via methane catalysis, the emergence of decarbonated hydrogen produced from low-carbon energy sources is notable. Hydrogen's high energy release upon combustion, emitting primarily water as a byproduct, underscores its potential. However, its high flammability, propensity for detonation, and impact on material structures, elevate accident risks [1], [2]. Additionally, studies indicate that environmental hydrogen release can indirectly exacerbate global warming by extending the atmospheric lifetime of other greenhouse gases, such as methane.

In this project, we have developed microstructured, high-porosity materials designed to convert leaked hydrogen into water vapor through autocatalytic processes. These composite materials allow to convert more effectively the hydrogen into water vapor than the simpler and costly use of bulky metallic palladium and platinum of the Passive autocatalytic recombiners (PARs) [3]. The use of appropriate metallic oxides doped in catalysts enhances reaction efficiency at room temperature even at low concentration [4]. The exothermic nature of this reaction accelerates hydrogen consumption while allowing its detection. In confined spaces, this technology significantly reduces the risk of hydrogen accumulation. Moreover, the resultant water vapor saturation decreases the flammability risk of hydrogen-oxygen mixtures, as delineated in the Shapiro diagram [2]. For outdoor storage or pipeline operations, these materials can be applied to prevent environmental hydrogen release whilst allowing its leakage screening.

Our research focuses on both the chemical composition and physical structure of the material. We optimize the selection and ratio of metallic oxides and catalytic components to enhance reaction kinetics. Additionally, microstructuring techniques are employed to maximize the specific surface area, achieving surfaces exceeding 50 square meters per gram of material allowing efficient neutralization and detection of hydrogen leak.

This approach aligns with current advancements in catalyst technology for hydrogen applications, emphasizing the importance of material selection and structural optimization to mitigate associated risks.

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Atom probe tomography and advanced thermal desorption spectroscopy for atomic scale characterisation of hydrogen in materials

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D4_2, Z4 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Hydrogen detection at the atomic scale has long challenged materials researchers, primarily due to pervasive background contamination within conventional atom probe systems. In this work, we present a transformative approach that significantly reduces spurious hydrogen signals and enables unprecedented clarity in imaging hydrogen–metal interactions. A central innovation lies in our newly developed ultra-low hydrogen atom probe, featuring a titanium vacuum chamber coupled with non-evaporative getters (NEGs), cryopumping, and optimized vacuum protocols. This novel configuration—departing from the standard use of austenitic stainless-steel chambers—cuts the background hydrogen level by orders of magnitude. In comparative studies using low-field metals (e.g., aluminum), we observe a near-absence of artifact peaks, ensuring that any hydrogen detected indeed originates from the sample itself.

An equally noteworthy aspect of the research is the pivot from traditional electrochemical hydrogen charging to gas-phase exposure, including deuterium. Though electrochemical routes are well-established, challenges such as transient hydride formation, tip fracture, and unpredictable yield drove the adoption of more controlled gas environments. We developed miniaturized “cube” and “cartridge” chambers to safely expose specimens to pressures up to 10 bar and 90 °C, while a specialized high-pressure bunker facility extends exposures to 1000 bar and 300 °C. Importantly, cryogenic transfers preserve hydrogen content, enabling direct atom probe analysis without the risk of out-diffusion. By eliminating electrolyte-induced surface damage and providing well-characterized thermodynamic conditions, this gas-phase method yields more reproducible and accurate data.

In this talk, we will also introduce pulsed laser experiments in the titanium atom probe, significantly expanding the usefulness of atom probe tomography for the investigation of hydrogen in materials.

As a complement, we also introduce a novel thermal desorption spectroscopy method with significantly improved thermal/energetic resolution. This system works in the UHV regime and has improved diffusion dynamics over conventional approaches. This complements the atom probe to provide statistically significant data on hydrogen-defect interactions, especially in fcc systems, where sluggish diffusion limits the interpretability of the TDS data.

Influence of Synthesis Parameters on the Microstructure and Porosity of Hydroxyapatite

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Hydroxyapatite, due to its ability to easily replace cations and anions, is widely used in several areas, such as the pharmaceutical and especially in the area of biomaterials [1]. Also, hydroxyapatite has significant applications in the environmental area, mainly in water and soil treatment. When associated with porosity, it becomes ideal for catalytic processes [2]. For these purposes, it is essential to produce porous materials, since porosity increases the specific surface, favoring the contact area, improving absorption and facilitating the transport of substances. Given the wide applicability of hydroxyapatite, several synthesis methods are used. In this work, the precipitation method was used, widely adopted due to its simplicity [3]. This method basically consists of adding phosphate ions to a suspension containing calcium ions. For this, a variation in the dripping speed of phosphoric acid was performed. Slow addition rates allow gradual nucleation and growth of larger crystals, which can result in lower porosity, since the crystallites tend to compact more organized. On the other hand, a fast addition rate generates excess nuclei, leading to the formation of smaller, less organized particles and, consequently become more porous. This work aims to analyze the influence of the synthesis method on the porosity of hydroxyapatite, by controlling the parameters of the synthesis process. For this, the phosphoric acid was dripped at two different speeds, resulting in two types of hydroxyapatite. The characterizations performed on the hydroxyapatites were Transmission Electron Microscopy (TEM) for morphology and structures; Brunauer-Emmett-Teller (BET) measurements, to evaluate the influence on porosity; and X-ray Diffraction (XRD), to identify the phase formation. For Hydroxyapatite, the goal is to achieve a surface area similar to that studied by [4], in the BET, which is 144 m²/g.

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Restoration of physiological conditions in the assessment of the biocompatibility of SiO₂ coatings deposited on Nitinol cardiovascular implants through electrophoretic deposition

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D5_1, Albéniz Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

The materials under investigation concern implants designed for heart muscle regeneration. The development of such materials requires comprehensive research, from basic studies to physiological simulations, in vivo testing, and the preparation of certification documentation. Inadequate planning and improper testing techniques can lead to failure. Due to the critical impact of medical devices on human health, this field is heavily regulated.

Nitinol, a widely used material in cardiovascular implants, is known for its excellent properties, including shape memory and superelasticity. However, its biocompatibility remains a challenge due to the potential release of nickel ions. In this study, surface-modified Nitinol was evaluated with silica (SiO₂) coatings, applied via electrophoretic deposition (EPD). The objective of the coatings was to create a protective barrier between the Nitinol substrate and the biological environment.

To optimize the deposition parameters, the zeta potential of the EPD electrolyte was measured. This analysis confirmed stable colloidal dispersions resistant to aggregation. Wettability of surfaces was assessed through water contact angle measurements. Enhanced wettability is beneficial for promoting protein adsorption and cell attachment, which are crucial for better tissue integration.

The microstructure was examined using transmission electron microscopy (TEM) and energy-dispersive X-ray spectroscopy (EDS) to assess the morphology, composition, uniformity of the coatings. Thin foils for TEM were prepared via gallium ion milling. These techniques enabled detailed analysis of the coating's structure, critical since both microstructural and chemical properties influence biocompatibility and cytotoxicity.

Cytotoxicity was assessed according to ISO 10993-5. Extracts were prepared by incubating coated Nitinol samples in culture medium for 24 hours. Following this, the medium was replaced with the extracts, cells were incubated for 48 hours. Cell viability and proliferation were assessed by monitoring cell growth. Confocal laser scanning microscopy (CLSM) and live/dead fluorescent staining were used to visualize cell viability and confirm reduced cytotoxicity of the coated samples.

The genotoxic potential of the SiO₂-coated samples was evaluated using the Xenometrix Rapid Micronucleus MoA assay. This assay detects DNA damage in cells exposed to the extracts. Preliminary results indicated the coatings effectively reduced both cytotoxicity and genotoxicity compared to bare nitinol.

The results of zeta potential optimization, improved hydrophilicity, and microstructural analysis contributed to enhancing the biocompatibility of SiO₂-coated nitinol implants. These coatings showed promising results in reducing nickel ion release and fostering a surface conducive to tissue interaction, offering a potential solution for cardiovascular applications.

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Biomechanical and Microstructural Characterization of Biocompatible Metamaterials for Surgical Applications

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D5_2, Albéniz Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Advancements in medical technologies require innovative materials that enhance surgical precision, improve patient safety, and support sustainable practices. This study presents the biomechanical and microstructural characterization of biocompatible metamaterials for next-generation surgical instruments, particularly for CardioVascular and Thoracic Surgeries (CVTS). These materials ensure controlled force application, real-time stress sensing, and extended durability under clinical conditions. The developed tools incorporate 3D-printed titanium (Ti6Al4V) metamaterials with reversible deformation properties, preventing excessive clamping forces. Integrated piezoelectric sensor arrays (PyzoFlex technology) enable real-time force monitoring, while soft biocompatible coatings minimize tissue trauma. Fluorinated wear-resistant coatings enhance sustainability, allowing over 100 sterilization cycles without degradation. Biomechanical performance was evaluated using an MTS universal testing machine to simulate vessel compression. A prepared vessel model replicated in vivo conditions by applying an external load while maintaining internal pressure. The metamaterial inserts deformed upon exceeding a force threshold, ensuring controlled occlusion and preventing excessive closure. Post-experimental samples were analyzed using scanning electron microscopy (SEM) to assess deformation mechanisms and surface integrity. Imaging was performed using in-lens detectors (Trinity) on a DualBeam SCIOS II microscope (ThermoFisher), with thin foil preparation via AutoTEM 4 software. Transmission electron microscopy (TEM) using a THEMIS (200 kV) FEG microscope enabled high-resolution imaging, selected area electron diffraction (SAED), and energy-dispersive X-ray spectroscopy (EDS) for phase and composition analysis. Integrating biomechanical validation with microstructural analysis highlights the potential of these metamaterials in addressing key CVTS challenges, such as uneven pressure distribution and excessive clamping forces leading to arterial stenosis and tissue damage. The study demonstrates overload protection accuracy exceeding 90% for clamping forces of 2.2–2.7 N, a pressure sensor resolution below 3 mm per unit with over 98% signal accuracy, and reduced tissue trauma validated histologically. The materials comply with ISO standards (10993, 13485) for biocompatibility and safety. This work advances surgical instrument development by combining biomechanical performance with microstructural engineering, improving surgical outcomes while promoting sustainable medical device design.

Acknowledgements:

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Advanced biomaterials for pediatric miniatural heart pumps – characterization and modelling

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D5_1, Albéniz Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

Introduction

The heart, this amazing organ can fail, either due to congenital and genetic problems such as inherited heart muscle disease (cardiomyopathy) or secondary to congenital arrhythmias. The intended target was minimal invasive paediatric pump prototype introduced via vascular access, such placement in an aortic vessel would prevent burdensome invasive surgery at the opened chest for short-term heart support (<4 weeks).

Materials

The coatings dedicated for the pump parts were elaborated full filling the following features: ultra-low friction & fully hemocompatible fullerene/diamond-like carbon hard coatings with surface functionalization for high adhesion of athrombogenic oligoproline & polydopamine with superior properties to heparin.

Modelling

Numerical simulations of the testers were performed before testing the materials. As part of the evaluation of the biological suitability of materials dedicated to cardiac support pumps, multi-analyses were performed on several alternative testers and the flow properties as well as the interactions between the analyzed surface in cells were recalculated theoretically and only in the next step verified experimentally.

Experimental verification

The experimental verification consisted of an originally developed and executed blood-material interaction scenario under the „Organ-on-chip” technique. The high speed rotors normalized testers dedicated to evaluate of whole human blood quality changes under dynamic conditions were developed. The aggregates of leukocyte-platelet, platelet-platelet, monocyte-platelet formation and platelets activation were evaluated using the flow cytometry and confocal microscopy. For the group of selected coatings, the adhesion efficiency of blood morphotic elements was determined under a shear stress by the radial flow chamber assay. This multistep material selection was based on the broad materials characterization. To evaluate the developed materials in the sample scale a new prototype of a bio-pump dedicated for the 3D shape substrate testing was developed. The system enabled the testing of cardiac assist devices under normal and dysfunctional heart conditions.

Results

In most cases, tested coatings showed good or very good haemocompatibility. Type “nano-onion” fullerene/diamond-like carbon PVD hard coatings with coating proved to be superior in terms of activation, risk of aggregation, and the effects of generating microparticles of apoptotic origin, and also demonstrated excellent mechanical properties. The Surface additional surface functionalization for high adhesion of athrombogenic oligoproline & polydopamine resulted in the achievement of activation parameters at the level of the negative control, i.e. disactivated blood.

Acknowledgement

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Modelling and Experimental Verification of the Freezing Process in Ice Templating

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Introduction

Novel material solutions in cardiac surgery are highly anticipated, due to the multitude of complications and the need for fast and efficient regeneration. Advances in materials engineering and its link to tissue engineering may offer promising tools for creating a new type of prosthesis for the heart. The work has a basic character and focuses on the development of a new concept of myocardial regeneration in the form of porous materials

Goal

The work involved the scientific development of correlative microscopy technique to control the process of porous material creation based on ice templates. The porous scaffold was developed with the intended application in heart regeneration.

Methods

The porous structures were fabricated using an ice templating technique. The material prepared in this way has a controlled architecture depending on the freezing direction. To introduce a controlled temperature gradient during freezing, copper inserts with various inclination angles were used. Copper was chosen due to its high thermal conductivity, allowing for effective heat transfer and controlled ice crystal growth. In accordance with the angle between the surface of the insert and the bottom of the vessel, the conductive material influenced the degree of the material porosity. In this study, an alginate solution was used. The freezing process was carried out at three distinct temperatures: -20°C, -80°C, and -196°C (liquid nitrogen), to investigate the effects of different cryogenic conditions on the formation of porous structures. This approach aimed to create a tailored porosity gradient, which was a critical parameter for optimizing toward future tissue integration. The fabrication process was preceded by finite element modelling of the temperature distribution. In the work, porosity was controlled using complementary microscopy techniques, including digital microscopy, acoustic microscopy, scanning transmission electron microscopy and confocal laser scanning microscopy.

Results and discussion

The analysis of the relationship between temperature conditions and the resulting pore's shape and size, enabled to understand how ice templating can be tailored for tissue engineering applications. The simulations provided insights into how different inclination angles affected the temperature gradient, enabling better control over the material properties in subsequent fabrication steps. By adjusting the insert angles, it was possible to induce variations in the local cooling rate, leading to differences in pore size, distribution, orientation and overall microstructure.

Acknowledgement

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Microbiological techniques assessing the infection risk associated with materials designed for laparoscopic instruments

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D5_2, Albéniz Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Introduction

Laparoscopic surgery provided a giant leap in safety and recovery for patients over open surgery methods, robotic-assisted surgery (RAS) is doing the same to laparoscopic surgery. Laparoscopy is an essential diagnostic and therapeutic tool in modern medicine. It has become the primary method of diagnosing pathologies of internal organs. It is a minimally invasive method, allowing patients to recover quickly and leaving a good cosmetic result. The most common complications of the laparoscopic technique are associated with the insertion of Veress needles and trocars [1]. One of the resulting and possible risks is the development of a bacterial biofilm on the surface. Of course, nowadays this risk is of low severity, but it is still necessary to develop tools towards the detection of bacterial biofilm. Another factor indicating the need to develop microbiological techniques in this direction is the increasing complexity and sophistication of instrument arms, which can also promote microbial growth. Hospital-acquired infections and the increasing resistance of bacteria to antibiotics represent a critical challenge in contemporary medical practice. One strategy to reduce the likelihood of severe infections is the application of antimicrobial coatings on surgical instruments. This study focuses on the microbiological evaluation of the potential for bacterial infection development on the surface of materials designed for tools used in vascular surgery, specifically the flow closure clamp. This paper offers a correlative analysis of the interactions between bacteria and the surfaces of materials intended for surgical instruments. In order to achieve this goal, contact tests in accordance with ISO 22916 and bacterial biofilm formation analyses were carried out. That included Fluorescence In Situ Hybridization (FISH) staining that was analysed using Confocal Laser Scanning Microscopy (CLSM) and furthermore the surfaces were evaluated by Scanning Electron Microscopy (SEM).

It can be noted that the application of various techniques may yield distinct outcomes. Integrating conventional microbiological methods, such as dilution spotting, with contemporary diagnostic technologies proves to be advantageous for evaluating the antibacterial properties of intricate material surfaces.

Acknowledgement

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Tunable nano-Rare Earth oxides for pAthogen mitigation (TREAT)

Prof. Sudipta Seal¹, Craig Neal, Elayaraja Kolanthai, Candace Fox, Dr. Griff Parks, Abinaya Sindu Pugazhendhi, Melanie Coathup, Marco Molinari, Katarzyna Stan-Glowinska, Joanna Wojewoda-Budka, Natalie Sobczak

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D5_1, Albéniz Room (Level -2), septiembre 18, 2025, 10:30 - 13:10

Since COVID 19 pandemic, there is a huge demand for effective disinfectants to combat pathogens including deadly Viruses and bacteria and has grown significantly. This need extends to addressing both community-associated and hospital-acquired infections, which continue to pose major global challenges to human health. Therefore, novel strategies offering broad-spectrum and non-specific protection are urgently required.

In this talk we will explore design of the nanomaterials for radical generating/scavenging nanozyme surface redox chemistry of metal substituted rare earth (ceria)-based materials; the charge transfer behavior and review documented antiviral and antimicrobial properties. Various formulation efficacy studies will also be presented. Most importantly, we will present In situ electroanalytical measurements (impedance spectroscopy, equivalent circuit analysis) highlighted these biological activities with particles from each formulation showing substantial anti-microbial activities towards both enveloped and non-enveloped virus species via physical or chemical inhibition mechanisms. Furthermore, the surface chemistry and morphology of these nanoformulations have been thoroughly examined using high-resolution transmission electron microscopy and X-ray photoelectron spectroscopy. To optimize nanozymatic activity, a combination of ab initio and classical computational modeling, alongside experimental validation, has been employed in designing these potent nanostructures.

(Some of the TEM examination was financially supported by the Institute of Metallurgy and Materials Science of the Polish Academy of Sciences within the MOU between the University of Central Florida Board of Trustees and Institute of Metallurgy and Materials Science Polish Academy of Sciences)

Advanced multifunctional biomaterials supporting bone tissue regeneration and healing

Prof. Elżbieta Pamuła¹

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D5_2, Albéniz Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

Although bone has considerable ability to regenerate, infected or critical size bone defects do not heal spontaneously and need special therapies and/or tissue engineering approach. Biomaterials that support bone tissue regeneration and healing should be designed to eradicate pathogenic bacteria, followed by facilitating osteogenic cell signalling and bone tissue expression processes. In our research, we design multifunctional biomaterials that provide mechanical support and are integrated with bone tissues (titania and zirconia ceramics) [1,2] or are made of biodegradable polymers, so their disappearance from the treated lesion is correlated with the ingrowth of native tissue [3,4]. Both types of biomaterial can be modified to deliver drugs or biologically active substances to support bone tissue regeneration. We found that the deposition of calcium phosphate, collagen, or sulphated hyaluronan on polymer scaffolds promotes cell osteogenic differentiation and the healing of osteochondral defects [3,4]. We also develop biomaterials dedicated to infected bone in the form of antibiotic-loaded polymeric micro- / nanoparticles [1,2,5,6]. They can be used as a component of injectable matrices [5,6] or be immobilised on the pore walls of scaffolds, to obtain implantable medical devices, when mechanical support is particularly essential [1,2]. The developed biomaterials release the drugs in a controlled manner to be adapted to the clinical needs. Thus, they are promising for bone tissue regeneration and healing.

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Bridging In Vitro and In Vivo Degradation of Biodegradable Implants: An ODE-Driven DoE and Uncertainty Quantification Approach

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Developing biodegradable implants requires extensive in vitro and in vivo experimentation, yet a clear correlation between these degradation scenarios remains unresolved. The inability to establish a robust correlation hinders the prediction of in vivo degradation based on in vitro studies, making experimental validation highly restricted due to strict ethical and regulatory limitations on animal testing. The challenges arise from biological variability, anatomical constraints, and dynamic degradation mechanisms, making the selection of representative sampling points and optimal experimental time points particularly difficult.

To address these limitations, we introduce a hybrid computational-experimental framework that integrates ordinary differential equation (ODE) models with a Design of Experiments (DoE) approach under uncertainty. Our methodology not only predicts degradation kinetics of Mg-based implants but also provides a systematic strategy to optimize experimental design, ensuring that the most informative time points for data collection are selected. This is achieved by integrating uncertainty quantification (UQ) and scenario modeling, expanding the parametric space of key influential parameters using surrogate models to ease the limitations of scarce experimental data.

Previously, we derived a time-independent correlation ratio for Mg-xGd implants using a multi-fidelity model and data-driven surrogate modeling, demonstrating its potential in bridging in vitro–in vivo gaps. However, the computational cost and complexity of multi-fidelity models restrict their applicability. Here, we propose an efficient and interpretable ODE-based framework that leverages data-driven optimization, accounting for both experimental noise and inherent model uncertainty while refining parameter selection and improving predictive robustness.

A key innovation of this approach is its ability to guide experimental planning by identifying the most informative sampling points, reducing experimental redundancy, and minimizing the number of required animal studies. By establishing a quantitative correlation between in vitro and in vivo degradation, this framework enhances the predictive capability of digital twins in biomaterials research, accelerates the clinical translation of biodegradable implants, and improves the efficiency of preclinical evaluation.

Keywords: Biodegradable Implants, ODE Modeling, Design of Experiments, in vitro-in vivo Correlation, Uncertainty Quantification, Scenario Modeling, Magnesium-Based Implants.

Engineering Biocompatible Surfaces with Oligoproline: A Powerful Anti-Biofouling Peptide

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The surfaces of medical devices are in direct contact with their surrounding environment, making them critical in determining key properties such as durability and functionality. When implanted in the body, the interactions that occur within the first few seconds between the device surface and biological components including proteins, cells, and blood, are decisive in the long-term success or failure of the implant. Therefore, surface engineering technologies that regulate biological interactions play a crucial role in the performance of implantable medical devices. To prevent unfavorable biofouling leads to the blood coagulation, an anti-biofouling surface minimizes biological recognition, allowing the device to function without triggering adverse reactions. To prevent unfavorable biofouling, which can lead to blood coagulation, an anti-biofouling surface minimizes biological recognition, allowing the device to function without triggering adverse reactions. Here, we designed and characterized a novel non-ionic anti-biofouling peptide, oligoproline, inspired by the collagen backbone structure.

Oligoprolines (Ac-CP_n-NH₂, n= 6 or 9) were synthesized by Fmoc solid-phase procedure and immobilized on the Au-sputtered coverslip via Au-SH bonding. Oligoproline-immobilized (OP) surfaces were characterized by water contact angle measurements and X-ray photoelectron spectroscopy (XPS). Subsequently, protein adsorption, fibroblast adhesion, platelet activation, blood cell interactions, and bacterial adhesion on OP surfaces were evaluated.

The OP surfaces were successfully prepared with a smooth topology ($R_a \approx 6$ nm) and a low water contact angle ($\theta \approx 30^\circ$). Serum protein adsorption was significantly reduced upon oligoproline immobilization, with albumin and fibrinogen adsorption levels below 10 ng/cm² and 40 ng/cm², respectively. Fibroblast adhesion was strongly suppressed in vitro. After 5 minutes of whole-blood exposure under dynamic in vitro conditions, the surface coverage by blood elements including platelets and blood cells on OP surfaces was markedly lower than that of clinically available polyurethane. Adhesion of CD62P⁺ platelets and CD45⁺ leukocytes was also significantly suppressed. Furthermore, OP surfaces effectively prevented the adhesion of *E. coli* and *Staphylococcus aureus*, both of which are known for secreting prolyl aminopeptidase.

Characterization of osteoarthritis bone changes with nano-CT observation

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The musculoskeletal system is made up of bones, muscles, joints, tendons, ligaments, fascia, and neuromuscular junctions. It is responsible for maintaining stable posture and movement of the body. Musculoskeletal disorders (MSDs) are defined as diseases of locomotor system or injuries to bones, cartilage, joints, tendons, ligaments, muscles, and nerves. In total, they include more than 150 disease entities. The most common MSD include: pain and functional failure of joints as a result of previous injuries, chronic overload, and degenerative joint disease (osteoarthritis – OA). The treatment of MSD, regardless of the cause, should be interdisciplinary. To be effective therapy, it is necessary to evaluate the tissues forming and surrounding the upper and lower limb joints: muscle, cartilage and bone tissue. One of the methods that allows for the assessment of tissue condition is computed tomography (CT), and interdisciplinarity may consist of conducting detailed research with engineering units using the most modern solutions, such as nano-CT systems. However, there is a limit to the size of tissue samples that must be taken from the already removed long bone epiphysis during surgery (total knee arthroplasty – TKA; total hip arthroplasty – THA; reverse shoulder arthroplasty - RSA).

In the current modern approach to treatment, a thorough and meticulous analysis of the tissues involved in the disease process is indicated. In our work, due to the increase in the number of patients suffering from degenerative joint disease, we focus mainly on the methodical evaluation of bone and cartilage tissue.

The aim of this study was to determine whether nano-CT analysis of samples (taken from the epiphyses of the proximal tibia obtained during TKA) is an appropriate tool to assess changes in the structure of the subchondral bone plate and bone trabeculae as a result of the development of OA. Research has the consent of the relevant Ethics Committee to conduct the study (KB-0024/150/11/2024). Observations using Zeiss Xradia 510 Versa nano-CT allowed assessment of the degree of mineralization of the subchondral bone plate and changes in the arrangement and density of trabeculae bone in this zone. Furthermore, changes in the cancellous bone was also observed. The results will be the basis for the development of personalized implants using additive technology and medical instruments.

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New generation copper-based coatings of improved antimicrobial resistance to pathogens

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The use and abuse of antibiotics for many years has created very unfavourable living conditions for bacteria, forcing microorganisms to create many defence mechanisms and selecting strains best suited to these conditions. The appearance of bacteria resistant to many antibiotics, so-called "Super bugs" or MDR (multi drug resistant) has been noticed not only by patients, medical doctors, but also by epidemiological services in many countries.

Antimicrobial copper can be used to produce parts often touched by people in hospitals and clinics but also in public places. Copper ions penetrate into bacterial cells and damage nucleic acids, which leads to disruption of the helical structure and DNA denaturation. Copper ions can also bind informational RNA and thus inactivate viruses, whereas copper complexes form radicals that inactivate viruses.

Therefore, in the proposed study, viability of various bacteria and viruses were examined on variety of copper and copper-based coatings. Innovative copper-based composite coatings obtained through the addition of TiO₂ or CeO₂ particles during the deposition process, will constitute an even more effective weapon in the fight against the spread of pathogenic organisms.

It is known that the rate of copper's antibacterial activity depends on the percentage of copper in the alloy. Thus, the use of durable and wear-resistant coatings, in which the copper content is as high as possible, is an economical solution. Three copper deposition technologies are proposed to be applied: electroplating, electroless plating and selective plating. The common advantages of the considered technologies are their simplicity, wide application in industry, economic attractiveness, the possibility of using complicated product shapes and partial or total versatility, when it comes to the base material on which these layers can be embedded. Synergy of expertise of all partners will contribute to in-depth understanding of the relation between the plating process, microstructure, properties and anti-pathogenic response of the copper and copper-based coatings, which will translate into the development of optimal technology to produce surgical instruments, in particular for dental applications.

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Biodegradable polymer coatings release active ingredients in implantology

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Currently, the primary purpose of using implants is to provide conditions for proper tissue regeneration. Regardless of the application, implants are intended to stabilize tissues. However, the effect of implantation may be inflammation and postoperative complications. They may be caused by a natural reaction to a foreign body or the release of their degradation products. Unfortunately, postoperative wound infections caused by microorganisms contaminating the wound during or after surgery remain a problem.

The main direction of research aimed at reducing inflammation and postoperative complications is to modify the material selection from which the implant is made and the modification of its surface, specifically metal implants. A very interesting direction for modifying the surface of implants is to apply coatings of biodegradable polymers to them. These polymers will play a protective role by limiting the adverse effects of the tissue environment and body fluids and, thus, the process of their degradation. In addition, they can be a matrix for active substances with anti-inflammatory or regenerative properties that can be released locally to the tissue. Depending on the time of tissue regeneration, it is possible to support these processes by adequately selecting the type of polymer and active substances. The basis for selecting the type of polymer is its degradation time, which depends on its chemical composition and structure, as well as the environmental conditions of the body. Designing and applying mono- and multi-layer coatings consisting of various polymers with different active substances is possible. Using implants with coatings with controlled kinetics of the release of active substances may be an alternative to the commonly used systemic pharmacotherapy. Direct, local delivery of active substances to the tissue regeneration area should have a beneficial effect on the process of regeneration.

The applied biodegradable single or multilayer coatings should be characterized by an even distribution of active substances. These conditions are necessary for controlling the kinetics of their release. The ultrasonic spray method enables the application of such external coatings.

The paper presents research results on a multilayer PLGA coating composed of inner layers containing hydroxyapatite, intermediate layers of pure PLGA, and outer layers containing dexamethasone. Studies of the substrate-coating system's physicochemical properties were carried out for samples in their initial state and after long-term exposure to PBS solution. The obtained results indicate good protective properties of the coating and controlled release of active substances.

Influence of UV polymerization conditions on the physicochemical properties of temporary dentures fabricated by the Digital Light Processing additive manufacturing

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Dynamic technological developments have not only allowed existing manufacturing processes to be improved but have also contributed to the emergence of entirely new manufacturing methods. One of these is 3D printing, which enables the creation of three-dimensional objects layer by layer based on a digital model. This technology was mainly used for rapid and cost-effective prototyping. Currently manufacturing technologies vary in layer application, curing methods, and materials used. The wide range of possibilities has contributed to their application in medicine, among other fields. One area in which 3D printing has potential is dental prosthetics, where DLP (Digital Light Processing) is being used. This method involves the selective curing of successive layers of liquid resin using light. The greatest advantage of DLP over time-consuming traditional manufacturing methods is a significant reduction in production time for temporary dentures. In addition, the use of 3D printing makes it possible to produce more accurate and customized dentures, which is crucial in terms of treatment efficiency and improving the patient's quality of life. Although the DLP method and the resins used in it have proven themselves in dental prosthodontics, their application in this area is relatively new and continuous research is needed to improve knowledge of their capabilities and limitations.

Therefore, the aim of this study was to evaluate the influence of the curing time and conditions of resin processed by DLP technology on the physicochemical properties of temporary dental prostheses. For these medical devices, an analysis of the influence of the time and type of gas atmosphere used during post-processing curing in UV ovens on their physicochemical properties was carried out. Polymerization was used in a UV oven in air for 10, 20 and 30 minutes, in a UV oven with a nitrogen protective atmosphere for 10 minutes. The control group consisted of 3D-printed samples not subjected to the curing process. The morphology, topography, surface roughness and wettability, hardness, compressive strength and abrasion resistance were studied. The samples were tested both before and after the accelerated ageing process, which was carried out using a thermocycler. The samples were subjected to 5000 cycles of transition from 5 °C to 55 °C, which corresponds to 6 months of in vivo use of temporary dentures.

The results indicated that specimens cured in nitrogen atmosphere for 10 minutes had higher post-ageing durability compared to all alternative curing options used without a protective atmosphere regardless of their duration.

Effect of Post-Processing Parameters on the Surface Properties of Ti6Al4V Scaffolds Manufactured by SLM

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Additive manufacturing technologies based on selective sintering of metal powders can be used to produce implants with appropriate mechanical properties and favorable conditions for osseointegration by providing space for bone tissue penetration into the implant. While powder-based additive manufacturing allows for precise control of the implant's pore structure, modifying the surface properties—especially in the central regions—remains challenging. These properties are crucial for the final functionality of the implants.

The aim of this study is to evaluate the effect of post-processing parameters, namely annealing and etching, on the surface properties of scaffolds made from Ti6Al4V using selective laser melting (SLM, 3D EOS M100). The designed porous structure, based on a diamond-shaped lattice with a pore size of approximately 600 μm , featured an open architecture with spherical pores. The manufactured samples were initially cleaned with compressed air and then subjected to ultrasonic cleaning. After cleaning, the samples were weighed, and their true porosity was determined using helium pycnometry (Micromeritics® 1305).

The samples were vacuum annealed for 2 hours at 800°C, 900°C, and 1000°C, followed by vacuum cooling. Subsequently, they underwent single-step etching for 9 minutes and sequential etching (3 $\times$ 3 min) in 50 ml of HF/HNO₃ solutions at different concentrations (1%/10%, 2%/5%). After each immersion step, the scaffolds were ultrasonically cleaned.

The surface topography of the modified samples was analyzed using scanning electron microscopy (SEM, Tescan Vega) and optical profilometry (3D Surface Metrology Microscope, Leica DCM8), performed globally and on selected small areas. Surface wettability was assessed by measuring the static contact angle (CA) of a 5 μl water droplet using an optical tensiometer with a topography system (Theta 3D). Additionally, to determine the effect of thermal treatment on the material structure, metallographic sections were prepared and etched with 8% HF to reveal the microstructure. Metallographic analysis was conducted using a Leica DMI8 A microscope.

The conducted research demonstrated the influence of annealing temperature on the metallographic structure and grain size. However, the grain elongation along the OZ axis, characteristic of additive manufacturing technologies, was preserved. Annealing did not affect the observed surface topography. Sequential etching minimized the mass loss of the scaffolds, which is crucial for maintaining their potential mechanical strength. The applied modifications positively influenced the surface wettability of the tested scaffolds.

Artificial staining of 3D X-ray virtual histology of bone implants through deep learning

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D5_2, Albéniz Room (Level -2), septiembre 18, 2025, 17:00 - 19:00

3D X-ray virtual histology (XVH) techniques leverage the benefits of X-ray tomography (non-invasive, 3D volume-based measurements) for the correlative imaging of biological samples traditionally visualised through conventional 2D histology, thereby removing the need for labour-intensive sample preparation steps including sectioning and chemical staining. However, such XVH approaches yield greyscale 3D data sets characteristic of X-ray imaging, and cannot replicate the same biological specificity provided by different histological stains directly visualised through the selective colouring of biological tissue components. Concurrently, within the separate field of digital pathology, advances in machine learning have led to the emergence of ‘virtual staining’ whereby histological stains may be virtually transferred onto non-stained (visible light-based) images through the training of neural networks.) In this work we bridge the two concepts of X-ray virtual histology and virtual staining (previously used for visible light-based histology), by applying image-to-image style-transfer models to generate artificially stained X-ray 3D virtual histology data. As part of our multimodal correlative characterisation studies of biodegradable metal implants in bone, we have performed multiple synchrotron-based x-ray micro-CT and toluidine blue histological measurements sequentially on the same samples. We co-registered more than 50 sets of micro-CT and histology image pairs, which were then used for training on a patch-based modified cycleGAN model network suited for limited pair data. Training results were optimised with the goal to replicate the colours present in the histology images whilst retaining most of the high contrast and resolution features.

Hemocompatibility Assessment Method Based on the Principles of a Radial Flow Chamber

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The hemocompatibility assessment of biomaterials and implants is a crucial element in their qualification for clinical applications. Any material in contact with blood must meet stringent requirements to prevent complications such as thrombosis, hemolysis, or excessive platelet activation. Improper interaction between a biomaterial and blood can lead to severe health complications and even pose a life-threatening risk to the patient. Therefore, it is extremely important to use precise research methods to assess the compatibility of blood with biomedical materials under conditions as close as possible to physiological ones.

In research practice, a widely used method for evaluating hemocompatibility is the Impact-R test, which enables the analysis of dynamic interactions between blood and the biomaterial's surface. To expand the capabilities of this method, an innovative device called SYMMED has been developed, allowing for a more advanced evaluation of the impact of shear stress on the interactions between implants and blood. This method is particularly important in the context of modern coatings used in vascular and cardiac implants, where dynamic blood contact plays a crucial role. Under physiological conditions, shear stresses occurring at the implant-tissue interface can lead to undesirable reactions, including hemolysis or the initiation of thromboembolic processes. Precise regulation of experimental parameters, such as rotational speed, gap width, and the exposure time of the sample to flowing blood, enables controlled analysis of platelet activation, hemolysis levels, and the thrombotic potential of the biomaterial under study. The methodology used in SYMMED is based on advanced diagnostic techniques, such as confocal microscopy to detect platelet activation using specific antibodies, hemolysis analysis, and other quantitative methods that assess the compatibility of the biomaterial with the circulatory system. The results provide comprehensive information about the biocompatibility of the analyzed materials, which is crucial for their further development and clinical application.

In conclusion, the development of modern methods for assessing hemocompatibility, such as the extended version of the Impact-R test using the SYMMED device, represents an important step toward ensuring the safety and effectiveness of new solutions in medical biomaterials. By precisely replicating physiological conditions, reliable results can be obtained, which are crucial for evaluating and optimizing modern materials used in medicine.

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Biomimetic Composite Heart Valve with AI-Enhanced Hemocompatible Coatings: Integrated Simulation, Fabrication, and Preclinical Evaluation

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The bioVALVE project addresses the critical challenge of thrombo-emboli formation in pulsatile ventricular assist devices (VADs) by developing an innovative biomimetic heart valve based on a metal–polymer composite. Current mechanical valves suffer from suboptimal blood flow dynamics and elevated shear-induced platelet activation, which promote thrombogenesis and compromise patient outcomes. To overcome these limitations, our interdisciplinary approach integrates advanced fluid-dynamic simulations, state-of-the-art material processing, and rigorous in vitro and in vivo testing. A flexible heart valve was fabricated via injection moulding of thermoplastic polyurethane (TPU) with an embedded, delicate titanium mesh insert, combining microscale elasticity akin to native blood vessels with the macro-scale mechanical stability required for effective valve function.

In parallel, ultra-thin, biofunctional coatings were developed using physical vapor deposition (PVD) and plasma-assisted chemical vapor deposition (PACVD) techniques. The coatings, primarily based on diamond-like carbon (DLC) materials, were systematically optimized through nitrogen and silicon doping and further refined via post-deposition fluorination. These tailored coatings exhibit exceptional uniformity, minimal particulate contamination, and precisely tuned surface wettability, thereby enhancing the “washing” effect on blood-contacting surfaces and significantly reducing shear-induced platelet activation.

A distinguishing feature of our project is the integration of artificial intelligence (AI) methods within the material design and evaluation process. Advanced machine learning algorithms were employed to refine numerical simulations, predict material properties, and accelerate high-throughput screening of coating parameters. This AI-enhanced approach not only reduces reliance on traditional trial-and-error methods but also enables simultaneous multi-attribute optimization—addressing mechanical stability, biocompatibility, and hemocompatibility concurrently.

Mechanical characterization via nanoindentation and scratch testing confirmed that the optimized coatings deliver superior hardness, ductility, and wear resistance under cyclic loading. Complementary hemocompatibility assays under dynamic conditions demonstrated marked reductions in platelet adhesion, aggregation, and activation compared to conventional carbon disc valves. The promising preclinical results underscore the potential of this integrated, AI-driven design framework to advance the performance and safety of VADs, thereby improving clinical outcomes and reducing healthcare costs.

MECHANICAL BEHAVIOUR OF BIO-COMPATIBLE LATTICE STRUCTURES CANCELLOUS BONE REALISED BY FUSED FILAMENT OF Z-ABS MATERIAL UNDER COMPRESSIVE TEST

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Designing and manufacturing replacement cancellous bone structures by lattice structures and Additive Manufacturing (AM) techniques is an effective method to create lightweight orthopedic implants while ensuring that they are mechanically bio-compatible and their osseointegration ability with the host bone.

In this work, we suggest a new design based on three lattice structures from triply periodic minimal surfaces (TPMS) with a different volume porosity to replace cancellous bone based on predicting the mechanical stiffness. To predict the mechanical stiffness, the relationship between the effective modulus of elasticity and different porosity ratios of the lattice structures was determined by using three methods, finite element modeling (FEM) simulation, Gibson and Ashby method and a uniaxial compression test after manufacturing the lattice structures by using Fused Filament Fabrication (FFF) Technology. To demonstrate the efficiency of our approach, the comparison of both numerical and experimental results showed that the effect of structure difference and porosity ratio of lattice structures on the mechanical stiffness values effectively match the cancellous bone in terms of elastic modulus and porosity ratio.

Machine Learning and Kinetic Monte Carlo Models of Transport in Concentrated Alloys

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With the increasing interest in so-called high entropy, multi-principal component, or compositionally complex alloys, there is a greater need to understand how

transport is affected by the complex chemistry of these materials. As compared to a simple elemental solid, in which every lattice site is identical and transport can be described by a handful of saddle points, these materials exhibit a very rugged potential energy surface in which every site has a unique chemical environment. This means that every site exhibits a different defect formation energy and corresponding migration barriers for motion to neighboring sites. As the number of elements in these systems increases, it becomes increasingly challenging, and soon impossible, to enumerate the energetics of every site in the system. Alternative approaches are necessary.

Machine learning has become a popular choice to describe the chemistry-dependent properties of defects in these alloys. By training on atomistic data, machine learning models can predict the energetics of defects in unseen environments and be subsequently used in kinetic Monte Carlo simulations of defect transport. However, for the transport simulations to be thermodynamically valid, the underlying machine learning model must obey detailed balance.

Here, we describe various ways that detailed balance can be enforced in a machine learning model of defect formation and migration energies. Specifically, we consider a brute force model, a “soft constraint” model in which penalty associated with detailed balance is added to the loss function, and two “hard constraint” models in which detailed balance is explicitly included in the architecture of the model. We find that these physically-constrained models exhibit superior performance in maintaining detailed balance. This is demonstrated by determining the error in the energy of the system as defects traverse closed loops. We conclude that detailed balance must be considered to obtain valid trajectories. We implement this approach to investigate various materials science problems with inherent constraints.

Influence of material strength on microshear bands formation through crystal plasticity simulations

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D6_5, Andalucía III Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Capturing highly localized deformation features in a deformed microstructure is critical for further recrystallization simulations. Quite often recrystallized nuclei originate from such localized deformation zones. The highly localized deformation in such zones can lead to formation of texture components different from regular deformation/rolling texture components on a very local scale. From the basis of crystal plasticity simulations (DAMASK) of different aluminium alloys, we show that propensity of such localized deformation is a function of material strength and deformation temperature. Higher material strength and lower deformation temperatures lead to more localized deformation resulting in micro-shear bands. This holds relevance for hot-rolling, where the rolling temperature can control the localized deformation in material and thus, eventually affecting the recrystallized microstructure. The full-field crystal plasticity simulation data will be used to understand the mechanisms behind the phenomena. Also, it will be investigated as to which texture components form in these localized deformation zones and if they have potential to be recrystallized nuclei.

The Role of Plastic Deformation in Martensitic Transformation of Low Carbon Steel

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D6_5, Andalucía III Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The complex interplay between the rapid martensitic transformation and the plastic relaxation during martensitic transformation in low-carbon steel is investigated using a combined phase-field and phenomenological crystal plasticity approach. The large transformation-induced deformations and local lattice rotations are rigorously described within the finite strain framework. The study reveals that plastic relaxation plays a crucial role in accommodating the transformation-induced deformations of martensite in the parent austenite phase. By systematically varying the plastic slip rate, imposed cooling rate, and carbon content, the simulations provide insights into the interdependence between these factors, contributing to a better understanding of the martensitic transformation process and the resulting microstructures. The phenomenological crystal plasticity model effectively relates the plastic relaxation rate to the rate of martensitic transformation with a significant time scale difference between the two processes. The findings contribute to a deeper understanding of the interplay between the rapid martensitic transformation and the requirement for plastic deformation.

First principles investigations of metastable group IV transition metal diboride solid solutions

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D6_6, Andalucía III Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

A prominent class of refractory ceramics, transition metal diborides, has recently attracted scientific attention – both in their bulk and thin film form – due to their high-temperature stability and extreme mechanical properties. The thin film community has primarily focused on metastable solid solutions, where alloying with silicon leads to massively enhanced oxidative properties combined with only minor drawbacks in hardness. However, theoretical investigations of TM-Si-B₂ based systems have been limited until now.

Therefore, this study employs ab initio methods to shed light on the physical fundamentals of metastable solid solutions of TiB₂, ZrB₂, and HfB₂ with silicon. Utilizing Density Functional Theory (DFT), the structural and mechanical properties were investigated and compared well with experimental thin films. Methods such as Crystal Orbital Hamilton Populations (COHPs) allowed to couple chemical stability and elemental bonding properties, whereas Radial Distribution Functions (RDFs) and simulated XRD patterns unraveled a direct connection between experimentally explored Si solubility limits and AlB₂ type structure loss. Moreover, a novel ab initio-based statistical technique was explored to investigate maximal solubilities in the metastable solid solution state. Furthermore, a structural instability of ternary diborides concerning transition metal vacancies was found, in contrast to low variations of the chemical stability at high silicon contents.

Phase-field simulations of grain and dendritic-scale microstructures under additive manufacturing solidification conditions

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D6_3, Andalucía III Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Investigations of directionally solidifying melt pools during metal additive manufacturing (AM) reveal that the resulting subgrain cellular structures often grow along crystalline orientations different from the temperature gradient direction, some of which are not even along preferred crystallographic directions. It is well-known that dendrite orientation results from the growth competition between the heat flow direction and preferred crystallographic orientation. Specifically, the competition between interfacial anisotropy and process anisotropy (thermal gradient and interface velocity) during directional solidification leads to rich morphological diversity of the resulting dendritic structures, including columnar dendrites, tilted dendrites, and seaweed patterns. The orientation selection mechanisms of such patterns remain unexplored at high velocity in the frame of AM. We study the tilted growth of cellular-dendritic arrays as a function of the misorientation angle between the thermal gradient and crystal lattice directions and other relevant control parameters. First, we explore dendritic-scale microstructure evolution during high-velocity binary alloy solidification using two-dimensional phase-field simulations. We find marked effects of thermal gradient, growth velocity, alloy composition, and anisotropy parameters on the possible growth directions and the primary arm spacing, constitutional undercooling, microsegregation, and secondary phases that arise during dendritic-scale melt-pool solidification. Then, growth competition among favorably- and unfavorably-oriented dendrites was simulated as a function of misorientation within a bicrystal setup. Finally, we perform simulations of grain-scale solidification within a full-melt pool to shed light on the formation of cellular microstructures, stray grains, and competitive grain growth, among others. The results reasonably agree with analytical and experimental measurements. Our findings should have qualitative relevance for controlling the subgrain structure, chemical segregation, and texture randomization in various commercial dendrite materials relevant to AM.

Phase field simulation of segregation in single crystal Ni-based superalloys and its influence on creep properties

Mr. Sean Böhm¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Ni-based superalloys exhibit inhomogeneous microstructures dependent from the manufacturing route, thus resulting in inhomogeneous properties such as tensile strength and creep strength. Hence, combined FEM and phase-field simulation models are developed. The simulation models allow to determine the influence of casting parameters and subsequent heat treatment parameters on local microstructures of Ni-based superalloys.

The combined simulation models are calibrated on the Ni-based superalloy CMSX4. CMSX4 contains gamma-prime-forming elements Al, Ti and Ta, which segregate in the interdendritic regions, and slow diffusing elements Re or W, which segregate in the dendrites. The segregations influence the solid solution hardening and gamma-prime precipitate structure, resulting in local differences in crystal properties.

The combined simulation models predict local i.e. position dependent creep properties as well as global creep properties. The combined simulation models thus establish a link between process and heat treatment parameters and creep properties

On Neural Networks for Grain Boundary Segregation

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D6_4, Andalucía III Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Most structural and functional materials are polycrystals; they are composed of crystalline grains that are joined at grain boundaries (GBs). Such interfaces play a critical role in controlling many engineering and functional properties. Understanding GB physics is, therefore, a key aspect of materials discovery and design efforts. Owing to their local atomic environments, GBs provide preferential sites for alloying elements to occupy. Indeed, the direct manipulation of GB chemical states has been found to influence a host of materials properties and processes, such as cohesion, electrochemical response, and electrical conductivity. Of particular interest is the impact of GB solute segregation on boundary dynamics, as it influences microstructure formation and evolution pathways during processing treatments or under operating environments. For example, GB segregation has been used to mitigate grain coarsening and thermally stabilize nanograined structures. While GB solute segregation has been the subject of active research, most existing studies focus on the thermodynamics of GB segregation and the kinetic role (i.e., dynamic solute drag) remains unexplored. GB solute drag results when segregated alloying elements exert a resistive force on migrating GBs hindering their motion. The challenge here is that solute drag depends on several properties, such as alloy thermodynamics, and dynamic processes including solute diffusion and boundary migration; solute drag is a hypersurface. In this talk, we unravel GB dynamic solute drag through theoretical analysis, mesoscale modeling, and machine learning studies. We establish design maps relating drag effects to relevant bulk alloy and GB properties. We find that solute drag is dominant in immiscible alloys with far-from-dilute compositions in agreement with experimental observations of GB segregation in metallic alloys. Further, asymmetric GB segregation is found to greatly influence solute drag values. On the whole, our work provides future avenues to employ GB segregation to control GB dynamical processes.

Analysis of STEM diffraction patterns with multiple ML algorithms

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 17, 2025, 13:10 - 14:30

Machine Learning (ML) assisted image analysis is applied in various fields of material science to gain knowledge about microstructures of different material classes. Since microstructures substantially influence the materials' properties, a deeper understanding of their interaction is necessary to optimize these properties. Even though a manual study of their interplay might be possible for single microstructural parameters, it gets almost impossible if multiple parameters are considered. These parameter restrictions are insignificant for ML studies, which are also less computationally expensive. In this presentation, I show the prediction of grain orientations in energy material LiNiO₂ (LNO) with different ML algorithms and compare their performances. In our study, we used the classical image analysis ML model convolution neural network (CNN), its enhancement dense convolutional network (DenseNet) and a model of the transformer class, called SwinT transformer.

As the first step, diffraction patterns (DP) of an LNO particle are gathered by scanning the particle with transmission electron microscopy. The grain orientations of the DP are determined by template matching and both, processed DP and corresponding grain orientation labels, are used to train the neural networks. All algorithms can then predict the Euler angles (correlate with grain orientation) of a single diffraction pattern and the predictions for a whole dataset can be visualized as an inverse pole figure (IPF).

Automizing the analysis of huge amounts of DP, the trained models are computationally more efficient, than the extensive template matching previously used. In addition, there are differences in performance between the ML models.

Development of neural network interatomic potentials for molecular dynamics: Application for martensitic nickel-titanium

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D6_2, Andalucía III Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Machine learning based potentials represent a new powerful tool for accurate modelling of complex interatomic interactions in materials. In our work, we apply the high-dimensional neural network (HDNNP) methodology using the atom-centred symmetry function descriptors for the shape memory alloy NiTi in the martensitic phase [1].

NiTi is a system that poses significant challenges for both experimental and theoretical modelling, and an accurate atomistic scale model is required to fully understand all of its mechanical properties. Recent experimental results from thermomechanical testing and microstructural analysis of polycrystalline NiTi shape memory alloys have provided a qualitatively new picture of the plastic deformation mechanisms of this most common shape memory material. In particular, they challenge the widely accepted paradigm that austenite is a phase more susceptible to dislocation slip and plastic deformation in NiTi than B19' martensite, despite the fact that only a single [100](001)M dislocation slip system is observed in martensite. The simultaneous activation of [100](001)M plastic slip and reorientation of martensite between two variants sharing the (010)M plane results in kink banding and twinning, forming the so-called "kwink" bands [2].

We show that our newly developed interatomic potential is suitable for simulating the evolution of the martensitic microstructure, is close in accuracy to density functional theory, preserves the strong plastic slip anisotropy of NiTi in the martensitic phase, and has all the prerequisites to simulate the new kwink mechanism.

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Extending Grain Boundary Phase Diagrams to Multi-Phase Boundary Diagrams

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D6_4, Andalucía III Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Phase diagrams serve as fundamental blueprints for comprehending material behaviour and guiding material design. However, the phase diagrams are largely available only for the bulk phases. The thermodynamic properties and phase behaviour of defects, such as grain boundaries (GBs) and phase boundaries (PBs), are equally important for the safe design of materials. Recently, we developed CALPHAD-integrated density-based phase field model (DPF) to calculate the thermodynamic data of GBs. In the model, the GB was represented by a continuous relative atomic density field with reference to a single bulk density and a Gibbs free energy functional was derived. In this work, we extend the DPF model by re-deriving the Gibbs free energy functional for PBs lying between heterogeneous bulk phases of different atomic densities. Here, we use phase-specific atomic densities to normalize the phase properties on either side of the PB such that the relative density fields are continuous across the interface. Using the model, the multi-phase interfacial thermodynamic data are obtained and related phase boundary diagrams are constructed. We study binary and ternary Fe-Mn-X alloy systems. In the Fe-Mn multi-phase boundary diagram, a shrinkage in the α -ferrite region is observed. Integrated with CALPHAD databases, the developed model may be used to calculate the segregation of solute to the PBs, paving way to manipulate segregation behaviour for microstructure design.

Advancements in DFT methods for the investigation of complex transition metal oxides

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D6_6, Andalucía III Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Methods based on Density Functional Theory (DFT) play a central role in designing advanced functional oxides, allowing the identification of promising materials through property prediction, and the understanding of the underlying structure-composition-property relationship. In the last decades, the DFT+U method has enabled the investigation of transition metal oxides with strongly interacting d-electrons. However, progress in the modelling of correlated TM oxides demands the enhancement and assessment of improved exchange-correlation functionals. This is particularly defying for complex oxides combining different TM ions. [1,2] This communication discusses the performance of the strongly constrained and appropriately normed (SCAN) meta-GGA functional and its SCAN+U derivative to model the basic physical properties of Fe⁴⁺-based perovskite oxides.

Going into property prediction, DFT serves to identify oxides with catalytic activity for the dissociation of water into hydrogen (HER process) and oxygen (OER process), as well as the combination of oxygen and hydrogen to produce water (HOR and ORR processes). Electronic descriptors, such as the oxygen 2p-band center or the intermediate absorption energies, show strong correlations with properties that directly influence the catalytic activity, such as the area-specific resistance (ASR) for ORR, and the OER overpotential in Alkaline Electrolyzers (AEL). [3,4] While previous studies have mainly focused on simple perovskite ABO₃ oxides, this communication explores complex Fe⁴⁺-based perovskites. Complementary experimental investigation on SrFe_{1-x}MoxO_{3-δ} perovskites [5] allows for discussing the reliability of electronic descriptors for property prediction.

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[3] Electronic Structure-Based Descriptors for Oxide Properties and Functions. L. Giordano, K. Akkiraju, R. Jacobs, D. Vivona, D. Morgan and Y. Shao-Horn, Accounts of Chemical Research, 55, 2022

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Ab-initio informed CALPHAD modelling of SIGMA7 grain boundary phases in the Mg-Ga system

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D6_1, Andalucía III Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The study of defect phases is of crucial importance when it comes to the design of nanostructured metals and alloys. Grain boundaries (GBs), a significant class of defects, influence key material properties such as deformability and strength. It has been demonstrated that alloying can induce GB phase transformations and thus alter mechanical performance. Employing defect phase diagrams facilitates the identification of phase transformations in the Mg-Ga system, e.g. from the SIGMA7-T to the SIGMA7-A structural type of the GB, alongside a systematic transition in segregation site preference. [1]

Consequently, Ab-initio simulations were conducted on various grain boundary structures to parametrize a CALPHAD model of the bulk phase and the grain boundary phases, SIGMA7-T and SIGMA7-A. The grain boundary phases are described using a virtual system component for defects. This enables the inclusion of grain size as an input parameter to a CALPHAD calculation and thus enables the quantitative treatment of partitioning of the elements at the grain boundary.

By integrating the bulk phase diagram with defect phase energetics, a defect phase diagrams with temperature, chemical potential, grain boundary energy, composition or grain size as axes can be drawn. These diagrams delineate the formation of distinct grain boundary structures as functions of temperature, composition, and grain size, under both stable and metastable conditions. The theoretical predictions align well with experimental microstructural investigations performed via transmission electron microscopy and atom probe tomography.

The integration of complementary thermodynamic modelling approaches engenders a holistic perspective on the prediction of grain boundary phases and segregation effects in defect structures. This methodology can be expanded to examine interactions among various structural imperfections. The results demonstrate a very good agreement with experimental observations, underscoring their broader implications for defect-engineering in metallic alloys.

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Data-Driven Prediction of Thermal and Mechanical Properties in Composite Materials Using Machine Learning and Computational Simulations

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D6_4, Andalucía III Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The effective design of composite materials with tailored thermal and mechanical properties requires a fundamental understanding of the underlying structure-property relationships (SPR). However, establishing accurate SPR models is challenging due to the complexity of microstructural features and the high cost of experimental characterization. To address these challenges, this study employs data-driven methods, combining machine learning (ML), computational homogenization, and finite element simulations to predict thermal and viscoelastic behaviors of composite materials. For thermal conductivity prediction, an ML-based approach is developed using microstructural features extracted from scanning electron microscopy (SEM) images. The microstructure is reconstructed using a diffuse interface method, facilitating accurate interpolation of phase and interface properties. Principal Component Analysis (PCA) is utilized to condense two-point statistics, which serve as input descriptors for the ML model. A dataset of 1440 synthetic microstructures is generated to train the model, with effective thermal conductivity values obtained from simulations.

In parallel, a deep learning-based framework is proposed for predicting the viscoelastic behavior of composites. A recurrent neural network (RNN) is leveraged to capture the time-dependent stress-strain response under varying loading conditions. This approach integrates microstructural descriptors with applied loading histories, enabling the prediction of viscoelastic behavior beyond traditional constitutive models. The ML-based surrogate model efficiently maps complex structure-property relationships in ceramic composites and provides a computationally efficient alternative to direct finite element simulations.

This study highlights the potential of ML-driven approaches in accelerating the design of advanced composites by reducing reliance on expensive experiments and computationally intensive simulations. The integration of data-driven modeling with physics-based simulations paves the way for the rapid discovery and optimization of materials with enhanced thermal and mechanical performance. The trained ML model demonstrates high predictive accuracy and applicability for sensitivity analysis and inverse design, enabling the optimization of composite microstructures with desired properties.

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First-principles and machine learning-accelerated molecular dynamics for complex disordered materials in energy applications

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D6_2, Andalucía III Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The accurate modeling of disordered materials is essential for understanding their potential impact and applications in energy applications. This work leverages first-principles molecular dynamics (FPMD) and machine learning interatomic potentials (MLIP) to bridge the accuracy of quantum mechanical methods with the efficiency of large/long-scales simulations. These advances enable us to accurately describe highly complex disordered systems—such as chalcogenides, transition metal-containing oxides, and antiperovskites—that have so far been approximated only by classical interatomic potentials.

We apply this approach to sodium vanadium phosphate (NVP) glasses and glass-ceramics, promising electrode materials for sodium-ion batteries; amorphous Na₃OCl, an emerging solid-state electrolyte; and disordered chalcogenides (GexSy, GeSe_y, GexSbyTez) for multifunctional applications, including thermal management in PCM devices. A crucial requirement for optimizing these materials is a detailed, quantitative description of their intricate structure and bonding, which in turn enables the accurate prediction of key functional properties such as ion dynamics, thermal conductivity, and electronic/magnetic behavior.

For NVP glasses and glass-ceramics, FPMD reveals the intricate interplay between V coordination, phosphate network polymerization, and Na-ion mobility, while MLIP simulations extend time and length scales, capturing percolation pathways critical for ion conduction [1-3]. Similarly, in Na₃OCl, our simulations establish the structural characteristics of the amorphous phase, validating MLIP models against FPMD-derived structure factors, structural features, and ion transport mechanisms [4-6]. The ability of MLIP-driven simulations to achieve near FPMD accuracy while reducing computational cost by orders of magnitude makes them indispensable for designing next-generation functional materials. Additionally, we highlight advances in data-driven approaches for improving MLIP performance. Multikernel similarity-based clustering methods provide an optimized database construction framework, enhancing the representativity and transferability of MLIP for complex amorphous chalcogenides and enabling accurate predictions of their thermal properties at the nanoscale [7-10]. By integrating these advancements, our study establishes a powerful and efficient methodology for modeling disordered materials, paving the way for predictive materials design in energy applications.

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Modelling exploration of contact area and stress in the deposition of a pathogen in an antimicrobial MIRIA nanocoated surface

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D6_4, Andalucía III Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Innovative biocidal nanocoatings constitute a relevant option for preventing the spread of infectious diseases. Understanding their interaction with the pathogens they aim to eliminate is, therefore, essential for enhancing their efficacy and design.

The model works with an elastic triangular mesh acting as the pathogen and immersed in a computational Lattice-Boltzmann fluid. The coated substrate is also modelled as a triangular mesh, and the interaction between both objects is introduced through a Lennard-Jones potential. The simulations performed cover the deposition of the pathogen on the nanocoated substrate, revealing the stress endured by the pathogen upon deposition and measuring the contact area between the pathogen and substrate. Additionally, simulations are performed for variations in the substrate roughness and dispersion of the surface at hand, introduced by scaling the surface in the z-direction, or in the (x,y)-plane. This enables an analysis of how these surface properties could affect the antipathogenicity of the substrate.

It is expected that for large dispersion values, as we initially consider, a higher roughness would lead to a higher contact area and, in theory, to lower stress, as the forces on the pathogen should be more distributed. Similarly, for static roughness, lower dispersion should lead to a lower contact area, presumably implying higher stress. This thesis is put to the test in the study, and the obtained results are presented, establishing the relationship between stress endured by the pathogen, contact area, surface roughness and dispersion. The main conclusion of the study is that there is a direct correlation between contact area and stress.

Machine learning potentials for simulations of defects in TiN and TaN

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Transition metal nitrides (TMNs) are widely recognized for their exceptional hardness, thermal stability, and electrical conductivity, making them irreplaceable in numerous industrial applications such as protective coatings and high-performance materials. Among these TMNs, titanium nitride (TiN) and tantalum nitride (TaN) have gained significant attention for their versatility and performance in wear-resistant coatings. The increasing demand for advanced materials has driven the exploration of methods to fine-tune their mechanical properties, such as through the introduction of structural defects.

In this study, we investigate defects in the cubic and hexagonal phases of TiN and TaN using molecular dynamics (MD) simulations. MD provides atomic-level insights into the structure and behavior of materials under well-controlled conditions, which can be challenging and resource-intensive for experiment. To speed-up MD simulations and access length scales beyond that typical for ab initio modeling, we develop machine learning potentials (MLPs), combining computational efficiency with accuracy for defect modeling.

To train these MLPs and validate their predictive power, we generate data through finite-temperature density functional theory (DFT) calculations. Our dataset encompasses a wide spectrum of defect types, including vacancies, grain boundaries, and twins. This approach facilitates the development of robust MLPs while enabling direct comparisons between MD simulations and DFT results, ensuring both reliability and accuracy.

Our work aims to advance the understanding of defect-driven property modifications in TiN and TaN, paving the way for improved materials design with applications in wear-resistant coatings and high-performance materials.

Microstructural control of aluminum alloys under high pressure

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D6_7, Andalucía III Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Pressure is one of the canonical thermodynamic variables which control the equilibrium conditions of a physical system. Precipitation strengthening in Al alloys is hindered by the limited solid-solubility, while it can be enhanced under pressure. In this work, the Al-Mg phase diagrams at 0 and 4 GPa of hydrostatic compression were constructed by first-principles calculations. The enthalpy and internal energy of configurations was obtained by density functional theory. Cluster expansions were fitted to account for the relationship between internal energy and atomic occupation while the PV term was only sensitive to alloy concentration. Monte Carlo simulations were performed to obtain the Gibbs free energy of solid phases while that of liquid were obtained from CALPHAD. The entire phase diagrams under 0 GPa and 4 GPa were constructed, and the increment in solid solubility due to the hydrostatic pressure was ascertained. Finally, a solid solution heat treatment was performed under hydrostatic pressure, followed by precipitation experiments to ascertain the precipitate structure and volume fraction. The influence of enhanced solid-solubility under high pressure was also verification with Al-Si alloy and Mg-Li alloy.

Machine learning and Bayesian calibration of multiphysics simulations of crystal growth

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D6_3, Andalucía III Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Material development and optimization inherit the need to understand and control processing-structure-property relationships. Of particular interest is SiC, which is utilized in power electronic devices due to its exceptional properties such as a wide bandgap, high breakdown voltage, and high thermal conductivity. The most common method to produce SiC single crystals is through physical vapor transport (PVT) where the SiC boules are grown within a closed reactor. Process temperatures around 2000 °C as well as pressure close to 5 mbar make it not only challenging to acquire experimental data but also complicate the quantification of physical material properties of the system.

In order to improve process knowledge and reduce the need for expensive experimental trials, multiphysics FEM-based crystal growth simulations are frequently utilized. Reliable models not only facilitate the production of high-quality crystals as well as high output and resource-saving processes, but they can also aid in optimizing growth conditions or scaling the process appropriately. However, models must consider complex coupled physics phenomena, accurately representing the key aspects of the growth environment within reasonable computational efforts. A further challenge arises from uncertainty in the materials parameters of the furnace which need to be calibrated precisely to achieve reliable simulation results. Novel techniques from machine learning (ML) offer great opportunities in this respect.

We present an approach providing a computational and time-efficient active learning algorithm, that sequentially builds an ML model that can replace the COMSOL multiphysics calculation to access relevant quantities in the reactor. Training data are generated by sequential design of experiment combined with Gaussian Process Regression. Based on real PVT furnace data, ML models in combination with Bayesian inference, particularly with Markov Chain Monte Carlo, are used to calibrate the unknown physical material parameters. With this, our approach addresses several challenges simultaneously, i) improvement of execution speed of multi-physics FEM simulations ii) calibration of the FEM simulations to experiments iii) in-service determination of materials properties, and iv) material degradation monitoring. The adapted methodology is quite general and shows great potential to be used also for other calibration tasks and for different downstream tasks, like sensitivity and uncertainty analyses.

A multi-phase-field model for simulation of solid-state sintering

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D6_3, Andalucía III Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Particle sintering is a well-established and widely utilized powder-processing technique for manufacturing metal and ceramic components. Sintering induces morphological changes in the green compact, reducing surface area and increasing density. Understanding the mechanisms behind the densification and microstructural evolution during the sintering process is of immense importance because of its broad industrial applications. A model is developed based on the multi-phase-field approach to describe the microstructural evolution during solid-state sintering. This model integrates the multiphase Allen-Cahn equations to describe the evolution of different particle phases and the multiphase Cahn-Hilliard equations to characterise the behaviour of the vapour phase. The multiphase Cahn-Hilliard formulation enforces volume conservation of the sintering compact, ensuring physically realistic simulations. The model considers different diffusion mechanisms including volume diffusion, surface diffusion, and grain boundary diffusion together with grain boundary migration. To enhance computational efficiency, the model is implemented using parallel GPU-based computing, allowing for the simulation of multiple interacting particles. We validate the model by matching two-particle sintering simulations with the analytic solutions. We also investigate the relation between the dihedral angles and energy ratios of the sintered powder particles. Beyond two-particle interactions, we extend our investigation to large-scale sintering simulations involving multiple particles. The results of these large-scale sintering simulations of multiple particles are compared with an existing analytic model.

Advancing Binder Jetting: A Multi-Scale Numerical Approach to Minimize Residual Porosity

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Binder jetting has emerged in recent years as a promising Additive Manufacturing (AM) technique, featuring the typical advantages of AM—such as the ability to produce unconstrained geometries and reduce material waste—whilst avoiding the energy cost and challenges tied to rapid solidification and extreme thermal cycles common in fusion-based AM methods. Despite its potential, due to an incomplete understanding of the multi-scale and multi-physics nature of the process, the presence of defects, particularly residual porosity, still limit its broader adoption.

Numerical simulations offer a pathway to investigate binder jetting processes with exceptional spatial and temporal resolution, providing insights that would be extremely challenging to obtain (if feasible at all) through experimental approaches alone. To advance the understanding of sintering mechanisms contributing to residual porosity, this study proposes a novel integrated approach combining the Discrete Element Method (DEM) and Phase Field (PF) models.

The DEM is utilized to predict the powder bed's characteristics post-spreading, such as particle packing density and coordination, which serve as critical inputs for the PF model. The PF model, based on a grand potential approach, is employed to examine the evolution of porosity during sintering under the thermal conditions of the process. The effects of binder residues on diffusion mechanisms—including volume, surface, and grain boundary diffusion—are explicitly incorporated by locally modifying mobilities, offering a more comprehensive depiction of sintering dynamics.

Accurate calibration of model parameters is essential to faithfully represent the underlying physical phenomena. While some parameters can be derived directly from the literature, others require detailed calibration. To address this challenge, a Bayesian calibration framework is implemented in ACBICI (A Configurable Bayesian Calibration and Inference package), an open-source Python library, to identify the most probable parameter distributions for governing DEM and PF models. This probabilistic approach not only refines parameter determination but also quantifies uncertainties in the models and calibration procedures, enhancing their predictive reliability.

The combined framework of DEM and PF models, augmented by Bayesian calibration, establishes a robust methodology for investigating binder jetting processes. By elucidating the underlying mechanisms of defect formation and quantifying uncertainties, this work contributes to the development of strategies to minimize residual porosity, ultimately advancing binder jetting toward the production of high-performance, defect-free components.

First-principles-based description of segregation in steel

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D6_1, Andalucía III Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

This study presents a first principles investigation of the paramagnetic α/γ interface in iron. The research is divided into two main parts. The first part focuses a methodology for interface calculations in Green's functions codes using coherent potential approximation. This methodology enables DFT calculations of α/γ interfaces in the paramagnetic state, leveraging the disordered local moment (DLM) approach. The methodology is used in a combination with VASP supercell calculations of interfaces in iron, which are also used calculate the fundamental properties of a representative α/γ interface.

The second part addresses an evaluation of available first principles methods for solute segregation to grain boundaries in combination with recent machine-learning models and their potential for application to segregation calculations in paramagnetic and concentrated alloys. We present a methodology to evaluate the composition of interfaces in the dilute limit and necessary methodological steps for its extension towards concentrated alloys. This research work aims at providing insights into the segregation phenomena in steel, contributing to the development of advanced materials with optimized properties.

First principles modeling of short-range order in Fe-Si-Al alloys

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D6_1, Andalucía III Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Unique electromagnetic properties of steels with silicon and aluminum make them a perfect choice for the production of transformers and electric motors. These so-called electrical steels have enhanced energy efficiency due to reduced core losses and enhanced magnetic permeability. However, increasing the concentration of silicon and aluminum beyond a critical amount leads to significantly worse ductility, which makes production very challenging.

The theoretical origin of these embrittlement effects is still not fully understood, as ab-initio modeling based on Density Functional Theory (DFT) are rather challenging, due to requiring large supercells and complex magnetic interactions. Such first principle simulations frequently use Special Quasirandom Structure (SQS) approaches to simplify the problem, as they are designed to describe a fully random distribution of the alloying elements. However, real systems are not perfectly random, due to atomic interactions, which result in short range ordering (SRO) of the atomic sites. We investigate atomic SRO phenomena using accurate, DFT based full potential methods, as well as the Generalized Perturbation Method (GPM) to account for the magnetic state dependence of the effective cluster interactions and study their hierarchy. We introduce thermal atomic displacements to investigate the effect of temperature on magnetic exchange interactions in selected electrical steels. We discuss how accurate modeling of thermodynamic properties of these materials close to the Curie temperature should take such thermal effects into account, and that a semiclassical approach using thermal displacements is a computationally efficient way of achieving this.

Decoupling chemical and vibrational contributions to vacancy formation at high temperatures in MoTaNbWV high-entropy alloys

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D6_2, Andalucía III Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

We calculate the temperature-dependent vacancy formation energies in the refractory high-entropy alloy (HEA) MoTaNbWV and its unary, binary, and quaternary subsystems using machine-learning-based interatomic potentials. This study systematically examines the chemical, configurational, and vibrational contributions to vacancy formation over a broad temperature range of up to 3000 K. The results show that while temperature strongly influences vacancy formation energies, vibrational contributions remain largely independent of the local chemical environment, even at high temperatures. This finding reveals a decoupling between chemical and vibrational contributions. Leveraging this insight, we develop a general phenomenological model that treats these entropic contributions separately, enabling accurate predictions of vacancy formation energies across all investigated subsystems and the MoTaNbWV HEA. These findings provide a foundation for improving diffusion models and optimizing the design of multicomponent alloys.

Unveiling the Origin of the Yield Stress Anomaly in L12 Intermetallics via Multiscale Atomistic Approaches

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D6_7, Andalucía III Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

We investigated the yield stress anomaly (YSA) in L12 intermetallics using a multiscale atomistic approach, bridging electronic-scale calculations with large-scale molecular dynamics simulations through machine-learning-based interatomic potentials. An ab initio database of temperature-dependent Gibbs energy for relevant planar defects in L12 Ni₃Al was developed, covering the full temperature range of the YSA. Machine-learning interatomic potentials, trained and benchmarked against DFT results, achieve accuracy comparable to ab initio calculations. Key dislocation mechanisms, such as cross-slip and dislocation jumps, were successfully observed and analyzed. These MD results enabled the development of a phenomenological model that captures the YSA characteristics, providing deeper insights into the high-temperature performance of Ni- and Co-based superalloys.

A Phase-Field Study on the Effect of Nanoparticle Size, Concentration and Type on Columnar Growth during Electrodeposition

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D6_3, Andalucía III Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Electrodeposition is a complex process in which a metal or alloy accumulates onto the surface of another material via reduction and oxidation reactions in the presence of an electric current. However, the properties of the resulting coating depend strongly on the final surface texture and solidification dynamics. In this presentation, we introduce how the incorporation of nanoparticles into a polycrystalline matrix during electrodeposition significantly influences the solidification process, affecting both columnar growth and surface texture, and study the effect of nanoparticle size, shape and type via Phase-Field modelling. We observed that relatively large concentrations of spherical metal oxide nanoparticles like MgO or Al₂O₃, which enhance interface wettability, and 2D nanomaterials like MoS₂ or graphene, thanks to their capability to reduce drag and promote smooth interface movement, show up as perfect candidates to control columnar growth during electrodeposition.

Investigation of Carbide Effects on the Mechanical Properties of AISI 420 Steel by Crystal Plasticity Simulation

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D6_5, Andalucía III Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Understanding the role of precipitates in determining the mechanical properties of metallic materials is essential for optimizing their design and performance. This study investigates AISI 420 stainless steel, which consists of ferrites with carbide precipitates in its annealed state. A virtual laboratory framework is developed using a multiphase crystal plasticity (CP) model to systematically explore the effects of carbide—including their volume fraction, distribution at grain boundaries, average size, and quantity—on the steel's mechanical response across scales. The methodology involves constructing representative volume elements (RVEs) from microstructural characterization of the as-received material, calibrating material parameters within the CP model, and validating the model against experimental texture and mechanical properties. A series of RVEs were generated by systematically altering carbide characteristics to evaluate their influence on stress-strain behavior, anisotropy, and micromechanical interactions between the ferritic matrix and carbides. This research underscores the effectiveness of a virtual laboratory in bridging microstructural attributes with macroscopic mechanical behaviors and demonstrating its feasibility for studying microstructural influences. The insights gained are not only relevant to AISI 420 steel but can also be extended to other steels containing hard, elastically distinct precipitates, offering a broader perspective on microstructure-property relationships.

Fluid Flow and Heat Transfer Control in Spray Forming: Toward Improved Steel and AM Powder Production

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Spray forming is an advanced manufacturing technique that integrates metal atomization and deposition to produce high-quality steel and metal powders. Despite its potential advantages, such as refined microstructures and reduced segregation, its adoption in steel production remains limited compared to traditional continuous casting methods, primarily due to economic considerations and process difficulties. However, spray forming offers a unique capability to produce metal powders suitable for additive manufacturing (AM) applications. Achieving desired material properties in both bulk steel and powders necessitates precise control over the spray forming process. Critical parameters include fluid flow dynamics, heat transfer characteristics, primary and secondary atomization, and solidification patterns, all of which significantly influence the final microstructure and properties of the products. For instance, to ensure a uniform microstructure in the deposited ingot, it is essential to maintain a consistent top surface temperature during spraying, which requires full control over the different process parameters. In this study, we employ a comprehensive multi-scale and multi-physics numerical simulation approach using advanced CFD techniques to model the entire spray forming process. The simulations begin with the molten metal's transfer from the furnace to the tundish, followed by its flow through the tundish to the nozzles. At the nozzle exit, high-pressure nitrogen gas atomizes the molten metal into fine droplets. These droplets either deposit onto a substrate to form ingots or are collected as powders for AM applications. By analyzing and optimizing fluid flow and heat transfer throughout these stages, we aim to enhance control over the process, thereby improving the material properties of both the produced steel and powders. Our objective is to develop a well-designed and controlled spray forming process that minimizes impurities and inclusions, resulting in high-quality steel and powders tailored for AM applications. This research contributes to advancing spray forming technology, highlighting its potential as a viable method for producing superior materials for various industrial applications.

Ab initio machine-learning unveils strong anharmonicity in non-Arrhenius self-diffusion of tungsten

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D6_2, Andalucía III Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Understanding diffusion mechanisms in materials is essential for predicting their high-temperature behavior and stability, yet accurately capturing the underlying physics, particularly thermal effects, remains a challenge. In particular, the experimentally observed non-Arrhenius diffusion behavior has long been difficult to explain due to the lack of effective computational approaches. Here, we introduce an efficient ab initio framework for computing the Gibbs energy of the transition state in vacancy-mediated diffusion, incorporating relevant thermal excitations at the density-functional-theory level. Leveraging a tailored machine-learning interatomic potential, we demonstrate that the temperature-dependent vacancy formation and migration Gibbs energies in body-centered cubic (BCC) tungsten are significantly influenced by anharmonic effects. This insight provides a fundamental explanation for the non-Arrhenius self-diffusion behavior observed in experiments. Our results exhibit remarkable agreement with experimental self-diffusivity data, accurately capturing both the temperature dependence and its curvature. Furthermore, the robustness and versatility of the framework are highlighted through preliminary applications to a hexagonal close-packed (HCP) multicomponent high-entropy alloy. These findings establish a reliable path toward an accurate ab initio diffusion database, enabling predictive modeling across diverse material systems.

Machine learning-enhanced modeling of interactions between diamond surfaces and protein sequences

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This work presents an investigation into the application of machine learning (ML) methods for modeling protein structures of microcystin-LR (MC-LR) and diamond-based surfaces for advanced biosensing applications. MC-LR, a highly potent toxin produced by cyanobacteria, necessitates innovative detection strategies to ensure safe water supplies. In response, our research combines computational protein modeling with diamond surface optimization, showcasing the predictive capabilities of modern ML algorithms. Initially, we established a comprehensive dataset of homogeneous and heterogeneous diamond surfaces using QuantumATK software. The heterogeneous diamond structures were simulated as boron-doped diamond (BDD) functionalized with hydrogen, hydroxyl, or oxygen terminations to generate relevant terminations. The Moment Tensor Potential (MTP) was then trained and optimized using an active learning approach, allowing the model to refine itself iteratively as it encountered new or challenging configurations. By selectively adding data and calibrating parameters, the trained MTP exhibited enhanced robustness and predictive accuracy, effectively mitigating overfitting. In the second phase, we employed AlphaFold to predict protein sequences capable of detecting MC-LR. The predicted structures demonstrated high confidence scores, lending credence to the proposed folding motifs and providing a strong basis for subsequent experimental validation. Complementary simulations were performed for DNA aptamers designed for MC-LR detection, highlighting their potential for highly selective and sensitive biosensing applications. Collectively, these results underscore the promise of ML-driven approaches in bridging materials science and biotechnology for water remediation. The primary application of our findings is the development of optimized diamond-based electrodes, which can be seamlessly integrated with protein- or aptamer-based sensing elements to enable reliable detection and further degradation of MC-LR. This work drives innovation in the creation of cost-effective, durable, and scalable biosensors that enhance water quality monitoring and help protect public health. By uniting advanced ML-optimized materials modeling with biomolecular engineering, we provide a blueprint for addressing complex environmental challenges — particularly the urgent need for efficient and sustainable water safety technologies.

Energy barrier of twinning and transformation induced plasticity in titanium alloys - extension to the classical electronic based approach of TWIP/TRIP materials design with modulated yield strength

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 17, 2025, 13:10 - 14:30

Twining and transformation induced plasticity (TWIP/TRIP) are novel deformation mechanisms of metastable β -Ti alloys characterized by extremely high work hardening and great ductility [1]. The main limitation of this materials group is relatively low yield strength governed by the energy barrier of $\{332\}\langle 113 \rangle$ twinning (TWIP) and stress induced $\beta \rightarrow \alpha''$ transition (TRIP). Recent investigation of TWIP/TRIP phenomena revealed that both lattice reconfigurations share the same shear-shuffle mechanism indicating their polymorphic nature [2]. Based on these findings we introduce the original, first principles-derived, extension to Bo-Md phase diagram focusing on the energy barrier (ET) of TWIP/TRIP transformation. To this end, a series of Ti-X (X = V, Nb, Ta, Cr, Mo, Mn, Fe and Re) alloys with different stoichiometry was analyzed to calculate the influence of particular solutes on ET. As a result, the solution strengthening of TWIP/TRIP has been parametrized for individual alloying elements with respect to atomic concentration, average electron-to-atom ratio e/a , Bo and Md values. Ultimately, determined hardening parameters were successfully used to estimate the Ti-X compositions of model alloys with TWIP/TRIP effects and to improve the yield strength of experimental ternary system. Presented study will be highly useful for designing new TWIP/TRIP alloys where apart from phase composition, the level of critical stress triggering the phase transformations can be also controlled.

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A phase-field model of CALPHAD stoichiometric phases of Aluminum alloys

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D6_3, Andalucía III Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The phase-field method is widely recognized as one of the most effective tools for simulating meso-scale material phenomena due to its robust interface tracking capabilities. It allows for the modeling of complex interfacial dynamics, including arbitrary interface shapes, with minimal computational effort. By incorporating the equal diffusion potential condition and anti-trapping currents, the method significantly reduces numerical artifacts associated with diffusive interfaces. However, challenges remain, particularly in accurately modeling stoichiometric phases. A key difficulty arises from the use of point-wise free energy expressed in terms of composition, which often lacks the necessary composition dependencies. This limitation forces the introduction of artificial composition variations to apply the equal diffusion potential condition. In this study, we address these challenges by developing a phase-field model that is both computationally efficient and easy to formulate for stoichiometric phases and phases with limited solubility. Our approach builds upon the existing relaxation-based equal diffusion potential condition, which has proven effective for simple soluble phases. We extend this framework to more complex systems, including general stoichiometric compounds and phases with restricted solubility ranges. By refining the model in this way, we aim to improve the accuracy and efficiency of phase-field simulations for a broader range of material systems, ultimately enabling better predictions of meso-scale material behaviors in diverse contexts. This work represents a step forward in the development of practical, versatile phase-field methods for complex material phenomena.

Machine Learning-Based Predictive Model Integrating Experimental Data and Multiphysics Simulations for Product Quality Assessment in Metallic Laser Powder Bed Fusion: Deformation, Surface Roughness, and Part Density

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D6_7, Andalucía III Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Product quality is a key metric for evaluating the performance of LPBF machines. Among various indicators, deformation, surface roughness, and part density are closely interconnected. Higher deformation often leads to surface irregularities, affecting overall part quality. Similarly, lower density caused by porosity or incomplete fusion results in a rougher surface due to balling effects and uneven solidification. In contrast, high-density parts exhibit smoother surfaces, as uniform melting and solidification reduce surface defects. Part density also plays a crucial role in deformation. Lower density weakens structural integrity, making the part more susceptible to warping and distortion. Conversely, high-density parts provide better mechanical stability, reducing residual stress and minimizing deformation. This interdependence highlights the need for optimized process parameters to achieve the desired balance between deformation, surface quality, and density in LPBF manufacturing.

This work focuses on rapid quality prediction using a machine learning model. Since direct measurement of the aforementioned quantities is challenging, a validated finite element-based part-scale thermo-mechanical model serves as a data generator. This model simulates 3D displacement and stress maps under varying laser process parameters, including laser power, scan speed, hatch spacing, powder thickness, and beam shape profile. Meanwhile, data for other quality criteria, such as surface roughness and part density, is obtained through in-house experiments, measurements, and an FVM-based thermo-fluid dynamic model, ensuring a comprehensive dataset for training the machine learning model. The proposed approach consists of two parallel predictive models: The first model, a sequence-to-sequence learning framework, takes 3D geometry and laser settings as inputs to predict residual stress and displacement profiles. The second neural network model uses laser process parameters to first predict surface roughness (S_a , S_q , and S_z) and texture (Str). These surface characteristics are then used as inputs to predict part density, given their strong correlation. Finally, the model optimizes the process parameters to minimize defects and enhance overall quality. This framework enables efficient, data-driven process optimization, significantly reducing the need for extensive simulations and experiments.

Modeling complex diffusion phenomena in compositionally-graded single-crystal Ni-based superalloys

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D6_6, Andalucía III Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The present work consists of modeling various complex diffusion-related phenomena in single-crystal Ni-based superalloys including CMSX-10 and CMSX-4, under isothermal annealing and composition gradient. The simulated diffusion events include multi-component diffusion of elements and vacancies, phase transformations, dissolution of precipitates and Kirkendall pores nucleation, growth and their morphological instability.

The applied methodology combines novel quantitative phase-field models coupled with thermodynamic and diffusion parameters based on the CALPHAD approach.

For all simulated efforts, the achieved results are compared with experimental data such as measured interdiffusion profiles, SEM analysis of microstructure and synchrotron X-ray tomography of the Kirkendall pores.

Understanding structure and wetting behavior of nickel-based coatings in contact with liquid tin droplet: atomistic simulations vs. experiment

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 Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The elimination of lead-based solders from electronics application (EU Directive 2002/95/EC) forced to search for new technological solutions, including alternative solder and coating technologies. Lead-free alloys (the alternative solders) react much faster with Cu substrates due to their high Sn content and increased soldering temperature, resulting in the uncontrolled growth of intermetallic compound (IMC) layers [1]. Ni-based coatings, obtained by electrodeposition and electroless techniques, are used to prevent Cu dissolution and limit excessive IMC growth, acting as diffusion barrier layers between Cu substrates and Sn solder[2,3]. The modification of chemical composition and structure of Ni-based coatings can further enhance coatings' thermal stability, wetting properties and limit the formation of undesired phases at coating/solder interface by slowing down the interfacial reaction rate.

Herein, we provide insight into the structure and wetting behavior of nickel-based coatings in contact with a liquid tin droplet by combining molecular dynamics simulations and sessile drop experiments. The impact of Ni-based coating structures ranging from amorphous to nanocrystalline, on the wetting mechanism of a liquid tin droplet was simulated. The structure, chemical, and phase composition changes of the interface zone formed between coatings and the solder were explored experimentally (using scanning and transmission electron microscopy techniques) and computationally [4,5]. 3D height profile maps were computed and compared with experimental results obtained using a non-contact confocal profilometer and atomic force microscopy techniques.

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Metastable defect phase diagrams as roadmap to tailor chemically driven defect formation

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D6_1, Andalucía III Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Thermodynamic bulk phase diagrams have become the roadmap used by researchers to identify alloy compositions and process conditions that result in novel materials with tailored properties. Recent experimental studies show that changes in the alloy composition can drive not only transitions in the bulk phases present in a material, but also in the concentration and type of defects they contain. Defect phase diagrams in combination with density functional theory provide a natural route to study these chemically driven defects. Our work reveals, however, that direct application of equilibrium bulk thermodynamics can fail to reproduce experimentally observed defect formation. Therefore, we extend the concept to metastable defect phase diagrams to account for kinetic limitations that prevent the system from reaching equilibrium. In this regard the exothermic formation of defect phases can be explained. We apply this concept to successfully (1) design suitable conditions for synthesis, which we subsequently realized experimentally, successfully validating the formation of the predicted defects in Mg-Al-Ca alloys. Finally, we (2) resolve the discrepancy between bulk phase diagrams and experimental observations regarding the formation of Mg-rich C14 and Al-rich C15 Laves phases in MgAlCa alloys at moderate temperatures and (3) clarify, the effect of the thermodynamic state of alloys on the competition between solute-rich hcp-like planar defects and stoichiometric basal stacking faults. The concept of metastable defect phase diagram offers new avenues for the design of materials performance by tailoring defect structures.

Unraveling Atomistic Mechanisms of Pressure-Induced Phase Transitions in Silicon and Germanium

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D6_6, Andalucía III Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Silicon and Germanium are some of the most studied materials for their importance in the microelectronic industry, but they have been studied so far mainly in their most stable phase: the diamond cubic. However, they also exhibit several metastable allotropes, some of which are very promising for their superior optoelectronic properties. These allotropes can be experimentally synthesized starting from the dc by inducing solid-solid phase transitions driven by pressure, like the BC8/R8 phases and the hexagonal diamond [1].

In this work, we advance the understanding of the atomistic mechanisms underlying pressure-induced Phase Transitions in Si and Ge by combining state-of-the-art techniques for the atomistic simulations of kinetic processes in solid-solid phase transitions. In particular, we exploited massively parallel Molecular Dynamics simulations [2] based on Machine Learning potentials, like the GAP potential for Si [3] and an ad-hoc developed Neural Network potential for Ge [4]. We complemented such simulations with the solid-state Nudged Elastic Band [5] calculations. Particular focus is devoted to the search for transition processes showing the local nucleation and growth of a phase inside a hosting matrix. We explicitly show the improved estimation of the transition rates considering the local nucleation process compared to the more simplified full-cell transition models [6]. Examples will be provided for several phase transitions in both silicon and germanium.

Finally, we exploited a high-throughput search method for exploring possible transition paths based on the solid-state Dimer method [7] and the adaptive Kinetic Monte Carlo scheme in order to automatize the search process for physically relevant phase transitions.

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[7] P. Xiao, JCP 140, 174104 (2014)

Unraveling the Plastic Deformation Mechanism in Oxide Glasses via Atomistic Simulation and Coarse-Grained Analysis

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D6_5, Andalucía III Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Amorphous materials, valued for their optical transparency, insulation, and oxidation resistance, are indispensable in applications ranging from architectural glass to electronic displays. However, their limited mechanical performance, particularly the absence of a robust plastic deformation mechanism, restricts their widespread utility. Recent experimental studies have revealed that amorphous alumina ($\alpha\text{-Al}_2\text{O}_3$) thin films exhibit remarkable plasticity at room temperature, challenging traditional perceptions of amorphous materials' mechanical behavior.

This study investigates the plastic deformation mechanisms of $\alpha\text{-Al}_2\text{O}_3$ using molecular dynamics simulations and complementary characterization methods targeting medium-range order (MRO). Our findings demonstrate that viscous flow governs the deformation behavior of $\alpha\text{-Al}_2\text{O}_3$ under mechanical stress, distinguishing it from other amorphous oxides. The unique structural characteristics of $\alpha\text{-Al}_2\text{O}_3$, attributed to its harsh preparation condition, likely underpin its enhanced plasticity.

To expand the scope of our understanding, we developed a coarse-grained analytical model that bridges atomic and mesoscopic scales, enabling a quantitative evaluation of medium-range structural features. This model reveals the critical role of MRO in dictating the plastic deformation capacity of amorphous oxides, including amorphous alumina and silica. Our approach provides a versatile framework for assessing and predicting the mechanical performance of amorphous materials, paving the way for designing amorphous systems with improved mechanical properties.

This work offers a deeper insight into the deformation mechanisms of amorphous oxides and broadens the potential for their application in mechanically demanding environments.

Multiscale simulations and experimental analysis of polytypism and ultrafast growth rates in semiconductors using SiC nanowire synthesis as model.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

NanoWire (NW) synthesis holds tremendous potential for a wide range of applications in energy, catalysis, composites, and electronic devices. One of the main methods for synthesising NWs is through Chemical-Vapour-Deposition (CVD) growth, an industrially scalable method that enables control over polytypism, aspect ratio, and integration on devices. One of the main methods for synthesising NWs is through Chemical-Vapour-Deposition (CVD) growth, an industrially scalable method that enables control over polytypism, aspect ratio, and integration on devices. Within the family of CVD methods, we use a variant termed Floating Catalyst Chemical Vapour Deposition (FCCVD), in which Liquid Metallic NanoParticles (LMNP) embedded in a gas stream function as catalyst, solvent, and growth medium. Gases precursors are incorporated into the LMNP, leading to supersaturation and subsequent nucleation via the Vapour-Liquid-Solid (VLS) mechanism. The growth conditions in FCCVD enable ultrafast growth of NWs, resulting in micrometre-long NWs within a minute residence time. Growth from the gas phase allows for direct assembly of NWs into macroscopic ensembles (e.g. yarns or fabrics).

NWs synthesised with FCCVD typically exhibit aspect ratios of between 12 and 2200. However, in the same NWs mixed polytypes, stacking faults can usually occur which degrades the electronic properties. Since the available information of the FCCVD method is scarce, it limits the synthesis to new materials and the use of other catalysts. The present study focuses on polytypism selection and growth rate, exploring several models and compared their results to experimental data reported in the literature. The input data was obtained with a wide variety of methods, from precise and costly methods such as ab-initio calculations to analytical models, as well as values reported in the literature. A high-throughput screening of different semiconductors was also carried out, using various materials and thermodynamics databases.

For SiC nanowires, which were successfully synthesised in the laboratory using Au catalyst, we have use ab-initio calculations for calculating critical parameters as the surface energy of different planes. We critically assessed the validity of different model and their sensitivity to the source of input data to calculate growth rate and polytypism selectivity. We have implemented a workflow to extend the approach to other semiconductor NWs. Finally, we also found a correlation between polytype selectivity and growth conditions in an FCCVD reactor that can be described from analytical equations to advance kinetic model and validated with experimental data.

Numerical Investigation on the Laser Absorptivity in Laser Additive Manufacturing of Copper using Beam Shaping

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D6_5, Andalucía III Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Copper has been widely used in various engineering applications due to its excellent thermal and electrical conductivity properties. The laser powder bed fusion process (PBF-L) involves multiple physical phenomena, e.g. phase change, evaporation, melting, solidification, microstructural evolution, etc.

This work simulates the PBF-L process of copper under infrared laser irradiation at the deposition scale using the finite volume (FVM) solver OpenFOAM, including various physical effects such as buoyancy, surface tension, evaporation, and the Marangoni effects. The simulation results have been verified by a decent agreement with experimental measurements in terms of melt pool profile at different combinations of laser, ranging from conduction to transition and keyhole modes.

For copper PBF-L, there has been disagreement in the literature regarding the correct absorption rate of laser power, especially in simulation-related work.

Here, we investigate the influence of laser power, scanning speed on the absorptivity, and provide a reference for the contour of global absorptivity V.S. process settings.

Beam shaping generally has an influence on the melt pool shape and the printing quality, and here we apply two types of laser beam shapes, one with Gaussian and one with Ring-shaped profiles as input heat sources, to investigate their effects. This work is performed for simulating the melt pool at dense substrates at single track, single layer, shedding light on the fundamental impacts of the process settings on melting and global absorptivity.

Keywords: Additive Manufacturing, Copper, Absorptivity, Melt Pool, Beam Shaping

Foundation Models For Aluminium Alloys

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D6_2, Andalucía III Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Foundation models have proven very popular in recent years, with new record-breaking models coming out every month. But how accurate are they, and can they replace "bespoke" potentials? In this talk I will present the state of the art in both categories.

First, I will show that using the GRACE2L-OAM foundation model we can achieve very high accuracy across a broad range of metallurgically-relevant benchmarks "out of the box" with no further modification or fine-tuning. Overall these models are able to produce results that are almost as accurate as a collection of custom BP-NNPs for aluminium developed over the course of several years by hand.

I will then show how the ACE model can be used to create a class of very powerful next-generation custom potentials. Some techniques, such as ladder learning, and training on individual elements first will be discussed. A performance evaluation showing how while foundation models can produce very impressive results, for the greatest accuracy and speed one should still use 'bespoke models'.

This talk will include the challenges in computing material properties: elastic constants, lattice constants, surface energies, generalized stacking fault energies and dilute solute interactions. I will also cover how to select and evaluate foundation models and reasons why any of the most popular datasets (at time of writing) are insufficient for aluminium metallurgy. Computational considerations, such as how to design effective 'unit tests' for interatomic potentials, and computational performance issues regarding the ASE python interface vs directly computing with LAMMPS.

While the focus will be on aluminium alloys, the author will also mention the use of foundation potentials in the context of designing new batteries and magnetic materials.

Uncertainty in the era of machine learning for atomistic modelling

Dr. Kevin Rossi¹

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D6_7, Andalucía III Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Machine Learning Potentials (MLPs) have revolutionized the simulation of complex material systems by offering high efficiency and accuracy. However, their reliability can be compromised when simulations explore configurations not well-represented in the training data. [1]

In this presentation, I will then focus on how to assess the accuracy and precision of MLPs. First I will define the concept of robust and non-robust extrapolation, and of transferability, in the context of machine learning potential validation and exploitation. I will then discuss extrapolation metrics that enable to quantify the reliability of a MLP prediction. [2] Next, I will elaborate on how to estimate the uncertainty in MLPs predictions, and how to rigorously propagate the latter when estimating a physical observable from molecular dynamics sampling. [3].

I will conclude my talk with a reflection on: i) how uncertainty estimate and propagation is central to other machine learning for science application as well, ii) what our community can do to foster the development of workflows and models, which rigorously account for sources of error and uncertainties [4]

[1] Digital Discovery 3 (1), 113-121 (2024)

[2] Physical Review B 105 (16), 165141 (2022)

[3] The Journal of Chemical Physics 154 (7), 074102 (2021)

[4] <https://www.cost.eu/actions/CA22154/>

Mesoscale Modelling of Phase Transformations via Cellular Automata: The Role of Artificial and Physical Anisotropy in Ferrite Growth Kinetics

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D6_4, Andalucía III Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

This contribution presents a mesoscale modeling approach for the austenite-to-ferrite transformation in Fe–C–Mn steels, highlighting how both artificial and physical anisotropy can influence ferrite growth kinetics. The mesoscale model employs a Cellular Automata (CA) method to simulate phase growth, coupled with a finite difference (FD) method to model the diffusion of solute elements. Thermodynamic data are incorporated through the CALPHAD methodology, ensuring a robust calculation of the local driving force for phase transformation across heterogeneous compositions.

Artificial anisotropy stems from the microstructure discretisation using a regular CA grid, where a nominally isotropic interface migration velocity can generate non-spherical growth morphologies. On the other hand, physical anisotropy arises from a range of factors, including grain boundary curvature, crystallographic orientation, preferred boundary diffusion pathways, spatial variations in local chemical composition, and anisotropic diffusion coefficients sensitive to changes in carbon content. These phenomena collectively alter the local growth rate of ferrite, underlining the necessity of carefully accounting for microstructural heterogeneities and their thermodynamic implications.

By focusing on relatively simple Fe–C–Mn alloy compositions, the model effectively isolates and elucidates the impact of the aforementioned anisotropic effects. This approach not only provides more accurate predictions of ferrite kinetics but also paves the way for higher-fidelity simulations in modern steel-processing routes.

Simulation of the homopolymerisation of bismaleimide monomers using tailored reactive Molecular Dynamics

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Even if they were initially developed for the electronic industry, bismaleimide resins are widely used in high-performance composite applications, particularly when high temperature is the primary stress factor. Derived from the polyimide chemistry, bismaleimides resins are easier to process, more affordable, and emit fewer volatiles during their polymerization. Despite many decades of research aimed at evaluating their performance, the various chemical reactions involved in the formation of the polymeric network are not fully understood.

The reactions between bismaleimide monomers – including crosslinking via homopolymerization (1) and linear cyclo-polymerisation (2) - as well as their interactions with diallyl co-monomers through Alder-ene and Diels-Alder1 cyclization reactions, can be thermally or photochemically. However, due to a lack of solid-state analytical methods capable of distinguishing the specific carbon-carbon bonds formed in the cured resin, their respective contributions to the final polymer remain unstudied.

Molecular modeling, and more specifically reactive Molecular Dynamics can be a useful as a valuable tool for identifying the fundamental structure-property relationships in such systems. However, most reactive Molecular Dynamics approaches struggle to accurately describe the relevant reactions, especially concerted mechanisms such as Diels Alder reaction, where reactive groups cannot be easily differentiated using SMARTS notation with simple reaction formula $AB+CD=AC+BD$ proposed most of the time.

This work presents an alternative approach for describing the reactive behavior of a single-component bismaleimide resin, specifically 4,4'-bismaleimidodiphenylmethane (MDAB). The study explores two types of possible reactions, their impact on the polymeric network's topology, and estimates the fundamental properties of extreme simulated systems.

Two MDAB amorphous systems were considered: one consisting of 24600 atoms (600 molecules) and another with of 49200 atoms (1200 molecules). The reaction simulations and predictions of the network's thermomechanical properties were conducted using the Schrödinger Suite program with the OPLS4 force field.

A comparison of between linear MDAB systems with and without cyclic structures shows that the presence of cyclic structures has a minor impact on the mechanical properties when compared to the more significant changes induced by crosslinking. Overall, the simulations highlight emphasize the strong impact of crosslinking on enhancing the mechanical integrity of MDAB polymers, leading to a substantial increase in polymer moduli.

(1) High temperature and toughened bismaleimide composite materials for aeronautics, PhD Thesis G. Fischer, 2015, HAL Id: tel-01368436

(2) A. Wagner, et. al., Cure kinetics of bismaleimides as basis for polyimide-like inks for PolyJet-3D-printing, J. Appl. Polym. Sci. 2019, 47244

Comparative Analysis of Bainitic Microstructures under Varying Heat Treatment Conditions: Microstructure, Mechanical Behavior, and Yield Surface Estimation

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Bainitic steels are widely recognized for their exceptional combination of strength and toughness, making them essential in advanced engineering applications. This study presents a comparative evaluation of two distinct bainitic microstructures produced through varying heat treatment conditions. Microstructure evaluation was performed to analyze phase distribution and grain morphology. Tensile tests were conducted to evaluate the mechanical properties, including ultimate tensile strength and yield strength providing insights into the performance variations induced by the differing heat treatments. Additionally, yield surface estimations were performed to investigate the anisotropic stress-strain response and local deformation behavior of the bainitic microstructures. The findings reveal significant correlations between the heat treatment parameters, resulting microstructural features, and mechanical performance metrics. This study underscores the critical role of heat treatment in tailoring bainitic microstructures to achieve desired mechanical properties. The insights into yield surface behavior offer a deeper understanding of localized stress distribution and deformation mechanics, which are crucial for optimizing the design and application of bainitic steels in high-stress environments. These findings contribute to advancing the development of high-performance bainitic materials through precise heat treatment control.

A unique authenticator for additively manufactured parts derived from their microstructure

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The international research community is currently devoting extensive resources to the development of digital material data spaces and the associated digital twins and product passports of materials and components. A common weak link in these projects to date has been the connection between physical components / samples and their digital data and documents. This is where the concept of the unique identification comes in. Components produced using additive manufacturing can be marked for unique identification and secure authentication [1,2]. Serial numbers and machine-readable codes can be used to identify the component, and link digital product-related data (i.e., a digital product passport) to the actual components. The most prevailing solution consists of local process manipulation, such as printing a quick response (QR) code [3] or a set of blind holes on the surface or the internal cavity of hollow components. However, local manipulation of components may alter the properties, and external tagging features can be altered or even removed by post-processing treatments.

This work provides a new methodology for identification, authentication, and traceability of additively manufactured (AM) components using microstructural features that are unique to each part. X-ray computed tomography (XCT) was employed to image the microstructural features of a batch of AlSi10Mg parts. Based on size and geometry, the most prominent features were selected to create a unique digital authenticator. We implemented a framework in Python using open-access modules that can successfully create a digital object authenticator using the segmented microstructure information from XCT. We show that this method allows to authenticate individual parts from the build cycle based on its microstructural fingerprint. This is our contribution to enhancing the security and product protection of additively manufactured components.

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Advancing Digital Transformation in Material Science: The Role of Workflows Within the MaterialDigital Initiative

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D7_3 Materials Platforms & Data Spaces, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The MaterialDigital initiative represents a significant effort to advance the digitalization of material science. In addition to developing a prototype infrastructure for a shared data space and addressing semantic interoperability, the Platform MaterialDigital (PMD) emphasizes the utilization of workflows to encapsulate data processing and simulation steps in accordance with FAIR (Findable, Accessible, Interoperable, Reusable) principles. Through collaboration with the funded projects of the initiative, the Workflow Working Group is focused on establishing shared standards to enhance the interoperability and reusability of scientific data processing workflows. Central to this effort is the Workflow Store, a platform designed to facilitate the dissemination of workflows within the community, thereby enabling the exchange and replication of scientific methodologies. This presentation will discuss the challenges associated with adapting workflow concepts, offer insights into their development and application across the domains of the funded projects, and highlight the role of the Workflow Store within the initiative. Furthermore, it will outline the future roadmap for the PMD Workflow Group, aiming to further refine and expand the role of scientific workflows in advancing digital transformation and fostering collaborative research in material science.

A User-Friendly Application for Seamless Material Science and Engineering Knowledge Integration: The Graph Designer App

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

In the rapidly evolving field of Material Science and Engineering, ontologies play a significant role in digitalizing data and ensuring adherence to FAIR principles (Findability, Accessibility, Interoperability, and Reusability). They enhance interoperability among diverse data sources and formats, enabling the development of automated workflows tailored to specific applications across institutions. However, the implementation of this advanced technology often necessitates data science skills that many production engineers and materials scientists may not possess.

To bridge this gap, we present the Graph Designer App, a user-friendly web-based application designed to make ontology-based semantic digitalization accessible. This app empowers users to create domain-specific knowledge graphs utilizing pre-loaded ontologies (e.g., the PMD-co). Users can visualize these graphs, populate them with process data, and convert them seamlessly into RDF format for storage in graph databases or further processing through SPARQL queries.

A key feature of the Graph Designer App is its application of consistent graph patterns, which support the creation of generic SPARQL algorithms for complex processing tasks, such as generating and retrieving digital process chains. By simplifying intricate ontology workflows, the Graph Designer App enables users to harness semantic technologies without extensive data science knowledge.

The app functionality is illustrated through a dataset focused on high-temperature materials, featuring a use case derived from the Material Digital 2 project, funded by the German Federal Ministry of Education and Research (BMBF). This dataset is utilized to calibrate sophisticated inelastic deformation models. In this context, an ontology domain module is developed to digitalize deformation models and simulation processes, making specialized material knowledge accessible to component design and optimization engineers.

Moreover, the ontology-based knowledge graph ensures traceability of model parameters to individual data points, providing a comprehensive description of the material state. This traceability offers a solid foundation for model validation and further refinement, significantly improving reliability and reproducibility in Material Science and Engineering applications.

A Generative Adversarial Networks (GANs)-based data augmentation in the context of material testing and predicting strain rate effect

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D7_2 Semantic Interoperability, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The aerospace industry is showing increasing interest to accelerate the certification process of composite aero-structure using machine learning (ML) models since certification often requires extensive testing to validate the safety and reliability. For example, the number of experimental tests, especially at the coupon level, can be reduced using ML models by identifying patterns and relationships while still ensuring the necessary levels of reliability in material characterisation.

However, a large amount of data is essential to train ML models for learning the patterns to correctly predict the target values. The acquisition of training data, more particularly for the identification of strain-rate effects in composite materials, solely through material testing is often difficult due to high costs and time constraints, which often result in data scarcity. The lack of data presents considerable challenges when training ML models, as it can lead to overfitting and poor generalisation.

This study reports the development of a data augmentation technique with a generative model Generative Adversarial Networks (GANs) as one of the potential solutions to alleviate the issues of data scarcity. Firstly, the capabilities of the GANs model are investigated for the generation of synthetic material test data, which should capture realistic physical phenomena. Secondly, the quality of the generated data and its similarity to available experimental datasets are evaluated. Evaluation metrics based on Principle Component Analysis (PCA) are developed to determine the acceptability of the generated synthetic data. Finally, the strain-rate effects on carbon/epoxy composites are exemplarily predicted using a Gaussian Process Regression (GPR).

Furthermore, the management of a high number of heterogeneous datasets raises additional challenges to guarantee FAIR principles. In this work, experimental and synthetic data are parsed and converted into structured JSON data and labelled using an internal ontology. The storage in the research data management system of DLR, Shepard, allows to increase data findability and interoperability.

The predicted results indicate that GPR can accurately forecast the in-plane shear strength of carbon/epoxy composites across various strain rates. This accuracy is achieved using a training dataset generated through a developed data augmentation technique. This framework supports a data-driven approach for creating synthetic data and establishes its acceptance criteria while also facilitating the prediction of the mechanical properties of carbon/epoxy composites.

Semantic Technologies for Digital Transformation in Materials Science: From PMDco 3.0 to Prototypical Applications

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D7_2 Semantic Interoperability, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The digital transformation of Materials Science and Engineering (MSE) is accelerating the adoption of structured, interoperable, and FAIR data practices, in particular with respect to an advanced research data management. Semantic technologies play a pivotal role in this transformation, as they enable the integration, contextualization, and automation of diverse data sources across experimental, computational, and simulation domains. Central to these efforts is the Platform MaterialDigital Core Ontology (PMDco), now in version 3.0, which provides a robust mid-level semantic framework tailored for MSE. PMDco bridges abstract high-level ontologies, such as the Basic Formal Ontology (BFO) standardized in ISO/IEC 21838-2, with domain-specific terminologies to ensure consistency and interoperability across applications.

This presentation explores the application of PMDco and its integration into workflows within the Platform MaterialDigital (PMD) initiative. Through its deployment in electronic laboratory notebooks (ELNs), PMDco enables semantic representation of experimental data, such as tensile test results compliant with ISO 6892-1:2019-11, transforming them into machine-actionable knowledge graphs. Prototypical implementations demonstrate how semantic technologies enhance laboratory processes, improve data reuse, and streamline documentation which offers opportunities for automation and education.

Further extending its versatility, PMDco serves as a linking point for semantically representing simulation data, enabling comprehensive integration of experimental and computational datasets. This creates structured data spaces that support advanced digital workflows. Beyond PMDco, the presentation highlights the design of graph patterns and semantic shapes, showcasing generalizable methods for managing diverse data in MSE being based on data structuring and formatting.

By presenting best practices in ontology development, data acquisition, and knowledge graph generation, this talk underscores the transformative potential of semantic technologies in MSE. It offers a forward-looking perspective on the role of structured data spaces as a driver for innovation, ensuring that materials science continues to advance through rigorous, interoperable, and automated digital methodologies.

From unstructured to structured data – semantics-driven workflows for multimodal characterization of materials properties

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D7_2 Semantic Interoperability, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

A meaningful characterization and understanding of material properties depends on structured data from experiments and simulations. To combine information from both sources, a formal language enables the standardization of workflows for meaningful comparisons.

Our strategy to enable this comparison efficiently involves two main steps. First, we curate a dataset of unstructured literature sources that includes results from studies of experimental and simulation origin related to a defect property known as stacking fault energy (SFE). To structure them, we use multiple large language models (LLMs), such as GPT-4o and Mistral Large 2, within the llama-index framework. These models are used to identify key entities and extract their relationships within the structure-process-properties paradigm. The extraction process is ontology-guided, using the computational material sample ontology (CMSO) [1] and atomistic simulation methods ontology (ASMO) [2] for simulation-based studies. For experimental information we use the platform material digital (PMD)-core [3] and PMD-application. To improve the accuracy and relevance of extracted information, we employ prompt engineering techniques. This results in a structured and domain-aware organization of knowledge from literature.

Second, we have a simulation workflow with an ontological track using CMSO and ASMO with the help of the atomRDF [4] package to perform stacking fault energy calculations. This workflow incorporates a variety of computational methodologies, including gamma surface analysis, axial next-nearest neighbor Ising (ANNNI) model, and tilted cell approaches, all implemented in LAMMPS [5]. With the ANNNI model, we explore the composition and temperature dependency of SFE. The simulations are carried out on pure magnesium and aluminum as well as aluminum-magnesium alloys.

By integrating literature-based knowledge extraction with ontology-driven simulations, we construct a comprehensive knowledge graph that allows to connect data from existing experimental and simulation sources as well as new results. Within the llama-index framework, we further improve the usefulness of this knowledge graph by employing a retrieval-augmented generation (RAG) approach. This allows us to systematically extract the different steps of a workflow while preserving the correct sequence of operations. Additionally, the RAG approach enables us to determine the necessary parameters associated with each process step and allows reproducibility.

Ultimately, such a knowledge graph can serve as a robust framework for linking experimental findings, computational workflows, and materials properties, thereby improving our understanding of stacking fault energies and their dependencies across different materials and conditions.

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Advanced materials characterization tools: The development of Harmonised documents (CHADA) for Liquid Nitrogen Adsorption and SAXS results on hierarchical porous carbons.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Energy storage devices such as batteries and supercapacitors are key side-components of tomorrow's European power grid fed with a largely increased share of inherently intermittent renewable energies. Currently, nanotechnology offers several tools towards the decarbonization. Despite the already established commercial use of electrolyzers, huge efforts are required to minimise their critical content (e.g. noble metal), increase the efficiency and improve their cost-effectiveness. Therefore, a global method for widening, deepening, and accelerating the finding of sustainable technologies is needed. Addressing these challenges, KNOWSKITE-X project aims at a science-driven method to develop fine-tunable active materials relevant to energy conversion and storage. Nowadays, hierarchical porous carbon-based have attracted much attention as materials for supercapacitors. The hierarchical pores can exhibit the advantages of each pore size with a synergistic effect during the electrochemical charge–discharge process. On the other hand, the development of relevant characterization methodologies and tools for assessing key properties are critical. Due to the variety of materials and their properties, common terminologies, metadata and documentation are needed. Thus, protocols for sample handling, running characterisation and tests were developed and turned into harmonised documentation (CHADA). In this work, the CHADA scheme for liquid nitrogen adsorption (LN2) and Small Angle X-rays Scattering (SAXS) techniques were built considering: (1) Sample; (2) Method; (3) Raw data and (4) Data processing parameters, enabling the construction of the metadata structure for the specific material's characterization technique. Thus, the LN2 and SXAS characterization metadata of the developed hierarchical porous carbon were prepared and uploaded to project's data platform.

Funding

This work is part of the project entitled 'Knowledge-driven fine-tuning of perovskite-based electrode materials for reversible Chemicals-to-Power devices (KNOWSKITE-X)' funded by the European Union, and granted by the European Health and Digital Executive Agency (HaDEA) [Grant Number 101091534] as part of the "Horizon Europe" framework program (HORIZON-CL4-2022-RESILIENCE-01-19).

An Exploration of Specification Methods and Standardization Bodies and their Impact on FAIR Research Data Management in the MSE Domain

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D7_3 Materials Platforms & Data Spaces, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Materials scientists and engineers (MSE) aim to share their research findings within their communities to validate, discuss, and highlight their relevance. The current emphasis on rapid and precise material development has driven the field of integrated computational materials engineering (ICME), which relies strongly on computational support for data generation. The resulting data from such research is often large in volume and multiscale, necessitating effective summarization and abstraction methods to ensure the findings are findable, accessible, interoperable, and reusable (FAIR).

A spectrum of venues and formats for representing computationally assisted research findings exist today. As publications of research results often are intended to be FAIR, this intention necessitates representing research results in appropriate formats, complete with necessary metadata, to ensure they are reproducible and understood by other scientists for years to come. These requirements can be satisfied by appropriate specifications or standards in support of semantic interoperability and corresponding data formats tailored to the application. Yet the key question remains: which type of specification or standard is most useful for my specific application and publication?

This presentation elaborates on different aspects and perspectives to that question: (a) Stand-alone specifications are typically chosen by stakeholders who have reached a consensus within the context of a specific application. De-facto standards typically come with a proven track record of usefulness and applicability, while national or international standards have survived the scrutiny of rigorous review processes that can span many years. (b) The number and quality of authorities contributing to a standardized model can range from a central, well-vetted and well-vetting authority to standard designs that allow for multiple authorities contributing independently to the same domain. (c) The qualities of data representations for research results range from inherited requirements of "human readable", over extensibility, post-processing constraints, processing effort, and data size to convey (e.g., using JSON for material databases?).

Exemplary standards-defining organizations (SDOs) are illustrated, and corresponding approaches to registration authority models for interoperable semantics are highlighted. The advantages and disadvantages of registration authority models and data representation formats, as well as the impact of the number of authorities on design and registration procedures, are discussed in detail using examples of SDOs such as ISO, W3C, or IETF, and data representations, such as OWL, JSON, or CBOR.

While there is never one solution that fits all applications and requirements, some guidance is provided to help navigate the options in the semantic interoperability landscape presented.

Accelerating Discovery of Corrosion-Resistant Alloys Using a Self-Driving Laboratory and Closed-Loop Optimization

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The development and commercialization of novel corrosion-resistant alloys through conventional experimental approaches is often slow and costly. To accelerate this process, global efforts have focused on creating self-driving laboratories, known as Material Acceleration Platforms (MAPs). These platforms integrate automated material synthesis, characterization, and testing into closed-loop workflows, leveraging artificial intelligence (AI) and machine learning (ML) to optimize experiment design, predict material properties, and analyze data efficiently.

We have developed a MAP for corrosion research by automating liquid handling, electrochemical testing, and data evaluation. The electrochemistry module supports both the electrodeposition of various alloys and subsequent electrochemical corrosion testing. Through a closed-loop optimization framework, test results inform the selection of the next set of deposition parameters autonomously until predefined objectives are met. This iterative optimization is powered by active learning strategies and Bayesian optimization, to efficiently explore the parameter space (bath composition incl. metal ion and additive concentrations as well as the current density) to identify promising alloy compositions. In this project, we utilized the MAP to design new multi-principal element alloys (MPEAs) as corrosion-resistant electrode materials for H₂O, NO₃ and CO₂ electrolysis. The development of the MAP workflow also includes the optimization of electrochemical testing sequences, ensuring that the experimental design maximizes data efficiency, minimizes redundancy and uses multiple metrics for performance evaluation. In one optimization run, open circuit monitoring, electrochemical impedance spectroscopy (EIS), linear polarization resistance (LPR) and chronoamperometry (CA) measurements can be configured in a sequence. In each campaign, the MAP selects promising leads for upscaling, either by means of electrodeposition or powder metallurgy and arc-melting. Spectroscopic and electrochemical characterization techniques are then employed with selected systems to validate the MAP-driven leads.

This presentation will provide an overview of the MAP's design, its integrated modules, and workflow implementation. We will also highlight key findings from our FeNi-X MPEA system and discuss how closed-loop optimization strategies enhance the rapid discovery of corrosion-resistant alloys.

ML-driven optimization of corrosion inhibitor mixtures with an automated platform

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The CorRobot initiative is a pioneering project in materials science that automates corrosion protection material discovery through an AI-driven workflow, integrating Bayesian Optimization (BO) with neural networks. Traditional discovery methods for corrosion inhibitors are often slow, costly, and inconsistent due to variations in testing methodologies and environmental conditions. CorRobot streamlines this process by optimizing the automation platform with intelligent decision-making, enabling efficient and precise inhibitor formulation discovery.

The CorRobot workflow leverages neural networks to model complex electrochemical relationships, while BO intelligently selects the most informative experiments, reducing the number of trials required. This adaptive learning system refines experimental conditions in real time, prioritizing promising formulations and improving the efficiency of corrosion inhibitor screening. By integrating predictive modeling with automated laboratory processes, CorRobot minimizes human intervention while maximizing data-driven optimization.

A key breakthrough of the CorRobot project is the identification of an effective low-concentration mixture of cerium nitrate and sodium fumarate for iron corrosion protection. This result underscores the power of AI-enhanced workflows in uncovering novel inhibitor synergies often overlooked in conventional methods. The seamless integration of BO and neural networks accelerates discovery cycles and enhances reproducibility in corrosion science.

Beyond improving efficiency in corrosion inhibitor discovery, CorRobot aligns with the FAIR data initiative to enhance predictive simulation tools for material properties. By optimizing workflow automation and data utilization, CorRobot's AI-driven platform has the potential to revolutionize materials science applications beyond corrosion protection. This project paves the way for intelligent, sustainable advancements in surface technology and industrial chemistry.

Keywords: Automation, Corrosion Inhibition, Artificial Intelligence, Bayesian Optimization, Neural Networks, Workflow Optimization, Materials Discovery, Electrochemical Characterization.

Materials Data Infrastructure and Ontology Development for Exemplary Reference Dataset

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The development of new engineered materials relies on high-quality reference data and material standards. Especially mechanical properties at high temperatures, such as creep resistance, are crucial for potential structural applications of new alloys. Within NFDI-MatWerk, the exemplary reference dataset uses data from creep experiments on a single crystal Ni-based superalloy with benchmark material properties, along with a detailed experimental description and relevant information on material provenance and condition.

The FAIR (Findable, Accessible, Interoperable, and Reusable) principles are applied when distributing the reference datasets along with their metadata. FAIR Digital Objects (FDOs) are created to support machine readability and accessibility using Persistent Identifiers (PIDs). Our proposed workflow highlights two aspects: creation of FAIR DOs and ontology development. The experimental data generated is stored in repositories, such as Coscine or published on, for instance Zenodo. We develop a data schema to define a structured approach for collecting all the required information on a creep experiment. The entries are grouped according to their content and summarized under respective headlines, thereby forming a hierarchy of concepts. Based on this schema we create FDOs to make the reference dataset and its metadata interpretable for the external material scientists' community. Moreover, we develop a semantic description in the form of an ontology and a metadata schema to make the information explicit, and to enable interoperability between databases, automated analysis, and integration into simulation workflows. The reference dataset ontology (RDO) provides a formal description of concepts, which define reference data, e.g., standard, validation, curation, etc. and are based on the exemplary reference dataset. Thus, classifies the RDO as a top-level ontology with universal concepts. The experimental workflow and material characteristics, which are important for the interpretation of research data, must be described in an application-level ontology or mapped to other related ontologies, e.g., PMD (Platform Material Digital) Application Ontologies.

This approach ensures the FAIRness of the data and accelerates research in the field of Material Science and Engineering by providing high-quality reference datasets and material standards for the development of new alloys for high-temperature applications. The workflow, part of an overarching framework for management of reference data, has been successfully implemented for an example use case and will be supported by easy-to-use tools in the future.

Acknowledgments: This work is part of the consortium NFDI-MatWerk, funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under the National Research Data Infrastructure – NFDI 38/1 – project number 460247524.

Digital representation of physical metallurgical knowledge

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D7_2 Semantic Interoperability, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

We will here present a framework for digitally documenting materials knowledge addressing all levels of semantic documentation, including cataloguing as well as structural, contextual and semantic documentation. It ensures that the documented data becomes FAIR with a special emphasis of making it meaningful, linked and actionable. The documentation itself is stored in a knowledge base, while the documented resources (e.g. datasets) may be stored elsewhere. All types of resources (datasets, materials, processes, samples, instruments, models, researchers, etc...) can be documented and related to each other using the Elementary Multiperspective Material Ontology (EMMO) and its domain ontologies. It ensures consistency of data documentation with materials science knowledge. Datasets are furthermore documented using the DCAT-AP vocabulary (making them accessible and useful for DCAT-aware data services) and preferably also with formalised data models mapped to the ontologies (to document their structure and achieve interoperability at a numerical level).

The framework is developed with the perspective of the data producer focusing on making the documentation process as seamless and simple as possible, while ensuring that all aspects of the FAIR principles are addressed. The data producer is only exposed to well-defined keywords that may either refer to literal values or other resources in the knowledge base. Behind the scenes, the keywords are mapped to ontological data properties (literals) or object properties (resources) using a JSON-LD context. The set of available keywords can be extended with a custom JSON-LD context. To keep the required input for the data documentation to a minimum, the framework reuses the mappings and data models to prepopulate all input fields that can be inferred from the documented resource. Complex (potentially nested) inferences and transformations are achieved with the help of so-called mapping functions. They are functions typically implemented in Python, whose input and output are defined from the ontologies. They are documented like any other resource and applied transparently by the framework whenever transformations are needed between different literal representations.

To document a series of similar resources, the framework offers a spreadsheet-like interface. This allows the data producer to prepare the documentation using a familiar tool like Excel and commit the documentation of all the resources in one go.

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Enhancing FAIR Data Management in Materials Science and Engineering (MSE): Integrating FAIR Digital Objects into the MSE Knowledge Graph

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The Materials Science and Engineering Knowledge Graph (MSE-KG) [1] serves as a central knowledge base for integrating and structuring research data within the NFDI-MatWerk [2]. It provides a semantic backbone that connects datasets, research outputs, institutions, and infrastructures, ensuring interoperability and enhanced data discovery. The MSE-KG facilitates a unified and structured approach to manage heterogeneous data. Despite its structured approach, challenges remain in ensuring that research objects remain machine-actionable, persistent, and interoperable across different domains. To address these challenges, the integration of FAIR Digital Objects (FDOs) has been proposed as a solution for enhancing machine-actionability and interoperability of digital research assets in the MSE domain.

In the context of NFDI-MatWerk, with the integration of FDOs into the MSE-KG we aim to enhance the findability, accessibility, interoperability, and reusability of research data. This work investigates the representation of FDOs within the knowledge graph, addressing key questions such as the availability of FDOs, their association with datasets, provenance records, and licensing terms. By linking datasets, publications, and software to their respective FDOs, the MSE-KG provides structured access to research objects and ensures their long-term usability. The study further explores how FDOs are referenced within the knowledge graph, their accessibility via persistent links, and the implications of integrating semantic descriptions for enhanced machine-actionability.

References

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Improving the data-driven experimental materials science: PASTA-ELN electronic laboratory notebook

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Electronic laboratory notebooks (ELNs) revolutionize research data management in experimental materials science by streamlining workflows and improving efficiency. Unlike traditional manual methods of documentation and sharing research data, ELNs save scientists valuable time and effort, allowing them to focus on the core aspects of their work. This presentation introduces PASTA-ELN, a customized ELN solution designed specifically for experimental materials science.

One of the standout features of PASTA-ELN is its innovative approach to raw scientific data storage. By storing raw data locally on the researcher's hard drive, PASTA-ELN ensures data accessibility and application of further analysis protocols, while safeguarding data confidentiality and security. Additionally, metadata related to measurements, samples, etc. is stored in a dynamic SQLite database, which functions like a document database for efficient data management.

PASTA-ELN also includes extractor add-ons that automatically process raw measurement files by scanning the working directory. These add-ons capture thumbnails, data, and metadata, integrating them seamlessly into the project. Researchers can customize these extractors to suit their specific requirements for data and metadata processing.

As a member of "The ELN Consortium", PASTA-ELN facilitates data exchange and collaboration through the RO-Crate standard via a compatible (.eln) file format. This feature enables effective data archiving, migration across platforms, and ensures long-term data interoperability, fostering collaboration across research teams and institutions.

EMMO: an ontology based on universal materials science concepts

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D7_2 Semantic Interoperability, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The task of building a 'materials science knowledge graph' is intriguing but also appears daunting. However, in materials science we can build on fundamental physical science principles and foundations. That is how the EMMO ontology has been constructed from the bottom up. The paper will discuss these foundational requirements in relation to the ISO standard for Top Level Ontologies, and how materials science desiderata are fulfilled by EMMO. Based on these solid foundations, examples of the EMMO discipline and domain ontologies will be showcased. In particular, we highlight the CHAMEO ontology for materials characterisation, which underlies the updated "CHADA" CWA 17815:2025. Finally the application of CHAMEO to industrial applications including battery testing and automotive coatings will be demonstrated.

This work received funding from the European Unions Horizon 2020 programme, Grant Agreements n. 952869, 862136 and 953167

pyiron - Developing and managing materials science workflows

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

To support and accelerate the development of simulation workflows in computational materials science, the pyiron Integrated Development Environment (IDE) (<https://pyiron.org>) has been introduced with a focus on FAIR (findable, accessible, interoperable and reusable) workflows. The pyiron IDE covers the whole simulation life cycle in a single software platform and provides both developers of simulation workflows and their users with an intuitive and easy to use Jupyter notebook based interface that shields them from the underlying data and job management. Using a generic input and output format rather than code specific ones allows incompatible simulation codes to directly communicate, e.g., to exchange key quantities such as energies and forces of an atomistic configuration at every timestep of a molecular dynamics trajectory. Further, these simulation workflows can be applied for highthroughput screenings over the whole periodic table. This is enabled by the pyiron job management system, which allows an easy up-scaling from interactive Jupyter notebooks to HPC handling thousands of parallel simulations.

Within this presentation following a short introduction of the fundamental concepts behind the pyiron IDE, the focus will be on the user experience with this platform as the pyiron development is primarily driven by these applications to accelerate Materials Design. Some concepts that turned out to have a particular impact on the usability and gained traction with the pyiron users will be emphasised. This includes the generic interface for atomistic simulation codes, the interactive coupling of simulation codes during their execution, the up-scaling of simulation workflows for high-throughput screenings, and the extendability of pyiron which enables the integration of new simulation codes with minimal overhead. The presentation will end with an outlook on future innovative developments in order to further improve the attractiveness of pyiron for a broad range of users and simulation topics.

Building a Legacy Lab for Advanced Functional Materials: Integrating Synthesis and Characterization Capabilities

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The rapid evolution of Materials Acceleration Platforms (MAPs) requires robust, interconnected research infrastructures to speed up the discovery and optimization of new materials. In this context, we are developing a distributed MAP that connects multiple legacy laboratories by integrating the expertise and experimental capabilities of the Solid-State Group through a data pipeline. This initiative aligns with the EU-MACE framework, fostering a data-driven and AI-assisted approach to materials research.

The distributed MAP will encompass various synthesis and characterization facilities, including:

High-Temperature Synthesis and Crystal Growth Laboratory – focused on the preparation and single crystal growth of inorganic-based materials.

Molecular and Electrochemical Synthesis Laboratory – specialized in the synthesis of molecular-based materials with unconventional electrical and magnetic properties.

Polymer Synthesis Laboratory – leveraging expertise from the Organic Electronics Laboratory (IT) to explore organic conducting materials.

Magnetic and Electrical Characterization Laboratory – equipped for measurements at low temperatures and high magnetic fields.

Mössbauer Spectroscopy Laboratory – providing insights into hyperfine interactions and electronic structures.

By digitally connecting the synthesis and characterization laboratories, we aim to create a highly efficient research environment that enhances reproducibility, data sharing, and machine-learning-driven material discovery. This initiative will serve as a strategic step toward implementing MAPs within the EU-MACE framework, strengthening Europe's leadership in the field of advanced functional materials.

Interoperable workflows as an enabler for data-driven materials design

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D7_1 Workflows, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Material science problems have intrinsically multiscale and multiphysics characters, and require us to employ a combination of methods on different time and length scales to resolve critical features. Normally creating workflows that connect data in multiple scales and various methods is a cumbersome task. pyiron, an integrated development environment (IDE) for material science, contains modules for the atomistic as well as continuum scale that make a seamless connection possible. To this end, it provides a high-level coherent language in a unified workflow platform to study materials, for example, with LAMMPS simulations in the same framework as crystal plasticity codes such as DAMASK. The latter is integrated such that all required input files can be generated, the analysis can be executed and the routines of the DAMASK post-processing library can be employed.

One example of a multi-scale workflow is the simulation of a multi-stage cold rolling process using pyiron. As with every DAMASK simulation, pre-processing includes the creation of the representative volume element and the material definition. It contains elastic properties that are obtained from LAMMPS calculations. To simulate the actual rolling process, the rolling subclass was implemented in the pyiron-job class. Since the total height decrease in technical rolling processes can be very large, the implementation provides for optional regridding between rolling passes. This is also required for the coupling with OpenPhase for simulating recrystallization using pyiron. To ensure interoperability between evaluation and simulation tools, work was done on a semantic representation of pyiron

A seamless dataflow combining material, virtual engineering workflows and production data in the project lifecycle

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D7_3 Materials Platforms & Data Spaces, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Advancing industrial efficiency in high-mix/low-volume production requires innovative digital solutions that seamlessly integrate simulation workflows, process control strategies and data-driven optimisation algorithms. The development of an open innovation platform and an interoperable digital pipeline is designed to enable a design-by-simulation optimization framework. The approach integrates feedback and inline feedforward control strategies to enhance the performance of industrial systems by linking materials modelling, materials characterization, simulation-based digital twins, and data-driven models. The framework dynamically updates through distributed production data collected from embedded IoT edge devices and product quality metrics.

A unified methodology is established and demonstrated through two case studies. The first focuses on multidisciplinary optimization to ensure certified path-planning strategies for manufacturing topology-optimized structural elements via Wire-Arc Additive Manufacturing (WAAM) in the construction sector, exemplifying a low-volume production scheme. The second explores optimized design and manufacturing strategies for producing Carbon Fibre Sheet Moulding Compound (CF-SMC) components in the automotive sector, representing a high-mix production scenario. These demonstrations highlight the framework's potential to drive efficiency and innovation across diverse industrial applications.

Enhancing Data Acquisition in Manufacturing: LLMs for Effective Material Property Databases

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D7_3 Materials Platforms & Data Spaces, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Large Language Models (LLMs) facilitate the development of up-to-date material property databases, offering significant potential for identifying materials with target properties, resolving discrepancies in reported values, and automating inputs for tools like Finite Element Analysis. This work explores Retrieval-Augmented Generation (RAG) for extracting material data, particularly from tabular formats in PDFs with varying formats. Parsing methods were evaluated for robustness, and extracted data was processed into structured formats, incorporating automatic conversion into SI units to ensure consistency. LLM-generated outputs were assessed using standard metrics, while a custom metric was designed to assess domain-specific accuracy and reliability.

Laboratory Automation Aiding the Design of Multifunctional Nanocomposites

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D7_3 Materials Platforms & Data Spaces, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Advanced polymer nanocomposites are relevant to a broad spectrum of applications, from clean and efficient industrial separations through innovative medicine to safe commodity products with low-impact life-cycles. We specifically focus on sustainable and multifunctional nanocomposites, which incorporate bio-based polymer matrixes and multiple advanced functional components such as 2D materials and/or metal-organic frameworks. Formulating the composition of such nanocomposites tuned to a specific application poses a significant challenge as they need to include the appropriate components to ensure desired performance while simultaneously addressing constraints regarding the physicochemical compatibility between them as well as the overall dependence on the processing involved. We are streamlining this process by the development of a dedicated material acceleration platform (MAP). The MAP is a closed-loop experimental setup where laboratory work related with preparation and characterization of samples is performed by a robot while machine learning algorithms dictate what experiments to make in order to achieve desired results with minimal number of experiments. Unlike other emerging MAPs that work with solution or thin-film chemistries, our MAP focuses on thermoplastic materials, which are processed in a pelletized form and require solid specimens for property testing.

Our presentation will introduce the concepts behind our nanocomposite MAP and summarize the recent progress in its development, which for far have included (i) an automated twin-screw extrusion process for nanocomposite preparation, (ii) a nested Bayesian optimization loop for 3D printing of testing specimen executed on a pellet 3D printer farm, (iii) a collaborative robot-operated analogue Charpy impact test instrument and (iv) an outer Bayesian optimization loop for navigating the nanocomposite formulation space. Such organization of the MAP allow fairly easy extension to other properties such as tensile tests, thermal conductivity, degradation profiles, etc, which are the subjects of on-going work. The latter will also be highlighted in the presentation.

Accelerated steel development on the ALPmat platform

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D7_3 Materials Platforms & Data Spaces, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The development of novel steels is highly demanding due to their complexity in terms of chemical composition and the strong dependence of their mechanical properties on the processing route. Moreover, the development process involves a series of experimental steps, including synthesis, sample preparation, multi-scale structural characterization, and mechanical testing. Therefore, the usage of AI-based methods for optimizing chemical compositions and process conditions, the integration of data-driven and physics-based modeling, and advanced FAIR data management solutions are key to success.

The ALPmat is an Active Learning Platform for MATerials design. A hybrid approach is followed for optimal exploitation of the available knowledge, where physical models and expert knowledge are combined with data from observations. The resulting hybrid models are used for an Active Learning Loop (ALL) to improve the addressed properties iteratively via optimization of the material's chemistry and processing conditions while minimizing the number of new samples.

We will present the details of the ALPmat in terms of hardware and software for the platform backbone, the FAIR database, the framework for running physical modeling and Bayesian optimization algorithms, and integrated software services. Moreover, we will present the data model for bainitic steels. This data model is linked to the state of the investigated sample and is used to uniquely identify use case-specific synthesis, processing, and characterization steps. It serves as a basis for ingesting comprehensive metadata and ensures the data are fully FAIR.

Finally, we will demonstrate the capabilities of ALPmat for running ALLs and present our results for bainitic steels, where we did a multi-objective optimization of the uniform elongation and the yield strength as a function of chemical composition and processing conditions.

Automating Knowledge Graph Composition for Multi-Scale and Interdisciplinary Research

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D7_2 Semantic Interoperability, Seminario 1 + 2 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

In multi-scale modeling and interdisciplinary research, the integration of heterogeneous data and domain knowledge is essential for achieving comprehensive insights. Ontology-driven knowledge graphs (KGs) serve as a powerful framework for structuring and connecting information across different disciplines and scales. However, manually constructing and updating KGs is a time-consuming and error-prone task. This talk introduces semantikon, a software package designed for automating the composition of knowledge graphs based on user-defined workflows. By leveraging ontologies, reasoning mechanisms, and workflow-driven orchestration, semantikon ensures semantic consistency, enhances interoperability, and facilitates dynamic knowledge integration. This approach enables researchers in materials science to efficiently model complex systems, bridge disciplinary boundaries, and accelerate data-driven discovery. We discuss methodologies for workflow-based KG automation, key challenges, and potential applications in materials science.

The Platform MaterialDigital Workflow Store - Sharing Scientific Workflows within the MSE community

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembere 17, 2025, 13:10 - 14:30

The MaterialDigital Platform (PMD) project, launched in 2019, aims to advance digitalization in material science and engineering in Germany. The project focuses on creating a robust infrastructure for managing and sharing material-related data.

The PMD Workflow Store is a key component of this initiative. It serves as a repository where scientists and engineers can access, collaborate on, and upload workflows for material simulation and analysis. The platform features centralized access and sharing, automated validation, a searchable index, and a commitment to continuous enhancement based on user feedback.

Here, we introduce the PMD Workflow Store and demonstrate how it streamlines collaboration and knowledge sharing within the scientific community. We show that this platform simplifies access to diverse workflows, ensuring high standards of quality and consistency. The Workflow Store accelerates research and development by providing a single entrypoint to discover and share workflows and workflow modules from and with the MSE community.

We highlight the transformative impact of the PMD Workflow Store on the material science community. This platform not only meets current needs but also aims to incorporate tools for future advancements. As digital workflows become indispensable in material science, the PMD Workflow Store aims to become a vital resource for researchers and engineers.

Representing MSE Research Metadata Using the NFDI MatWerk Ontology: Patterns and Use cases

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

NFDI-MatWerk (National Research Data Infrastructure for Materials Science and Engineering) is a German initiative focused on developing a digital infrastructure that integrates decentralized data, metadata, workflows, and a materials ontology to improve interoperability and reproducibility in materials science and engineering (MSE) research data processing. The NFDI MatWerk Ontology (MWO) is a unified framework developed by the Task Area Ontologies for Materials Science (TA-OMS) within the NFDI-MatWerk initiative. Its primary goal of MWO is to standardize the representation of materials data, ensuring consistency and interoperability across diverse datasets and research activities. By creating structured vocabularies and frameworks, MWO facilitates efficient data discovery, integration, and reuse, thereby enhancing researchers' ability to find, share, and utilize materials data effectively. The newest version of MWO (V3.0.0) has been mapped to the Basic Formal Ontology (BFO) and NFDIcore ontologies and integrated well with Platform MaterialDigital Core Ontology (PMDco v3.0.0). This talk showcases example ontology design patterns (ODPs) developed using MWO and their application in representing practical MSE-based use cases, highlighting their capacity to enable scalable, reusable, and semantically robust knowledge frameworks. ODPs are reusable and modular components that encapsulate best practices for solving common challenges in ontology development, thus help domain experts and developers to create consistent, efficient, and extensible ontologies. The example structural, content-based, and presentation ODPs were designed to define foundational arrangements of entities, address domain-specific knowledge, and optimize user interaction with ontologies. To illustrate the practical utility of ODPs, we presented several use cases within the MSE domain, such as representing metadata for materials, instruments, large-scale facilities, researchers, organizations, educational events, resources, datasets, data portals, and material research software. Through these cases, we emphasize how ODPs facilitate development by offering standardized templates for tasks such as hierarchy modeling, semantic relationship management, and data source integration, while also supporting ontology-driven solutions that are technically sound and adaptable to changing domain requirements.

High-Throughput SEM for Microstructural Analysis in Additive Manufacturing

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D8_1, Machado Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

High-throughput microstructural characterization is critical for understanding and optimizing the complex, inhomogeneous microstructures formed during metal additive manufacturing (AM) processes such as Plasma Arc Additive Manufacturing (PLAAM). Rapid thermal cycles in these processes leads to microstructural heterogeneities, including defects (e.g., lack of fusion, porosity, cracks) and complex grain structures, which significantly impact material performance.

This study focuses on optimizing data acquisition speed in scanning electron microscopy (SEM) while resolving critical microstructural details. By optimizing the selection of critical imaging parameters, such as dwell time and pixel size, acquisition times are significantly reduced while maintaining a controlled error rate. This approach enables large-area imaging comparable to optical microscopy but with the significantly higher resolution of SEM.

A Python-based framework automates defect detection in secondary electron (SE) images, extracting key metrics such as defect area, roundness, and orientation. Meanwhile, backscattered electron (BSE) imaging leverages channeling contrast to analyze grain structures. A deep-learning model, trained on electron backscatter diffraction (EBSD)-derived labels, facilitates grain segmentation and detailed assessments of grain area and aspect ratio. This method eliminates the need for chemical etching, preserving the sample surface for further analysis while providing comprehensive insights into grain structures.

The proposed high-throughput SEM framework integrates automated defect detection and grain segmentation to deliver comprehensive microstructural insights. By balancing data acquisition speed and accuracy, this scalable approach improves our understanding of microstructural evolution in additive manufacturing by uncovering the underlying relationship between processing parameters and resulting microstructure and properties.

Microstructure and micromechanics evolution of β -Ti gum metal (TNTZO) during cyclic loading using synchrotron diffraction

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

β -Titanium alloys have gained interest in the past few years for their excellent mechanical properties, including high strength and low elastic modulus. A considerable number of these alloys are a perfect fit for medical applications as they consist of elements with excellent biocompatibility, such as Ti-Nb-Ta-Zr alloys known as TNTZ. TNTZ alloys offer elastic modulus values as low as 56 GPa and strength up to 1 GPa. Using additive manufacturing techniques, such as LPBF, to build customised TNTZ medical implants increases the potential for a better patient-specific healthcare concept. However, inevitable oxygen pickup during powder atomisation and the LPBF process results in a high-oxygen version of these alloys referred as TNTZO (Gum metal) with altered mechanical properties and deformation mechanisms, as oxygen is found to block the stress-induced phase and twinning transformations during loading. Post-processing heat treatments have been found to alter the microstructure and the micromechanics of TNTZO alloys, leading to a wide range of macro-mechanical properties. The fact that most loading on load-bearing implants, such as hip and knee joints, is cyclic loading raises special concerns about the material response to this loading case. These changes in the micromechanical behaviour of the material under cyclic loading are crucial for fully enhancing the predictability and reliability of the alloy for medical applications.

In this study, synchrotron diffraction was used to analyse the microstructural properties of the as-built TNTZO in comparison with the solution-treated and aged versions of the alloy. The effect of heat treatments on the lattice-scale elastic moduli and dislocation density of the alloy was analysed. Moreover, the microstructural texture evolution and the dislocation density of the different samples were assessed along with cyclic loading using the Williamson-Hall technique for peak analysis. The structure-property relationship was studied by examining the aforementioned micromechanical changes against the measured elastic modulus softening through successive loading cycles. Similarly, the presence of α -phase after aging is related to a noticeable increase in the recoverable strain value along the test accompanied with hysteresis loop between the loading and unloading elastic regions. These findings provide insight into the deformation mechanisms governing cyclic superelasticity in β -Ti alloys and highlight the role of microstructural refinement in optimising mechanical performance. The results contribute to the broader understanding of fatigue behaviour in β -Ti alloys and their potential for high-strain applications requiring enhanced recoverable deformation.

Temperature Gradients for data mining

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Experimental data on phase diagrams, chemical and thermal diffusion and interfacial energies are required for reliable alloy and database development, the prediction of microstructural evolution and materials properties. Considering the number of alloy systems and alloying elements, efficient experimental methods are needed to characterize metallic materials. Experiments with concentration gradients offer a high throughput. Widely known are methods with diffusion couples and multiples or thin films. Less common are methods that combine temperature and concentration gradients.

At the university of Jena, methods for effectively obtaining thermodynamic, kinetic, and thermal data have been developed over the past 20 years. The early methods are related to directional solidification, where temperature gradients are used to adjust microstructures. In sample regions where solid and liquid phase co-exist, locally separated, temperature-dependent phase equilibria are formed and accessible to subsequent characterization. In this way, large sections of solidus, solvus and liquidus lines in binary alloys or paths in multicomponent systems can be determined with a highly reduces experimental effort. The concept also allows for the synthesis of pure intermetallic phases as bulk materials for measuring and modelling heat capacities. Recently, the method development focused on analyzing non-equilibrium or transient states. The efficient characterization of thermal properties is one application, another is the measurement of interfacial energies of alloys from metastable microstructures. The poster gives an overview of the methods and introduced basic concepts.

Combinatorial Screening of Magnesium-Scandium Thin Film Alloys

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D8_2, Machado Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Mg-Sc thin film library was produced by thermal evaporation technique focusing a compositional spread of Sc up to 20 at.%. Microstructural investigations were carried out by scanning electron microscopy (SEM), X-ray diffraction (XRD) and Atomic Force Microscopy (AFM) analyses and the results demonstrated that microstructures primarily consisted of hexagonal facets corresponding to (0002) basal planes. The wall size of these facets showed a significant alteration with increasing Sc concentrations. Nanoindentation tests revealed that the hardness of Mg showed enhancements up to around 10 at.% of Sc, above which it decreased. Electrochemical characterizations were conducted through Scanning Droplet Cell Microscopy (SDCM) performed at specific Sc concentrations. Potentiodynamic polarization and Electrochemical Impedance Spectroscopy (EIS) tests showed that increasing Sc content up to specific composition shifted corrosion potential of Mg toward positive direction and improved the corrosion resistance of Mg. Sc led to the improvement on the protectiveness of the surface layer formed during their exposure to the electrolyte.

Deformation Mechanisms in Ti-Nb Graded Materials: Insights from High-Throughput Analysis

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septembre 15, 2025, 13:15 - 14:30

β -metastable alloys have attracted growing interest in recent years thanks to their great work-hardening, allowing to combine strength and ductility. These properties are obtained by triggering the transformation-induced plasticity (TRIP) and twinning-induced plasticity (TWIP) effects, that are related to the metastability of the β -phase, and thus the composition of the alloy. However, despite their promising properties, a large development of these alloys remains. Current design approaches to target compositions of this family are mostly semi-empirical or empirical and rely on a large dataset resulting from numerous papers. The inherent drawback of this approach is that papers do not necessarily study the alloys in the same microstructural conditions (grain size, processing conditions...) or do not provide all the characteristic of the material (oxygen content...). Thus, exploiting such datasets leads to uncertainties. which might limit or postpone the development of this family of materials.

To tackle this problem, we propose using compositionally-graded materials. The Ti-Nb binary system is selected as a case-study. Indeed, depending on the Nb-content, it displays all the deformation mechanisms of interest, and is well documented in the literature. The graded material is prepared by diffusion couple with the two end-compositions Ti-18Nb and Ti-30Nb (at.%), framing the compositions of interest. Triggering the deformation mechanisms is done thanks to a single tensile test, and subsequent analysis of the deformed microstructures is done by electron microscopy. The results demonstrate that this approach allows us to quickly identify the compositional domains where a certain deformation mechanism is obtained. As all the compositions contained in the sample have undergone the same processing route, one sample leads to one solid dataset. The efficiency of the approach, in terms of time, is also discussed by comparing the tensile approach used here, to another one using micro-indentation.

High-throughput hard X-ray reflectometry to investigate interfaces in materials

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D8_2, Machado Room (Level -2), septembre 15, 2025, 10:50 - 13:10

The ability to probe interfaces in complex hetero-materials is paramount to fully understand and control the properties of the materials in question. Yet, accessing such interfaces is usually difficult as they represent only a small volume fraction of the samples of interest. Typically, phase fronts or grain boundaries have often been studied using direct-space imaging techniques, such as electron or X-ray microscopy or tomography. Even though spatial resolution has much improved over time, imaging at the ultimate resolution comes either at the cost of sample preparation (e.g. TEM lamellae, FIB milling) or complex measurements (e.g. ptychography), severely hindering high-throughput considerations.

In this presentation, we will discuss how recent developments on the GMT instrument at beamline BM32 at the European Synchrotron Radiation Facility have enabled the investigations of solid-solid or solid-liquid interfaces with a high resolution and at a high sample rate, using Hard X-ray reflectometry (HXRR). HXRR basically consists in measuring the reflection of X-rays on an interface between two materials of different refraction index (i.e. different electron density), as a function of the angle of incidence. The hard X-rays used (27 keV, 0.4592 Å) easily penetrate matter and can access buried interfaces, i.e. going beyond the limitations to surfaces. The measured HXRR signal probes of the electron density gradients across interfaces, with a resolution across the interface that is a fraction of the wavelength, effectively achieving sub-Angström resolution.

We will show how the principal requirement of reflectometry, namely well-defined interfaces, can actually be harnessed to investigate a broad range of topics, from model systems to evidence surface reactivity, to industrially relevant materials for advanced microelectronics substrates. The technical developments recently funded by the French DIADEM program now offer the opportunity to mount up to 650 samples on a single sample stage, enabling the high-throughput, fast screening of interfaces at the sub-atomic monolayer scale. Examples in a broad range of application fields, ranging from chemical separation of strategic elements to interfacial reactivity in electrolytes or direct bonding interfaces in semiconductors, will illustrate the new capabilities of the GMT instrument, open to the community.

High-Throughput Materials Informatics Integrating Ab Initio, Machine Learning, and CALPHAD Data

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D8_2, Machado Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Traditional CALPHAD modelling (CALculation of PHase Diagrams) has been proven effective in accurately predicting phase stabilities and material properties as functions of temperature, pressure and composition. However, this approach has notable limitations, including the significant time required to develop comprehensive databases and a scarcity of available relevant experimental data. To address this challenge, we present a Machine Learning (ML)-enhanced, high-throughput approach that leverages the aiMP and aiOQ databases to bridge the gap between first-principles calculations (DFT) and CALPHAD-based metallic alloy design.

The aiMP and aiOQ databases integrate ML predictions of entropy and heat capacity, derived from large-scale datasets of thousands of compounds, offering a significant advantage over typical models trained on more limited datasets of only hundreds of compounds. These databases facilitate three key applications that align with high-throughput materials discovery:

1. Data Cleaning & Reliability assessment: Anomaly detection in curated databases, as well as inconsistencies within aiMP itself, ensuring more robust predictions for CALPHAD modeling.
2. High-Throughput Alloy Screening: Enabling the rapid evaluation of a wide range of material compositions to identify promising candidates for further experimental and computational investigation.
3. Phase Diagram Estimation and Optimization: Providing an efficient starting point for phase diagram development through traditional CALPHAD optimization approaches.

While curated databases continue to hold an advantage in terms of accuracy and reliability for specific applications, aiMP and aiOQ represent a transformative approach to materials data management. These databases bridge the gap between DFT 0 K data and the need for 298 K data for CALPHAD modelling, while maintaining a relatively small error margin, which is likely influenced primarily by the functional used in DFT calculations, the machine learning models, and errors in experimental values. By supporting highly automated workflows and encompassing a far broader range of materials than is feasible in manually curated databases, aiMP opens new possibilities for large-scale materials discovery and thermodynamic analysis.

To illustrate the practical impact of this approach, we demonstrate the combined application of curated CALPHAD databases and aiMP in the high-throughput design of a novel Fe-based hardfacing alloy.

Optimized Electrodeposition of Multi-Principal Element Alloys through Automation by Material Acceleration Platform

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D8_1, Machado Room (Level -2), septiembre 15, 2025, 9:20 - 10:20

Multi-Principal Element Alloys (MPEAs) are garnering significant academic and industrial interest due to their exceptional mechanical and anti-corrosion properties, making them promising materials for engineering applications. Characterized by a disordered atomic distribution within their crystal lattice, MPEAs offer high catalytic efficiency, excellent thermal stability, and sluggish diffusion kinetics, depending on their composition and crystal structure. Notably, several MPEAs, such as the CrCoNi alloy, exhibit excellent corrosion resistance and potential for electrocatalytic applications.

This project aims to develop an automated optimization process for the electrodeposition of first-row ternary MPEAs, investigating their electrochemical properties and testing their application as electrodes in electrocatalysis within a lab-automation loop. While binary and ternary alloy electrodeposition has been achieved, the electroplating of MPEA films with desired bulk properties remains in its infancy. The vast compositional space of MPEAs and the development of respective electrodeposition methods add to the complexity of this topic. Achieving MPEA films with inherent bulk alloy properties requires precise bath compositions and the selection of appropriate additives.

Initially, the development and selection of bath components is based on existing literature to identify bath compositions that facilitate the deposition of the desired MPEA film. However, the challenges of system optimization reported in the literature for MPEA electrodeposition present an opportunity to utilize an automated lab approach. Consequently, initial bath compositions are refined based on the performance of the MPEA film in terms of composition, electrochemical properties, and surface-specific parameters.

The characterization of the deposited films is both automated and manual. Key electrochemical characterization methods include Electrochemical Impedance Spectroscopy (EIS), linear resistance polarization, and potentiodynamic polarization. Scanning Electron Microscopy (SEM) is primarily used for surface morphology analysis, while in-situ Atomic Force Microscopy (AFM) is conducted on optimized electrodeposition systems to investigate deposition mechanisms. Film compositions are determined using Glow Discharge Optical Emission Spectroscopy (GDOES). Additionally, PM-IRRAS and Raman spectroscopy data on additive adsorption at the metal surface support the automation process database. The results of this study will be presented herein.

Phase transformations during post-processing of metastable β titanium alloys fabricated through additive manufacturing

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D8_2, Machado Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

The microstructural evolution and phase transformations in the metastable β titanium alloys, widely used in aerospace applications such as aircraft frames and landing gear, were investigated in the context of wire arc additive manufacturing (WAAM). This alloy offers exceptional strength and corrosion resistance with an elastic modulus of approximately 110 GPa, making it a promising candidate for advanced manufacturing techniques. Due to the unique microstructural characteristics produced by WAAM, including large columnar β grains and the absence of the nodular and acicular α -phase typically observed in forged alloys, mechanical properties may deviate from standard values to lower strength values of approximately 800 MPa and an elastic modulus of ~ 80 GPa.

This study analysed the as-deposited WAAM microstructure to characterise grain size, morphology, and phase composition. Also, post processing heat treatments were optimised to bring the mechanical properties of the alloys closer to the nominal values. The β microstructure of WAAM-ed parts was found to be clean and free of significant element segregation, allowing shortening of the solution treatment stage to minimise unnecessary grain growth and further reductions in alloy strength. Aging treatments promoted the precipitation of fine α -needles within the β matrix, significantly enhancing mechanical strength. TEM analysis confirmed the careful selection of the aging temperature avoided the formation of the isothermal ω phase during aging, which can deteriorate the deformation range of the alloy. The optimised Heat treatment parameters controlled α -phase growth in β grains while limiting the formation of α -phase at grain boundaries, which has a detrimental effect on the ductility of the alloy. The heat-treated samples achieved a broad range of tensile strengths comparable to the forged alloy while maintaining an acceptable strain range of up to 5%, providing flexibility for tailored mechanical performance in specific applications.

The findings highlight that the introduction of optimised heat treatments can achieve near-forged mechanical properties in WAAM-ed metastable β titanium alloys with reduced energy and time investment. This work underscores the potential of WAAM for manufacturing aerospace-grade components while minimising the need for extensive machining and multi-step thermal processes.

CALPHAD-Based High-Throughput Assessment of Scrap-based Metal Powders Printability for L-PBF

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Steel manufacturing is an energy-intensive process with a significant CO₂ footprint. Scrap recycling plays a significant role in reducing the environmental footprint of steel manufacturing. While the use of scrap in steelmaking is a long-established and widely accepted practice, its variable chemical composition and presence of contaminants often limit its application to steel grades that are less sensitive to composition and microstructure, such as structural steels used in long products like reinforcing bars. However, using steel scrap for manufacturing high-performance, near-net-shape products, (such as additively manufactured (AM) parts) is an ongoing research topic, focusing on understanding the effects of chemical composition variations, impurities, and the development of impurity-tolerant alloys [1,2].

In this work, we perform high-throughput computational thermodynamics (CalPhaD) simulations to evaluate the manufacturability of metal powders derived from steel scrap for the laser powder bed fusion (L-PBF) process. By analysing the phase evolution and material thermal properties across a range of chemical compositions, we assess potential printing issues such as hot cracking, keyholing, balling, and lack of fusion using phenomenological criteria in the literature [3]. This study explores the admissible range of chemical composition for scrap-based steel powder, which could be used to lead the strategies for different scrap selection and mixing and pre-atomization impurity/contamination removal procedures.

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Gas adsorption meets deep learning

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Metal-organic frameworks (MOFs) are promising materials for gas adsorption due to their ultra high porosity and surface area. However, their vast combinatorial space makes traditional material discovery methods inefficient. Recently, machine learning (ML) approaches have been proposed for large-scale screening of MOF databases but their efficacy rely heavily on hand-crafted features.

We propose a deep learning (DL) framework [1] for predicting gas adsorption properties of materials, using as one and only descriptor the potential energy surface (PES). The latter uniquely combines the structural properties and the electronic structure of a material in real space, rendering the proposed scheme applicable in any host-guest system for predicting any adsorption property of interest.

Furthermore, we have developed a generalized deep learning framework [2] that predicts gas adsorption properties from raw structural information using a point cloud representation of the material. Combining this simplified yet complete representation with DL, introduces a versatile paradigm for data-driven material science, bypassing the obstacles of manually crafted descriptors.

Our algorithms were tested for CO₂ adsorption in MOFs, outperforming conventional ML models in the literature, which rely on geometric descriptors. The proposed methodologies were further validated across different host-guest systems, demonstrating broad applicability in diverse materials and properties.

[1] Sarikas, A.P., Gkagkas, K. & Froudakis, G.E. Gas adsorption meets deep learning: voxelizing the potential energy surface of metal-organic frameworks. *Sci Rep* 14, 2242 (2024). <https://doi.org/10.1038/s41598-023-50309-8>

[2] Sarikas, A.P., Gkagkas, K. & Froudakis, G.E. Gas adsorption meets geometric deep learning: points, set and match. *Sci Rep* 14, 27360 (2024). <https://doi.org/10.1038/s41598-024-76319-8>

Laser metal deposition additive manufacturing combined with high-flux in situ X-Ray analysis for high-throughput materials characterization

Prof. Thomas Niendorf¹

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D8_2, Machado Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

Additive manufacturing (AM) is characterized by the evolution of unique microstructures upon processing. Due to the distinct thermal history imposed by rapid solidification and intrinsic heat treatment, i.e., layer-wise re-heating of already solidified volumes, microstructures of well-established alloys such as Ni-base superalloys, austenitic steels or Ti-base multi-phase alloys differ significantly from their cast and forged counterparts. In several alloys, properties of AM-processed conditions are characterized by superior properties, however, numerous alloys suffer from process induced cracking, residual stress and presence of unwanted phases. To overcome prevailing challenges, novel alloys being adapted to the specific boundary conditions of AM have to be developed.

To be able to fully exploit these boundary conditions, in situ and operando techniques are the key toward in-depth understanding, e.g. in research studies conducted at synchrotron facilities. Here, radiography and diffraction allow to not only study melt pool dynamics but also phase changes occurring during any specific process step. Unfortunately, beam time at such research facilities is very limited and, thus, the investigation of entire material libraries in one campaign is hardly feasible. As a consequence, availability of lab-based equipment allowing for such kind of studies is urgently required. The present work focuses on the design, realization and implementation of a novel system being installed at University of Kassel. Laser metal deposition, combined with in situ X-Ray analysis using a high-flux source will allow for tackling prevailing gaps in this field. Initial experiments are presented and prospects as well as limitations are discussed.

Combined high-throughput computational and experimental screening of aluminum alloys suitable for additive manufacturing from scraps

Dr. Katrin Bugelnig¹, Dr. Tobias Strohmamm¹, Dr. Maïke Becker¹, Nuria Navarrete¹, Dr. Florian Kargl¹, Dr. Janis Ganzenmüller¹, Julie Villanova², Elodie Boller², Pierre Lhuissier³, Dr. Guillermo Requena^{1,4}

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D8_2, Machado Room (Level -2), septiembre 15, 2025, 10:50 - 13:10

To meet societal goals like climate neutrality by 2050 and a circular economy, material discovery must be faster and more flexible, especially as raw material costs and supply chain issues increase. Advanced technologies like computational screening, 3D/4D characterization, and machine learning enable rapid responses to these challenges.

A new Al-based alloy suitable for additive manufacturing (AM) derived from scrap metal mixtures was developed using high-throughput alloy screening paired with synchrotron radiation based experimental validation. The new alloy is intended for aerospace applications and has to meet requirements such as low sensitivity to hot-cracking, minimal solidification interval, appropriate strength and elongation, etc.

In high-throughput computational screening, up to 10k alloy compositions were generated by mixing the scrap alloys at different ratios. The CALPHAD method was used for equilibrium and non-equilibrium simulations to assess key parameters, including phases, solidification intervals, and mechanical properties like yield strength and hot-cracking sensitivity. A random forest model predicted properties from simulations and literature, while a multi-objective evolutionary algorithm filtered alloys with target characteristics. Uncertainty calculations addressed compositional variations in scrap, ensuring robust designs.

For experimental validation, selected alloy compositions were synthesised by conventional casting, remelted and subjected to laser line scan testing to investigate the effect of different solidification rates on the material. Satic synchrotron tomography scans were taken to analyse the microstructure in 3D. Finally, a potential composition suitable for additive manufacturing was selected for powder production and in-situ laser powder bed fusion experiments were performed during microtomography to confirm the processability of the alloy.

Artificial intelligence-enhanced atom probe microscopy: Local chemical ordering analysis

Dr. Yue Li^{1, 2}

¹Max-planck-institut Für Nachhaltige Materialien GmbH, Düsseldorf, Germany, ²University of Kassel., , D9_2 - AI for Materials Characterization, Seminario 6 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

In solids, chemical short-range order (CSRO) refers to the self-organisation of atoms of certain species occupying specific crystal sites. CSRO is increasingly being envisaged as a lever to tailor the mechanical and functional properties of materials. CSRO is typically characterized indirectly, using volume-averaged (e.g. X-ray/neutron scattering) or through projection microscopy techniques that fail to capture the complex, 3D atomistic architectures. Quantitative assessment of CSRO and concrete structure-property relationships have remained so far unachievable. Herein, we showcase how machine learning-enhanced atom probe tomography (APT) can mine the near-atomically resolved APT data and jointly exploit the technique's high elemental sensitivity to provide a 3D quantitative analysis of CSRO in a series of metallic materials, including Fe-Al, Fe-Ga, and CoCrNi medium-entropy alloys. We reveal multiple CSRO configurations, with their formation supported by state-of-the-art Monte-Carlo simulations. Quantitative analysis of these CSROs allows us to establish relationships between processing parameters and physical properties. The proposed strategy can be generally employed to investigate short/medium/long-range ordering phenomena in a vast array of materials and help design future high-performance materials.

Heat Treatment Simulation of Normalized Steel 9310

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

This presentation addresses a computational approach to simulate the heat treatment process of Steel 9310. The aim is to validate the heat treatment process with experiments and use that validation to help to create a digital twin of the heat treatment process, which can be used to mimic the heat treatment of any new steel alloy. Heat treat process includes copper plating, stress relieving, vacuum carburizing, annealing, copper plate stripping, hardening & quenching, cold treat, and temper. First, the finite element model is validated with experiments, and then a parametric study is carried out to identify the critical process parameters. Then, the results of the parametric study are used to establish a relationship between the critical process parameters and the output hardness, residual stress, and distortions. This research also aims to find the effects of critical process parameters on the final hardness, residual stress and distortions during heat treatment of Steel 9310. The usage of virtual but validated physics-based models in the steel gear manufacturing drastically reduces cost and time and saves energy.

Machine Learning Prediction of magnetic properties for Fe-based and Pt-based alloys

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Fe-Pt intermetallic alloys represent a group of solid-state materials that exhibit interesting physical and chemical properties dependent on their chemical compositions.

For instance, Fe-Pt alloys can experience various types of phase transitions, including atomic and magnetic ordering and martensitic transformation, across a wide range of concentrations and temperatures.

Different phase transitions can coexist, and their interactions may alter material properties.

Meanwhile, Pt-based alloys undergo magnetic transitions along with atomic ordering.

Fe- and Pt-based alloys are utilized in high-density magnetic storage devices, magnetic recording media, and optical and electronic devices.

There are two different approaches to determining the Curie temperature. The classical method involves preparing an alloy of a specific composition and measuring the Curie temperature through experimental techniques. In contrast, the second approach predicts the Curie temperature before performing experiments, based on the known physical and chemical properties of the material.

In this research, we adopt the second approach and apply machine learning techniques to predict the Curie temperature (T_c) for Fe-based and Pt-based alloys. Control factors include atomic order (formation of the L12-type of superstructure) and variation of the chemical composition of the alloy by adding a small amount of a third element (up to 5 at.%).

The feature set for supervised machine learning includes the alloy's composition, atomic order state, and the atoms' properties.

We identified the best-fit mathematical model and validated the results using experimental methods to measure the Curie temperature.

Our findings indicate that the Voting Ensemble model, combined with the Monte Carlo cross-validation method, achieves the best performance and provides the most accurate predictions. "Normalized root mean squared error" is used as the primary metric for evaluation obtained results.

For our technical toolkit, we select the Azure machine learning framework due to its robust capabilities in machine learning and its user-friendly design.

This study can be extended to include different doping elements in Fe-Pt alloys, as well as applications to Fe-Pd-based and Fe-Ni-based bulk alloys and nanoparticles.

Machine Learning Assisted Dark Field X-Ray Microscopy Data Analysis

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 POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
 Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Mapping dislocations is essential to understand the mechanical behaviour of crystalline materials, as they critically influence mechanical, electrical, magnetic, and optical properties. Dark Field X-ray Microscopy (DFXM) is a diffraction imaging technique that enables three-dimensional mapping of dislocations in millimetre-sized samples with a spatial resolution of 100 nm and superior angular resolution compared to Transmission Electron Microscopy (TEM). However, analysing DFXM datasets is data-intensive and requires significant supervision. Moreover, dynamical diffraction effect can influence reconstructed maps in thick crystals, rendering data interpretation difficult. To address these challenges, we propose a workflow using machine learning techniques to facilitate DFXM data analysis. Specifically, we introduce:

1. A data reduction approach based on labelling DFXM rocking curves to identify the weak beam condition for defect analysis, followed by dislocation segmentation.
2. An artificial neural network coupled with geometrical optics simulations to predict the Burgers vector of the dislocations.

This workflow offers an efficient, automated, and rapid approach for analyzing dislocations in DFXM data, achieving a data size reduction of 70%. Beyond its application to DFXM images, the methodology is versatile and can be implemented agnostically for X-ray topography and TEM, broadening its potential impact across various imaging modalities. These advancements pave the way for more streamlined and accessible analysis in crystallographic research.

Machine Learning Approach in Aluminium Melt Quality Control

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D9_6 - FAIR Data, Interoperability, and Digital Workflows, Seminario 6 Room (Level +1), settembre 16, 2025, 14:30 - 16:30

To support sustainability, industries aim to reduce energy use and emissions. Primary aluminium production is energy-intensive and relies on bauxite, facing strict regulations. Achieving high-quality aluminium casting relies significantly on melt preparation, influencing the occurrence of wide variety of casting defects. While traditional methods face challenges in assessing melt quality online due to time and energy constraints, recent innovations present a practical evaluation system. This advancement holds promise for improving final product quality and operational efficiency by minimizing suboptimal molten material and subsequent scrap. A patented system offers real-time insights during alloy solidification, reducing the carbon footprint and enhancing casting quality. When combined with advanced machine learning algorithms, this system rapidly detects impurities, improving production processes and alloy reliability.

This research explores the integration of machine learning (ML) methodologies to revolutionize melt quality assessment. By establishing correlations between rapidly obtainable non-equilibrium thermodynamic data and critical melt parameters, predictive models will enable estimations of chemical composition and solidification processes. Leveraging fundamental melt composition data and cooling regimes, these models aim to predict diverse solidified part characteristics, aiding process engineers.

This project aims to elucidate crucial connections between cooling curves and solidified part characteristics using predictive models, thus advancing melt quality control. Integration of various ML techniques such as simple linear regression, Multiple Linear Regression, Lasso regression, Elastic Net regression, Ridge Regression, Polynomial, SVR, Random Forest, Decision tree and Gradient Boosting regression represents a significant step forward, promising rapid, real-time estimation of melt quality parameters. Results obtained from the evaluation of the mentioned models highlighted the higher accuracy of the Gradient Boosting Regression model followed as the best candidates to be used for the prediction of magnesium content during aluminium alloy preparation because magnesium is the main alloying element for alloy 5754.

Design optimization through a DNN-based FE surrogate model by developing a design and analysis automation

Mr. Dongwoon Han¹, Dr. Seongtak Kim¹

¹Korea Institute of Industrial Technology, Wonju-si, South Korea

POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Developing an appropriate design and manufacturing process that achieves optimal performance while satisfying functional requirements is crucial for ensuring the quality of the product. This study proposes a design optimization method that reduces time and cost in traditional finite element analysis (FEA)-based design optimization by developing a deep neural network (DNN)-based finite element (FE) surrogate model. An algorithm for automatic geometry generation and mesh automation was developed for the creation of an FE surrogate model. Additionally, an algorithm was developed to automatically assign boundary conditions, perform FEA, and collect data automatically. A FE surrogate model was developed using a DNN-based framework incorporating Bayesian optimization and k-fold cross-validation techniques. Optimal design factors were derived using the simple additive weighting (SAW) method and validated using FEA. The optimization results suggest that our surrogate model replicates the high-fidelity FE model at a lower cost and promptly provides accurate optimal results.

ACBICI: An Open-Source Python Library for Bayesian Calibration of Complex, Data-Scarce Models

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D9_3 - Bayesian and Advanced Optimization for Materials, Seminario 6 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Standard techniques for model calibration typically focus on minimizing the fitting error between model predictions and experimental data. While straightforward, this approach overlooks errors present in the available data and can lead to parameter estimations that are local error minimizers, heavily dependent on the given samples. This is especially problematic when data is scarce, and model testing is resource-intensive or expensive.

A powerful and well-established methodology that can overcome some of these limitations employs Bayesian inference to obtain probabilistic distributions for the model parameters while accounting for the scatter caused by experimental errors. These types of calibrations profit from preexisting knowledge about the parameter values -- whether from past experience or published data -- and can provide detailed information about the uncertainty of parameters. The latter can be exploited to ascertain the confidence of the calibration, for example, but also to guide experimental campaigns and optimize resource allocation.

In our group, we have developed a framework for the calibration of complex, data-scarce models based on Bayesian inference approaches, called ACBICI, following the pioneering work of Kennedy and O'Hagan [1]. This open-source Python library can be used in a variety of applications since it is designed for ease of use, and employs Gaussian process surrogates to simplify the calibration of extremely costly models.

In this talk, we will introduce the ACBICI library, highlighting its capabilities and demonstrating its utility in practical applications. As a specific example, we will showcase its use in calibrating a complex model for creep in steel. Through this example, we will illustrate how ACBICI can provide valuable information to modelers and material scientists.

[1] M. Kennedy, A. O'Hagan (2001). Bayesian calibration of computer models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 63: 425-464.

Understanding microstructure-property correlation of pearlitic steel by machine learning-based modeling

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¹Forschungszentrum Jülich, Jülich, Germany

D9_4 - Structure-Property Relationships and Synthetic Data, Seminario 6 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Understanding and predicting the structure–property relationship is a cornerstone of materials science, particularly for designing advanced materials with tailored properties. The mechanical behaviors of pearlitic steel, widely used in demanding applications, are often dominated by the lamellae spacing, the colony shape and grain size [1, 2] while several other aspects concerning its microstructure-related properties have not yet been studied in detail.

In this study, a novel data-driven framework was proposed to predict localized hardness in 100Cr6 steel based on the integration of advanced imaging techniques, nanoindentation measurement and machine learning-based modeling. The workflow begins with the acquisition of high-resolution Scanning Electron Microscopy (SEM) images and Electron Backscatter Diffraction (EBSD) data to capture the morphology of ferrite crystallite lattices and cementite lamellae. Convolutional Neural Networks (CNNs) are employed for automated image segmentation, enabling precise identification and quantification of microstructural features such as lamellae spacing and colony morphology. These segmented features are then integrated with corresponding nanoindentation hardness data to train predictive machine learning models.

The results demonstrate that the morphology of ferrite and cementite phases significantly impacts localized hardness at the nanoscale. The developed model provides quick, cost-effective predictions of hardness, validated by detailed experimental measurements, and reveals new insights into the relationship between pearlite microstructure and mechanical properties.

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AI-Driven Multimodal Analysis of Microstructure and Phase Composition in a 3rd Generation Medium Mn Steel Using 4D STEM and X-ray Diffraction

Dr. Seyedeh Leila Panahi¹, Dr. Marc Raventós¹, Dr. Oleg Usoltsev¹, Dr. Marcel Carpio², Dr. Nuria Cuadrado², Dr. Simone Kaar-Schickinger³, Dr. Michael Schwarzenbrunner³, Dr. Nuria Bagués¹, Dr. Edgar E. Villalobos-Portillo¹, Dr. Lucia Aballe¹, Dr. David Frómeta², Dr. Joaquín Otón¹

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D9_2 - AI for Materials Characterization, Seminario 6 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The complex microstructural characterization of Advanced High-Strength Steels (AHSS) demands innovative analytical approaches to fully understand their multiphase nature. We present a novel artificial intelligence framework for analyzing 4D Scanning Transmission Electron Microscopy (4D-STEM) data, where, in combination with the Automated Crystal Orientation Mapping (ACOM) procedure, enabling precise visualization of grain boundaries and texture variations. This development addresses a critical challenge in the automotive industry, where AHSS materials are increasingly utilized for lightweight, high-performance auto body components due to their exceptional combination of strength and ductility. The microstructure of AHSS, typically comprising phases such as austenite, ferrite and/or bainite, presents significant challenges for traditional characterization methods due to its complexity and fine-scale features.

In this study, we developed and implemented machine learning algorithms for the automated analysis of the microstructure and morphology of medium manganese steel (Mm1000), produced by Voestalpine. Our approach combines advanced data analysis from both X-ray diffraction (XRD) and 4D-STEM electron diffraction patterns. The AI-driven analysis pipeline integrates crystallographic information from both techniques, enabling rapid and detailed phase identification along with grain orientation and stress mapping. Additionally, Energy dispersive X-ray Spectroscopy (EDS) was employed to analyze the elemental composition across the depth of the bulk regions, providing complementary chemical information to validate our AI-based structural predictions.

These results demonstrate the power of combining advanced characterization techniques with artificial intelligence, providing not only valuable insights into the microstructure of medium manganese steels but also establishing a new model for automated materials characterization. This approach paves the way for improved manufacturing processes and enhanced performance in next-generation AHSS materials, while significantly reducing the time and expertise required for complex microstructural analysis

References

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- [2] Raabe, D., Sun, B., Kwiatkowski Da Silva, A. et al. Current Challenges and Opportunities in Microstructure-Related Properties of Advanced High-Strength Steels. *Metall Mater Trans A* 51, 5517–5586 (2020)

High-throughput analysis of loop dynamics in irradiated MPEAs using deep learning

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D9_2 - AI for Materials Characterization, Seminario 6 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

With the modernization of in situ transmission electron microscopy (TEM) irradiation experiments [1], there is a latent need to establish high-throughput data segmentation of TEM micrographs. To address this necessity, we evaluate the performance of Mask-CNN [2] — a popular computer vision model that enables simultaneous object detection, classification, and pixel-level segmentation — to identify dislocation loops in TEM video frames.

The use of deep learning in materials science has grown in recent years. The work of Jacobs et al. [3] is a pioneer concerning the application of Mask R-CNN to identify defects in TEM images of irradiated BCC FeCrAl alloys. The authors showed that the model successfully categorizes $\langle 100 \rangle$ loops, $\langle 111 \rangle$ loops, and black dots. In 2024, T. Bilyk demonstrated that a similar strategy could convey insights into overlapping perfect, faulted, or on-edge loops in irradiated Multi-principal element alloys (MPEA) alloys [4].

In the present work, we focus on segmenting black dots in bright-field TEM images. Our model was trained on five annotated snapshots from a video with nearly 3600 unique features of the same class. Such video records an in situ ion irradiation experiment performed within the JANNuS Orsay facility [1] of austenitic stainless steel 316L with the following parameters: Fe⁺ irradiation at 2 MeV for 60 min at 550 °C; total flux of 10^{15} ions/cm². After training, the model helps interpret a second video concerning a similar experiment with the 16Cr-37Fe-13Mn-34Ni (at.%) MPEA alloy, with slightly different irradiation conditions.

The model performs well and segments images with a mean average precision (mAP) of around 80%. The digested data points to a rapid increase in dislocation loop density after 2 minutes, reaching values close to $8 \cdot 10^{14}$ 1/m², which is consistent with the expected behavior for this system. In conclusion, the proposed framework may help researchers extract critical data on the dislocation loop dynamics from in situ experiments, even in the case of low-magnification or low-resolution videos. The talk will also include the characterization of radiation defects formed in situ in high-purity FCC metals at low temperatures, providing insights into their energetics.

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Data driven reduced order modelling of metal casts with induction-heated feeders and a parameterized geometry

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Energy efficiency and innovation are key drivers in the energy intensive metal casting industry. Conventional casting processes rely on oversized feeders to prevent defects, leading to significant energy waste and additional work for handling, sawing, and re-melting of metal. Therefore, the Norwegian company EFFEE develops an induction-heated feeder that can be dimensioned much smaller. Early tests show induction-heated feeders can cut energy use by 30%, with feeder size reduced by 40% (e.g., 800kg to 100kg for a 1000kg casting), lowering overall variable costs by 3%.

With the innovation comes a need to understand the impact on material properties and to optimize the processes. Preventing potential issues and identifying opportunities where induction feeders can actively enhance the casting process are critical to build confidence in the casting industry. Current simulation software cannot effectively and accurately predict the effects of induction heating and Lorentz force stirring caused by electromagnetic fields on molten metal solidification process during casting, leaving unanswered questions about heat transfer, material structure, and defect prevention. To fill this gap, IFE is developing the Induction Feeder SIMulator (IFSIM) to get deeper insights and to analyze the new technology systematically. With the help of COMSOL and the in-house software Alsim, IFSIM provides predictions of melt levels and flow underneath the feeder, essential for optimally controlling induction heat input.

Detailed simulations can take hours, making parameter studies and automated optimizations expensive. We have developed a data driven surrogate model based on Non-Intrusive Reduced Order Modelling. It allows accurate predictions in split seconds even when training data is sparse. A given cast geometry is quickly approximated by a representative, simplified and parameterized geometry for which we have precomputed snapshots. The snapshots are reduced with a proper orthogonal decomposition (POD), and interpolation or machine learning in the reduced space allows to predict the reduced coefficients for new inputs in real time. The full system response can be obtained through a simple linear projection, and it is used to optimize the input of induction heat.

However, the mesh changes with time to account for solidification shrinkage, and because of the parameterized geometry, the mesh changes in the parameter domain too. The fact that spatial locations of the snapshot data don't match introduces significant challenges. Moreover, moving discontinuities such as the melt surface in the feeder are known to be difficult to represent with linear subspaces. We employ novel smoothing and desmoothing techniques to address this.

Microstructural characterization of stainless steels from distorted in-situ X-ray diffractograms by means of machine learning tools

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D9_2 - AI for Materials Characterization, Seminario 6 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The phase fractions and the dislocation densities during the heat treatment of stainless steels are determined by in-situ X-ray diffraction measurements. Due to comparatively fast cooling rates the diffractograms are frequently degenerated with a high signal to noise ratio. Asymmetric peaks caused by the slit system, peak broadening and peak overlapping further reduce the quality of the diffractograms. Then, these diffractograms are evaluated by using the Rietveld method including the fundamental parameter model with the Voigt profile, to estimate phase fractions and dislocation densities in martensite and austenite. Whereas classical least-squares optimizers frequently fail to find the peak positions, the Markov Chain Monte Carlo algorithm successfully overcomes the limitations of covariance matrix-based error estimation by providing robust uncertainty quantification. By means of L1 regularization methods the influence of the instrument on the diffractograms is deconvoluted. In addition, neural networks trained by synthetic diffractograms are used to calculate the initial values for the optimization problem. Thereby, the evolution of the microstructure during thermal processing can be elucidated from comparatively cost-effective X-ray measurements under industrial conditions.

Efficient Steel Creep Behavior Prediction with Bayesian-Calibrated Models

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D9_3 - Bayesian and Advanced Optimization for Materials, Seminario 6 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Steel production accounts for 20-25% of industrial CO₂ emissions[1], significantly contributing to global carbon emissions. Accurate and efficient prediction of steel creep behavior is essential for improving material performance and supporting sustainability goals. However, traditional predictive approaches face major challenges, including the high cost of experiments, computationally intensive models, and uncertainties in material properties and operating conditions. Overcoming these challenges is critical for advancing material science and reducing the environmental impact of steel production.

To tackle these challenges, we present a Bayesian calibration framework, following the original ideas of Kennedy and O'Hagan[2], which leverages Gaussian processes for robust uncertainty quantification. This method enables precise estimation of model parameters, hyperparameters, and system discrepancies. Using our open-source Python library, ACBICI (A Configurable Bayesian Calibration and Inference package), we calibrate and predict steel creep behavior based on experimental data and synthetic data generated through complex finite element simulations using the research code Lagamine[3].

Our application of this methodology demonstrates its effectiveness in predicting steel creep behavior under uncertain conditions. The Bayesian calibration framework provides probability distributions of the physical creep model parameters and hyperparameters consistent with experimental data and simulations. Hence, quantifying underlying uncertainties. These results highlight the practical advantages of combining Bayesian methods with advanced computational tools for material modeling. Beyond creep modelling, this approach illustrates new avenues for dealing with calibration and uncertainties across a wide range of engineering and scientific domains.

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Deep learning based strategies for noise reduction of synchrotron X-ray nano-tomography images of light alloys: investigation on experimental extensive dataset.

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D9_2 - AI for Materials Characterization, Seminario 6 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

This research aims to develop and optimize deep learning algorithms to enhance the temporal resolution of X-Ray nano-Tomography (nanoCT) at the ID16B beamline of the European Synchrotron Radiation Facility (ESRF). By incorporating advanced artificial intelligence techniques, this study seeks to enable rapid data acquisition while preserving the quality of the reconstructed images. These innovations are pivotal for reducing exposure times, thereby minimizing radiation-induced artifacts and extending the applicability of nano-CT to in situ experiments, where precise and reliable imaging is essential for the characterization of light alloys elaboration and processing.

The methodology employed in this study revolves around the adaptation and evaluation of the Noise2Inverse algorithm, an unsupervised deep learning technique developed by Hendriksen et al. (2020)¹ tailored for denoising X-Ray Computed Tomography (XCT) data.

Datasets were carefully selected to include aluminum alloys with varying compositional and microstructural complexities, allowing the exploration of the algorithm's performance limits. These extensive datasets consist in nano-CT acquisitions of the same samples under about 200 diverse experimental conditions, including variations in spatial resolution (from 25nm to 250nm), number of projections (from 100 to 2000) and exposure times (from 0.28ms/proj to 40ms/proj), being last one the only variable relevant for the denoising task. This diversity ensured a robust evaluation of the algorithm across a wide range of scenarios on real data.

The Noise2Inverse algorithm was systematically studied in different domains: projections, sinograms, and reconstructed images. Its architecture, specifically evaluated using U-Net and MSD-Net models, was assessed in multiple configurations, including 2D, 2.5D, and 3D implementations, to determine its effectiveness in preserving spatial fidelity across various data dimensions and domains.

Noise2Inverse treated volumes are compared with holotomography high quality volumes (long exposure time, high number of projections) to assess the quality of the results and to ensure the faithful representation of material features critical for advanced analysis.

This work highlights the potential of deep learning techniques to significantly enhance nano-CT imaging by improving noise handling and facilitating faster data acquisition.

These advancements are critical for in situ experiments and broader multi-scale imaging applications in additive manufacturing and materials science. Future efforts will focus on integrating these algorithms into beamline operations for real-time use.

¹ A. A. Hendriksen, D. M. Pelt and K. J. Batenburg, "Noise2Inverse: Self-Supervised Deep Convolutional Denoising for Tomography," in IEEE Transactions on Computational Imaging, vol. 6, pp. 1320-1335, 2020, doi: 10.1109/TCI.2020.3019647.

Machine learning approaches for the determination of liquidus and eutectics

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Knowledge of the liquidus is crucial for designing and processing a wide range of materials. Local minima in the liquidus correspond to the composition of the eutectics which are particularly important for the design of alloys such as metallic glasses, solders, cast alloys, or phase change materials for energy storage [1] due to their properties such as low melting points and the absence of a solidification range. Liquidus data can be obtained from Calphad-based thermodynamic calculations, however, two challenges arise. The first is to be able to efficiently screen for eutectics in the immense compositional space offered by multicomponent alloys, since Calphad databases can include dozens of elements. The second is the lack of liquidus data to improve and enlarge the reliability of the calculations, starting with the binary systems that are the building blocks of Calphad databases.

In recent years, machine learning (ML) algorithms have demonstrated their power in various applications. In our work, we examine how liquidus determination can benefit from ML's ability to extend the information gained from the training sample to new observations.

In the first part we focus on exploitation of the Calphad databases guided by active learning and the subsequent interpolation of retrieved data in order to accelerate acquisition of the liquidus. Eutectics are then identified as local minima in the liquidus representation. Benchmark of different approaches for eutectic identification is performed.

The second part of work addresses the challenge of shortage of liquidus data in many binary systems. Using properties of the pure elements as well as thermodynamic properties of mixing that were also obtained by ML models [2], a model is developed to predict the liquidus in binary systems generated by 70 elements.

[1] G. Deffrennes, K. Terayama, T. Abe, E. Ogamino, R. Tamura, A framework to predict binary liquidus by combining machine learning and CALPHAD assessments, *Mater. Des.* 232 (2023) 112111. <https://doi.org/10.1016/j.matdes.2023.112111>.

[2] G. Deffrennes, B. Hallstedt, T. Abe, Q. Bizot, E. Fischer, J.-M. Joubert, K. Terayama, R. Tamura, Data-driven study of the enthalpy of mixing in the liquid phase, *Calphad* 87 (2024) 102745. <https://doi.org/10.1016/j.calphad.2024.102745>.

Multiscale modeling of microstructure formation in re-heating and quenching process for understanding creep related properties of large shaft

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Microstructure is the key for understanding the mechanical properties of a steel product. Microstructure formation can be simulated using models at different length scales that can include the desired level of resolution and physical phenomena involved in the manufacturing process. For example, the formation of microstructure during thermomechanical processing requires larger scale model which can simulate the conditions relevant to industrial operations and then provide the boundary conditions for the smaller scale models.

We apply heat transfer and conduction finite element simulations coupled with mean field phase transformation model to calculate the cooling of macroscopic objects. Phenomenological Cellular Automata (CA) models are used to calculate nucleation, growth and impingement of phase regions, as well as grain growth phenomena. Physically based phase field / level-set model is used for simulating partitioning diffusion, transformation strains, elasticity and plasticity associated with microstructure formation during cooling.

By combining the models with different length scales, we aim to bridge the industrial scale down to microstructure length scale. The aim of the microstructure formation model is to complement the experimental investigations and to provide relevant information for understanding the creep related properties of a large scale shaft.

Machine Learning-Driven Prediction of Mechanical Properties in Resorbable Magnesium Alloys for Biomedical Applications

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D9_4 - Structure-Property Relationships and Synthetic Data, Seminario 6 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Magnesium alloy wires exhibit significant potential for biodegradable medical applications, particularly in bone support, where they serve as cerclage and fixation wires [1,2]. This study establishes a quantitative relationship between the composition, processing history, heat treatment conditions, and mechanical properties of magnesium-based fine wires (diameter < 500 μm) by leveraging different machine learning (ML) techniques. A dataset comprising approximately 100 samples compiled from literature sources was utilized to develop predictive models, including support vector regression (SVR), linear regression (LR), polynomial regression (PR), decision tree regression (DT), random forest (RF), and CatBoost regression. These models were employed to predict key mechanical properties, namely ultimate tensile strength (UTS), yield strength (YS), and elongation (EL), with high accuracy. Notably, the CatBoost model demonstrated superior predictive performance, achieving coefficients of determination (R^2) exceeding 0.92 for UTS and 0.98 for YS on the testing dataset. The evaluation of various statistical metrics, including R^2 , mean squared error (MSE), root mean squared error (RMSE), and mean absolute error (MAE), confirms the reliability and robustness of the proposed models in predicting the mechanical properties of resorbable magnesium alloy for biomedical applications.

Using Computer Vision and Microstructure Informatics to Characterize Dendrite Growth in Ni-base Single Crystal Superalloys

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D9_1 - Opening Session and Keynote, Seminario 6 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Microstructure informatics combines traditional quantitative metallography with computer vision, algorithmic geometry and data science. It uses automated procedures to retrieve statistically relevant information from micrographs. Its power is demonstrated in a case study which focusses on competitive dendrite growth during directional solidification of single crystal Ni-base superalloys (SXs). The method presented in this work relies on three basic components: (1) A deep learning object detection network for detecting dendrite core positions. (2) A 3D image reconstruction routine for tracing dendrite paths. (3) And an ontological database of relational geometric data, documenting relationships between individual dendrites. To develop this method one had to assess the performance of different deep learning classification architectures (AlexNet, GoogleNet and MobileNetV2) in combination with a subdetection network (YOLOv2). In parallel the network hyper parameters (anchor box sizes, confidence scores) needed to be optimized to achieve a detection better than 99%. And, most importantly, an ontological data base had to be designed.

Deep learning architectures were trained using manually annotated reference images. Detection performances were evaluated based on manually curated ground truth data. The best performing network consisted of the first 30 layers of a MobileNetV2 architecture combined with a YOLOv2 sub-detection network. Optimum results were obtained when combining this architecture with an anchor box size of 35 x 35 px using a confidence score (CS) of 0.4. A central element of the proposed procedure is a microstructure specific relational geometric ontology database (RGO) which provides a foundation for further quantitative evaluation. It represents a digital replica of all relevant morphological features of the 3D dendritic microstructure. A cylindrical SX bar with 12 mm diameter of the alloy CMSX4 was investigated. Optical wide field micrographs from 1 mm spaced cross sections were taken over a length of 76 mm. Each cross section contained close to 3000 dendrites. The method presented here allows to follow the growth paths of all dendrites in the test volume (16,631 objects). It moreover provides new quantitative insight into competitive growth with a focus on branching and extinction events and neighborhoods (156,735 relations). The method also provides specific results which account for crystal mosaicity, individual dendrite growth directions, competitive interactions between dendrites and groups of dendrites and interaction between dendrites and mould walls. The proposed methodology and especially the developed database scheme can be fully generalized. It can act as a foundation for digital infrastructures for microstructure characterization in the future.

Optimal Discovery of multi-dimensional Pareto Sets in High Entropy Alloys

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D9_3 - Bayesian and Advanced Optimization for Materials, Seminario 6 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Recent advancements in materials discovery have shifted from traditional, labor-intensive methods to data-driven, informatics-based approaches. High-throughput (HTP) experimentation and computation dominate current efforts but are constrained by practical limitations such as resource availability and human decision-making bottlenecks. To address these, framing materials discovery as an optimal experimental design problem has emerged as a promising paradigm. In this talk, I will explore the application of Bayesian Optimization (BO) in the targeted exploration of the CoCrFeNiVAl FCC high-entropy alloy space. This integrated framework identifies Pareto-optimal solutions across performance metrics, including strength, hardness, and strain rate sensitivity, while leveraging advanced cyber-physical workflows. By utilizing only 0.15% of this vast design space, our iterative synthesis-characterization-testing loops achieved unprecedented acceleration in discovering optimal alloy compositions. The results highlight the efficiency of Bayesian-guided discovery in navigating complex, multi-objective spaces and the insights gained into the underlying chemical and microstructural drivers of alloy performance. I will also discuss current challenges, the impact of these findings on alloy optimization processes, and future opportunities for integrating AI/ML-assisted simulations with experimental workflows. This approach represents a significant step toward autonomous materials design and scalable multi-objective materials optimization.

MicrostructureDB: An AI-Powered Open Data Platform for Materials Characterization

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D9_6 - FAIR Data, Interoperability, and Digital Workflows, Seminario 6 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

We present MicrostructureDB, a new platform that demonstrates how AI can enhance metallurgical data analysis and laboratory management. This beta release introduces practical tools for automating common challenges in materials characterization: identifying experimental anomalies, filling missing data, and finding related samples across datasets. The platform includes an integrated metallurgical AI assistant that helps researchers interpret results and maintain consistent documentation standards. Using our curated steel microstructure collection, we demonstrate how these tools can streamline laboratory workflows, improve data quality, and accelerate the analysis of experimental results. Through practical examples, we showcase the platform's capabilities in enhancing materials research while maintaining rigorous scientific standards, illustrating the potential of AI-assisted materials characterization.

From accelerated creep tests to performance parameters: Efficient dataset generation, creep curve representation, and performance prediction using machine learning and numerical simulations

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D9_3 - Bayesian and Advanced Optimization for Materials, Seminario 6 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Creep is an industrially significant material behavior that describes the time-dependent deformation of materials under constant stress, particularly at elevated temperatures. Understanding creep performance is crucial for the design and longevity of components in high-temperature applications, such as in power plants or aerospace applications. However, standard creep tests are traditionally time-consuming and cumbersome, posing significant challenges in the conduction of tests and slowing down materials and component design processes. In contrast, accelerated creep tests provide faster results; however, these tests do not allow for direct identification of creep performance parameters as is the case with standard creep tests. To address this gap, machine learning models can be employed to predict creep performance parameters from accelerated creep test data. This contribution focuses on the fundamentals and key challenges of developing such machine learning models using data from numerical simulations. Critical issues to be addressed include defining a suitable parameter space, efficient dataset generation, and representing creep curves in a lower-dimensional feature space. From this, we will derive and present concepts for mapping accelerated creep test data to creep performance parameters and discuss their applicability to experimental data. Ultimately, our aim is to accurately predict creep performance parameters from accelerated creep test data, enabling a faster evaluation of the creep performance of metallic materials.

Effect of microsegregation on phase transformation behaviour and microstructural evolution in a continuously cooled 1CrMoV bainitic steel

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

This study aims to understand the effect of microsegregation on phase transformation behaviour and the corresponding microstructural evolution at different cooling rates in an oil-quenched 1CrMoV bainitic steel used for turbine applications in power plants. Samples for dilatometer measurements were subjected to heat treatment in a Gleeble 3800 thermomechanical simulator, where the samples were heated at 5 °C/sec to 950 °C and held at this temperature for 30 minutes to achieve an austenite grain size comparable to that of industrial conditions. Following this, the samples were continuously cooled at different linear cooling rates in the range 0.03 – 50 °C/sec. The Ar₃, Ar₁, Bs, and Ms temperatures were identified as a function of cooling rate based on the inflexions in the dilatation curves, and a continuous cooling transformation (CCT) diagram was constructed. Presence of microstructural features such as quasipolygonal ferrite, lath bainite/upper bainite, coalesced bainite, and lath martensite were confirmed using both confocal laser scanning microscopy (CLSM) and scanning electron microscopy (SEM). Due to the effect of microsegregation in the steel, the impact on austenite grain size and phase transformation behaviour differed between prior alloy-rich (interdendritic) and alloy-lean (dendritic) regions. To identify bainite and martensite phase constituents more comprehensively in these complex microstructures, electron backscattered diffraction (EBSD) technique was utilized to construct band contrast maps. Phase fractions were measured in both alloy-rich and alloy-lean regions, which revealed discernible variances. The high-hardenable alloy-rich regions were more prone to the formation of harder martensite phase, compared to the significant formation of bainite along with martensite in the alloy-lean regions. The microstructural observations corroborated the result of the dilatation tests over a broad cooling range between 2.5 and 50 °C/sec. Additionally, the electron probe microanalyzer (EPMA) was utilized to confirm the microsegregation pattern in the steel. Elements such as Cr, Mo, V, Mn, and Ni were found to be enriched in the alloy-rich (originally interdendritic regions), whereas the alloy-lean dendritic regions were depleted of these elements. The EPMA results further corroborated the predictions of the thermodynamic modelling. The partition coefficients measured using the EPMA further verified the thermodynamic predictions.

Materials Design and High-throughput Screening of Multicomponent High-temperature Coatings Accelerated by Artificial Intelligence

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The MCrAlY systems (where M represents Ni, Co, Fe, or their mixtures), along with nitride and diamond-like carbon (DLC) coatings, are widely employed in high-temperature, heavy-duty surface protection applications due to their exceptional resistance to thermal corrosion, high strength and hardness, superior wear and friction resistance, and versatile selectivity. These coatings effectively mitigate challenges such as high-temperature oxidation and impact failures in harsh environments, including extreme temperatures and high-speed conditions. Guided by the concept of data-driven intelligent material design, this study employs machine learning, CALPHAD phase diagram calculations, and first-principles simulations across different computational scales to predict the structure and performance of coatings. The study provides insight into the effects of various alloying elements on the oxidation resistance, phase structure, and friction and wear behavior of the coatings.

For the MCrAlY multicomponent coating system, high-throughput experimental preparation and performance testing were carried out on the selected MCrAlY compositions using physical vapor deposition (PVD) techniques. The results reveal that temperature, exposure time, and alloying elements (such as W, Ti, Nb, Co) are strongly correlated with the high-temperature oxidation rate. The addition of Si enhances the coating's resistance to marine environments, while its synergistic interaction with Ta improves the mechanical properties and optimizes oxidation and corrosion resistance. Based on these findings, a novel NiCrAlYSiTa multicomponent alloy coating was designed, demonstrating exceptional oxidation resistance and mechanical properties. Furthermore, a dual-migration machine learning strategy was employed to extract elemental and phase transition features related to the evolution of metastable nitride phase structures. This approach achieved an impressive prediction accuracy of 0.95 for the phase transition interfaces of typical ternary nitride metastable phases. Additionally, machine learning was integrated with large-scale molecular dynamics simulations (involving thousands of atoms on the nanosecond scale) to maintain the accuracy of density functional theory (DFT) calculations. The resulting deep potential model exhibited an error margin of approximately 10 meV, which was then used to simulate the surface structure evolution of DLC coatings under friction. A quantum effect correction method was also applied to calculate thermodynamic quantities, and when combined with the deep potential model, it provided a more generalized friction model capable of accurately predicting friction force changes over a range of temperatures and speeds.

In conclusion, this study demonstrates that data-driven material design and screening approaches can significantly accelerate material development, reducing iteration cycles and associated costs.

Can AI Clean Up Your Characterization Data? Modern Approaches to Historical Dataset Curation

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D9_4 - Structure-Property Relationships and Synthetic Data, Seminario 6 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Materials characterization datasets, both historical and modern, often suffer from inconsistent documentation, varied formats, and unclear metadata. This presentation introduces a systematic AI-driven approach to transform such datasets into well-organized, standardized resources for materials research. Using self-supervised learning and specialized clustering algorithms, we demonstrate how modern machine learning techniques can extract meaningful patterns and relationships from poorly documented data while preserving physical validity. Our case study focuses on a historical metallurgical dataset, showcasing how contrastive learning methods, guided by materials science domain knowledge, can automatically organize microstructures. The developed framework establishes best practices for both retroactive dataset curation and future data collection, enabling more efficient knowledge extraction from materials characterization archives.

AI for Materials Industry: An Open Online Course

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

We present AI4MI, an open-access educational initiative bridging the gap between materials science expertise and modern AI capabilities. Designed for materials scientists and metallurgists, this curriculum transforms complex AI concepts into practical tools through industry-relevant case studies. The course combines hands-on experience with real industrial datasets and foundational machine learning theory, featuring applications such as automated steel defect classification, materials discovery, and sensor data visualization. Through carefully structured modules, participants learn to identify suitable AI applications in their work, understand implementation requirements, and avoid common pitfalls. Special attention is given to data preparation, model validation, and model insight, ensuring participants gain both theoretical understanding and practical implementation skills.

Real or Fake? Evaluating synthetic Electron Microscopy Data in Materials Science

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D9_4 - Structure-Property Relationships and Synthetic Data, Seminario 6 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The growing adoption of AI in materials characterization demands increasingly large, unbiased datasets, yet acquiring comprehensive steel microstructure data through electron microscopy remains resource-intensive and often leads to sampling biases. While generative AI offers a promising solution through synthetic data creation, validating these artificial microstructures raises fundamental questions about authenticity and scientific utility. Using the Ultra High Carbon Steel Database (UHCSDB) as our foundation, we investigate the effectiveness of current validation approaches for synthetic metallographic images. Our study critically examines standard AI-based metrics in both real and Fourier space, questioning their ability to guarantee preservation of physical properties. By comparing these computational assessments with expert metallurgists' evaluations, we explore whether conventional similarity metrics align with domain expertise in distinguishing real from synthetic microstructures. This comprehensive analysis aims to establish whether current validation methods can ensure physically meaningful synthetic data, addressing the fundamental question posed in our title: can we reliably determine if a metallographic image is real or fake, and what criteria should guide this determination?

A common workflow description for experimental and computational materials science

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D9_6 - FAIR Data, Interoperability, and Digital Workflows, Seminario 6 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Workflows in experimental materials science often rely on informal, textual descriptions with minimal standardization, which limits their machine-readability and interoperability. Typically, these workflows are structured in two layers: the top layer provides an abstract description, while the bottom layer details the technical aspects of the operating procedure. Similarly, also computational workflows follow a two-layer structure, with the top layer commonly represented by a Jupyter script that chains function calls, and the bottom layer comprising individual functions.

This presentation introduces a workflow description concept designed to support both experimental and computational materials science, facilitating interoperability. The pyiron workflow software enables users to graphically combine building blocks. Experimental scientists can access instrument operating procedures via custom workflow software on various devices. Despite the use of different software, the workflow descriptions remain consistent, allowing execution on a single engine. We will present various workflows and illustrate how experimental and computational scientists can collaborate using shared workflows, thereby bridging different materials science disciplines.

EMMO Ontology enabling AI-based innovative advanced materials development: the CoBRAIN Knowledge Base for Hardmetal Thermal Spraying Coatings

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D9_1 - Opening Session and Keynote, Seminario 6 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

EMMC is a community of stakeholders covering all types of materials models, computational methods and applications. Improved methods integration and digitalisation are of particular relevance to advancing and accelerating materials design in a way that takes multiple dimensions of properties, performance and circularity into account. To that end, EMMC has been facilitating workflow integration, data documentation and semantic interoperability. Multiple projects have been collaborating under the EMMC banner in the development of the EMMO ontology for applied sciences and manufacturing. EMMO provides a strong semantic framework for all the datasets generated by experimental, modelling and characterisation activities.

We give an overview of pertinent EMMO ontologies, including characterisation, manufacturing and their industrial applications. In more detail, we highlight the CoBRAIN project, demonstrating the impact of integrating computational and experimental data through semantic interoperability. It enables the development of intelligent tools that (a) propose novel materials from the class of high entropy alloy-based “hardmetals” for direct deposition by Thermal Spraying techniques, and (b) are capable to estimate their impact on the economy and the environment.

Development of new materials with high wear and good corrosion resistance is usually based on experimental trial-and-error and operational feedback. Combining data coming from modelling and experimental approaches provides an advancement but is limited by the fact that the final coating properties depend on too many materials and process factors. Hence obtaining reliable results from physical modelling as well as experimentation are in conflict with the response time and cost containment required for industrial innovation. Here, the application of modern AI techniques can speed up the innovation process when used as complementary tool to existing experimental, modelling and characterisation activities. It can also enhance decision systems integrating all aspects of the materials and production process, taking account of economic and environmental factors.

In order to facilitate such a system, all the CoBRAIN generated data are collected into a single end-point via a full conceptual model based on the EMMO ontology. Datasets from the various areas of expertise within the project have been integrated thanks to the interoperability provided by the EMMO framework and made available to the users through a triple store Knowledge Base. Besides dramatically improving the FAIR level of the project results, it facilitates the creation of meaningful and coherent dataset for AI training and verification.

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Effects of cooling rate and tempering on the microscale mechanical properties of heat resistant steel (30CrMoNiV5-11)

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Ferritic/martensitic heat-resistant steels used for high-temperature applications typically have a multiphase microstructure containing ferrite, martensite, and/or bainite, as well as carbides. This microstructure is controlled by the cooling rate during quenching and by tempering parameters. Various microstructural constituents exhibit different mechanical properties, which, along with the microstructural architecture, define the mechanical properties on the macroscale. This work focuses on the effect of local microstructure on the local mechanical properties of 30CrMoNiV5-11 heat-resistant steel.

Samples machined from the as-received material were austenitized at 950 °C for 30 minutes, followed by controlled cooling at the following rates: 0.05, 0.5, 5, and 50 °C/s. Scanning electron microscopy (SEM) and electron backscatter diffraction (EBSD) analyses were performed to identify individual microstructural constituents and conduct their quantitative analysis. Nanoindentation tests were carried out using a Hysitron TriboIndenter TI 950 with a Berkovich indenter, performing measurements on EBSD scans to correlate local microstructural architecture with nanohardness values.

The results showed that higher cooling rates (50 °C/s) produced a martensitic microstructure with the highest average nanohardness (6.1 GPa). As the cooling rate decreased, the microstructure changed, and average nanohardness values also decreased as follows: 5 °C/s resulted in a martensitic-bainitic microstructure with a nanohardness of 5.8 GPa; 0.5 °C/s yielded a ferritic-bainitic microstructure with 4.8 GPa; and 0.05 °C/s produced a ferritic microstructure with the lowest average nanohardness value of 4.5 GPa.

Subsequently, simulating an industrial manufacturing process, tempering was performed at 680 °C for 45 minutes, followed by rapid cooling in water. EBSD and nanoindentation analyses were repeated to evaluate the effect of tempering on local mechanical properties in comparison to the quenched material. It was found that the average nanohardness values decreased after tempering. Specifically, the tempered martensitic microstructure (50 °C/s) exhibited an average nanohardness of 4.5 GPa, followed by the tempered martensitic-bainitic microstructure (5 °C/s) with an average nanohardness of 4.7 GPa, the tempered ferritic-bainitic microstructure (0.5 °C/s) with 3.9 GPa, and the ferritic microstructure (0.05 °C/s) with 3.7 GPa. The microstructure-property relationship on the microscale is discussed.

Bayesian Active Learning for Physics-Informed, Multi-Constraint, Multi-Objective Alloy Design: A Probabilistic Approach

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D9_3 - Bayesian and Advanced Optimization for Materials, Seminario 6 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Given the diverse performance criteria in materials development, alloy design is better approached as a simultaneous optimization and constraint satisfaction problem rather than a straightforward optimization task. In this work, we introduce a Bayesian closed-loop framework that concurrently identifies feasible alloys—those meeting all predefined performance constraints—and alloys that are Pareto-optimal across multiple properties. Unlike traditional optimization approaches, our method assigns probabilistic scores to candidate alloys based on their likelihood of satisfying constraints and achieving Pareto optimality. Moreover, Bayesian principles are employed to update low-fidelity prior models with limited high-fidelity data, thereby expediting the active learning process. We demonstrate the efficacy of this framework through a multi-constraint, multi-objective high entropy alloy design case study.

Leveraging AI and Genetic Algorithms for Self-Healing Alloy Design

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D9_4 - Structure-Property Relationships and Synthetic Data, Seminario 6 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The well-studied 9–12% Cr steels are an economical and highly versatile material choice, making them suitable for power generation and other demanding industrial applications. However, prolonged exposure to high temperatures inevitably leads to creep damage. In this context, self-healing (SH) mechanisms have emerged as a promising approach to enhancing the steel's resistance and extending its service life under extreme conditions. While precipitation-based SH processes have been primarily identified in binary and ternary alloys, their underlying mechanisms in multicomponent systems remain unclear. To address this challenge, we propose a design strategy that leverages data science tools and genetic algorithms to optimize and predict self-healing behaviour in complex alloy systems. Building on this premise, our strategy begins with a novel data extraction workflow designed to automatically collect key attributes from scientific journal articles, including material properties, chemical composition, heat treatments, and reinforcement particle size. Given the complexity and variability of scientific literature, traditional data mining approaches often struggle to extract structured data effectively. To overcome this limitation, we employ a large language model (LLM)-driven workflow, which offers superior adaptability in text classification and structuring. Notably, models such as GEMINI-AI, GPT, and DeepSeek were employed without pretraining or fine-tuning for the selected characteristics. The resulting dataset, which comprises information from approximately 15,000 scientific articles on 9–12% Cr steels accessed via the ELSEVIER API, was structured with achieved an average precision of 85% and systematically organized within an SQL database.

Genetic algorithms were chosen for their effectiveness in exploring large, high-dimensional search spaces and optimizing multi-objective problems, making them particularly well-suited for designing complex alloy systems with self-healing capabilities. The structured database enables advanced data mining analyses to uncover patterns that drive the optimization of genetic algorithm parameters, individual genes, and go/no-go criteria. Additionally, an existing fitness function was chosen to optimize precipitation and solid solution reinforcements, contributing to the self-healing capability of the alloys.

Advancing Interoperability and Digitalization in Materials Science and Manufacturing: A Semantic Workflow Module for Standardized Data Management

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D9_6 - FAIR Data, Interoperability, and Digital Workflows, Seminario 6 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Inconsistent experimental procedures, diverse modelling methodologies, and insufficient protocol reporting present significant challenges in materials science, hindering reproducibility and data validation. The standardization of data offers a promising approach to addressing these issues; however, integrating data from disparate sources, a common scenario in the field of materials science and manufacturing, introduces complexities. While applying ontologies facilitates data harmonization and interoperability, the associated overhead can be substantial. Moreover, effective tools for managing these challenges are scarce and often inadequate for production environments.

This talk introduces a novel semantic workflow module, developed as part of the Dataspace Management System (DSMS) technology stack, to address critical gaps in managing material-related processes such as manufacturing and characterization. A key challenge we address is that users are typically not ontology experts, which can hinder efficient interaction with complex data. The intuitive interface of the module simplifies this process, enabling users to easily engage with the system without requiring deep knowledge of the underlying ontologies.

We illustrate the module's powerful and user-friendly approach with a practical use case derived from the ongoing AID4GREENEST project. There we leverage the CHADA (CHAracterization DATA) framework for standardizing characterization workflows as well as its ontological representation, the CHAMEO ontology, a module of the European Multiperspective Material Ontology (EMMO). We assert that this development contributes to the critical effort of optimising product development in the manufacturing industry.

Multiscale mean-field framework for process-structure-property prediction in large-scale component manufacturing: A case study of turbine shaft forging

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D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The manufacturing of large-scale components for energy applications presents significant challenges in terms of material efficiency, energy consumption, and sustainable use of critical raw materials. In response to these challenges, we present a comprehensive mean-field material model for predicting microstructure evolution during the hot forging of large turbine shafts, developed and utilized within the framework of the Horizon Europe project AID4GREENEST.

Our model is founded on fundamental thermodynamic principles and addresses the complex interplay between various physical phenomena occurring during hot forming. The framework simultaneously accounts for work hardening, dynamic recovery, recrystallization, and grain growth through a physics-based approach. A key strength of our methodology lies in its ability to couple microstructural evolution with thermo-mechanical material behavior, enabling accurate predictions of local microstructure development throughout the entire forging process.

We have implemented the model within the FORGE finite element software environment, facilitated by the DynamiX GUI, which allows for practical industrial applications. The simulation framework has been specifically calibrated for turbine shaft steels containing critical elements such as Mo, Nb, and Ni. Our validation approach combines extensive thermo-mechanical experiments with detailed metallographic analyses performed on industrial-scale components, ensuring robust and reliable predictions under various processing conditions.

The model demonstrates particular strength in optimizing process parameters while considering the desired microstructural and mechanical properties. Our results show that the implementation successfully predicts local microstructure evolution across multiple length scales, from grain interactions to macroscopic property development. This capability enables more efficient process design and optimization, potentially reducing the material and energy consumption associated with traditional trial-and-error approaches in large-scale forging operations.

Furthermore, our work provides a foundation for sustainable manufacturing practices in the energy sector. By enabling precise prediction of microstructure evolution based on varying process parameters, the model supports the development of optimized processing routes with reduced energy consumption and more efficient use of critical raw materials. The methodology significantly reduces the time and resources required for process design through numerical simulations, representing a substantial improvement over conventional approaches in the forging industry.

This research contributes to the ongoing digital transformation of the metallurgical industry by providing a robust, physics-based tool for process and material optimization. The developed framework represents a significant step toward more sustainable manufacturing processes for critical energy sector components, aligning with the industry's goals of reduced environmental impact and improved resource efficiency.

Advances in Modelling, Simulation, and Digitalization for Material and Process Design of Metallic Materials

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D9_6 - FAIR Data, Interoperability, and Digital Workflows, Seminario 6 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The manufacturing of materials and their transformation into products in a sustainable and environmentally friendly manner is one of the major challenges currently facing industry in order to enable a greener society. In the fields of materials science and the mechanics of materials, the last few decades have been dominated by innovations in modelling and simulation as well as characterisation techniques. The determination of process-structure-property relationships plays an increasingly important role. Notably, the chemical composition and the microstructure of materials is identified as a pivotal factor, with the potential to markedly accelerate the design of materials, processes, and products while substantially minimizing experimental requirements. The talk proposes a paradigm shift, advocating for an integrated approach underpinned by the Integrated Computational Materials Engineering (ICME) framework, the digital transformation of diverse data into knowledge, and the strategic application of artificial intelligence to expedite processes and generate actionable recommendations. The digital representation of materials and processes by using semantic technologies to enable FAIR (Findable, Accessible, Interoperable, Reusable) data as well as the solving material and process design challenges via machine learning are key elements of the change of paradigm. The talk will demonstrate how the three central elements will be linked to accelerate the material and process design.

Machine Learning Approaches for Predicting Engineering-relevant Material Properties

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¹Ansys, Cambridge, United Kingdom

D9_5 - Process Modeling and Simulation, Seminario 6 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

AI and machine learning (ML) are playing an increasingly important role in materials science, offering new ways to accelerate discovery and optimize material properties. Much of the focus has been on applications such as crystal structure prediction and the development of ML interatomic potentials; however, these techniques are largely limited to idealized or simplified systems. In contrast, despite their practical significance, AI/ML applications to real engineering materials have received less attention. With the rapid expansion and democratization of AI/ML tools in recent years, it can be difficult to select the most suitable approach for the intended application, as often best practices from more established fields, e.g. finance, do not fully translate to the world of materials.

Engineering materials, with their complex microstructures and processing-dependent properties, present unique challenges that require specialized ML methods. This work explores AI/ML techniques for predicting the properties of real materials, addressing key challenges such as data scarcity, microstructural effects, and the influence of state and environmental variables. We discuss strategies including validation, uncertainty quantification, and the integration of domain knowledge to improve predictive accuracy and reliability. This will be illustrated using a number of examples. By adapting ML methods to the specific challenges of engineering materials, this research aims to support their broader adoption in materials design and development.

Advanced Correlation Analysis of Process-Microstructure-Property Relationships in LPBF AlSi10Mg: Beyond Traditional Metrics

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D9_2 - AI for Materials Characterization, Seminario 6 Room (Level +1), septembre 15, 2025, 10:50 - 13:10

Recent advances in Laser Powder Bed Fusion (LPBF) of AlSi10Mg have underscored the need for more comprehensive analyses that link processing parameters, microstructural features, and mechanical properties. In this study, we present an in-depth correlation analysis that clusters and quantifies interactions among key variables, including laser power, scan speed, porosity (Archimedes vs. XCT), sub-grain cell dimensions, and mechanical performance indicators such as ultimate tensile strength (UTS) and elongation at fracture.

Our results show that certain microstructural descriptors—particularly solidification cell size—are strongly correlated with mechanical response in near-dense parts (<0.5% porosity), suggesting that strength and ductility can be better predicted when both porosity metrics and cell structures are considered. Interestingly, the figure also reveals how large, irregular pores affect overall ductility more than finer round pores, reaffirming that defect morphology plays a major role in fracture initiation. Conversely, when samples remain below a critical porosity threshold, the effect of cell size can dominate, leading to both higher strength and a potential decrease in ductility.

Additionally, we confirm that laser energy density and hatch spacing do not act independently: certain parameter combinations drive either lack of fusion or keyhole porosity, which in turn governs overall mechanical performance. By visually clustering these parameters, it sheds new light on specific “safe zones” for optimal density and mechanical properties, beyond the simplified process windows typically reported.

In conclusion, our correlation-based approach identifies strategic pathways for parameter tuning to achieve targeted mechanical behavior. Future work will integrate these findings with advanced in situ monitoring and machine learning models to predict and control defect formation in real time, thereby pushing the envelope of performance in LPBF-manufactured AlSi10Mg.

nanoHUB services for FAIR simulations and data: ResultsDB, Sim2Ls, and AI research assistant

Prof. Alejandro Strachan¹

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D9_6 - FAIR Data, Interoperability, and Digital Workflows, Seminario 6 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

nanoHUB is an open cyber platform for online simulation, data, and education that seeks to make scientific software and associated data widely available and useful. This presentation will describe recent developments in our infrastructure to address modern data needs. nanoHUB's Sim2Ls (pronounced sim tools) make simulation, modeling, and data workflows discoverable and accessible to all users for cloud computing using standard APIs. In addition, published tools are findable (with digital object identifiers), reusable (via documented requirements and services), and reproducible via containerization. In addition, all Sim2L runs are automatically cached, and their results are indexed in a global and queryable database (ResultsDB). We believe this infrastructure significantly lowers the barriers to making simulation/data workflows and their data findable, accessible, interoperable, and reusable (FAIR). These information resources can be easily invoked as needed by domain experts to advance their fields. I will demonstrate the use of the ResultsDB and Sim2Ls as information sources to power an autonomous research agent based on a large language model for end-to-end scientific discovery.

Experimental investigation of tire-wear particle sizes

Mr. Alexander Schmiedhofer¹

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E1_3, Z3 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

The electrification of personal vehicles is a crucial step in combating climate change. One significant initiative driving this transformation is the implementation of the new EURO 7 emission standards. This regulation addresses exhaust emissions and targets non-exhaust sources, particularly tire wear, which is recognized as the largest contributor of microplastic particles to the environment.

While extensive research has focused on tire abrasion and determining abrasion rates, relatively little attention has been given to the distribution of particle sizes generated during this process. The size of microplastic particles plays a vital role in determining their environmental impact. Therefore, it is essential to understand how driving parameters—such as slip, velocity, and normal force—affect the size distribution of these particles.

This study utilized a mini traction machine to replicate tire abrasion under real-world conditions. In this scaled-down experiment, the tire was represented by a ball made from the same material, while the road surface was simulated with an asphalt disc composed of small-grain gravel and bitumen. In this experimental setup, multiple tests were conducted with varying normal loads, slip ratios, and velocities. The generated particles were carefully collected with a brush and analyzed using microscopy to classify them by size, and EDX to determine their chemical composition.

This approach provides valuable insights into how driving parameters influence the size distribution of microplastic particles, contributing to a deeper understanding of their environmental implications.

Ni-9%P+(a:C-H)DLC multilayer coating: a solution to improve the tribological behaviour of complex-shaped AlSi10Mg components produced by Powder Bed Fusion-Laser Beam for automotive industry

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The interest of the industrial and scientific community in Powder Bed Fusion-Laser Beam (PBF-LB) technology stems from its innovative approach to the design and manufacturing of high-performance and complex-shaped components. AlSi10Mg alloy is widely used to produce lattice structures and thin-walled parts by PBF-LB technology for the automotive industry, as it combines good mechanical properties and corrosion behaviour. However, it is characterized by poor tribological behaviour, especially under severe environmental conditions.

The application of the Ni-9%P+(a:C-H)DLC multilayer coating is a promising solution to improve the tribological behaviour of PBF-LB AlSi10Mg components: the deposition conditions (time and temperature) are compatible with the as-built microstructure, preserving its mechanical performance, and can be integrated with heat treatment cycles used to optimize bulk tensile properties. In addition, the Ni-9%P interlayer is able to coat complex geometries and surface-connected defects, typical of the PBF-LB process, ensuring uniform thickness, good adhesion and continuity, and providing load support to the (a:C-H)DLC topcoat, which is characterised by high wear resistance and low friction. Barrel finishing can be implemented before the deposition of the Ni-9%P+(a:C-H)DLC multilayer coating to obtain a controlled surface finish over the entire surface, ensuring uniform functional properties.

To demonstrate the effectiveness of the whole post-process cycle (barrel finishing + multilayer coating deposition), a complete microstructural and micromechanical characterization was carried out on a motorcycle steering plate in PBF-LB AlSi10Mg alloy. Optical profilometry and cross-section observations using FEG-SEM/EDS and ion milling were used to analyse the surface roughness and the quality of the multilayer coating, substrate and interfaces. The adhesion of the Ni-9%P layer on the substrate was evaluated by Rockwell indentation ("Mercedes test") and the practical adhesion of the (a:C-H)DLC on the Ni-9%P interlayer was tested by progressive load scratch testing. Instrumented indentation was used to measure the hardness of both layers (Ni-9%P and (a:C-H)DLC) on the micro/nanoscale.

The results obtained from the microstructural and micromechanical characterization demonstrated the applicability of the Ni-9%P+(a:C-H)DLC multilayer coating on real automotive components produced by PBF-LB. This will enable the production of innovative components with sustainable materials and processes, supporting the ecological transition in the automotive sector.

Effects of different surface treatments on the fatigue behaviour of AlSi10Mg alloy produced by Powder Bed Fusion-Laser Beam: a comparison between machining, sandblasting and Ni-9%P+(a:c-H)DLC multilayer coating

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E1_2, Z3 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The demand for sustainable mobility is growing and the use of innovative materials and processes is essential to support the ecological transition. The AlSi10Mg alloy produced by Powder Bed Fusion-Laser Beam (PBF-LB) is widely used in the production of lattice structures and thin-walled parts in electric and hybrid vehicles due to its high strength-to-weight ratio. However, poor surface finish and high defect density in the surface area of the as-built components can significantly reduce the fatigue performance of structural parts. In this perspective, surface treatments can be useful to improve the fatigue strength of PBF-LB-produced components, reducing the negative effects of process-induced defects and as-built surface.

In this work, rotating bending fatigue tests were carried out on the PBF-LB AlSi10Mg alloy subjected to two different heat treatments (direct aging (T5) and T6 solution treatment), used to maximize the mechanical properties, and in three different surface conditions: (i) machined, (ii) sand-blasted, (iii) Ni-9%P+(a:c-H)DLC coated. A detailed microstructural, mechanical and fractographic characterization was performed to evaluate the effect of heat treatments and surface treatments on the fatigue strength of the material.

The results showed significant and comparable improvement in fatigue strength achieved by both sandblasted and Ni-9%P+(a:c-H)DLC coated samples: approximately 55% for the T5 alloy and approximately 25% for the T6 alloy compared to the machined samples. The residual compressive stresses in the superficial and sub-superficial zone and the change in type and distance from the surface of the “killer” defects induced by sandblasting and multilayer coating deposition were identified as the main causes of the improved fatigue performance of the PBF-LB AlSi10Mg alloy. In addition, machining reduced the distance of killer defects from the surface by removing part of the contour zone, thus limiting the fatigue strength achievable by the material. The T5 alloy showed better response to surface treatments: (i) the ultrafine cellular microstructure was more susceptible to sandblast-induced work hardening than the T6 microstructure, resulting in higher and deeper surface compressive residual stresses, and (ii) the multilayer Ni-9% P+(a:c-H)DLC coating improved the defect tolerance of the T5 microstructure, increasing the distance from the surface of the possible crack initiation zone and the surface hardness.

This study demonstrated that sandblasting and Ni-9%P+(a:c-H)DLC multilayer coating can be good solutions to improve the fatigue performance of complex-shaped PBF-LB AlSi10Mg components for sustainable mobility, avoiding the need for mechanical processing to improve the surface finish and defect tolerance of PBF-LB-produced structural parts.

Environmental impact assessment of battery module lifecycle: a comparative evaluation of components replacement in the circular economy concept

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E1_3, Z3 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

This study explores the environmental implications in the lifecycle management of batteries for electric vehicles, with a specific focus on a single module. The goal is to evaluate the possibilities of circular economy strategies to mitigate environmental challenge associated with batteries life cycle, focusing on reuse and repair strategies, as an alternative to complete disposal.

In order to analyze the life cycle stage of a single battery module, to be introduced to the second life application during the testing process, the gate-to-gate scope has been assigned by the Life Cycle Assessment (LCA) methodology. The Ecoinvent 3.8 database and the SimaPro software were used to measure various environmental impact categories, particularly climate change. Three different scenarios, according to the output of the module's technical and electronical test, have been identified. Defined scenarios measured the environmental impacts, driven by a single cell and electronic components, adopting a repair strategy, compared to the full module disposal scenario and to the production.

Obtained results highlighted that the complete discard highly effect on eutrophication in marine ecosystems and climate change, while adopting the inserted strategies reduce the effect notably in the considered categories, as well as material and resource use. Performed studies highlighted several challenges, such as discrepancies between industrial and laboratory data, variations in recycling processes and methods, differences in battery chemistries, manufacturing technologies, and regional energy mixes. These data can affect results derived from the LCA methodology, confirming the need for a harmonized LCA methodologies to ensure consistent evaluations of environmental impacts.

Outcomes align with the three pillars of circular economy, showing that even partial reuse reduces the demand for new raw materials and mitigates the ecological consequences of critical material extraction. By maximizing the interval between manufacturing and recycling phases, industries can reduce environmental impacts, and promote a sustainable industry, along with the circular economy strategies, in the full battery life cycle manufacturing process. Several possible second life applications have been identified for the battery module under study, allowing to maximize the livability and reduce the need for critical material extraction for the new battery production.

KEY WORDS: Lithium-ion battery, Electric vehicle, Environmental impact, Life Cycle Assessment, Batteries second life application, Circular Economy.

Sustainable Recovery of Critical Raw Materials through Advanced Hydrometallurgical Recycling

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E1_2, Z3 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The emerging shift of the linear raw materials value chain to circular economy in the automotive sector entails the recycling of strategic and critical raw materials (CRMs) from End-of-Life (EoL) vehicle components and devices. Two innovative approaches have been developed focusing on recovering valuable materials from automotive catalysts, hydrogen fuel cells, permanent magnets, and lithium-ion batteries of electric vehicles (EVs), all essential for future mobility and sustainable transportation. The underlying research aims at closing the loop in the value chain of these EoL devices by utilizing two concepts; i) chlorine hydrometallurgy using HCl, and solvometallurgy using Deep Eutectic Solvents (DESS).

Both processes begin with pre-processing of the EoL device, followed by selective leaching and refining of CRMs, and is completed by reusing the recovered CRMs in new products. The hydrometallurgical leaching process has been developed and upscaled by MONOLITHOS in one-step, offering energy-efficiency and achieving very high CRM recovery rates from the aforementioned waste streams, i.e. 100% of Pt, 92% of Pd and over 61% of Rh from three-way catalytic converters (TWC) [1]. Characterized as environmentally friendly, the solvometallurgical leaching process developed by YS Cypriot Catalysts, utilizes biodegradable lixiviants [2] to extract over 81% of Pt, 95% of Pd and 79% of Rh from EoL TWCs. Both processes can be tailored to meet the specific requirements of the different automotive waste streams, offering flexible and sustainable solutions for CRM recovery. The chlorine hydrometallurgy approach offers high efficiency in extracting metals from spent materials like autocatalysts but involves the use of acids, raising environmental concerns. In contrast, recycling using DESs is more environmentally friendly with low toxicity, but it has lower extraction rates and is presents challenges during upscaling for industrial operations. However, process optimization and parametrization through computational modeling can provide the potential for DES processing to achieve comparable metal extraction yields to chlorine hydrometallurgy. Thermodynamic modelling on DES systems can provide insights on the chemical interactions and process mechanism, towards resolving upscaling bottlenecks and the recycling of more EoL feeds beyond TWCs.

Aiming to reduce the EU dependency on virgin raw materials in the automotive sector, both recycling processes promote a sustainable, resilient and resource-efficient ecosystem aligned with the transition to “green mobility”.

[1] I. Yakoumis, A. Moschovi, M. Panou and D. Panias, J. Sustain. Metall., 2020, 6, 259–268.

[2] O. Thoda, E. Svinterikos, K. M. Sakkas, A. M. Moschovi and I. Yakoumis, Separations, 2023, 10, 445.

Additive manufactured complex cooling channels for High Pressure Die Cast (HPDC) electric power train components for automotive applications

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E1_3, Z3 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Several components of the electric powertrain require solutions for cooling or temperature control. These include electric engine as well as power electronics housings, or battery cases, which are typically realized as cast aluminum components, with HPDC as the production process of choice based on its high productivity. However, realization of cooling channels in HPDC is a difficult business, as many lost core techniques are not applicable to this process due to the high forces acting on the cores during the filling as well as the intensification phase. An alternative is the integration of aluminum hollow profiles. According to the state of the art, this is e.g. possible based on the Combicore® or the ZLeak Tube® technology. However, both approaches require a filler which stabilizes the cooling channel during casting, and thus affords an additional process step, which is the removal of the filler. The alternative approach suggested by the BioniCast project is the use of additively manufactured cooling channels. The advantage of this concept is that cooling channel design can be optimized for stability, heat transfer and flow resistance, and varied along the length of the channel if necessary.

The present study outlines approaches to determine, by means of casting and finite element simulation, the stability of given cooling channels made via the Laser Powder Bed Fusion (LPBF) additive manufacturing process from AlSi10Mg alloys in different heat treatment states, namely stress relieved for 2 hours at 350°C and warm aged for 6 hours at 170°. We use the MAGMASOFT® casting simulation package to extract the thermal loads acting on the cooling channels and transform them directly into a stability criterion based on a simplified equation for tube stability under external pressure. As the relevant moment in time, we identify the freezing of the gates, as we must assume that intensification pressure can only be transferred to the cavity until this moment in time. We add a finite element simulation assuming (a) homogeneous temperatures within the insert and (b) the temperature distribution derived from the casting simulation to compare this data with the aforementioned MAGMASOFT® user result as well as experimental data based on casting of actual test components. The prerequisite for all analyses is the detailed characterization of temperature-dependent properties of the additively manufactured AlSi10Mg alloy in both heat treatment states, which has been done in a range from room temperature to 450°C using a Gleeble system.

Advanced Laser welding processes for joining of High Pressure Die Casting (HPDC) components made from secondary aluminum alloys

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E1_2, Z3 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The automotive industry is subject to the necessity of reducing the carbon footprint of their products. With the transition of from internal combustion engine to electric drive, the focus in this respect has moved from the use to the beginning-of-life, i.e. the production phase. At the same time, the production of rear and front underbodies as well as battery cases as single-piece castings (often termed Mega- or Gigacasting) has the potential of drastically increasing the amount of cast aluminum in automotive body structures. As a primary material, aluminum production carries the burden of a considerable energy input, and thus, depending on the energy source, a carbon footprint in a range from approx. 2 (hydro power, Norway) to 8.6 (Europe, average sourcing) and 20 kg (fossil fuels) CO₂eq./kg primary Al. The focus thus moves to the possibility of using secondary aluminum alloys. These are typically characterized by an accumulation of specific elements like Cu, Fe and Zn, which have an impact on structural characteristics, corrosion etc., plus a higher likelihood of other types of impurities. Several studies are currently addressing the issue of material characteristics, however, the question of joining techniques is of similar importance and has so far largely been neglected in terms of the impact of using secondary alloys.

The present study attempts to partially close this research gap by addressing the laser beam welding process. Since HPDC is mostly considered unsuitable for welding due to high hydrogen contents and trapped gases from the casting process an excellent welding process and the desired high quality cannot be guaranteed. By modifying conventional laser welding with the dynamic beam modulation approach, the welding process can be stabilized and the joint quality significantly improved. In experimental studies covering high pressure die cast AlSi10MnMg alloys with secondary material content levels ranging from 0 wt.-% to 89 wt.-%, castability and weldability were investigated and the structural and mechanical properties of the joint determined. The paper shows how the developed approach of dynamic beam modulation can be used to combine die casting with semi-finished products in order to achieve lightweight construction and produce a cost-effective car body. In combination with the use of secondary casting, this opens up the possibility of producing almost CO₂ neutral components.

Multiscale models combined with LCA design framework to conceive sustainable and circular energy storage systems

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E1_3, Z3 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

The transition toward sustainable and circular energy storage solutions is a key challenge in the transport sector. In this work, we present a simulation-guided design framework for hybrid battery packs that integrate lithium-ion cells with high-energy-density supercapacitors. Developed within EU founded projects and validated on an e-scooter case study, our approach combines multiphysics and multiscale simulation with cradle-to-cradle life-cycle assessment (LCA) to support the entire value chain—from material development and process optimization to component design and upscaling.

At the material level, atomistic models have been used to guide the fabrication of carbide-derived electrodes from recycled plastics. By bridging experimental observations (e.g., TEM characterization) with fundamental electrochemical behavior, these models can shed light on the complex interactions between key structural properties (i.e., pore size distribution) and interfacial interactions with electrolytes and ionic liquids, thereby reducing the need for costly trial-and-error investigations. At the mesoscale, microstructure models coupled with discrete and continuum simulations can capture the effects of electrochemical, thermal and mechanical processes on cell performance and selected ageing mechanisms, thereby linking the main operating and manufacturing parameters to performance metrics. At the system level, simplified models, such as equivalent circuit representations calibrated on synthetic data from continuum simulations, enable prediction of battery pack performance under realistic operating conditions. These models also support the development of control logic and monitoring strategies that account for ageing effects and ensure reliable operation in the field.

The integration of this multiscale and multiphysics simulation chain with LCA analysis allows design decisions to be informed not only by performance targets but also by environmental impact and cost considerations. This is critical in electrochemical systems, where the use of critical raw materials or polluting techniques may jeopardize the goal of producing environmentally-conscious products.

In summary, our work demonstrates that the combined use of atomistic, mesoscale, system-level simulations, and a systematic life-cycle assessment, can effectively guide the design and optimization of hybrid battery packs. This simulation toolchain provides a robust basis for accelerating material selection and process improvements while ensuring high performance, reduced charging times, steady power delivery, and extended driving range in sustainable transport applications.

Towards material circularity and manufacturing sustainability in the automotive industry

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E1_1, Z3 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

Although materials and manufacturing are the backbone of the global economy, they also pose a significant climate liability. In 2023, 59 gigatons (Gt) of CO₂eq were emitted, with nearly 40% of industrial emissions coming from iron and steel, aluminum, and plastics. Decarbonizing these sectors by increasing circularity and reducing energy use is essential for achieving a carbon-neutral, circular economy. For example, steel production (1,700 Mt annually) uses only 45% scrap input, emits 3.7 Gt CO₂eq, and generates 425 Mt of scrap; aluminum production (94 Mt annually) relies on 30% scrap, emits 0.7 Gt CO₂eq, and produces nearly 40 Mt of scrap; while plastics account for 4.5% of global emissions with just 18% recycled, and their production is expected to rise as petroleum feedstocks shift to material applications. On the other hand, fossil fuels currently supply 84% of global energy and 90% of transportation energy, yet automotive OEMs worldwide are committing to carbon neutrality by 2035–2050. With California banning new gasoline-powered cars and Canada requiring all new vehicles to be zero-emission by 2035, the automotive industry in North America is shifting from internal combustion engines to electric and hydrogen fuel cell vehicles. This electrification presents major opportunities for achieving material circularity and sustainable manufacturing.

This paper reviews emerging technologies that promote material circularity and manufacturing sustainability in the automotive industry, using aluminum sustainability as a prime example. Although aluminum is increasingly employed for lightweighting in transportation to reduce energy consumption and carbon emissions, its primary production is highly energy-intensive and generates substantial CO₂ emissions. In contrast, re-melting aluminum scrap consumes only about 5% of the energy needed for primary production, markedly reducing emissions and ensuring a sustainable supply chain. Additionally, renewable materials such as “super wood”—densified natural wood with metal-like mechanical properties—offer further promise. Advances in energy-efficient large thin-wall die casting (mega/giga casting) support the sustainability of automotive manufacturing, especially as alternative energy vehicles adopt simplified body structures that enable the use of consolidated castings, thereby minimizing welding and assembly operations. Moreover, reclaiming high-value battery materials from electric vehicles remains challenging; however, a patented “Hydro-to-Cathode” direct precursor synthesis process effectively leaches impurities and retains valuable metals, streamlining recycling by eliminating multiple processing steps. Ultimately, the integration of recycled/renewable materials with energy-efficient manufacturing techniques is key to driving the automotive industry toward a circular and sustainable future.

Sustainability Assessment of Hydrometallurgical Recovery of Platinum Group Metals from End-of-Life Hydrogen Fuel Cells and Electrolyzers

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E1_3, Z3 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

The transition to green and sustainable mobility is accelerating as the automotive sector shifts toward electrification and hydrogen-powered technologies to reduce greenhouse gas emissions and dependence on fossil fuels. Fuel cells and electrolyzers are key components in this transition, enabling hydrogen-powered transport and energy storage solutions. However, these technologies rely on Platinum Group Metals (PGMs), which are both scarce and economically critical. Developing efficient End-of-Life strategies to recover PGMs from fuel cell and electrolyzer components is essential to ensuring resource security, cost efficiency, and environmental sustainability.

This study evaluates the sustainability, safety, and economic feasibility of a patented, eco-friendly, and industrial-scale hydrometallurgical process developed by MONOLITHOS Ltd. for the recovery of PGMs from End-of-Life Membrane Electrode Assemblies (MEAs), achieving high recovery efficiencies (Pt >99% and Ir >60%) [1,2]. The assessment integrates Life Cycle Assessment (LCA), safety risk analysis, and cost modeling to evaluate energy consumption, greenhouse gas emissions, human health impacts, and resource depletion.

Preliminary results indicate an 80% reduction in CO₂ emissions compared to traditional PGM extraction methods, demonstrating the process' environmental benefits. Additionally, an economic analysis highlights the cost advantage of the recovered materials, showing a 30% lower cost compared to commercial PGM components for hydrogen devices. Further optimization efforts aim to reduce the overall environmental impact by at least 15%, while maintaining high material purity and ensuring process scalability.

The LCA was conducted using SimaPro and the ecoinvent database, ensuring transparent process modeling and benchmarking against conventional end-of-life PGM recovery routes. Workplace safety risks—including chemical exposure, reagent handling, and waste management—are analyzed to support industrial-scale implementation.

This research contributes to sustainable hydrogen mobility and clean energy technologies, providing a scalable and environmentally responsible solution for PGM recovery in hydrogen fuel cells and electrolyzers. By integrating LCA, safety assessment, and cost modeling, this study aligns with the EU's circular economy objectives, supporting the transition to low-emission transport and energy systems.

This research has received funding from the European Union's Horizon programme and the Clean Hydrogen Partnership through the HERAQCLES project under grant agreement No 101111784.

[1] Patents: Greek Patent, Appl. No: 20210100765 (2021); European Patent, Appl. No. EP22204905.8 (2022); Greek Patent, Appl. No: 20240100540 (2024).

[2] A. Moschovi, E. Zagoraiou, E. Polyzou, and I. Yakoumis, IOP Conf. Ser. Mater. Sci. Eng., 2021, 1024, 012008.

Multi-material Lightweight Design with Aluminum-Steel Hybrid-Casting: Process Parameters and Influencing Factors

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E1_2, Z3 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Multi-material Lightweight Design with Aluminum-Steel Hybrid-Casting: Process Parameters and Influencing Factors

Introduction

Steel and aluminum remain key materials for lightweight design, especially in automotive applications. Both materials have different advantages in their mechanical and physical properties as well as their processing technologies. The presented aluminum-steel hybrid-casting process enables metallurgical bonding between aluminum cast components and steel sheets or profiles. It combines the specific advantages while eliminating the need for costly mechanical joining or adhesive bonding. The resulting hybrid structures are lightweight, space-efficient, and optimized for load conditions.

The metallurgical bonding is achieved by a unique Al-Si coating on steel inserts and optimized high-pressure die casting (HPDC) parameters. Casting simulations and experimental trials identified optimal process parameters, validated through mechanical tests.

Methodology

Steel inserts were coated with a 20-25 μm Al-Si layer by physical vapor deposition (PVD), forming a dual-layer structure. The first intermetallic sublayer ($\sim 2\text{-}3\ \mu\text{m}$) contains Fe-Si-Al phases, while the thicker Al-Si layer on top ensures bonding with molten aluminum, inhibiting brittle phases.

Cold-forming and dual-phase steels were paired with an AlSi10MnMg aluminum cast alloy. Extensive casting trials were conducted using a HPDC machine. Key parameters varied were:

- Melt temperatures: 685–750 °C
- Gate velocities: 20–60 m/s
- Die temperatures: 180–280 °C
- Insert preheating: 20–500 °C

Numerical casting simulation supported parameter optimization. Mechanical testing on produced samples included tensile shear, pull-out, cross-tension, and fatigue experiments to evaluate joint strength.

Results

Die temperature and insert preheating significantly influenced bond strength, with higher values creating superior results. Higher gate velocities also improved bonding, whereas lower melt temperatures were favorable. Simulation data correlated well with fracture patterns and measurements.

Shear strength tests yielded an average of approximately 16 MPa, with low deviation ($<1.2\ \text{MPa}$). The ductility of the bond was evident from significant necking in the steel insert and heavily deformed honeycomb fracture surfaces in SEM images.

In pull-out tests, failure occurred in the steel component rather than at the joint. Similarly, fatigue tests under cyclic tensile loading showed crack propagation within the steel insert, without premature joint failure.

Conclusion and Outlook

This study establishes key process parameters for a reliable aluminum-steel hybrid-casting process, achieving a strong and ductile metallurgical bond. Future work aims to scale the technology from test samples to automotive components. Planned demonstrators include a hybrid aluminum-steel beam

for torsion, bending, and crash testing, as well as a hybrid strut tower, pushing the technology towards industrial application.

3D-Printed integrated circuits for adhesive joints disassembly and locally thermal curing

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E1_3, Z3 Room (Level -3), settembre 15, 2025, 14:30 - 16:30

Various directives, including ELV, WEEE, Directive 2008/98/EC, and subsequent regulations regarding the prescribed recovery and re-use of various industrial waste products, have come into force through the European Parliament. In response to these new European sustainability directives emphasizing design for disassembly and waste reduction in manufacturing, the integration of printed electronics into structural components offers novel opportunities for localized heating applications. This study explores the development of 3D-printed integrated circuits within adhesive joints, enabling precise and efficient heating. By embedding conductive pathways directly into the printed structure, controlled heating can be achieved in the overlap region of adhesive bonds, enhancing adhesion performance and curing processes while aligning with circular economy principles.

Two experimental approaches demonstrate the feasibility of this technology, highlighting its dual functionality. First, printed circuits can be exploited for disassembly purposes: in thermoplastic-based adhesives, localized heating enables bond release through polymer softening, allowing for easy separation or even repair of joints without replacing the adhesive. In thermosetting adhesives, controlled thermal degradation facilitates separation without damaging the substrate. Second, these integrated circuits can be used to enhance joint strength by localized curing, reducing stress concentration effects. This targeted reinforcement allows for optimized material distribution, leading to lighter and more resource-efficient components without compromising structural integrity.

Preliminary results demonstrate the effectiveness of these approaches. Heating circuits embedded within thermoplastic joints achieved adhesive softening and bond release at temperatures as low as 120 °C. Additionally, thermoplastic-based joints could be repaired up to five times while retaining more than 50% of their original strength. In thermosetting adhesives, controlled degradation at 180 °C enabled clean substrate separation. Furthermore, localized curing processes increased the maximum joint strength by up to 60%, reducing peak stress concentrations. These findings highlight the potential for integrating printed electronics into adhesive bonding processes, fostering sustainability and efficiency in industrial applications.

Beyond adhesive bonding, this approach can be extended to broader industrial applications, i.e. for automotive components like batteries, lights and electronics. The integration of modular, additive-manufactured circuits with enhanced recyclability can facilitate more sustainable production and disposal methods. By focusing on repairability, reusability, and material recovery, these technologies support circular economic principles while maintaining high performance. Furthermore, embedding heating circuits into structural components can contribute to innovative urban regeneration strategies, where sustainability, technological advancement, and design converge to optimize resource efficiency and promote environmentally conscious manufacturing practices.

Aluminium matrix composites with recycled alloys for lightweight automotive brake discs

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E1_2, Z3 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Aluminium-based metal matrix composites (MMCs) are promising materials for automotive brake discs, and aluminium provides an opportunity to use secondary alloys in the production of MMCs. Interest in the sustainability of composites is increasing steadily, and further investigation is needed when secondary aluminium alloys are included as the matrix. The drawback is that secondary aluminium alloys usually include several impurities and oxides that can harm the mechanical and thermophysical properties. Given the promising results of the preliminary studies, the present work focuses on the characterization of Al-Si-based MMCs reinforced with 20 wt. % of SiC particles. The brake discs are produced by squeeze casting using 0 %, 50 %, 70 %, and 100 % secondary AlSi9Mg alloy for the matrix.

The critical material properties for brake discs are good thermal conductivity, a suitable mechanical response at high temperatures, and a coefficient of friction that guarantees an acceptable braking performance. The microstructure of the MMC produced with the secondary alloy was comparable to that of the reference composite (0% recycled alloy), indicating good incorporation of SiC particles in the melt. The intermetallic phases present are linked to magnesium and iron, with Chinese script and lamellar morphologies, especially in MMCs containing recycled alloys. The presence of these phases had a limited effect on the thermal conductivities of the composites produced with secondary alloys. Similarly, the compression strength up to 470 °C is in line with that of the reference composites, indicating that the microstructural features related to the secondary alloy have a limited impact on the mechanical performance. The evolution of the microstructure with different strain rates and temperatures was investigated by SEM, EDS, and EBSD to describe the role of different microstructural features. The results of the present study confirm that these composite materials provide good mechanical performance and suitable thermophysical properties for automotive brake discs combined with a lightweight solution. The main challenge lies in the recyclability of the material at the end-of-life of the brake disc, which will be the focus of our future research.

Fe, Cu and Zn modification strategies in recycled AlSi10MnMg alloy: insights from high-pressure die casting (HPDC) and gravity casting processes.

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E1_1, Z3 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

The transition from internal combustion engines to electric vehicles has had a substantial impact on the automotive industry, particularly on foundries supplying high-volume products. There has been a decline in demand for traditional components such as engine blocks and gearboxes, which has led to a shift towards structural castings. Several of these castings are produced using Giga casting technology, which has been adopted by companies such as Tesla, Volvo, Nio, and XPeng. The fundamental idea behind this approach is to blow up the size of high pressure die casting (HPDC) equipment to levels that allow the production of large underbody parts or battery housings in a single operation. However, the increased use of aluminum alloys gives rise to concerns regarding their carbon footprint, with primary aluminum production emitting up to 20 kg CO₂eq per kg in China, compared to 8.6 kg in Europe. Recycled aluminum, such as AlSi10MnMg alloys, offers a lower carbon footprint but faces challenges due to impurities (e.g. Fe, Cu, Zn) in post-consumer scrap. The present study investigates the influence of such impurities on casting characteristics, microstructure and quasistatic mechanical properties with respect to an AlSi10MnMg base alloy. For this purpose, a DoE is developed covering, besides the reference alloy, stepwise compositional modifications with respect to the impurity content levels. A further comparison is made with two commercial alloys containing 58 and 89 wt.-% of secondary materials, respectively. The evaluation covers mold filling characteristics evaluated in gravity as well as high pressure die casting, metallographic studies based on light and scanning electron microscopy, and mechanical testing under bending and tensile loads. The aforementioned investigations are complemented by salt spray tests for evaluation of corrosion resistance. The results obtained are contrasted to corresponding data from the literature and recommendations are made with respect to the possibility of setting new compositional limits in order to facilitate the use of secondary aluminum casting alloys of the Al-Si-Mg type.

Designing Rubber for Mars Missions

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E3_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Mars missions involve progressively sophisticated equipment, which must operate in the harsh Martian environment. New designs of landers, rovers, and now helicopters push the performance levels beyond current boundaries. This includes the materials used for the construction of the new equipment.

Rubber is one of the most unique materials used in technology because of its viscoelastic properties. This means that rubber exhibits viscous and elastic behavior simultaneously. Because of this, it is currently an irreplaceable material in the construction of tires, vibration dampers, or seals.

With the constantly growing performance of Mars equipment, material requirements increase as well. This will be especially important when considering manned Mars missions. Astronauts will have to wear properly sealed Mars suits and crewed rovers will have to drive at much higher speeds than the current rovers, generating more vibrations. To meet these expectations, an application of rubber elements seems inevitable.

This project aims to develop rubber compounds designed to withstand the Mars environment while simultaneously preserving their viscoelastic properties in the highest possible temperature range. To meet these requirements, blends of Butadiene Rubber (BR) with Vinyl-Methyl Silicone Rubber (VMQ) are used as the polymer matrices because of their very low glass transition temperature assuring flexibility in a broad range of temperatures. BR provides better mechanical properties and wear resistance than VMQ, which in turn exhibits better flexibility at low temperatures and UV resistance. It is expected that BR/VMQ blends exhibit a synergistic improvement of properties in comparison to both rubbers alone. The blends are filled with various types of carbon black improving their mechanical properties and homogeneity. Also, different curing systems are used in the blend design, as well as oil replacement with non-volatile BR oligomers.

This paper presents the most important advancements in Mars rubber development achieved during the RED 4 MARS project [1].

[1] Rubber & Elastomer Development for MArtian enviRonment applicationS (RED 4 MARS), <https://cordis.europa.eu/project/id/101025756> (accessed 10.12.2024)

Enhancing thermal performance of micro-nano Al/SiC/cBN hybrid composites made for satellite applications via nitride-induced self-forming method

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E3_2, Press Room (Level +2), septiembre 18, 2025, 14:30 - 16:30

The aerospace industry, especially in the satellite environment, requires low thermal expansion, high heat dissipation, and lightweight materials for maintaining structural integrity and effective thermal management in harsh space conditions. Achieving this combination of properties is more challenging for aluminum metal matrix composites (AMCs) with a single reinforcing phase than for hybrid composites, which provide synergistic properties from multiple reinforcements. Therefore, it is essential to explore AMCs with various grain structures and multiple reinforcements to control the mechanical and thermal properties of hybrid composites.

In this study, SiC- and cBN-reinforced aluminum matrix hybrid composites were fabricated to examine their mechanical and thermal properties. Pure aluminum powder (108–150 μm) was blended with 5 vol.% SiC (1 μm) particles using attrition milling at 550 rpm for 12 hours to create nanocrystalline powders (n-Al/5% SiC). This attrition-milled powder was then mixed with pure aluminum (10 μm), 8.55 vol.% SiC (10 μm), and 10-30 vol.% cBN (36-54 μm) to form various hybrid composite powders. For instance, 5 vol.% of n-Al/5% SiC powder was combined with 65 vol.% pure aluminum and 30 vol.% cBN using a turbula mixer to create a 5% (n-Al/5% SiC)/30% cBN/65% mAl hybrid composite powder. Additional hybrid composite powders were developed similarly. These composites were manufactured using the nitride-induced self-forming process at 660 °C for 1 hour in a nitrogen atmosphere and subsequently densified by hot pressing at 580 °C for 1 hour under a 24-ton load.

After hot pressing, the hybrid composites were examined to analyze their mechanical and thermal properties, including microstructure. This study achieves a relative density greater than 98% for all composites. The uniform distribution of SiC particles and microstructural integrity of reinforcements with Al matrix was analyzed using SEM micrographs. Hardness and tensile strength were increased with the increasing vol.% of nanocrystalline powders and reinforcements. Most importantly, the thermal performance of these hybrid composites was investigated by measuring the conductivity (TC) and coefficient of thermal expansion (CTE). The highest TC and low CTE have been achieved for a hybrid composite of 10% (nAl/5% SiC)/30% cBN with 60 vol.% of mAl. According to preliminary results, composite materials' thermal and mechanical behavior is greatly influenced by the addition of reinforcements and tailored nitridation levels, which may result in innovative approaches for satellite systems. Further investigation is required to understand the interaction between microstructure and thermal properties, aiding the development of high-performance materials for future satellite applications.

Gravity independent Additive Manufacturing of an Al-Si alloy by Molten Metal Deposition (MMD)

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E3_2, Press Room (Level +2), septiembre 18, 2025, 14:30 - 16:30

Space exploration missions continue to push the boundaries of technology into far future. Additive manufacturing (AM) enables on-demand production, maintenance and repair in space, offering a valuable capability and bringing the possibility for deep space exploration closer to reality. The concept of in-space manufacturing (ISM) is driven by the need to overcome the severe constraints of payload capacity, design complexity increasing the risk for failure and the excessive costs associated with launching materials from Earth. Since 2014, extrusion-based 3D printers on the ISS have produced over 200 parts, highlighting AM's potential for space missions. However, metals AM's, particularly Laser Powder Bed Fusion, faces challenges due to powder handling in microgravity.

Molten Metal Deposition (MMD), the technology used in this research, is a liquid metal printing process where wire feedstock is melted and deposited as molten metal tracks. This study examines gravity independence by printing samples in standard and inverted orientations (with print head and substrate flipped). Support from the European Space Agency (ESA) enabled setup modifications. The selected material is a 4xxx aluminium alloy, specifically AlSi5 (wt.%). Bulk samples were printed with different parameter combinations (nozzle temperature, substrate temperature, print speed, layer height and track width) to study their effects on materials properties and microstructure. Porosity, microstructure and mechanical properties are compared between both gravity orientations.

Dense and uncracked bulk samples (density>99%) were achieved. Gravity orientation showed any impact on metal density. The microstructural analysis of sample cross-sections revealed a cellular microstructure, suggesting solidification and cooling rate higher than those typical of conventional casting processes. However, the average grain size is smaller than that of AlSi alloys produced by Laser Powder Bed Fusion. A reduction in grain size is observed from the bottom to the top of the sample section, without differences between regular and inverted samples. In the bottom layers, closer to the substrate, the thermal gradient during solidification is lower due to the influence of substrate preheating, leading to a lower cooling rate that in turn lead to coarser grains. Moreover, the layer deposited on top of the previously deposited layers, can contribute to grain coarsening, leading to a gradient microstructure. Microhardness tests were conducted, revealing variations corresponding to the material's microstructure. Hardness increased from the bottom to the top of the samples, with a rate of 0.18HV per millimetres of height, as grain size decreased. No notable differences in hardness were observed between regular and inverted samples.

Influence of Interfacial Characteristics on the Strengthening Mechanisms of B₄C-Reinforced Aluminum Matrix Composites

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Aluminum matrix composites reinforced with B₄C have garnered significant interest as radiation-shielding materials due to the unique properties of B₄C, including its high melting point, exceptional hardness, and effective neutron absorption capabilities via nuclear reactions involving ¹⁰B. Consequently, Al/B₄C composites exhibit superior specific strength, hardness, and radiation-shielding efficiency. However, the inherent poor wettability between B₄C and aluminum results in weak interfacial bonding, thereby compromising the mechanical performance of these composites.

In this study, aluminum matrix composites incorporating 1.5, 3, and 5 vol.% B₄C were fabricated through hot rolling of mechanically milled composite powders, followed by heat treatment to induce partial decomposition of B₄C. This process facilitated the intercalation of B and C atoms into the aluminum lattice, leading to localized lattice distortion. The present work systematically investigates the influence of interfacial characteristics, modulated by varying heat treatment durations, on the strengthening mechanisms governing the mechanical behavior of B₄C/Al composites.

High-Throughput Screening of Precipitates in Al-Cu Alloys Using Compound Big Data for Aerospace Applications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Aluminum alloys are widely used in aerospace applications due to their exceptional strength-to-weight ratio, corrosion resistance, and favorable thermal and electrical conductivity. Although high-strength aluminum alloys, including Al-Cu, Al-Si-Mg, and Al-Zn-Mg systems, have been extensively developed and applied in aerospace structures, their performance in space environments is often limited by precipitation-related challenges such as precipitation instability under prolonged thermal exposure. To overcome these limitations, there is a growing need for the discovery of entirely new precipitation-strengthening phases that can form in aluminum alloys while maintaining structural stability in space environments. Traditional alloy design approaches rely heavily on empirical trial-and-error methods, which are time-consuming and resource-intensive. To accelerate this process, we propose a novel high-throughput screening methodology utilizing materials big database to identify new precipitates that can form in aluminum matrices while effectively enhancing mechanical properties. By leveraging computational databases and predictive modeling, this approach enables the discovery of stable, high-performance precipitates, paving the way for the next generation of aerospace-grade aluminum alloys. Our analysis suggests that Al-Cu precipitates containing Lanthanum (La) or Strontium (Sr) may effectively enhance the strength of aluminum while also exhibiting high stability. To validate this further, we fabricated Al-Cu-La and Al-Cu-Sr alloys using casting and extrusion methods. Through differential scanning calorimeter (DSC) analysis, we explored the heat treatment profile for optimizing the formation of the desired precipitates. We will present the correlation between precipitate formation and mechanical properties under various heat treatment conditions.

Thermal conductivity and dynamic oxidation resistance of additive-free silicon carbide ceramics

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E3_3, Press Room (Level +2), septiembere 18, 2025, 17:00 - 19:00

Fully dense (t. d. > 99 %) silicon carbide ceramics without any sintering additives were successfully prepared by combination of freeze granulation of silicon carbide powder, annealing of granulated powder and subsequent rapid hot pressing at 1900°C with dwell time from 5 to 80 minutes under a uniaxial pressure of 70 MPa in vacuum. Different ratio of alpha and beta silicon carbide has been achieved by adjusting dwell time during sintering. Thermal diffusivity, specific heat capacity, thermal conductivity, density, microstructure of additive-free SiC with various α/β content has been investigated. The thermal diffusivity of additive-free SiC ceramics increased from 47.3 to 68.4 mm²/s with increasing holding time and therefore increasing α -SiC content from 63 to 94 % and increasing grain size. The highest thermal conductivity ($\lambda=165$ W/m.K) among the SiC ceramics sintered at temperatures $\leq 1900^\circ\text{C}$ was achieved for additive-free SiC sintered at 1900°C under vacuum for 80 minutes. To the best of our knowledge this is the highest value of thermal conductivity for silicon carbide ceramics sintered at $T \leq 1900^\circ\text{C}$ up to now. In addition, such prepared materials were tested in oxy-acetylene torch at 1700°C, 1800°C and 1900°C for 5 minutes. In the dynamic regime the ceramics sustained 1900 °C for 5 minutes. It seems that this material is suitable for ultra-high-temperature applications.

Acknowledgments

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In-space 3D printing of Li-ion batteries by Fused Filament Fabrication

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The Moon and Mars are the next targets for space exploration. However, launch costs and resupply delays have made inconceivable manned long-duration missions. In-Space Manufacturing (ISM) appeared as the essential breakthrough to remove these barriers. This approach would allow the production and repairs of critical systems to answer astronauts' needs independently from Earth resupply. Additive manufacturing processes (AM) are at the heart of this strategy thanks to their versatility, low cost, and ease of use (1). Indeed, Fused Filament Fabrication (FFF) has been successfully deployed in the International Space Station (ISS) to print spare parts and tools (2). 3D printing in microgravity of more complex systems is the next challenge to take up. In Space, energy supply is a critical issue as it is one of the main causes of the space systems lifespan limitation. Energy mainly comes from solar power so rechargeable Li-ion batteries (LIBs) are involved at all spacecraft levels : from the ISS primary power system to portable communications devices, going through life support systems (3). Thus, in-orbit manufacturing of batteries represent a necessary milestone to carry out the ISM approach.

This work aims to make in-space 3D printing of Li-ion batteries feasible. For seven years, our group has optimized composite filament formulations to successfully 3D print Li-ion batteries by FFF. The challenging task of this study was the transition from liquid electrolytes to solid polymer electrolytes suitable for microgravity. We have created and characterized new formulations to obtain a process that fits the security requirements of the spacecraft's environment (4). Materials choices, process parameters, and formulations have been ingeniously studied to obtain the best compromise between printability and electrochemical performances. 3D printing alleviating gravity constrain environments has been performed at European Space Agency (ESA) facilities to demonstrate in-space printability and to understand microgravity's influence on the morphology and the performances of our 3D-printed batteries.

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Unveiling δ Phase Strengthening Mechanisms in LPBF-Processed Inconel 718 at Elevated Temperatures

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E3_2, Press Room (Level +2), septiembre 18, 2025, 14:30 - 16:30

The highest-strength Inconel 718 alloy, widely used in aviation and increasingly in jet turbine engines (operating up to 650 °C), relies on high-temperature stable solid-state co-precipitation for strengthening. However, conventional co-precipitation is prone to service-induced degradation, particularly due to δ phase formation at elevated temperatures, which leads to significant deterioration in Inconel 718 alloys manufactured via transitional casting or laser powder bed fusion (LPBF). Here, we challenge the conventional understanding of δ phase precipitation in LPBF-produced Inconel 718 alloys, demonstrating that a high density of δ particles can actually enhance mechanical performance. Specifically, LPBF-induced δ phase promotes dynamic precipitation along cell boundaries within internal grains, leading to an optimal combination of strength (~ 1.2 GPa) and ductility ($\sim 23\%$) at 650 °C. We reveal that δ particles inside the grains exhibit temperature-dependent strengthening mechanisms: at room temperature, δ particles undergo shearing through dislocation slip, resulting in step formation along shear planes. In contrast, at 650 °C, dislocations bend δ particles without forming steps, instead accumulating at γ''/δ interfaces, which triggers a localized disordering transition of the δ phase. This novel δ bending and disordering mechanism arises from a combination of modulus mismatch and stacking faults. The high density of bent δ particles disrupts dislocation motion, inducing inhomogeneous deformation and reducing the yield strength and strain-hardening rate at 650 °C. Our findings provide new insights into the role of δ phase in LPBF-processed Inconel 718, offering a pathway for designing high-temperature stable alloys with enhanced mechanical performance.

PEEK composites with carbon nanoparticles for high performance applications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The industry finds itself at a crossroads with various trends related to the green transition (electromobility, hydrogen fuel cells, etc.) and the digital transition (connectivity, autonomous driving, software, etc.). These trends necessitate the development of innovative materials and products to meet the increasing demand for high-performance applications like sensors, composites, wire and cabling. As functionality increases and weight reduction becomes critical, embedded systems are also emerging. The demand for new materials that combine high mechanical performance, and functionality is one of the key challenges in aeronautics and mobility, driving innovation in lightweight structures, fuel efficiency, and advanced manufacturing technologies.

High-performance thermoplastics, such as polyether ether ketone (PEEK), which combine exceptional properties like a high strength-to-weight ratio, chemical resistance, recyclability, a low coefficient of friction, electrical isolation, and thermal stability, can be used in demanding applications such as high-voltage electrical connectors and insulation components, providing reliable performance in harsh environments for mobility and space applications. When PEEK is reinforced with carbon-based fillers, its electrical conductivity can be tuned, making it suitable for applications that require efficient electrical pathways.

This research focuses on designing new materials for high-performance applications such as mobility and aeronautics. Filaments of PEEK, combined with multi-walled carbon nanotubes (MWCNT) and exfoliated graphite nanoplatelets (xGnP), have been developed through extrusion compounding and melt-spinning technologies. These filaments demonstrate improved electrical conductivity values (~ 2 S/cm) and can be employed as heating systems to achieve high temperatures through the Joule effect. These nanocomposites offer significant advantages in terms of sensitivity and durability, making them ideal for integration into composite structures, providing functionalities like embedded sensors, heating elements and structural parts for mobility and aeronautics.

This work contributes to the advancement of technology by providing sustainable, efficient, and high-performance solutions that align with the industry's evolving needs. The findings have broad implications for the future of design and manufacturing, paving the way for more sustainable and technologically advanced systems.

TEMPUS - A microgravity electromagnetic levitation facility for parabolic flights

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E3_3, Press Room (Level +2), septiembre 18, 2025, 17:00 - 19:00

During the ~22s lasting free fall phase in an aircraft flying a parabola, the aboard installed electromagnetic levitation facility “TEMPUS” is used to investigate contactlessly and undisturbed of gravity induced convection thermophysical properties and microstructure formations of hot and highly reactive metal or semiconductor melts. The completely contactless handling and measurement of a liquid by the levitation technique keeps the melt free of contamination and enables the extension of the accessible sample temperature range far into the undercooled liquid state below the melting point. Additionally, the state of reduced weight during parabolic flights allows us to considerably decrease the strongly disturbing electromagnetic levitation forces acting in ground-based facilities on the suspended liquids.

The present talk explains the basic principle and the technical realization of the TEMPUS levitation facility and its attached measurement devices. Furthermore, it presents some typical experiments performed in TEMPUS, which also show the advantages resulting from the combination of reduced weight, electromagnetic levitation and contactless measurement techniques.

EML – Electromagnetic levitator onboard the ISS: investigation of thermophysical properties & solidification of liquid metals

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E3_3, Press Room (Level +2), septiembre 18, 2025, 17:00 - 19:00

EML is an electromagnetic levitation facility of the European Space Agency (ESA) onboard the ISS for the containerless processing of conductive materials under microgravity conditions, which is now since 10 years in operation in the Columbus module. Due to the absence of container walls the meta stable state of the undercooled melt can be reached and investigated. The facility allows the measurement of thermophysical properties as surface tension, viscosity, density, specific heat, emissivity & electrical conductivity. Solidification processes can be investigated by the measurement of the growth velocities, the delay time between metastable and stable phase formation and the investigation of the microstructure of the solidified sample after the experiments. In microgravity heating & positioning can be decoupled, so that measurements can be performed at reduced field strengths or the field and electromagnetic stirring can be used as parameter for the measurements. The presentation will give an overview of the technical aspects of the facility, the measurement principles and some results from the ISS experiments. It will be shown how the experiments are planned and performed and will present an overview of the experiments in the last decade.

Alloy Design for Magnesium Alloys in Aerospace Applications: Optimizing Strength and Thermal Conductivity

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E3_2, Press Room (Level +2), septiembre 18, 2025, 14:30 - 16:30

Recently, an interest in low Earth orbit (LEO) communication satellites is growing, and the miniaturization and weight reduction of satellite structures have become essential. Accordingly, the development of advanced lightweight materials with optimized performance characteristics in the space environment has become a critical challenge. Materials for satellite structures require multi-properties of high specific strength, low thermal deformation, and efficient heat dissipation. Fabricating metal matrix composite can be an effective way to enhance these multi-properties; however, the optimization of the matrix alloy is essential to fully exploit the potential of such composites.

In general, specific strength in magnesium alloys can be improved through alloying and precipitation hardening. However, the introduction of alloying elements significantly degrades the intrinsic thermal conductivity of pure magnesium (156 W/m·K), reducing it by up to 50%. To address this trade-off, this study systematically investigates the influence of alloying elements and heat treatment on the mechanical and thermal properties of magnesium alloys.

Thermodynamic simulations using Thermo-Calc Python were conducted to predict the thermal conductivity and mechanical strength of binary magnesium alloys. Based on these results, alloy systems with optimal strength and thermal conductivity balance were identified. Selected alloys were fabricated via a casting-extrusion-aging treatment route, and their microstructural evolution, specific strength, and thermal transport characteristics were thoroughly evaluated. Among the investigated matrix alloys, Mg-6Zn demonstrated excellent mechanical and thermal performance. Furthermore, metal matrix composites were fabricated using both commercial and newly developed matrix alloys, and their properties were comparatively analyzed.

Effect of the use of new aviation fuels on polymeric materials for use in aircraft

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E3_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The growing problem of environmental pollution and the current dependence on fossil fuels are generating interest in finding sustainable alternatives for the transport sector. Decarbonization has become the roadmap of regulations proposed by governments and institutions to reduce the carbon footprint, which has driven the development of sustainable aviation fuels (SAF). The physicochemical properties of SAF are like those specified in regulations for traditional fossil kerosene, but their fully paraffinic nature may affect the compatibility of these fuels with aviation materials with which they are in contact. This work analyses the effect on two thermoplastic polymers, nylon and high-density polyethylene (HDPE), which are used in fuel transfer systems and pipes, of two conventional kerosene fuels (Jet A-1 and JP-8) and a mixture of Jet A-1 and 30% (v/v) of SAF. For the development of the study, immersions were carried out at 71 °C for 28 days, as established by ASTM D4054. The properties evaluated to determine the compatibility between these polymeric materials and the fuels with which they are in contact are the stress at the elastic limit and the deformation at the breaking point. Additionally, other physical-mechanical properties such as hardness and dimensional and mass variation were measured to obtain a more complete evaluation of the behavior of the materials in service. Results showed that the influence of the three fuels on both materials was similar, which could mean that the 30% SAF blend would be equally compatible with those materials as with fossil kerosene fuels. These results confirm that, in addition to the known environmental advantages of SAF, the blend of kerosene fuels tested would not compromise the integrity of the materials used in fuel distribution systems.

Advanced Sustainable Composite Materials Based on Renewable Resources for Space Applications

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E3_2, Press Room (Level +2), septembre 18, 2025, 14:30 - 16:30

As the global population continues to grow, so does the demand for resources, making conservation and efficient industrial management more important than ever. A shift towards a sustainable economy is crucial, with bioenergy, biofuels, and bio-based materials playing a key role in reducing reliance on fossil fuels and addressing environmental challenges. This study focuses on developing eco-friendly composites reinforced with carbon or vegetable fibers, engineered to meet the strict requirements of industrial applications. These high-performance materials are particularly suitable for demanding environments, especially in aerospace and space exploration.

At the center of this innovation is a polymeric matrix derived from renewable sources, formulated with an aliphatic compound extracted from vegetable oils, such as epoxidized linseed oil (ELO). By reinforcing this matrix with carbon or vegetable fibers, the resulting composites achieve a unique combination of strength, durability, and adaptability. These materials can be recycled, repaired, and reshaped while maintaining their structural integrity, offering an environmentally responsible alternative to traditional petrochemical-based materials.

Comprehensive testing was conducted to assess their mechanical and thermal properties. Dynamic Mechanical Analysis (DMA) confirmed their exceptional stiffness, while mechanical strength tests demonstrated their durability under stress. The bond between the fiber and matrix was analyzed through Interlaminar Shear Strength (ILSS) tests and visually examined using Scanning Electron Microscopy (SEM), providing insights into the material's internal structure. Thermogravimetric Analysis (TGA) showed that these composites have good thermal stability, with a T5% (temperature at which 5% mass loss occurs) exceeding 300°C. Additionally, a Limiting Oxygen Index (LOI) above 30% highlights their strong fire resistance, making them reliable for applications where safety is a priority.

In space exploration, materials must withstand extreme conditions, including high temperatures, radiation, and vacuum environments. These composites offer promising solutions, as they are designed to endure the challenges of space environments.

In summary, these advanced polymeric composites present a sustainable, durable, and high-performance alternative to conventional materials. With their ability to combine environmental benefits with superior mechanical properties, they hold great potential for use in space missions and other high-tech applications, paving the way for innovative, long-term solutions in material science.

Pt nanonetwork coatings for spacecraft charging mitigation in photovoltaic solar arrays

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Spacecraft charging is a well-known charge accumulation process induced by the interaction of the space environment (plasma, solar radiation, and high-energy particles) with the surfaces of space vehicles. This phenomenon is the root cause of catastrophic electrostatic discharge (ESD) arcing on the non-conductive surface of spacecraft, as is the case of photovoltaic cover glasses. Therefore, it is a critical issue that compromises the integrity and limits the lifetime of space solar arrays. Within the framework of the ESA contract Ref. 40001139513/22/NL/CRS, the present research addresses this problem by developing a new type of transparent conductive nanocoatings consisting of percolated platinum-based nanonetworks developed by plasma processing techniques.

The fabrication approach combines the remote plasma-assisted deposition (RPAVD) of a hybrid platinum plasma-polymer nanocomposite with the room-temperature plasma etching of the resulting layer.[1]-[3] Both processes are consecutively carried in the same plasma reactor in a single fabrication run. This method exclusively involves vacuum deposition and plasma manufacturing techniques widely applied in different industrial sectors, including the development of optical coatings for photovoltaic applications. Thus, it can be scaled for either the large-area (up to a few m²) processing of windows and cover glasses or the mass-scale manufacturing of microelectronic/optoelectronic devices.

Recent studies addressed the development of solar cell photoelectrodes consisting of nanoporous TiO₂ optical coatings[2] and Pt nanostructured electrodes[3] developed by combined RPAVD and soft plasma etching at mild temperatures (~120°C). The current communication extends this approach to the room temperature fabrication of highly transparent and conductive nanoporous coatings (solar transmittance > 85 %) consisting of laterally interconnected Pt-nanonetworks. Process optimization provides a good balance between optical transmittance and sheet resistance. For a suitable spacecraft charging assessment, sheet resistance measurements were conducted in vacuum at different temperatures and complemented with advanced secondary emission yield and VUV photoemission measurements. This characterization was used to model, using SPENVIS' EQUIPOT and SPIS-6 simulation tools, the surface charge and potential developed in different orbits onto photovoltaics arrays coated with the Pt-nanonetworks. These analyses confirm the good performance of the developed transparent conductors for spacecraft charging mitigation applications in photovoltaic solar arrays.

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Fully-recyclable CNT sheets for multifunctional thermoset and thermoplastic composites

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E3_3, Press Room (Level +2), septiembre 18, 2025, 17:00 - 19:00

The carbon nanotube (CNT)-based high-tenacity fibres, multifilament yarns, nearly transparent nanotextiles, and thick paper-alike sheets can be synthesized in a single-step gas-phase chemical reaction via floating catalyst CVD process (FCCVD) [1]. With the most recent advantages in FCCVD synthesis conversion, international Carbon Hub R&D initiatives [2], and ongoing efforts in industrial scale-up, the annual capacity to produce CNT as high-performance macromaterials may increase from today's kilo ton per year to the megaton scale through co-production of CNTs in the generation of turquoise hydrogen [3].

These macroscopic CNT ensembles constitute a new class of carbon-based materials, combining the high graphitic carbonaceous nature with high structural ductility similar to high-performance polymers [4]. However, in contrast to conventional all-solid "monolithic" carbon fibres (CF), CNT macromaterials have hierarchical network structure built of ultralong interconnected CNTs, responsible for the remarkable fracture energy and through-thickness and longitudinal electrical and thermal conductivity, enabling their usage in novel multifunctional materials [3]. Such a unique combination of properties with the macroscale format (fibre, yarn, sheet) makes them prominent candidates for novel electrical conductors, thermal management, structural reinforcement, and other areas where they can displace CO₂-intensive materials. The CNT macromaterials could be used in 3D FFF printing and combined with AFP manufacturing of novel structural composites to leverage the design freedom and innovative multifunctional parts with integrated sensors for structural health monitoring, de-icing, lightning-strike protection, EMI shielding for aerospace, automotive, and other industrial sectors.

In this work, we discuss the structural features of macroscopic CNT sheets, their properties, composite processing with high-performance thermosets and thermoplastics (PAEK, PEI), and their recycling capability. The nanostructured CNT materials can be recycled from their thermoset [5] and thermoplastic composites without any notable chemical degradation and with nearly full retention of mechanical and electrical properties. The recycled CNT sheets retain their original shape and CNT alignment after polymer removal, which is hardly attainable for conventional CF recycled mainly as short discontinuous filaments. We correlate the high recycling potential with the intrinsic toughness and structural ductility of CNT sheets, which can be evaluated through the concept of the Essential Work of Fracture (EWF). We evaluate the EWF by testing the laser-cut double-notched samples of CNT sheets to pursue the models for predicting their behaviour and ductile fracture essential for understanding mechanics and recycling potential.

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[2] <https://doi.org/10.1073/pnas.2112089118>

[3] <https://doi.org/10.1016/bs.ache.2023.07.001>

[4] <https://doi.org/10.1016/j.carbon.2019.04.113>

[5] <https://doi.org/10.1016/j.carbon.2024.118851>

Space experiments on High-Temperature Molten Oxides, Metals and Alloys Using an Electrostatic Levitation Furnace on the International Space Station

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E3_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Assessing the thermophysical properties and solidification behaviors of melts at temperatures exceeding 2000°C, presents significant challenges due to reactions between the molten samples and their containers as well as heterogeneous nucleation. To overcome these issues, containerless techniques such as electromagnetic, aerodynamic, and electrostatic levitation have been developed. In electrostatic levitation, the Coulomb force between a charged sample and surrounding electrodes is utilized to precisely manipulate the sample's position. Our team have developed the Electrostatic Levitation Furnace (ELF), incorporating key technologies necessary for stable sample positioning and accurate scientific observation. In 2016, ELF was installed on the International Space Station (ISS). Using the microgravity environment, samples which cannot be electrostatically levitated mainly due to their poor charges could be precisely position controlled, melted, and their thermophysical properties such as density, surface tension, and viscosity were obtained. To date, 17 missions—excluding private commercial experiments—have been conducted. Of these, 13 missions related to molten oxides, metals and alloys were selected by JAXA and 4 by NASA. Nine missions have successfully completed space experiments, three are currently ongoing, and eight are in preparation on the ground. Among these experiments, the thermophysical property measurements of molten oxides, metals and alloys, which are strongly related to materials science, will be presented, and the obtained data will be discussed.

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Shaping the future of space exploitation with advanced materials and processes

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E3_1, Seminario 7 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Maturation of technologies based on advanced materials and their related process is a key aspect in the development of space mission. Driven by the necessity to improve performance, decrease system complexity and keeping high level of reliability or simply to reduce mass and cost, materials with enhanced (multi)functionalities by design and manufacturing process simplification are needed. However, nowadays it must be done implementing a sustainable approach whereas it targets ground based or out-of-earth/in space manufacturing processes.

In this paper, we will present a general assessment of new technology development based on advanced materials including polymeric materials (thermoplastic, thermoset, vitrimer), self-healing materials, composites and metals. Their added value will be associated with their related processing technologies and new design concept. In this respect, the recent advance on the use of 3D/4D printing concepts suitable for space application will be exposed and discussed with an emphasis on the role of meso-structuration and biomimetism. In the last part, the role of materials including several sources of feed stock (e.g. polymers, regolith) in the implementation and development of out-of-earth / In-space manufacturing capabilities will be put in perspective against the current state-of-the-art and available technology.

ISRU-approach on designing and fabricating successfully composite materials on the lunar soil

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

By the Artemis program, NASA will land the first woman on the Moon, using innovative technologies to explore more of the lunar surface than ever before and the first long-term presence on the Moon will be established. One of its basic strategy is to enabling the in situ resources utilization approach (ISRU) by focusing on how to process Lunar soil (regolith-a complex mixture of oxides) by using already terrestrial developed advanced technologies for extracting pure elements (i.e. Si, Al, Mg, Fe, Ti, etc.), to produce breathing air, growing plants, and whatever sustain Moon habitants in such extreme conditions, e.g. building materials, screens against radiations, etc. Under a great ISRU-focus is also the "space junk" mainly consisting of light weight alloys based on Al, Si and Ti. A preliminary investigation on using lunar soil (regolith) properly combined/processed with metal particles of the abovementioned alloys for fabricating composites feasible as building/functional materials will be introduced in this paper. In particular, as an example, preliminary results obtained by interactions tests between Ti64NPs/DNA-1 regolith simulant will be shown and discussed, even by comparing the observed microstructure and reaction products at the interface with thermodynamic calculations on phase stabilities obtained by using FACTSage.

Dendrite Growth on Aluminum Anodes in Non-Aqueous Aluminum Batteries: Influence of Alloying and Electrolyte Chemistry

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

99.99% Al (1xxx) is currently used as the negative electrode for aluminum-base battery. However, this high-purity 99.99% Al hinders the development of Al-based batteries in practice due to its high cost and complex manufacturing process. Therefore, 99.99% Al needs to be substituted with a suitable Al alloy. Additionally, the passivating oxide film covering the Al surface is another issue in Al-based batteries, as it impacts the plating/stripping process on Al in the battery. In general, the knowledge regarding Al negative electrodes in this context is insufficient and requires further detailed study. In this study, three aluminum electrodes from different alloy series—1xxx, 2xxx, and 5xxx, each with different surface and oxide film properties—were fabricated. Plating/stripping tests were conducted on symmetric cells of each alloy. The results demonstrate that the 5xxx aluminum alloy exhibited the best plating/stripping performance compared to the other alloys. Specifically, 5xxx alloys displayed the lowest voltage hysteresis throughout cycling, while 2xxx alloys showed the highest voltage hysteresis. Full cell studies of Al/graphitic cells revealed that cells assembled with 99.99% Al and 5xxx exhibited nearly identical performance throughout recorded cycling numbers. In contrast, cells assembled with 2xxx alloys exhibited a 38% lower efficiency in cycling performance compared to those constructed with 99.99% Al and the 5xxx alloy. These findings highlight the critical role of Al oxide and surface properties in influencing the behavior of Al-based batteries. The results are further discussed in terms of oxide film properties, surface microstructures, and the interphase layer formed on the Al surface. Furthermore, this work sheds light on the oxide film issue, which is recognized as a challenge in Al-based batteries.

Thermophysical and surface properties of Al-Sn miscibility gap alloys (MGA) phase change materials for Thermal Energy Storage applications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 17, 2025, 13:10 - 14:30

As compared to paraffin wax and molten salts, metallic phase change materials (PCM) offer attractive properties for thermal energy storage (TES) by providing high volumetric latent heat, high thermal conductivity, recyclability and non-toxicity. In this regard, a special attention should be given to so called miscibility gap alloys (MGA). The MGA are defined as a mixture of two metals that are strongly immiscible. Thus, they are characterized by a microstructure of high melting point continuous matrix and lower melting point particles embedded inside. Typical metallic systems are Al-Sn or Fe-Cu.

In this work, we present the results of investigation on thermophysical and surface properties of Al-Sn-based MGAs. Both model binary system (Al-Sn) and Al-based industrial alloys, are investigated. A set of key thermophysical properties (e.g. surface tension and density) was experimentally measured by sessile drop techniques and calculated by thermodynamic models. The samples and their final microstructures were analyzed by SEM/EDS and 3D-Computed Tomography. Furthermore, based on literature data and experimental observations, evaporation, oxidation and dissolution phenomena were described by using thermodynamic and fluidodynamic models.

Development and characterization of solid-liquid metal alloys phase change materials for high temperature thermal energy storage

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E4_2 - Energy Storage Materials: Development, Processing and Characterization 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The present work provides a study on the properties of metallic PCMs for integration into a TESS (thermal energy storage system) unit for heat storage at high temperatures. Al-Cu-Si alloys were selected in the temperature range 550°C - 850°C, and CALPHAD calculations were performed using FactSage 8.2 software (SGTE and FTLite databases). After optimal selection, the fabricated alloys were examined using a range of techniques to obtain the thermal properties and a full thermo-mechanical characterization. Thermal analysis was carried out using a STA 449 F3 JUPITER (Netzsch) with each sample placed in an alumina crucible (85 μ L). To avoid oxidation, the samples were heated with N₂ flow at 80mL/min. The samples density was measured using the Archimedes Principle and confirmed with a He gas pycnometer (Accupyc 1340 Micromeritics). The coefficient of linear thermal expansion (CLTE) was measured using a thermomechanical analysis equipment (TMA-SETSYS EVO SETARAM) which provides information on the solid-to-solid phase transitions. The CLTE measurements of the developed materials will help for later implementation of the metallic PCMs into any container for stress consideration at solid state.

The selected PCMs were thermally cycled 20, 40, and 100 times through the solid-liquid phase under air. DSC and LFA were used to assess changes in the thermal properties of the PCMs, such as melting point, latent heat, specific heat, thermal diffusivity, and thermal conductivity. Changes in the PCMs' thermal characteristics, including their melting point, latent heat, specific heat, thermal diffusivity, and thermal conductivity, were evaluated using DSC and LFA. The selected PCMs achieved the TES system's maximal energy storage density of 500 kWh/m³ for a temperature difference of 300°C. Finally, the materials examined in this study shown remarkable stability and energy storage densities, making them viable options for large-scale application. Afterwards, the PCMs will be inserted into a 3.5m height storage unit made of refractory bricks as mechanical support to prevent any leakage.

Melt-spun Cu-Al based ribbons as current collectors for Anode-Free cells in ASSBs

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E4_1 - Batteries and their components 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

All-Solid-State Batteries (ASSBs) were conceived to meet the need for a higher energy density and safety. Li-metal can be exploited in this type of cells, using a solid electrolyte, that reduces dendritic growth. Despite this, Li-metal is flammable, must be stored in a moisture-free atmosphere, and its production is environmental impacting. In this context, anode-free system emerged to avoid these problems: a current collector (CC), usually made of copper, is used as a support to plate Li-metal coming from the cathode. The optimization of the CC composition and the CC/electrolyte interface is essential to achieve high performances. [1]

The purpose of this study is the synthesis and characterization of new alloys to obtain greater lightness, lithiophilicity and lower production costs than traditional Cu-based CCs. In the Cu-Al system, a high percentage of Al leads to brittle alloys, due to the formation of intermetallic compounds. So, the specific goal of this work is to improve mechanical properties, thanks to the stabilization of the β phase. Aiming to inhibit the eutectoid decomposition and the formation of biphasic mixtures, some ternary alloys have been synthesized, by adding Ni and Mn, which enable to extend the field of existence of β phase, improving mechanical properties.[2] Various alloys, with different compositions, were synthesized from parent elements in an induction furnace, and then subjected to an annealing treatment. Moreover, the rapid solidification from the liquid phase was performed by melt-spinning, obtaining metal ribbons with desired size, to be directly used in anode-free cells. Prepared samples were characterized by SEM-EDX and XRD.

Melt-spinning has given better results than annealing. The formation of the β phase, with a martensitic structure, has been obtained in the 83-13-4%wt Cu-Al-Ni ribbon; in the case of Cu-Al (85-15 and 90-10 wt%) and Cu-Al-Mn (80-15-5 wt%) ribbons, XRD and SEM-EDX revealed a decrease in the intermetallic phase and an increase in the β phase. Future targets are the synthesis and characterization of lithiophilic Cu-Al-Mg ribbons, the creation of a surface coating to improve the Li-plating on the anode side and the demonstration of anodeless cells using a sulfide-based electrolyte and the developed CC.

[1] P. Molaiyan et al., "Optimizing current collector interfaces for efficient "Anode-Free" Lithium Metal Batteries", *Advanced Functional Materials*, 34 (2024) 2311301, doi: 10.1002/adfm.202311301

[2] C.C. Nwaeju et al., "Grain characteristics and mechanical properties of as-cast Cu-10%Al alloy: Effects of alloying additions", *Results in Engineering*, vol. 12, December 2021, doi: 10.1016/j.rineng.2021.100295

Containment of metallic phase change materials for latent heat thermal energy storage solutions

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E4_2 - Energy Storage Materials: Development, Processing and Characterization 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The transition to renewable energy sources like solar and wind is essential for a sustainable future, but their intermittency presents a significant challenge to energy grid stability. An energy storage solution is needed to store surplus energy and release it upon demand. Latent heat thermal energy storage (LHTES) is a promising technology for addressing this challenge. With the EU funded THERMOBAT and SUNSON projects we are exploring new phase change materials (PCMs). As LHTES systems evolve, the development of heat-to-electricity converters capable of operating at temperatures above 1000°C has highlighted the need for PCMs that can perform reliably under such demanding conditions. Ferrosilicon, a cost-effective and well-established material, shows significant potential due to its high volumetric latent heat, enabling energy storage capacities surpassing 1 MWh/m³. In this study, ferrosilicon is alloyed with boron to leverage boron's exceptionally high latent heat and further enhance energy storage performance. This study addresses the critical challenge of containing such Fe-Si-B alloys at temperatures between 1100°C and 1400°C, utilizing sealed graphite containers. The containment system must counteract the alloy's high reactivity and vapor pressure while preventing material loss and ensuring an inert atmosphere. A series of graphite-based crucibles, with different ceramic additions and with BN coating, were subjected to 100 thermal cycles and subsequently analyzed using computed tomography (CT scan) and scanning electron microscopy (SEM). Results indicate that bare graphite, despite forming SiC at the alloy interface, effectively contains the alloy over the 100 cycles with minimal degradation to both the PCM and the crucible. The BN coating provides an additional layer of protection, mitigating reactions at the interface, reducing the contact angle. These findings highlight the viability of sealed graphite containers as a cost-effective and robust solution for containing metallic PCMs in high-temperature LHTES systems.

Electrifying foil characterization – Mechanical characterization of electrode materials for simulation purposes

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

With the ever-increasing share of electric vehicles (EVs) in the global automotive market, the entire industry is gradually transitioning towards a more sustainable future. However, numerous reports of serious fires involving electric cars highlight the growing importance of ensuring the safety of Li ion batteries (LIBs). Additionally, the lifespan of these LIBs in the cars is a widely discussed topic, not only in the used car market but also among manufactures aiming to increase cell longevity. To address these challenges effectively, a detailed understanding of the behaviour of LIBs under critical thermo-mechanical loading conditions is essential.

The goal of our project is to provide a comprehensive modelling tool for the simulation of the thermo mechanical response of LIBs. Nevertheless, the most advanced modelling tool is only as good as its input parameters making reliable and repeatable measurements for the mechanical characterization of electrode materials essential. Even for conventional LIBs, this mechanical characterization is still a long way from being fully developed, which is mainly due to the sensitivity of the used foils materials. Existing standards as well as various testing methods from the literature for foil testing were compared and evaluated for their suitability. In addition, further refinements were made to suit the requirements of the existing machinery and sample materials. Initially, the electrode material was analysed for possible anisotropy in the foil plane to determine the necessary number of tests. In a next step, new processes were developed for the damage-free alignment and gripping of the samples in a testing machine for quasi-static tensile tests. Additionally, different methods for precise and gentle elongation measurement were researched for the tensile tests, since thin foils have a more varied fracture behaviour than their respective bulk materials due to their higher brittleness. Finally, various options for the accurate measurement of Young's modulus were compared.

Development of Additively Manufactured Anodes for Aluminum-Air Batteries: Influence of Microstructure on Performance

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E4_3 - Batteries and their components 2, Seminario 8 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Aluminum-air (Al-air) batteries are promising high-energy-density power sources for applications such as electric vehicles and portable electronics. However, conventional aluminum anodes face challenges including high self-corrosion, hydrogen evolution, and limited mechanical durability, which hinder their efficiency and lifespan. This study explores the electrochemical and microstructural properties of a 3D-printed AlMgScZr alloy as a potential anode material for Al-air batteries.

The AlMgScZr alloy exhibits a unique bimodal microstructure with a fish-scale morphology, characterized by equiaxed grains along the scales and a core of columnar grains. The grain size distribution ranges from 1 to 12 μm , contributing to enhanced mechanical strength and electrochemical performance. The addition of Sc and Zr promotes grain refinement, strengthening the alloy through grain boundary pinning and increasing its durability compared to pure aluminum.

Electrochemical testing was performed in a three-electrode setup using a platinum counter electrode in 4M KOH electrolyte. The open circuit potential (OCP) was measured at -1.7 V, confirming its suitability for Al-air battery applications. Additionally, the corrosion current density of 10^{-3} A/cm^2 indicates improved resistance to self-corrosion. A key challenge in Al-air batteries, the parasitic hydrogen evolution reaction (HER), was significantly mitigated by the presence of Mg, which stabilizes the structure and suppresses unwanted side reactions. Heat-treated alloys were also evaluated, demonstrating that microstructural optimization further enhances electrochemical performance.

The combined effects of microstructural control, alloying elements, and additive manufacturing contribute to improved electrochemical stability, reduced corrosion, and enhanced mechanical integrity. This study highlights the potential of 3D-printed AlMgScZr alloys as next-generation Al-air battery anodes, offering a pathway toward high-performance and long-lasting energy storage solutions.

Study of the degradation mechanisms of a thermal energy storage system based on molten metal

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E4_4 - Batteries and their components 3, Seminario 8 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Energy storage systems are an essential part of the energy transition towards more sustainable sources. In comparison to electric batteries, thermal energy storage can be a more competitive option depending on the characteristics of the system (applications involving heating, solar thermal energy, heat waste recovery, etc.). The quest of storing the biggest amount of energy possible goes through storage at higher temperatures. Metallic Phase Change Materials (mPCMs) can present high energy densities and high thermal conductivity which make them suitable for their use in high temperature energy storage systems, especially when the volume available for the storage is limited, or fast charge and discharge are required.

Many other criteria need to be considered when designing a high temperature thermal storage system beside the thermophysical properties of the storage material. Compatibility between the mPCM and the container must be ensured throughout the lifetime of the components. This also implies that the storage must be able to withstand a high number of charge/discharge cycles without compromising its performance.

In the present work, a methodology to estimate the lifetime of the components of a thermal storage system is developed. For that purpose, systems based in Al-12.5wt.%Si used as storage material and several iron-based container materials have been tested. The reaction rates between the mPCM and its housing were calculated by keeping the alloy molten for different durations inside a crucible of the container material. Post-mortem analyses were used to determine the extent of the reaction taking place. In parallel, the reaction rates when the system is submitted to numerous melting/solidification cycles were also studied, allowing to estimate the influence of cycling in the degradation mechanisms. This influence was also assessed by measuring the variation in the storage capacity of the mPCM using Differential Scanning Calorimetry. The combination of these experimental results served to establish a methodological first approach for the prediction of component lifetime in latent-heat based thermal energy storages.

Electrochemical Charging of MAX Phases and MXenes as Candidates for Hydrogen Storage Materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Hydrogen storage is a critical challenge in the transition to renewable energy systems, where hydrogen serves as a clean, efficient energy carrier. However, current storage methods face significant limitations in scalability, safety, and efficiency, highlighting the need for innovative solutions. MAX phases and their two-dimensional derivatives, MXenes, have emerged as promising materials due to their unique layered structures, which provide favorable hydrogen trapping sites; including interstitial spaces within carbide and M-A layers, interlayer regions between MXene sheets, and surface terminations. These materials exhibit the potential to store and release hydrogen under mild conditions while maintaining structural integrity, positioning them as strong candidates for practical hydrogen storage applications. Although theoretical studies have demonstrated the potential of MAX phases and MXenes for hydrogen storage, experimental efforts thus far have been limited, with only a few studies exploring gas-phase hydrogen charging. Electrochemical hydrogen charging presents an attractive alternative, enabling solid-state storage at room temperature and ambient pressure. Despite this potential, no studies have yet investigated electrochemical hydrogen charging of these materials, the mechanisms of hydrogen diffusion, or the effects of hydrogenation on their structural and functional properties. Herein, we address this gap by presenting the first demonstration of electrochemically charged MAX phases and MXenes, presenting associated challenges and evaluating their hydrogen storage capabilities. To characterize hydrogen trapping behavior, diffusion mechanisms, and microstructural effects, we employed a suite of advanced techniques, including hydrogen charging, thermal desorption spectroscopy (TDS), Kelvin probe (KP) measurements, in-situ X-ray diffraction (XRD), and scanning electron microscopy (SEM). By gaining deeper insight into hydrogen permeation and trapping mechanisms, this work lays the foundation for the development of sustainable and efficient hydrogen storage technologies for future energy systems.

Development of a Machine Learning Model for Estimating Microstructural Phase Fractions in Compacted Graphite Iron (CGI)

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This paper focuses on improving the process of prediction of the percentage composition of microstructural phases in vermicular cast iron using machine learning techniques. Vermicular cast iron is widely used in industry due to its high resistance to varying operating conditions, however, its mechanical properties depend on precise control of the microstructure. A key problem with traditional analysis methods is their time-consuming and subjective assessments, which limits their repeatability and efficiency in industrial applications. Therefore, the paper proposes an approach based on machine learning techniques, which allows for the automation of the microstructural analysis process.

The study used images obtained by scanning electron microscopy (SEM), which enabled accurate classification of ferritic, pearlitic and graphite phases. For segmentation and phase analysis, K-means clustering algorithms and the Gaussian Mixture Model (GMM) were used, which allow clustering of areas with similar properties without the need for manual labelling. However, the analysis showed that in some cases these algorithms had difficulty correctly distinguishing between phases whose color and intensity of pixels are very similar.

To increase the efficiency of classification, an iterative approach was implemented, consisting of selective detection and segmentation of specific microstructural phases. The results indicate that this approach allows for a significant improvement in the precision of the analysis compared to classical methods. Ultimately, the use of neural networks such as Mask R-CNN enabled more accurate recognition of phase boundaries and a more precise estimation of their percentage composition.

Ultimately, the presented approach allows for a significant reduction in the time needed to analyze microstructures, while increasing the precision and reproducibility of the results. Further work could focus on the use of even more advanced deep learning methods that will enable further optimisation and full automation of microstructural analysis of vermicular cast iron.

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Investigation of Processing and Microstructure on Electrode Materials for Fe-Air Battery Performance

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E4_1 - Batteries and their components 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Iron-air batteries are gaining attention as sustainable and cost-effective energy storage solutions, particularly for grid-scale applications, due to their high theoretical energy density, abundance of raw materials, and environmental recyclability. This study examines the electrochemical performance of three iron-based electrode materials—Fe bulk sheets, Fe₂O₃ powder pellets, and Direct Reduced Iron (DRI) pellets—for Fe-air battery applications.

Fe bulk sheets were fabricated by cold rolling iron sheets to varying thicknesses under different deformation levels. Increased deformation enhanced electrochemical performance by refining the grain structure and increasing surface area, which facilitated improved reaction kinetics.

Fe₂O₃ pellets were produced by compressing Fe₂O₃ powder with pore-forming agents and binders, followed by sintering to enhance mechanical stability. While these pellets exhibited moderate electrochemical performance, their effectiveness was limited by lower electrical conductivity and sluggish reaction kinetics.

In contrast, DRI pellets, prepared by compressing DRI powder with pore-forming agents, conductive additives, and binders, demonstrated superior electrochemical performance. Their high porosity, increased exposed surface area, and optimized microstructure enabled efficient ion transport and redox reactions. As a result, DRI pellets exhibited higher discharge capacity, lower charge transfer resistance, and improved cycling stability compared to Fe bulk sheets and Fe₂O₃ pellets.

This study highlights the importance of material microstructure and porosity in determining electrochemical performance. Among the investigated materials, DRI pellets with various additives emerge as the most promising electrode candidate for Fe-air batteries, offering a scalable and efficient energy storage solution.

Polymeric waste shells for developing new microencapsulated phase change materials (MPCM)

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E4_2 - Energy Storage Materials: Development, Processing and Characterization 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Polymers are one of the most produced materials in the last decades, due to its relatively good mechanical properties with low density and its extremely low cost of fabrication and processing. The polymers production comes principally from the refining of petroleum, that is the main fossil fuel. The main consequence of the high plastic production is that, in municipal solid wastes (MSW) and refuse derived fuels (RDF), the plastic fraction is in constant increase, being for polystyrene (PS) the 15 % of this fraction. This fraction is directly responsible for the presence of microplastics, which affects adversely the ecosystems. These wastes in natural environment cause different diseases including irritation and, in the worst cases, can lead to cancer.

On the other hand, energy consumption in buildings is in an increasing trend, being heating, ventilation and air conditioning (HVAC) systems one the main end-use sectors. HVAC contributes with approximately 7 % of global electricity, causing near of the 3 % of carbon dioxide (CO₂) annual emissions in the world. Thermal energy storage (TES) is a potential technology for more sustainable buildings, playing key role in saving energy. Phase change materials (PCM) are a kind of materials widely used in TES, which uses latent heat from phase changes to store or release energy. The possible phase transitions are solid-solid, liquid-gas, solid-liquid and their reverse paths, due their reversible nature. The most common system are solid-liquid transitions. Melting is an endothermic process and solidification is exothermic. Taking into account the above premises, melting is for heat storage, absorbing energy and solidification releases the energy in heat form. Microencapsulation of PCM is an extended technology for its preservation, resulting in microencapsulated phase change materials (MPCM). The microencapsulation brings to the PCM thermal, chemical and mechanical resistances for future uses as in building, inside cementitious materials. MPCM are constituted by a core/shell system where the core is PCM and the shell material depends on the future usage. The most produced MPCM are using polymeric materials as shell, like PS. To undergo a more sustainable process, production of polymeric shell microcapsules using plastic wastes is a possible way to study.

Multimodal Microscopy and Spectroscopy for Battery Characterization: Understanding Degradation Mechanisms

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E4_3 - Batteries and their components 2, Seminario 8 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Batteries play a crucial role in grid-scale energy storage and in powering modern technology, from portable electronics to electric vehicles. However, the gradual degradation of battery performance presents significant challenges to their reliability, safety, and economic viability. In this study, we combine high-resolution complementary analytical techniques to investigate the underlying causes of material degradation in solid-state metal-ion batteries after charge and discharge cycles. The resulting multimodal and multiscale data is analyzed and correlated using customized machine learning algorithms within the same software platform (XamFlow, Lucid).

Our focus is on lithium-ion battery stacks, a representative energy storage technology, consisting of a Nickel-Cobalt-Manganese (NCM) cathode, a polyethylene separator coated with an inorganic layer, and a graphitic anode. First, X-ray Microscopy (XRM) (Xradia 620 Versa, Zeiss) is utilized to non-destructively visualize the 3D micro- and nanoscale structure of NMC cathodes (spatial resolution ~ 500 nm). XRM data is then employed for the statistical analysis of NMC particle size and shape, porosity, as well as crack and void distributions. These are key parameters associated with degradation due to mechanical stress and cycling fatigue, which lead to increased interfacial resistance and reduced battery capacity.

Second, Scanning Electron Microscopy (SEM) (Crossbeam 550, Zeiss) provides even higher-resolution morphology and defect analysis in both 2D and 3D (spatial resolution ~ 10 nm). The 3D structure is reconstructed using Focused-Ion-Beam (FIB) milling in SEM, yielding high-resolution FIB-SEM tomography datasets. Additionally, elemental analysis is performed using Energy-Dispersive X-ray (EDX) spectroscopy, while Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) enables the spatial mapping of lithium distribution. This allows for the assessment of irreversible lithium ion loss, primarily attributed to degradation mechanisms such as electrochemical reactions and thermal effects, which contribute to Solid Electrolyte Interphase (SEI) formation, lithium plating, and electrode saturation.

Third, micro-Raman spectroscopy (spatial resolution ~ 1 μm) is employed for chemical analysis, enabling the precise differentiation between various crystalline phases of NMC and carbon materials, as well as lithium compounds such as lithium cobalt oxide (LiCoO_2), lithium carbonate (Li_2CO_3), and lithium hydroxide (LiOH), while also providing insights into lithium intercalation and deintercalation processes.

These characterization techniques are broadly applicable to other energy storage materials, including those requiring an inert atmosphere for sample preparation and analysis. In such cases, transfer shuttles are used to safely transport samples between different instruments for slicing, polishing, and measurements.

Mechanistic Insights into the Impact of Sulfide-Based Surface Treatments on Iron–Air Anodes

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Over the past few years, interest in iron–air battery technology has been reignited as a promising solution to large-scale, cost-effective energy storage. By relying on abundant, low-cost, and environmentally friendly materials (here iron) and a theoretical high energy density, both industry and academia have been making significant efforts to enable the widespread adoption of this technology. However, practical application is severely hindered by electrode passivation as well as hydrogen evolution reaction (HER), which serves as a competing reaction of iron-oxide reduction, reducing electrochemical efficiency and cycle life. Various studies have reported successful mitigation of such effects via surface treatments of iron particles with sulfide-based compounds (namely Bi₂S₃), by promoting the formation of a conductive and stable FeS layer on the anode. Said layer improves iron utilization, suppresses passivation and leads to improved cell stability. While published work has extensively explored the improved electrochemical performance, the underlying mechanistic behavior remains poorly understood.

The goal of this study is to present an in-depth characterization of sulfide-treated iron electrodes, to fully elucidate the exact effects of these treatments. This is achieved by utilizing various characterization techniques such as atom probe tomography (APT), X-ray photoelectron spectroscopy (XPS), and electrochemical impedance spectroscopy (EIS) and Transmission electron microscopy (TEM). A better understanding of the morphological and chemical changes induced by sulfide modifications, before and during cycling of the cells, shows that these treatments lead to enhanced charge transfer kinetics and increased cycle stability, shedding light on their role in improving iron-air battery performance. Our findings provide critical insights into the mechanistic origins of sulfide-induced enhancements, offering a pathway for optimizing electrode materials. By addressing key limitations, this work contributes to the advancement of iron–air technology for next-generation sustainable large-scale energy storage solutions.

Shape-stabilized phase change materials based on natural rubber

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E4_4 - Batteries and their components 3, Seminario 8 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

To target the problems related to the containment of organic solid-to-liquid phase change materials (PCM), research has led to several solutions mainly focused on their encapsulation at the microscale and macroscale. However, the leakage of liquid PCM can also be prevented by its embedding in a matrix such as porous aggregates or polymeric materials to form shape-stabilized PCMs (SSPCMs). Although thermoplastic polymers are usually chosen as a matrix, the use of elastomers brings the opportunity to obtain flexible and soft composite materials that can be potentially used as SSPCMs.

In this work, we investigate the feasibility of obtaining elastomer-based SSPCMs by incorporating commonly studied commercial organic PCMs with near room temperature phase change into a natural rubber (NR) matrix without the need for previous encapsulation. Thermal analysis of the prepared composites was performed to evaluate their performance as thermal energy storage (TES) material. A decrease in the melting point of the confined PCM was observed and was found to be dependent on the PCM concentration. Although this phenomenon is mainly attributed to the confinement of PCM in the NR network and its polymer-solvent interaction, further structural and thermal characterization of the PCM extracted from the matrix was performed with the aim of evaluating possible changes in its structure and thermal properties as a result of its interaction with the NR network.

Evaluation of the TES performance of the composites over time concluded that despite the initial ability of NR to incorporate great amounts of PCM in its network, the composite material tends to an equilibrium concentration of PCM at room temperature. Once the equilibrium is reached, SSPCMs were proven to be stable without leaking over time or melting-crystallization cycles, although the transition temperatures were shifted towards lower values in comparison to those of the bulk PCM.

The apparent difficulty in the prediction of the transition temperature range of the developed SSPCMs can be seen as a novel potential route for the design of SSPCMs with a customizable phase transition temperature.

Uncovering CSP-TES Synergies Aligned with Global and European Roadmaps in the COOPERANT Project

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E4_5 - Integration of Energy Storage systems: Emerging Materials and Hybrid Technologies, Seminario 8 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Global energy transition roadmaps include concentrated solar power (CSP) and thermal energy storage (TES) systems as key technologies in the decarbonisation of the energy sector and the development of renewable energies in the medium and long term. The global average LCOE (levelized cost of energy) of these promising technologies dropped by 70 % between 2010 and 2023 (from 0.38 to 0.11 €/kWh). However, this cost is still far from mature renewable technologies such as photovoltaics (0.04 €/kWh) and onshore wind (0.03 €/kWh)¹. In 2024, the global total CSP capacity exceeded 7 GW, and the International Energy Agency (IEA) estimates that 35 and 390 GW of CSP capacity should be added by 2030 and 2050, respectively, to achieve net zero emissions in the energy sector.

We have reviewed different European strategic roadmaps and identified the strategies that CSP-TES systems must follow to play a pivotal role in the uninterrupted supply of renewable electricity and high-temperature heat in alignment with the European Green Deal. The SET Plan includes specific targets to develop innovative and cost-effective systems unlocking the third-generation of CSP technologies.

In this vein, CSP-TES integration can significantly improve the dispatchability of solar energy, i.e., commercial molten salts-based TES achieve up to 18h storage capacity at 560 °C. We have identified and compiled current challenges linked to operation, compatibility and durability at high temperatures as well as reliable thermal cycling stability and concluded there is a need to develop new advanced materials, novel concepts and energy management technologies to ease CSP-TES integration across industrial sectors.

Aligning with the global and European roadmaps, the COOPERANT project introduces key innovations in a new CSP-TES conceptual design operating at high temperatures (>1000°C). To do so, a high-performance open volumetric receiver with a distinct cellular morphology made of silicon-carbon composites is used. Furthermore, the high-temperature hybrid TES with a large storage capacity (600 kWh/m³) will incorporate both latent and sensible heat storage mechanisms. Metal alloys and inorganic salts are investigated as phase-change materials (PCM) to operate up to 900°C while solid-state mixtures can withstand temperatures up to 1300°C. These innovations unlock the potential to reach an overall system efficiency over current benchmarks (>42%), accomplishing the second SET PLAN target.

Overall, COOPERANT's innovative energy storage solution will enable CSP plants to provide renewable high-temperature heat and power on demand, bridging the production/demand gap and aligning with EU and global climate and energy agendas.

Negative charged covalent organic framework (N-COF)-based Li ion filtering protective layer for stable Li metal anodes

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E4_3 - Batteries and their components 2, Seminario 8 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Lithium metal is considered as a promising candidate for the anode of next-generation batteries, such as lithium-sulfur and lithium-air batteries, due to its high theoretical capacity (3,860 mAh cm⁻³), low standard reduction potential (-3.04 V vs. Standard Hydrogen Electrode), and low density. However, it faces several challenges, including high reactivity, volume expansion, unstable solid-electrolyte interphase (SEI) layer, dendrite formation, and the formation of dead lithium.

To address these chronic issues, extensive research is being conducted, and one notable solution is the development of an artificial protective layer on the Lithium metal surface. In this study, an artificial protective layer was developed using a covalent organic framework(COF), which selectively allows the stable diffusion of lithium ions. Previously developed COF materials for lithium metal protective layer have been reported to enhance cycling stability by facilitating the uniform deposition of Lithium ions beneath the protective layer. However, their high initial resistance leads to poor initial performance, and low ion conductivity increases instability during high-rate charge/discharge cycles.

In this study, a COF material with high-ion-conductivity functional groups(N-COF) was developed to overcome the limitations of conventional COF materials. These functional groups enhance ion conductivity and impart a negative charge to the nanochannels.

To synthesize N-COF, a constant temperature was maintained to induce the spontaneous reaction of precursors, and its successful synthesis was confirmed through XRD, FTIR, Raman, and XPS analyses. Compared to other COF materials, N-COF features smaller pore sizes and is composed of abundant lithiophilic functional groups, which not only reduce overpotential during prolonged and continuous lithium plating/stripping but also promote uniform lithium deposition and dissolution. Furthermore, the mechanism of lithium anode behavior with N-COF was elucidated through first-principles calculations (DFT) and comprehensive electrochemical analyses. As a result, the N-COF protective layer facilitated stable lithium deposition beneath the protective layer, enhancing the long-term performance of lithium metal batteries. The symmetric cell and full cell tests demonstrated low overpotential and long-term stability. Additionally, due to its high ion conductivity and negatively charged nanochannels, stable cell performance was achieved even during high-rate charge/discharge cycles.

Self-healable polymer electrolyte for lithium batteries, targeting light-mediated and 3D-printable processes

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E4_1 - Batteries and their components 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

In the pursuit of enhancing the longevity and safety of lithium batteries, our research introduces a novel self-healing poly(urea-urethane) gel electrolyte. This dynamic covalent network, synthesized through the reaction of tris[2-(isopropylamino)ethyl]amine with hexamethylene diisocyanate followed by the addition of polyethylene glycol, exhibits remarkable self-healing properties activated at low temperatures. Notably, the gel electrolyte demonstrates higher ionic conductivity compared to conventional liquid electrolytes embedded in porous separators.

Electrochemical evaluations reveal that lithium symmetrical cells utilizing this gel electrolyte achieve homogeneous lithium plating and stripping, maintaining stability over extended cycles. Furthermore, even after significant mechanical damage, the electrolyte's self-healing capability ensures the recovery of electrochemical performance, sustaining over 100 charge/discharge cycles at a C/5 rate post-repair [1,2].

This innovative approach not only addresses mechanical vulnerabilities inherent in battery systems, but also aligns with sustainable practices by extending battery lifespan and reducing waste. Our findings suggest that integrating self-healing mechanisms into battery electrolytes holds substantial promise for the development of safer, more durable energy storage solutions.

Moreover, this Li⁺-conducting self-healing gel electrolyte extends its potential beyond conventional battery applications. Its high ionic conductivity and mechanical resilience make it an ideal candidate for Li-mediated electrochemical ammonia synthesis, a promising route for sustainable nitrogen fixation [3]. By stabilizing the Li-metal interface and preventing dendrite growth, this electrolyte enables efficient and prolonged operation under harsh reaction conditions. This breakthrough paves the way for next-generation ammonia production systems, leveraging lithium's reactivity while ensuring process stability and scalability.

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3D Simulations of Ultra-High Temperature Phase-Change Material Storage for Thermophotovoltaic Conversion: The SUNSON-BOX Approach

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E4_4 - Batteries and their components 3, Seminario 8 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

Searching for more efficient, high-temperature energy storage solutions, phase-change material (PCM)-based thermal energy storage (TES) systems have gained significant attention due to their ability to store and liberate heat on demand. As part of the Horizon Europe SUNSON project, we performed comprehensive 3D computational simulations in COMSOL Multiphysics® to investigate the thermal behaviour and energy conversion performance of a novel ultra-high-temperature PCM-TES prototype: the SUNSON-BOX. This system uses concentrated solar power (CSP) to store thermal energy, subsequently converting it to electricity via a thermophotovoltaic (TPV) unit (doi.org/10.1016/J.ENERGY.2016.04.048).

The developed model incorporates a multi-physics approach to account for all elements of this innovative system, investigating how different PCM properties and design modifications influence overall system performance, while providing essential data for optimising material selection, geometry, and operational strategies. The simulations combine heat transfer, radiation, fluid flow, and phase-change modelling under charging (with and without simultaneous discharge) and discharging (with and without active power production) modes. Various metal-silicon PCMs (doi.org/10.1016/B978-0-12-819955-8.00004-1) were analysed regarding latent heat capacity ($>1\text{MWh/m}^3$), melting temperature range ($>1150^\circ\text{C}$), and thermal conductivity, with the prototype having a 12l PCM volume. Results indicate that certain high-melting-point alloys, such as 24Mn-64Si-10B-2Cr, enable higher TPV operating temperatures, thus enhancing the electrical output. However, these attributes also increase heat losses, reducing system efficiency. Other alloys (43Fe-57Si, 41Fe-51Si-3B-5Cr) provided balanced performance by ensuring relatively high peak power output while limiting losses during extended storage periods.

The key performance indicators evaluated include solar-to-thermal conversion efficiency (ratio of accumulated heat in the PCM to total solar input), thermal-to-electric conversion efficiency (product of TPV absorption efficiency and TPV cell efficiency), and charge/discharge cycle times. In charging modes, the system stored up to 19kWh of thermal energy in one cycle, with melting durations of 0.5h-1.3h depending on the PCM alloy. During discharge modes, solidification times ranged from 3h-10h, with electricity outputs of 70-300W. Additionally, optimisation studies were conducted to evaluate the effect of design modifications (doi.org/10.2991/978-94-6463-455-6_18), such as varying crucible wall thickness and incorporating fins into the crucible walls. While adding fins slightly enhanced melting and solidification rates, the projected gains were insufficient to offset the added design complexity and cost.

Overall, this study provides essential insights into the interplay of PCM thermophysical properties, operating temperature, and system design in maximising energy conversion efficiency. These findings will guide ongoing refinement of the SUNSON-BOX prototype, support material selection, and ease subsequent experimental validation and scale-up for real-world renewable energy production.

Hybrid Sensible-Latent Heat Thermal Energy Storage for Concentrated Solar Power Applications

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E4_5 - Integration of Energy Storage systems: Emerging Materials and Hybrid Technologies, Seminario 8 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The integration of Thermal Energy Storage (TES) systems in Concentrated Solar Power (CSP) plants is crucial for enhancing their efficiency and dispatchability. This study presents a novel hybrid sensible-latent heat TES system designed for high-temperature CSP applications. The proposed system combines advanced solid-state materials with phase change materials (PCMs) to optimize thermal storage capacity and heat transfer performance. We aim to investigate innovative structured fillers, such as honeycomb designs, incorporating new solid mixture materials as PCM matrices and/or macroencapsulated PCM. These components are studied to be strategically arranged to maximize heat transfer and storage density.

Key aspects of the study include:

1. Defining input/output requirements and boundary conditions for the CSP-TES system, including energy flows, power, pressure, capacity, and temperature ranges.
2. Designing a volumetric receiver for efficient solar energy capture and transfer to the heat transfer fluid.
3. Developing alternative TES configurations with optimized material distribution and heat transfer enhancement techniques.
4. Establishing target requirements for storage materials, emphasizing cost-effectiveness and sustainability.

The study also considers key performance indicators (KPIs) to evaluate the TES system's effectiveness, including energy density, thermal efficiency, operational stability, and long-term durability. Various design alternatives are assessed to identify the most viable configuration for large-scale implementation. The work sets a foundation for future optimization efforts, ensuring the proposed system aligns with industrial scalability and economic feasibility.

The results of this study will be presented at the conference, focusing on design considerations, material selection, and performance benchmarks. This research contributes to advancing CSP technology by supporting the development of next-generation TES systems, this research supports the broader goal of improving CSP technology, making it more viable and cost-effective for widespread implementation.

Iron oxide-based catalytic structures as enablers of a thermochemical cycle based on solid sulphur for long-term storage of solar thermal energy

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

This work is part of a wider project aiming to demonstrate direct storage of solar energy into solid elemental sulphur. The concept, as originally proposed by General Atomics (Norman, J.H., US Patent 4,421,734, 1978), is a combination of three process steps that interconvert sulphuric acid to sulphur. In the first step, sulphuric acid (H_2SO_4) is first evaporated and then sequentially decomposed into sulphur dioxide and oxygen. This sulphuric acid splitting is the highest-temperature (650-1000°C) endothermic reaction step of the cycle. The heat needed can be supplied by Concentrating Solar Technologies (CST) since these temperatures are within the capabilities of state-of-the-art CST tower plants. In the second step, sulphur dioxide disproportionation, sulphur dioxide reacts with water to produce sulphuric acid and elemental sulphur. Hence, a significant proportion of the solar energy used to decompose the sulphuric acid is stored in sulphur for virtually unlimited time. In the third step, sulphur can be combusted on demand to release this stored solar energy as heat at temperatures in excess of 1200 °C, suitable for gas turbines and high-efficiency combined cycle power generation.

The present work comprises an integrated approach on catalytic sulphuric acid splitting. Typically, sulphuric acid is vaporized and driven first through a medium-temperature zone wherein it is thermally dissociated into steam and SO_3 ; the vapours mixture is then passed through a catalytic reactor at higher temperatures where the SO_3 splitting to SO_2 and oxygen is performed. Atomistic-scale simulations like Density Functional Theory (DFT) were employed to investigate the binding strength of SO_3 on various catalysts' surface, culminating to a plausible reaction mechanism. In parallel, a large number of iron oxide-based compositions - which are the state-of-the-art inexpensive splitting catalytic materials - single or mixed with other cations were investigated. They were shaped into spherical granules, catalytically tested and physico-chemically characterized before and after exposure to the reaction environment. Selected compositions were then shaped into larger-size honeycombs that underwent long-term (> 300 hours) catalytic testing in a suitably designed catalytic reactor test rig. Several of them demonstrated not only close-to-equilibrium conversion but also remarkable corrosion resistance under the reaction's "hostile" environment. The next goals are on the one hand to incorporate a large amount of iron-oxide-based inexpensive recycled materials into these catalytic structures and on the other hand to use the results for the design of a pilot-scale reactor for sulphuric acid catalytic splitting with renewable heat.

Efficient perovskite-based high-temperature hybrid sensible-thermochemical heat storage systems for integration with renewable energy sources

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E4_5 - Integration of Energy Storage systems: Emerging Materials and Hybrid Technologies, Seminario 8 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

The present work presents a holistic approach on development of efficient high-temperature heat storage systems for integration with renewable energy (RE) sources as well as industrial waste heat recovery. The concept pursued is that of hybrid sensible-thermochemical storage implemented on porous, flow-through ceramic monolithic structures like honeycombs and foams, manufactured entirely or substantially from earth-abundant, inexpensive, environmentally-benign perovskites. Ca-Mn-based perovskites in particular, are capable of cyclic, reversible reduction-oxidation (redox) under air atmosphere, accompanied by significant endothermal/ exothermal heat effects, according to the scheme: $\text{CaMnO}_3 \leftrightarrow \text{CaMnO}_{(3-\delta)+\delta/2} \text{O}_2$. The necessary “renewable” heat for the endothermic reduction step can be supplied from, otherwise to-be-curtailed, surplus electricity from PV or wind systems, concentrated solar energy or hot industrial waste gas streams. This heat is recovered by the inverse, exothermic oxidation of the reduced oxide when the RE-source is not available. With redox oxides, air can be used as both the heat transfer fluid and the reactant (O₂) coming into direct contact with the storage material (oxide).

The development of CaMnO₃-based redox structures is addressed starting from high-throughput computational screening of such A- and B-site doped perovskite compositions to extract via Density Functional Theory (DFT) theoretical key metrics like heat capacity (extremely important for sensible heat storage), redox reactions enthalpy and thermo-mechanical properties within the temperature range of interest, as a function of kind and concentration of dopant elements. The so-identified shortlisted multi-cation perovskite compositions are synthesized by scalable routes, optimizing selection of precursor powders and sintering conditions with respect to the targeted properties of merit like phase purity of the obtained perovskite, heat capacity, extend and reversibility of reduction, heat effects of the redox reactions, coefficient of thermal expansion, and dimensional changes due to thermochemical expansion/contraction, among others. Of significant importance is the absence of phase transformations, which, even though reversible during heating/cooling in the temperature range of 300-1100°C, are nevertheless detrimental on the thermomechanical strength and longevity of structured ceramics. Finally, rigid monolithic porous honeycombs and foams were manufactured from such optimized compositions in a variety of sizes spanning from few mm to tens of cm. Long-term cyclic redox tests (>200 cycles) on such structures have demonstrated for the first time the ability of a perovskite – or in general of a redox oxide operating via partial reduction (oxygen vacancies) mechanism - to generate repeatable heat effects manifested as sensible temperature rise of a working/heat transfer fluid upon cyclic redox operation.

A re-investigation of the phase diagram of the disodium hydrogen phosphate/water system and its consequences for latent heat storage applications

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E4_2 - Energy Storage Materials: Development, Processing and Characterization 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Latent heat storage (LHS) using Phase Change Materials (PCMs) has attracted the interest of researchers and policymakers as a promising technology to increase the share of renewables in contexts where space is either restricted, or a cost-limiting factor. The selection of suitable materials characterized by a reliable behaviour over long-term thermal cycling is the first essential criterion to the development of a LHS. Salt hydrates are a promising class of PCMs given their promising thermophysical properties such as high energy capacities, high densities and low cost. Disodium hydrogen phosphate dodecahydrate (DSPD) is particularly interesting due to its melting point over the range 30-32 °C – a temperature range for which there are fewer choices of PCMs. Despite its attractive properties, data on the melting point and phase change enthalpy of DSPD appear inconsistent in the literature, and concerns over its usage as PCM have also been highlighted because of reports of polymorphic behaviour.

In this study, a systematic investigation of the phase diagram of DSPD was performed using a wide variety of techniques, including differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), single crystal and powder X-ray diffractometry coupled with DSC (PXRD-DSC), hot-stage microscopy (HSM) and X-ray computed tomography (XCT). Different compositions of disodium hydrogen phosphate in water were produced and studied to clarify whether the phase diagram derived from previous studies is correct. In addition, single crystals of DSPD were successfully obtained.

The results showed evidence of polymorphism in DSPD, but this was not found to influence the overall phase diagram or long-term behaviour and stability. More notably, a strong tendency to dehydrate was observed, leading to a general instability and tendency to produce a mixture of the dodecahydrate and heptahydrate forms, rather than pure DSPD. This had been mistakenly labeled as a polymorphic phase transition in the phase diagram. A new methodology was developed using XCT, which enabled the in-situ observation of the solvent-mediated dehydration process, while a new approach to DSC data analysis allowed quantification of the ratio of disodium hydrogen phosphate dodecahydrate and disodium hydrogen phosphate heptahydrate present in samples at different compositions.

This work challenges the currently accepted phase diagram of the disodium hydrogen phosphate/water system. The use of different techniques to understand the behaviour and stability of salt hydrates paves the way for more reliable latent heat storage solutions.

Back to Basics: using conventional techniques to characterize graphite blends components for applications as anode in batteries

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E4_3 - Batteries and their components 2, Seminario 8 Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Graphite blends are rapidly gaining popularity in anode production for batteries, due to their ability to optimize performance, cost, and durability. By combining different types of graphite, manufacturers can enhance conductivity, life cycle, and structural stability, while maintaining low cost. Additionally, blends offer customization of electrode properties and supply chain flexibility. These advantages make graphite blends a key focus for advancing next-generation energy storage solutions. Understanding the structural properties of selected graphite is essential for the characterization of these blends.

Graphite exists in two crystalline forms: hexagonal and rhombohedral [1]. The hexagonal form is the most common and thermodynamically stable, while the rhombohedral form is unstable and always found mixed with the hexagonal one. The rhombohedral features, such as (101) and (012) reflections in powder X-ray diffraction (PXRD), are observed in natural graphite. On the contrary, they are absent in synthetic varieties, due to the high temperature of the production process, which leads the rhombohedral phase to gradually convert into the more stable hexagonal phase when heated above 1300 °C [1]. These structural differences influence the electrochemical properties of graphite blends, highlighting the need for advanced characterization techniques to clearly identify the components of graphite' blends.

The aim of this study is to standardize routine analysis methods for characterizing graphite blends. We synthesized 15 graphite blends with varying natural-to-artificial ratios using ball milling under different conditions, including varying milling times and using wet (water, ethanol) or dry milling. Blends were characterized using synchrotron PXRD, at the ID22 beamline at ESRF. Data analysis revealed that a unique method for distinguishing the components within graphite blends involves examining defects in the crystalline structure. Specifically, we investigated how stacking fault density and interplanar distance vary in the blend, using structural parameters of both natural and artificial graphites as standards. This approach allowed us to quantify the percentage of natural and synthetic graphite present in the blends. The PXRD data were complemented with pair distribution function (PDF) analysis to examine how the C···C distances vary in the blends, while FE-SEM measurements provided insights into observed morphologies. The combination of data from applied techniques was used to simulate and validate the crystal structure of the graphite blends. The impact of stacking faults was further explored through atomic-scale simulations, using XaNSoNS software [2]. Preliminary results suggest that using defects as unique fingerprints of different graphites could be a winning strategy.

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Environmentally sustainable alternatives to Portland cement optimized with phase change materials (PCMs) for low temperature thermal energy storage

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E4_4 - Batteries and their components 3, Seminario 8 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

The production of one of the base materials in modern construction, Portland cement, is associated with significant emissions of polluting gases, mainly CO₂, and with an important demand of water and fossil fuels. Thus, the search for ecological alternatives to Portland cement (PC) has intensified, leading to the development of new systems that allow not only to reduce the impact of the contamination but also to reutilize industrial wastes and to open up these systems to new applications. The recent studies on this field explore the potential of several alternatives, such as alkali activated and hybrid materials based on the use of blast furnace slag or blends of limestone and calcined clay (LC³ materials). Moreover, these alternative materials are observed in recent studies to serve as potential thermal energy storage (TES) systems, taking advantage of similar thermal conductivity and specific heat and better mechanical properties compared with PC, serving as bases for the development of renewable energies [1].

In the study of the optimization of these systems, phase change materials (PCMs) exhibit great thermal properties that make them attractive for the development of TES applications due to their ability to undergo a phase transition, absorbing or releasing a significant amount of heat during this process [2]. This allows the development of medium-to-low temperature TES systems with higher thermal storage capabilities for several applications. The research carried out consists of the study of the effect on thermal and mechanical properties of the PC and alternative systems doped with nylon and of their viability in construction and TES applications. For that purpose, the systems were exposed to low temperature cycles as well as to constant temperatures to determine their performance, stability and viability. The research highlights the potential of PCMs when integrated in both traditional and alternative cementitious systems, being a promising pathway towards a more sustainable and efficient construction.

Characterization of microencapsulated phase change materials developed from waste for sustainable constructive materials.

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E4_4 - Batteries and their components 3, Seminario 8 Room (Level +1), septiembre 18, 2025, 14:30 - 16:30

This study presents advancements by the DIOPMA research group in developing sustainable construction materials (SCM) and optimizing Microencapsulated Phase Change Materials (MPCM). With science, technology, and innovation as key drivers toward the 2030 Agenda's Sustainable Development Goals (SDG), our research explores alternatives to Ordinary Portland Cement (OPC), focusing on Magnesium Phosphate Cements (MPC) incorporating waste-derived raw materials and MPCM.

We investigate MPCM with polymeric shells from waste materials such as polyethylene terephthalate (PET), polystyrene (PS), and acrylics (PMMA), evaluating their compatibility with MPC for enhanced building performance. Key requirements include resistance to pH and temperature fluctuations, as well as mechanical strength to withstand the mixing processes. The materials undergo comprehensive chemical, physical, thermal, mechanical, and environmental assessments, including porosity analysis. A life cycle analysis (LCA) is essential to ensure these materials support climate change adaptation and decarbonization efforts in the building sector at both national and European levels. By reducing raw material consumption, enhancing thermal comfort, and lowering reliance on HVAC systems, this research contributes to energy efficiency and the circular economy, driving a sustainable transition in construction.

NEWIRONAGE: IRON AS A FUEL IN NEW ENERGY STORAGE CYCLES

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E4_5 - Integration of Energy Storage systems: Emerging Materials and Hybrid Technologies, Seminario 8 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

Metallic iron can serve as an energy-dense fuel, CO₂-free producing a regenerable oxide in combustion. The regeneration of the oxide to FeO through an industrial process of reduction with H₂ from renewable sources allows the direct storage of energy in the form of metallic iron. In this way, metallic iron falls into the category of recyclable electro-fuel, also called 'energy carrier'. The process of self-sustaining combustion of iron has been studied and demonstrated at laboratory and pilot plant scale, however there are still some uncertainties about the behaviour of the materials in realistic cycles.

The NewIronAge project studies the realistic combustion for industrial implementation in combustion boilers, and the behavior of particles in successive cycles, which is a novelty compared to theoretical and thermobalance scale studies. We have described the detailed physicochemical evolution of iron particles burnt under controlled, realistic conditions. In addition, the use of alternative iron sources is studied. The characterisation of the particles after the successive stages is carried out by XRD, SEM-EDX, TGA and size distribution. The results obtained under the appropriate conditions to ensure the viability of the decoupled storage cycles are presented.

Improvement in Performance of Energy Storage Technologies through Online Acoustic Emission Sensor-Based Battery Mixing

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E4_1 - Batteries and their components 1, Seminario 8 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The progress in battery technology is propelled not only by enhancements in materials and energy density but also by the optimization of manufacturing processes. A key element of battery production is the mixing process, as the uniformity of the mixture greatly affects both the stability of the final product and its overall performance. This study presents a real-time analysis technology designed to assess the homogeneity of battery slurry mixing. It proposes strategies to enhance the consistency of slurry viscosity and boost the efficiency of the mixing process.

The ongoing research and development of inline monitoring technologies and analysis have led to significant advancements in the methods used for analyzing battery mixing processes. The previous method as ex-situ approaches have been continuously refined. Leverage real-time analytics to improve electrode uniformity and minimize material waste and energy consumption to increase production efficiency and further optimize battery performance. A real-time optimization method that incorporates artificial intelligence (AI) and machine learning (ML) to reduce manufacturing defects, ultimately enhancing the quality and reliability of energy storage devices.

In this study, we propose a method to analyze the homogeneous mixing of cathode slurry in real time to evaluate the performance of energy storage devices. For real-time process evaluation, we utilize acoustic emission sensors and ultrasonic sensors, complemented by domain-specific signal processing algorithms to accurately detect the homogeneity of mixture and optimize endpoint of mixing. Data collection involved experiments using an IoT sensor developed at Korea University attached to a NETZSCH PMD mixer, along with a differential-pressure viscometer from NETZSCH for auxiliary viscosity measurements. This methodology enables the early identification of quality degradation factors in battery manufacturing early and respond quickly.

The technology developed in this study is anticipated to facilitate the realization of eco-friendly processes and advance sustainable battery manufacturing technologies. Such technological advancements are crucial for reducing production costs and minimizing environmental impact. This ultimately contributing to a transition to a sustainable energy system through next-generation energy storage manufacturing innovation.

Joule-Heated Perovskite Metal Oxides for Thermal Energy Storage

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E4_5 - Integration of Energy Storage systems: Emerging Materials and Hybrid Technologies, Seminario 8 Room (Level +1), septiembre 18, 2025, 17:00 - 19:00

High-temperature thermochemical cycles based on redox metal oxides offer great potential to utilize heat from renewable sources such as concentrated solar irradiation or produced from excess renewable electricity and industrial waste heat. All these have in common that the metal oxides are heated by an external heat source. In this work an innovative approach to power-to-heat conversion by joule heated perovskite metal oxides is presented. While typical thermal storage units required a heat transfer fluid such as air to be charged and discharged, joule-heated storage units neither require a heat transfer fluid nor an external source of heat to be stored in the unit. Instead, all it required is electric power and current flowing through the storage units. This concept can not only serve as a means to overcome the inherently fluctuating power supply by PV and wind, but also as solution to electrification of large scale heat supply to industry with high-temperature heat demand.

Perovskite metal oxides of the general formula ABO_3 are a versatile material class, which is considered for various applications due to its tunability and flexibility. Substituting elemental fractions on either A- or B-site can not only govern thermodynamic and kinetic properties, but also electrochemical properties and can improve structural and mechanical stability. Perovskite metal oxides are capable of fully reversible cyclic reduction and oxidation during thermal cycling at high temperatures, which they undergo non-stoichiometrically without any major phase transition. The large variety of possible composition allows precise fine-tuning of desired properties in multi-cation perovskites, including the electric conductivity. This allows perovskite metal oxides to be directly heated by electric current flow through the material, so called joule heating. The presented work investigates Mn- and Fe-rich perovskite compositions as functional materials for such a combined power-to-heat and thermal energy storage approach. From Density Functional Theory (DFT) calculations, a sophisticated doping strategy is derived and chosen material compositions are synthesized and characterized for validation. Electric conductivity, thermodynamic redox activity, heat capacities as well as reaction kinetics are determined experimentally in the desired temperature range of RT – 1100°C and are used to validate the previous theoretical calculations and evaluate the performance of novel material compositions for the described power-to-heat approach. Finally, based on this works results the potential of this novel concept is evaluated and outlook on follow-up work is drawn.

Processing Al-based MGA systems as phase change materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In energy storage applications, PCM (Phase Change Materials) stands in a sealed chamber near the heat source, exchanging thermal energy with the surrounding environment. In the Al-Sn system, aluminum (Al) serves as the housing material, while tin (Sn) is used as the phase change material. The theoretical phase change temperature of Sn is 232 °C, with a latent heat of 60.3 J/g, making this composite material suitable for medium-temperature thermal energy harvesting and storage applications. Due to the extremely low solubility of Al in Sn, the Al-matrix and the Sn-phase change material couple remain stable and do not react within the operating temperature ranges. Accordingly, composite microstructure should be long-term preserved even after several thermo-cycles. In this paper, preliminary study based on experimental observations, show the behaviour of selected Al-Sn alloys within heating and cooling processes, in view to find out the suitable process conditions for preserving microstructures and their performance under service conditions. Specifically, the behaviour and microstructure stability will be related to operating conditions and practical recommendations will be provided.

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PRODUCTION AND CHARACTERIZATION OF NEW MEMBRANES FOR HYDROGEN PURIFICATION BASED ON THE Nb-V-Pd SYSTEM

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E5_2, Z3 Room (Level -3), settembre 16, 2025, 10:30 - 13:10

Hydrogen is a universal, clean and efficient energy carrier, with a high calorific value (120MJ/kg), which can be used for storage and transportation of energy and converted into electricity via high-efficiency, emission-free fuel cells. Several processes, including biological-based ones, can be employed for hydrogen production but often these processes provide gas mixtures with high content of by-products (CO, CO₂, H₂S etc.). For this reason, a purification phase is necessary. Among the various separation technologies, membranes are a promising technology for hydrogen purification due to their operational simplicity, low energy consumption and the ability to work continuously.

Dense metallic membranes, in particular, show a high selectivity for hydrogen. The palladium-based membranes are widely considered the best for this purpose, due to their ability to dissociate and dissolve hydrogen into their bulk. However, besides its cost, Palladium has been identified as strategic critical raw material by the Critical raw material act of European Union in 2024. More recently, transition metals have been investigated, in particular V and Vb group elements, as alternative to Palladium-based alloys. In this work, the possible production of alternative membranes based on Nb-V-Pd system was studied to reduce the Palladium amount and so the total cost of the membrane, with acceptable overall performances.

High Power Impulse Magnetron Sputtering (HiPIMS) technique was employed as deposition method of a hydrogen-selective membrane film. In detail, multilayer films based on the Nb-V-Pd system were deposited by a combined HiPIMS/Direct Current (DC) magnetron sputtering process onto porous alumina.

The obtained membranes were characterized both on the surface and cross section through SEM-EDS analysis and phase composition was evaluated through XRD analysis. Membrane permeability measurements were carried out by means of a custom-built test station, to investigate hydrogen permeance, selectivity and resistance to hydrogen embrittlement.

The results were very promising, showing formation of a compact and uniform film, characterized by permeances higher than 1×10^{-6} mol m⁻² s⁻¹ Pa⁻¹ at 450°C and good stability to hydrogen embrittlement.

Acknowledgement: The authors would like to thank the Project PE0000021, Concession Decree No. 1561 of 11.10.2022 adopted by Ministero dell'Università e della Ricerca (MUR), Project title "Network 4 Energy Sustainable Transition – NEST" and the project "Research and development on hydrogen" financed by European Union – NextGenerationEU – M2C2 Investment 3.5 for financing these activities.

Study of RF Co-Sputtered $\text{ZnS}_{1-x}\text{Se}_x$ Alloys for Potential Photoelectrochemical Cell Applications

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E5_2, Z3 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Photoelectrochemical cells (PECs) are promising energy conversion devices that produce hydrogen (H_2) directly from solar energy using semiconductor materials. For efficient hydrogen production, semiconductors must have a band gap between 2–3 eV, with a conduction band minimum (CBM) more negative than 0 V vs. SHE and a valence band maximum (VBM) lower than -1.26 V vs. SHE. While ZnS has suitable CBM and VBM positions but an overly wide band gap (3.6 eV), ZnSe has a narrower band gap (2.7 eV) and compatible CBM and VBM positions. The potential of $\text{ZnS}_{1-x}\text{Se}_x$ pseudobinary alloys for PECs remains unexplored. In this study, $\text{ZnS}_{1-x}\text{Se}_x$ alloys were deposited by RF magnetron co-sputtering with varying ZnSe/ZnS ratios, followed by a post-annealing in Ar-H_2 at 300 °C. Morphological, structural, electrical, optical, and electrochemical properties were evaluated. AFM showed homogeneous film surfaces, and XRD revealed shifts in the (111) peak correlating with composition. XPS identified Zn interstitials and Se antisites, confirmed by Raman analysis of S-Se bonds. UV-Vis spectroscopy indicated tunable band gaps (2.74–3.57 eV), and photoluminescence revealed donor states. The alloys demonstrated favorable electronic properties for hydrogen production but also showed susceptibility to water oxidation, highlighting their potential for PEC applications.

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SAN and ABS polymers as binders for metal hydride pellets for hydrogen storage at the solid state

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E5_4, Z3 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Intermetallic compounds represent promising candidates for hydrogen storage applications under ambient conditions; however, their activation remains challenging.[1]The utilization of loose powder in metal hydride reactors often results in poor thermal conductivity and can cause the plastic deformation of tubes due to the volume changes during hydrogen charging and discharging cycles.[2] These issues can be alleviated by embedding the metal powder with a polymer to form pellets. The polymer should be homogeneously blended with the powder, be impermeable to oxygen but permeable to hydrogen, demonstrate elasticity to accomodate volume changes during hydrogen absorption/desorption cycles, and enhance thermal conductivity of the powder alone.[3]

This study examines styrene acrylonitrile (SAN) and acrylonitrile-butadiene-styrene (ABS) polymers, supplied by Versalis s.r.l., as binders for metal alloy pellets intended for hydrogen storage. Pellets were prepared by mixing polymers and metal powder with a general $\text{La}_{1-x}\text{Ce}_x\text{Ni}_5$ composition via ball milling and pressing. The pellets were characterized using X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS), differential scanning calorimetry (DSC), and Fourier-transform infrared spectroscopy with attenuated total reflectance (FTIR-ATR). Hydrogen storage performance was evaluated using a Sievert-type apparatus.

Both polymers yielded stable pellets with up to 95:5 weight ratio of metal powder and polymers at various pressures. XRD analysis confirmed that the crystalline structure of the metal powder remained unaltered, while FTIR-ATR spectra indicated no structural changes in the polymers. DSC analysis demonstrated no variations in the polymer glass transition temperature, suggesting thermal stability during pellet fabrication. Gas sorption tests enabled to assessment of the polymer's impact on the hydrogen storage properties of the metal powder, providing valuable insights into the compatibility and potential applications of these composite materials.

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Role of Co, Cu, Cr, and Al in Recycled TiFe Alloys for Hydrogen Storage

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E5_4, Z3 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Hydrogen has emerged as a promising solution to address environmental challenges posed by fossil fuels and to store excess renewable energy. Together with gas compression and liquefaction, the storage of hydrogen in suitable carriers is considered. TiFe-based alloys are particularly attractive for hydrogen storage, due to their storage capacity, although challenges remain regarding activation and plateau pressure stability. This study offers insights into the design of TiFe-X alloys for hydrogen storage, focusing on the use of commonly available elements found in scrap yards, and highlighting the potential of recycled materials to enhance sustainability. In this respect, this study is compliant with the innovation principles expressed by the Safe and Sustainable by Design approach for a responsible and sustainable production of chemicals and materials.

TiFe-X alloys were synthesized via arc melting of high-purity raw materials under vacuum, followed by suitable annealing. Obtained samples have been characterized by X-ray diffraction, scanning electron microscopy, and energy-dispersive X-ray spectroscopy. The hydrogenation properties of the alloys were assessed through Pressure-Composition-Temperature analysis and high-pressure differential scanning calorimetry.

The addition of Al and Cr was found to be particularly beneficial for the activation of the alloy. Al promotes compositional heterogeneity in the alloy, enhancing the number of fast hydrogen diffusion channels and improving the activation characteristics, while Cr forms secondary phases, that facilitate hydrogen absorption. Cr addition exhibited superior hydrogen uptake compared to other alloying elements, making it the best choice for maximizing storage capacity. In contrast, the inclusion of Co and Cu does not significantly improve either the activation or storage capacity of the TiFe alloy.

From an environmental perspective, the Life Cycle Impact Assessment of the arc melting production and annealing revealed that Co is the most impactful among selected elements, while Al is the most environmentally friendly, due to the lowest environmental impact during production. Although Cr introduces higher environmental costs compared to Al, it offers a balanced solution due to its superior hydrogen storage performance.

Thus, Cr can be regarded as an ideal compromise between hydrogen storage capacity (1.6 wt% of hydrogen compared to 1.1 wt% for the Al-substituted alloy) and environmental impact, positioning it as a promising alloying element for TiFe-based hydrogen storage systems.

Future work will involve an analysis of scaling up the production of these alloys from recycled metal sources and evaluating their performance in industrial-scale hydrogen storage systems.

Funds from Horizon Europe research, grant agreement No 101192503.

Molecular simulations of nanoporous carbon-based electrocatalyst for H₂ production

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E5_1, Z3 Room (Level -3), septembre 15, 2025, 17:00 - 19:00

This work focusses on the modeling of H₂ production assisted with porous carbons in a supercapacitor device configuration using a realistic model of electrodes texture. Using reactive meta-dynamics simulations in the constant voltage (N, V, T, Velec) ensemble, we reveal the synergic charge coupling between the electric double layer (EDL) at the external electrode surface or that of mesopores in contact with the electrolyte and sub-nanopores that are able to dock bare ions and induce a global electric charge redistribution toward topological and chemical defects such as surface species. In turn, this surface over-charging (induced by in-nanopores ion docking) that is the consequence of the electrode voltage polarization) leads to an ionic strength increase of the surface electric double layer (EDL) that is nanometric in thickness. Surface EDL then becomes the location of global strong electrostatic field that is able to induce chemical reactions such as electrolysis and cathodic H₂ production and can be seen as nanoreactor. Hence, this “reinforced” EDL leads to a boosted the hydrogen evolution reaction (HER) efficiency, in line with experimental results. This study reveals the crucial catalytic impact of ion docking, elucidating the fundamental mechanisms governing carbon-based electrocatalysis that is due to a collective, global, reinforced surface-polarization EDL effect initiated from carbon nanopores.

Fraunhofer High Performance Center Green Materials for Hydrogen – GreenMat4H2

Prof. Emanuel Ionescu, Dr. Sven Grieger¹, Prof. Dr. Saskia Biehl²

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E5_1, Z3 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

The Fraunhofer High-Performance Centers organise the close cooperation between university and non-university research and industry. Universities, universities of applied sciences, Fraunhofer Institutes and other non-university research institutions work together with companies and civil society players at a single location on specific topics in order to quickly put innovations into practice. High-performance centres stand for infrastructure, training concepts and expertise that can be used across organisations. They bring together suitable partners and support ideas as innovation pilots all the way to the market.

The GreenMat4H2 High-Performance Center was founded at the beginning of 2021 and is jointly managed by the Fraunhofer IWKS in Hanau and the Fraunhofer LBF in Darmstadt. The aim is to provide scientific and technological support for the development of a sustainable and reliable hydrogen economy in the federal state Hesse/Germany in order to make an important contribution to climate protection and ultimately strengthen Hesse as a high-tech federal state. Our aim is to consolidate a central contact point for the hydrogen economy in the Rhine-Main region and beyond. It promotes the application-orientated research and development of 'green' materials and technologies for the safe, sustainable and reliable production, storage, transport and use of hydrogen as well as for the conversion of existing structures to hydrogen applications. GreenMat4H2 focuses on the core competencies of the participating institutes Fraunhofer LBF and IWKS in the hydrogen sector.

This results in a coordinated, complementary portfolio of services in the four core areas of material development, reliability, sustainability and recyclability, particularly:

- Damage identification, damage development (degradation) on materials/components (e.g. cells)/systems (e.g. H₂-tank) under mechanical and electrochemical stress
- Characterisation of the operational stability and system reliability of components and systems (e.g. fuel cell) exposed to hydrogen under realistic conditions
- Recoverability/recycling of functional materials from fuel cell systems or electrolyzers: catalyst (platinum, iridium, ...) and membrane materials (PFAS) or bipolar plates from stacks, C-fibres from hydrogen pressure tanks
- Potential applications of secondary materials in components

In this presentation, the set-up and development of the GreenMat4H2 Center as a role model to establish a strong network of the relevant players in the regional hydrogen landscape, identifying the need for application-oriented research and expertise, developing specific transfer measures and initiating targeted research collaborations with partners from industry and science is shared. Furthermore, approaches for international cooperation in applied research are proposed to create synergies.

Effect of Different Dynamic Operating Conditions on the Materials of a PEM Electrolyzer

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E5_2, Z3 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Decarbonizing the energy matrix is a global goal driving the development of clean and sustainable energy solutions. In this context, hydrogen has emerged as a key energy carrier to support this transition. Among the available methods for hydrogen production, water electrolysis stands out as the most environmentally friendly, capable of producing hydrogen with a purity of up to 99.99%. Proton exchange membrane (PEM) electrolyzers are particularly notable due to their compact design, high current density (above 2 A/cm²), and low ohmic losses, achieving efficiencies between 50% and 80%. Their rapid response, operation at high pressures, and low temperatures further enhance their appeal as a promising technology.

However, PEM systems face challenges related to stability and durability under various operating conditions. The scientific community debates the optimal strategies for operation: some advocate for continuous operation to avoid performance fluctuations, while others recommend complete disconnection during intermittent periods. A third approach suggests operating at minimal currents, ranging from 10% to 25% of the nominal capacity, during these idle periods.

This study investigates the impact of different operating conditions on PEM cells: continuous operation, on/off cycles, and intermittent cycles with minimal current. Simulations were performed to represent one year of operation (365 cycles), and the cells were evaluated using polarization curves and Electrochemical Impedance Spectroscopy (EIS). Subsequently, the cells were disassembled to examine the degradation of their components at the microstructural level, employing techniques such as Scanning Electron Microscopy (SEM) and X-Ray Diffraction (XRD).

The results reveal that current interruption during idle periods mitigates degradation mechanisms, potentially extending the lifespan of PEM electrolyzers. The main contribution of this work lies in its comprehensive approach, integrating electrical, chemical, and microstructural analyses to provide a holistic understanding of the internal phenomena in PEM electrolyzers. Furthermore, this study highlights the importance of interdisciplinary collaboration between experts in electrical engineering and materials science, underscoring the value of joint efforts to improve the performance and sustainability of these technologies.

BiOCl microsphere-based photoanodes and the effect on DSSC performance

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E5_3, Z3 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

DSSCs stand out thanks to their ease and low cost of manufacture and ability to operate in low light conditions. These cells, generally manufactured with TiO₂, have limited efficiency, mainly due to the recombination processes that occur within the cell's photoanode. Among the strategies to reduce these processes is the doping of the semiconductor and the study of new materials; however, to date, these challenges have not been overcome.

Among the various semiconductors that could be used in DSSCs is BiOCl. This material presents a wide indirect band gap (close to 3.5 eV), low recombination rate, high electronic mobility, and non-toxicity, in addition to its ability to adsorb molecules of various dyes used in this device.

Despite its properties, few works are reporting the use of BiOCl in DSSC, so it is necessary to establish conditions for obtaining the semiconductor films to optimize the dye adsorption and its impact on the reduction of recombination processes and the overall efficiency of these devices. In this work, BiOCl powders were synthesized by coprecipitation, and films with hierarchical morphologies were obtained for the first time by screen printing. In addition, the impact on dye adsorption and efficiency of the cells fabricated with these BiOCl microsphere-based photoanodes was studied.

Metal-oxide ALD-coated electrospun nanofibers for fluorine-free and freestanding bipolar membranes

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E5_2, Z3 Room (Level -3), septembre 16, 2025, 10:30 - 13:10

As the demand for green hydrogen production grows, processes such as water electrolysis are among the most promising technologies. However, several limitations remain unresolved yet, Proton Exchange Membrane Water Electrolysis (PEMWE) relies on noble metal (IrO₂ for OER in acidic conditions) and Anion Exchange Membrane Water Electrolysis (AEMWE) can use earth-abundant metals for the OER in alkaline conditions, but HER is limited by the lack of available protons at the cathode. In this context, simultaneously achieving a high-pH OER and a low-pH HER is desirable and this is precisely one of the opportunities offered by bipolar membranes (BPM). When operated in reverse bias, BPMs can maintain a pH gradient across the electrochemical cell by dissociating water into protons and hydroxide ions. This allows for optimized reaction conditions at both anode and cathode, reducing catalyst costs. A BPM consists of two ion exchange layers of opposite polarity, separated by a catalytic layer. Water dissociation (WD) occurs at the interface of those two ion exchange layers known as bipolar junction. Water dissociation efficiency directly impacts energy consumption and overall cell performance. Additionally, while some catalysts have shown the ability to dissociate water effectively, the current deposition processes often produce a thick catalytic layer that can lead to delamination, catalyst leakage, further affecting long-term stability and performance. Therefore, our objective is to implement an efficient catalytic layer for WD, as thin as possible, in order to minimize catalyst usage while maintaining a strong bond to the polymer. A combination of Atomic layer deposition (ALD) and Electrospinning (ES) methods appears well suited to achieve this goal. ALD is a low temperature process that allows a precise control of thickness, conformity and uniformity of deposited layer, providing a chemically strong bonded layer even on polymer surfaces. ES is a cost effective method for producing high-surface-area, tunable, fluorine-free polymer nanofibers. By using quaternized poly(2,6-dimethyl-1,4-phenylene oxide) (Q-PPO) and sulfonated polyether ether ketone (S-PEEK), two ion exchange polymers of opposite polarity, TiO₂ ALD-coated nanofibers were produced and further processed to obtain a fully dense bipolar membrane. Bipolar membranes are tested in a two compartment H-cell, with a four probe electrode set-up and WD is studied through Current-Voltage (j-V) measurements. The nature, thickness and distribution of the catalyst will be studied to obtain optimal WD performances in the BPM as well as to ensure long-term stability and strong catalyst bonding in a BPMWE cell.

Modeling of the hydrophobic treatment of Gas Diffusion Layers to predict PTFE distribution after the drying step

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E5_1, Z3 Room (Level -3), septembre 15, 2025, 17:00 - 19:00

Proton Exchange Membrane Fuel Cell (PEMFC) is currently considered as a pollutant-free alternative to thermal engines, especially for Heavy Duty applications. The Gas Diffusion Layer (GDL) is a major component ensuring heat, mass (gas and liquid), and electrical transports thanks to its carbon porous structure [1]. GDL plays a crucial role on the performance of PEMFC and especially on the water management by ensuring a trade-off between drying (too low water vapor content) and flooding (too high liquid saturation).

To reduce the flooding risk during PEMFC operation, a hydrophobic treatment is applied to the GDL. The pristine carbon material is dipped into a hydrophobic ink (colloidal dispersion of PTFE) then dried and sintered. Experience shows that the resulting PTFE distribution is not uniform, depends on the drying conditions [2], and impacts the PEMFC performance. Interestingly, an ‘optimized’ PTFE distribution is still an open question and progress on this matter will help improving GDL.

In the spirit of GDL improvement, the most advanced models consider 3D volumes representing the GDL microstructure, which are obtained from X-ray microtomography or randomly generated. However, PTFE is rarely taken into account correctly, as it is not visible in X-ray tomography, or it is numerically added by morphological opening [3] for which the ‘deposition criteria’ are questionable.

Our research aims at modeling the main manufacturing steps of the hydrophobic treatment to predict more accurately the PTFE 3D distribution and the resulting (single and two-phase) GDL transport properties, which are key for the GDL performance. Based on characterizations of the hydrophobic ink and on SEM observations to locate the PTFE, a model of drying of the GDL is discussed and developed to simulate the final PTFE distribution in the microstructure. Numerical results are compared to experimental ones and the impact of PTFE treatment process is discussed on GDL transport properties. This research is part of the project “DECODE” which has received funding from the European Union’s Horizon Europe research and innovation program under grant agreement N° 101135537. More information on the project can be found at www.decode-energy.eu.

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Polymer-derived micro/macroporous Si-C-O-N-based ceramics with integrated catalytically active metal sites to stimulate superior oxygen and hydrogen evolution reaction activities

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E5_2, Z3 Room (Level -3), septembre 16, 2025, 10:30 - 13:10

Hydrogen (H₂) is considered as a promising energy carrier to assure the needs of humanity. Its combustion in a fuel cell (FC) emits only water and does not involve any noise pollution. However, in order to be used inside a FC, H₂ needs to be at a very high level of purity, which can be achieved by using the water electrolysis process. This clean reaction only represents 4% of the actual method of H₂ production around the world. The recent development of anion exchange membrane materials has led to the emergence of the anion exchange membrane electrolyzers allowing the use of non-noble transition metals in the composition of catalysts for hydrogen (HER) and oxygen (OER) evolution reactions in alkaline media. However, their nanoscale synthesis is highly challenging to limit the overpotential, particularly at the anode (OER).

The PDC (Polymer Derived Ceramics) route is a non-conventional way of designing ceramics by using preceramic polymers as precursors. The coordination (or direct reaction) of these precursors with metal complexes via the functional groups and/or ligands of the polymer makes it possible to trap transition metal nanoparticles in a micro-/mesoporous PDC matrix upon pyrolysis at low temperature. By considering the fact that preceramic polymers display an intrinsic ability to in-situ form and maintain a porosity at different length scales at low temperature pyrolysis, these metal nanoparticles become accessible while overcoming their stability issue during the catalysis process. Besides, the activity and selectivity can be simultaneously enhanced by taking advantage of the synergy between the metal nanoparticles and the encapsulating materials. This will be the content of this presentation that will introduce our very recent works on this topic.

Modified cryptomelane catalysts for OER

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E5_3, Z3 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

Environmental pollution and climate change have intensified the urgency of developing "green" alternatives to reduce the global carbon footprint. One of the most actively explored research areas is the production of green hydrogen via water electrolysis powered by renewable energy sources such as wind, solar, and hydroelectric power.

A major bottleneck in this process is the oxygen evolution reaction (OER), which has driven significant interest in the development of efficient catalysts for this half-reaction. Currently, commercial OER catalysts are primarily based on noble metals such as Pt, Ru, and Ir, which, despite their high catalytic efficiency, are associated with high costs due to their scarcity. Consequently, extensive research efforts are focused on developing cost-effective catalysts with catalytic activity comparable to noble metal-based systems. Among the most widely studied alternatives are transition metal-based catalysts, particularly those containing Mn, Co, Ni, and Cu, as these elements are more abundant in nature and therefore more economically viable.

In this study, we report preliminary results on the synthesis, characterization, and catalytic evaluation of Mn-containing catalysts. Specifically, we investigated the catalytic behavior of pure cryptomelane and cryptomelane doped with different concentrations of Co, Ni, and Cu, all calcinated at 500 °C.

The catalytic activity in the OER was assessed using electrochemical techniques. Thus, the catalytic activity has been determined through the measurement of the overpotential (η), measured at a current density of 10 mA·cm⁻², where lower η values indicate higher catalytic activity. The results show that pure cryptomelane exhibits an overpotential of 490 mV at 10 mA·cm⁻², while Ni- and Cu-doped cryptomelane catalysts display higher overpotentials. In contrast, cryptomelane catalysts doped with 5% Co, 10% Co, and 25% Co exhibit overpotentials of 430, 420, and 440 mV, respectively. These findings suggest that Co doping enhances the OER catalytic activity of cryptomelane, with the 10% Co-doped catalyst showing the best performance.

The role of precipitates in hydrogen embrittlement of precipitation hardened Al_{0.35}CoCrFeNi complex concentrated alloy

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The hydrogen embrittlement (HE) behavior of the precipitation-hardened Al_{0.35}CoCrFeNi complex concentrated alloy (CCA) was investigated as a function of microstructure. The cast alloy was thermomechanically processed and solution annealed at 1330°C to achieve a uniform distribution of equiaxed grains with single-phase FCC crystal structure. Consecutive precipitation annealing at 700°C (PA700) and 900°C (PA900) lead to the different phase compositions: FCC + B2 + L₁₂ (PA700) and FCC + B2 (PA900), with occasional formation of Cr-rich particles on the grain boundaries and inside of coarse B2 particles. Tensile tests were performed before and after electrochemical hydrogen charging at 70°C for 72 hours to evaluate the impact of hydrogen on mechanical properties. The PA700 samples exhibited the highest strength after hydrogenation (775 MPa) but suffered from severe hydrogen embrittlement, with ductility dropping from 25% to 8.3%, while the PA900 samples maintained moderate strength (684 to 659 MPa) and ductility (34% to 30.2%) after applied hydrogen charging. The single-phase FCC structure exhibited the best product of strength and elongation and maintained it also after hydrogenation. Fractographic analysis revealed that HE was associated with hydrogen-assisted crack initiation at the surface and on the grain boundaries with the prevalent cracking on the interfaces between B2 and Cr-rich particles in precipitation hardened alloy. The findings highlight the critical role of microstructural features in hydrogen-induced degradation of CCAs and provide insight into designing HE-resistant alloy systems.

A joint experimental and computational investigation of $\text{Sr}_{n+1}(\text{Fe}, \text{Ta})_n\text{O}_{3n+1}$ ($1 < n < \infty$) catalysts for the Oxygen Evolution Reaction

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The design of materials capable of catalyzing the water dissociation reaction is critical for green hydrogen production. Research efforts in electrode materials for alkaline electrolyzers (AEL) focus on (i) enhancing durability, as both the anode and cathode of electrocatalysts degrade over time, and (ii) improving electrocatalytic activity, particularly to accelerate the kinetics of the oxygen evolution reaction (OER). Transition metal oxides (MnO_2 , NiO , CuO , ZnCo_2O_4 , NiCo_2O_4 ...etc), known for their stability in alkaline media, are used as anodes for the OER process in AELs [1]. Oxides related to the perovskite ABO_3 structure (A = lanthanide, alkaline-earth; B = transition metal) are promising materials, and due to their high catalytic activity, cobalt-based perovskites have been extensively studied. However, one of the challenges in the energy transition is the scarcity of so-called critical materials, which drives the development of new OER electrocatalysts based on perovskite-derived structures, where Co is replaced by Fe/Mn. In recent years, Ruddlesden-Popper (RP) phases have emerged as potential alternatives to conventional perovskite electrocatalysts [2]. This work presents a combination of experiments and Density Functional Theory (DFT) calculations to investigate the $\text{RP-Sr}_{n+1}(\text{Fe}, \text{Ta})_n\text{O}_{3n+1}$ with $1 < n < \infty$. The materials are synthesized via solid-state reaction (ceramic method), and their structural characterization is performed using XRPD and HRTEM techniques. The catalytic activity of the materials for the OER process is confirmed through electrochemical measurements using a 1M KOH solution as the electrolyte. DFT calculations provide insights into the effects of composition (Fe substitution for Ta) and structure (n value) on catalytic performance.

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[2] X. Xu, Yi Pan, Y. Zhong, R. Ranc and Z. Shao *Materials Horizons*, 7, (2020) 2519-2565.

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Optimisation and scale-up of solid oxide fuel cells employing aqueous-based tape casting of anodes and spray pyrolysed active layers

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E5_3, Z3 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

In the current climate crisis, in which renewable energy must provide a larger share of the energy mix, green hydrogen is a promising solution for storing chemical energy for conversion to electricity, thus promoting the transition to a sustainable energy system. Solid oxide fuel cells (SOFCs), which work in the range 500-1000 °C, achieve this conversion efficiently, generating heat and power simultaneously, closing the energy cycle and promoting the circular economy. Even though performance at intermediate temperature (500-700 °C) is advantageous for long-term SOFC use and lower price, this reduces their efficiency considerably, mainly due to the higher polarisation resistance of the air electrode. In this sense, we have recently demonstrated that the addition of thin active layers of mixed-conducting materials between the electrolyte and the air electrode significantly improves the electrochemical performance at intermediate temperatures. This concept is based on the extension of the electrochemically active area through the adjustment of the ionic-electronic transport properties of the intermediate layers.

The present work demonstrates the scale-up of anode-supported SOFCs based on Ni-Ce_{0.9}Gd_{0.1}O_{2-δ} (CGO) and Ni-Zr_{0.84}Y_{0.16}O_{2-δ} (YSZ) cermets prepared by tape casting, with subsequent deposition of YSZ and CGO electrolytes, intermediate active layers and strontium ferrite-based cathodes by spray pyrolysis and screen printing. The preparation of water-based Ni-CGO and Ni-YSZ tapes and their thermal treatment have been optimised to achieve sintered anodic supports with suitable porosity and mechanical resistance. The thin electrolyte layers were deposited on the porous supports with the appropriate thermal treatment to obtain dense electrolytes with good adhesion to the anode. Scale-up of single cells of practical application with dimensions 5 cm x 5 cm involved the control of sintering to produce homogeneous, crack-free and delamination-free assemblies. The full single cells were analysed for electrochemical performance in a suitable test system for i-V characteristics and stability assessment.

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Alkali Metal-Promoted Ru/Al₂O₃ for Optimized NH₃ Decomposition and Electron Density Control

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Ammonia is considered a potential hydrogen carrier due to its higher volumetric hydrogen density than liquid hydrogen and its ability to be stored in a liquid state under stable conditions [1]. Hydrogen production through ammonia decomposition has gained significant research interest in recent years [2]. Since ammonia decomposition is an endothermic reaction, high temperatures are required to maintain efficiency. Recent studies have focused on the development of low-temperature catalysts, with Ruthenium (Ru)-based catalysts being reported as the most effective for ammonia decomposition [3].

Various support materials have been evaluated for catalytic activity, with Alumina being widely used in catalysis due to its high specific surface area and tunable physicochemical properties [3]. However, compared to MgO and rare-earth oxides, Al₂O₃ has been reported as a less effective support due to its lower Ru nanoparticle dispersion, which negatively affects catalytic performance in ammonia decomposition [4]. Recent studies have demonstrated that the incorporation of alkali metals into catalysts can induce surface basicity, significantly enhancing catalytic performance in ammonia decomposition [5].

In this study, Al₂O₃ was modified with various alkali metals to create highly basic surface sites. The Ru/Me-Al₂O₃ catalysts (Me = K, Na, Ca, Mg) exhibited enhanced activity in ammonia decomposition compared to Ru/Al₂O₃. A series of characterization analyses were conducted to investigate the correlation between the presence of highly basic surface sites and the catalytic performance of Ru/Me-Al₂O₃ catalysts. The NH₃ decomposition reaction over Ru-based catalysts is structure-sensitive, with catalytic performance highly dependent on the size of Ru NPs on the support. The formation of optimally sized Ru NPs on the surface of Me-Al₂O₃ in Ru/Me-Al₂O₃ catalysts was found to be beneficial for NH₃ decomposition. Catalytic activities were assessed at a weight hourly space velocity of 60,000 ml·gcat⁻¹·h⁻¹, and the temperature-dependent NH₃ conversion results are presented in Figure 1.

The addition of alkali metals (K, Na) significantly enhanced catalytic activity compared to unmodified Ru/Al₂O₃, whereas the incorporation of alkaline earth metals (Mg, Ca) led to a decrease in activity. These variations were attributed to differences in the super-basic properties induced by the respective metal additives, as confirmed by X-ray diffraction, Brunauer-Emmett-Teller surface area analysis, and CO₂ temperature-programmed desorption studies. The findings indicate that modifying Al₂O₃ with alkali metals can significantly improve its suitability as a support material for ammonia decomposition catalysts. Al₂O₃-based catalysts can be applied to various industrial processes, and their utilization is expected to enhance the diversity of ammonia decomposition catalysts.

Atomistic Modelling of Hydrogen Storage in Graphene Using LAMMPS Molecular Dynamics

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Hydrogen storage is a critical component for advancing clean energy technologies, and graphene has emerged as a promising material for this purpose due to its unique structural properties. In this study, we explore the hydrogen storage capabilities of graphene through atomistic modelling using the LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) molecular dynamics software. Our methodology involves simulating the adsorption process under various conditions to optimize hydrogen uptake. Specifically, we examine the effects of graphene defects, interlayer spacing, and external pressure to identify optimal parameters. The simulations demonstrate that graphene can achieve a hydrogen storage capacity of 2.8 wt% at room temperature and 10 bar. These findings highlight the potential of graphene for efficient hydrogen storage applications and provide insights for future experimental and theoretical studies in the field.

Advanced Transition Metal Vanadate Catalysts for Efficient Aqueous Electrochemical NRR

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E5_4, Z3 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

The Haber-Bosch process is a widely recognized methodology for the industrial production of ammonia, accounting for approximately 2% of global annual energy consumption and serving as a significant source of greenhouse gas emissions. To address these environmental concerns, electrochemical nitrogen reduction reaction (e-NRR) offers a promising alternative, utilizing nitrogen gas and aqueous electrolytes under ambient conditions for ammonia synthesis. Motivated by this, we investigate first-row transition metal-based vanadium oxide electrocatalysts for ammonia production. Zinc vanadate, synthesized via the sol-gel pyrochlore method, demonstrates vanadium as a highly active catalytic site, corroborated by density functional theory (DFT) calculations. Further efforts to incorporate lithium into the zinc vanadate framework aim to promote the formation of Li_xNy intermediates during the e-NRR process. This modification results in a composite of lithium vanadate and lithium zinc vanadate, which exhibits enhanced ammonia production activity compared to the individual phases. Our experiments explore the impact of transition metal incorporation into the vanadate matrix on ammonia synthesis in a basic aqueous electrolyte. The ammonia yield is quantified using the indophenol blue method and nuclear magnetic resonance (NMR) spectroscopy. This study highlights the potential of sol-gel-synthesized bimetallic oxide electrocatalysts for facilitating complex electrochemical reaction mechanisms and advancing sustainable ammonia production technologies.

Selective Dinitrogen Electroreduction to Ammonia on Zn₂V₂O₇ Pyrochlore

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Electrochemical ammonia synthesis offers a sustainable alternative to traditional nitrogen fixation, providing high energy density, low storage costs, and greenhouse gas-free combustion. However, the process faces significant challenges due to the slow kinetics of N₂ activation, highlighting the development of highly efficient electrocatalysts. This study investigates the sol-gel synthesis of bimetallic oxides, focusing on zinc pyrovanadate (Zn₂V₂O₇) for its potential in nitrogen reduction reaction (NRR). The pyrochlore framework of Zn₂V₂O₇ provides structural integrity through zinc, while vanadium serves as the active site, facilitating the reduction of molecular nitrogen (N₂), a thermodynamically stable molecule. Density functional theory (DFT) simulations indicate that Zn₂V₂O₇ facilitates the nitrogen reduction reaction (NRR) through a surface hydrogenation mechanism centered on vanadium active sites. The reaction intermediates were identified and characterized using in-situ attenuated total reflectance surface-enhanced infrared absorption spectroscopy (ATR-SEIRAS). The catalyst achieved selective ammonia production with a faradaic efficiency of 76.5 % and a yield of 101 µg h⁻¹ mgcat⁻¹ in 0.1 M Na₂SO₄ electrolyte, demonstrating its potential for practical applications in sustainable NRR processes.

Catalysts of Change: Advanced Ceramic Materials Steering Energy Transition

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E5_2, Z3 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Advanced materials are driving innovation across all fields of technology, ranging from construction and mechanical engineering, automotive and electromobility, to medical technology, energy storage and conversion technologies, and microelectronics. Given their technological impact, functional materials represent an essential segment of industrial technologies with significant value creation potential for both established markets and emerging technologies. Especially in the context of sustainable production techniques, substitution of critical raw materials, and energy- and resource-efficient manufacturing, tailored surfaces and interfaces are gaining increasing importance in the future. In this context, chemical processing of nanostructured ceramics in tuning the functional and interfacial properties for better charge transport, higher corrosion protection and enhanced performance. The examples will include the role of functionalized inorganic surfaces in electrolyzers for hydrogen production, and advances in photon-harvesting technologies for perovskite-based photovoltaics. This talk will emphasize the power of chemical synthesis in designing new materials for energy transition.

Optimising NiCoMn Electrocatalysts for Efficient Hydrogen Production

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Hydrogen evolution reaction (HER) is crucial for renewable energy, requiring the development of cost-effective electrocatalysts. Noble metals like Pt, Ru, and Pd are highly efficient HER electrocatalysts due to their exceptional catalytic activity.

Nevertheless, high costs and limited availability make them impractical choices, making it important to find more affordable and readily available alternatives.

This study proposes to utilise nickel (Ni), cobalt (Co), and manganese (Mn) synthesised and/or recovered from battery cathodes as electrocatalysts for the hydrogen evolution reaction (HER).

Ternary transition metals compounds (NiCoMn) obtained by hydrometallurgical processes for the treatment of waste lithium-ion batteries (based on Li, Ni, Co, and Mg oxide cathodes) were tested as electrocatalysts for HER in alkaline media and its performance compared with hydrothermal synthesised NiCoMn materials. NiCoMn materials supported in carbon black were also prepared by hydrothermal synthesis to promote synergy between the ternary transition metal compounds and the highly conductive carbon material.

While these metals individually exhibit catalytic activity, the use of NiCoMn complexes, particularly those derived from battery cathode leaching solutions, remains largely unexplored. The electrocatalytic performance of the NiCoMn materials reduced under H₂ flow at 200 °C shows the best electrocatalytic performance, with an overpotential of -0.5 V and excellent electrochemical durability for 100h. The enhanced catalytic stability of NiCoMn mixtures compared to the individual metal compounds is presumably related to the synergistic effect between the Ni, Co, and Mn and the increased number of active sites. Additionally, although carbon black decreases the catalyst overpotential, its general stability remains unchanged.

To the best of our knowledge, the use of NiCoMn compounds, mainly those derived from battery recycling, as HER electrocatalysts has not been previously reported. This approach offers a sustainable solution by minimising environmental impact, conserving resources, and fostering a circular economy.

Exploring a smart catalysts platform for the electroreduction of nitrogen species into ammonia: materials/performance correlation

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E5_3, Z3 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

The increasing demand for ammonia (NH₃) as a fertilizer precursor and alternative fuel has raised concerns about the sustainability of the primary production process, which relies on the well-established Haber-Bosch (HB) method. The HB process heavily depends on hydrogen (H₂) produced through methane (CH₄) steam reforming and uses reactors operating at high temperatures and pressures to facilitate nitrogen (N₂) triple-bond cleavage. Additionally, significant environmental impacts are associated with the transportation of the final product from centralized plants to end users. In recent years, various alternative approaches have been evaluated to reduce NH₃ production dependence on fossil fuels. The electrochemical nitrogen reduction reaction (E-NRR) in water-based electrolytes could potentially be carried out under milder temperature and pressure conditions. Despite its theoretical promise, several challenges - such as low selectivity at high current densities due to the unavoidable hydrogen evolution reaction (HER) - hinder its scalability. An alternative approach involves the electrochemical conversion of nitrate (NO₃⁻) and/or nitrite (NO₂⁻) present in polluted waters (e.g., groundwater, industrial, and nuclear wastewater) into NH₃. This reaction is thermodynamically favoured compared to E-NRR, and the NO₃⁻/NO₂⁻ hydrogenation reaction has a lower energy barrier than N₂ activation.

In this context, our research focuses on identifying electrocatalysts that are active for NO₃⁻ reduction in low-concentration aqueous streams, with the dual goal of denitrifying wastewater and producing a value-added product (NH₃). Specifically, we evaluate the activity of catalysts such as molybdenum disulfide (MoS₂), copper (Cu), and tin (Sn) in a flow cell reactor with a 10 cm² geometrical active area. Various parameters, including potential, catalyst loading, ions in solution, type of support for catalyst immobilization, and liquid flow rate, are varied to optimize the system performance with different materials. The process performance is assessed through Faradaic efficiency (FE) and NH₃ production over time. The ultimate goal of this investigation is to identify a catalyst and operational parameters that ensure high FE and production rates, even at high current densities, where the HER may dominate the process.

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Parametric investigation of the operation of an SO₂ depolarised electrolyser for hydrogen production

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E5_4, Z3 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Hydrogen is gaining momentum as a promising green energy carrier and different production routes are being intensely investigated. The hybrid sulphur cycle (HyS), or Westinghouse process, was developed as an alternative for the production of sustainable hydrogen. It consists of two main steps: a thermochemical (sulphuric acid decomposition to sulphur dioxide, water and oxygen in high temperatures, ~850-950°C) and an electrochemical (sulphur dioxide depolarized electrolysis - SDE). This electrochemical process, includes the oxidation of SO₂ to H₂SO₄ in the anode and the hydrogen evolution reaction in the cathode. The theoretical potential of the overall electrochemical reaction is 0.158 V, significantly lower than the one needed for direct electrolysis (1.23 V). This difference makes this hybrid approach an attractive alternative to conventional water electrolysis, as the same amount of hydrogen can be produced with lower electricity consumption, consequently lowering the operational costs. So far, research on SDE investigated the use of different catalyst materials and operating conditions, with most common catalysts being, platinum, palladium and gold-based. This work aims to experimentally investigate the performance of SDE in the lab-scale under different operational conditions, using commercial components designed for PEM electrolysers, in order to produce valuable insights and describe dependencies, useful for the process scale-up and the establishment of a baseline. This baseline will serve as a reference for comparison to the performance of SDE with custom modified components in future tests. The experiments utilize graphite monopolar plates and catalyst coated membranes, featuring a platinum loaded catalytic layer with a loading of 0.6 mg Pt/cm² at the anode side and 0.3 mg/cm² at the cathode, dispersed in carbon black. The pressure chosen for the long-term operation tests is close to ambient. The applied potential, operating temperature, concentrations and flowrates of the electrolytes are parameters of investigation. Results are extracted in a single cell setups of 5 cm², 10cm² and 25 cm² active surface area up to a stack with 100 cm² active surface area respectively. SO₂ consumption and H₂ production are evaluated in correlation with the electricity consumed, with specific energy consumption being used as a metric, while SO₂ cross-over from anolyte to catholyte and the parasitic actions in which it results, namely its reduction to H₂S and elemental sulphur is also assessed.

Strategic Needs, Market Opportunities and Technical Advancements in Large-Scale Manufacturing for Wind Turbine Components and Hydrogen Storage.

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E5_1, Z3 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

The global transition toward renewable energy has significantly increased the demand for large-scale manufacturing innovations in wind turbine components and hydrogen storage systems. Projections indicate that the global hydrogen market could reach approximately €1.3 trillion by 2050, while the global wind energy market is expected to attain €130 billion by 2030. Developing cost-effective, scalable, and high-performance manufacturing solutions has thus become a strategic imperative. This work explores how large-scale manufacturing capabilities, bolstered by academia-industry collaboration, can address the technical and economic challenges.

The National Manufacturing Institute Scotland (NMIS) has been instrumental in advancing next-generation manufacturing technologies for wind and hydrogen infrastructure. Through collaborative research and development, as well as technology transfer, NMIS has partnered with industry leaders to integrate digital manufacturing, AI-driven process optimization, and automated quality assurance into production workflows. These collaborations have resulted in enhanced efficiency, cost reductions, and improved material sustainability. Notably, NMIS has contributed to projects such as EnergyWorks, a €10.5 million energy incubator supporting advancements in offshore wind, hydrogen, and battery storage.

In the wind energy sector, large-scale manufacturing improvements are essential to achieving the global wind capacity target of 2,157 gigawatts by 2030.

Innovations in lightweight composite materials, turbine blade recyclability, and advanced forming techniques for substantial structural components are pivotal in enhancing efficiency and sustainability. Similarly, in hydrogen storage, advancements in high-pressure tank production, large-scale flow forming, and novel welding techniques are crucial for reducing storage costs, thereby making hydrogen a more viable alternative to fossil fuels.

The economic landscape is evolving, with over €1.1 trillion invested globally in renewable energy in 2023 alone, driven by favorable policy frameworks and industrial decarbonization incentives. This study also assesses the economic feasibility of manufacturing innovations, examining how cost-reduction strategies, supply chain readiness, and automation can enhance the competitiveness of wind and hydrogen technologies.

NMIS has established robust collaborations with industry leaders, including ScottishPower Renewables, BOC, and the European Marine Energy Centre (EMEC), fostering the development of Scotland's hydrogen economy. Additionally, NMIS's partnership with Ecomar Propulsion supports the transition to zero-emission shipbuilding, thereby extending the impact of large-scale manufacturing innovations.

This research demonstrates how strategic partnerships and cutting-edge manufacturing techniques can drive the scalable adoption of wind and hydrogen technologies, ensuring that the UK and Europe remain at the forefront of the renewable energy transition.

Fe/Mo bimetallic phases supported on TiO₂ for N₂ reduction into NH₃ by photo-processes

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E5_3, Z3 Room (Level -3), septembre 16, 2025, 14:30 - 16:30

As climate change and global warming are among the biggest challenges in the coming years, the main objective is to develop and use renewable energy sources like wind, solar and sea water to mitigate their impact. In our modern society, ammonia is considered as an unavoidable commodity chemicals, as well as an ideal H₂ storage and transportable material due to its green and high energy release capacity. This work consists in the use of solar power to catalytically produce NH₃ with low carbon emission, as the widespread conventional Haber-Bosch process requires so far high temperature and pressure conditions (typically 400°C and 100-200 atm), which is responsible of 300 million tons of CO₂ emission annually. Thereby the low-temperature photocatalytic N₂ fixation/reduction has become a hot topic in the recent years by allowing a green and environmentally-friendly way of production for ammonia using N₂ as cheap abundant reactants and photons as immaterial reactant under far milder and more sustainable conditions than the Haber-Bosch process.

In nature, the nitrogenase enzyme can convert N₂ to NH₃ at ambient conditions. The nitrogenase contains two key proteins, an Fe-based protein and a MoFe-based protein, working in tandem to convert N₂ to NH₃. The Fe-based protein hydrolyses the adenosine triphosphate (ATP) to adenosine diphosphate (ADP), hereby generating electrons that are subsequently transferred to the MoFe-based protein where N₂ is reduced to NH₃. As a consequence, our work is inspired from the natural enzymatic process based on the nitrogenase with MoFe active cluster sites for the development of novel photocatalytic systems for N₂ fixation/reduction to synthesis NH₃ under mild conditions.

This study deals with the assessment of both gas-phase photocatalytic and photo-thermal N₂ reduction using either H₂O or H₂ as H provider. Two different complementary methods were used to monitor the NH₃ production, respectively (1) a classical approach using indirect colorimetric tests (indophenol method) after accumulation in liquid phase and (2) a less common method based on direct measurement of gas-phase NH₃ production.

The present presentation will be focused on the elaboration, characterization and photocatalytic evaluation of Fe/Mo bi-metallic TiO₂-supported systems for both photocatalytic and photo-thermal NH₃ production from N₂ reduction. Structure/activity correlation will be discussed tuning the total metal (Fe+Mo) content, the Fe-Mo proportion and the Mo and Fe surface oxidation states.

Effect of bimetallic Fe-Co catalysts deposited on neodymium oxide on the properties and activity in ammonia synthesis

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Ammonia is a promising compound for hydrogen storage. It can be easily transformed from the gas to the liquid phase, and its decomposition does not produce carbon oxides. These advantages increase the interest in ammonia production [1]. Synthesis of ammonia is an industrial process that requires high temperatures and pressures. These conditions result in using 1,5% of the world's energy [2]. That is why new catalytic systems are widely being searched for. According to literature, metals that have the highest potential in ammonia synthesis are iron, ruthenium and cobalt. However, the high price of Ru is an obstacle to more frequent use of this metal, while iron and cobalt are often used in research [3]. The volcanic curve, which represents the activity of these metals in ammonia synthesis, shows that iron strongly binds the nitrogen molecule, and cobalt weakly binds this molecule. The combination of two metals, one that binds nitrogen molecule strongly and one that weakly does this, leads to the catalytic system showing much higher activity in ammonia synthesis than using only one metal [4]. Therefore, there is a considerable potential for obtaining active bimetallic catalysts using Fe and Co. This work aimed to obtain iron-cobalt bimetallic catalysts deposited on neodymium oxide using different ratios of Fe and Co.

The method of preparation of the neodymium carrier was precipitation using $\text{Nd}(\text{NO}_3)_3 \cdot 6\text{H}_2\text{O}$ in distilled water and solution of KOH and K_2CO_3 as a precipitating compound. Iron-cobalt catalysts with a metal content of 10 wt% were prepared using the wet impregnation method using $\text{Fe}(\text{NO}_3)_3 \cdot 9\text{H}_2\text{O}$ and $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$. Eight catalytic systems with different molar ratios of Fe/Co were received (1, 0.95, 0.9, 0.8, 0.7, 0.5, 0.2, 0). The obtained catalysts were tested in ammonia synthesis at 470°C and 6.3 MPa. All materials were subjected to physicochemical characteristics using N_2 physisorption, XRD, TPR, TPD- H_2 , TPD- CO_2 , and STEM-EDX.

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Composite electrodes and membranes for energy storage and conversion devices

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E5_2, Z3 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Composite materials are at the forefront of the modern conception and optimization of high technology storage and conversion devices, including anion exchange membrane fuel cells.

Complex multimaterials and their interfaces are important to increase the performances of catalysts at the triple phase boundary and ion conducting membranes (optimization of water uptake, ion conductivity, mechanical and degradation stability).

We intend to present here our work on electrodes and polymer electrolyte membrane development.

For electrodes, the combination of N-[1] or B-N co-doped[2] carbon quantum dots (CQD) with various anion exchange ionomers (AEI) is explored: AEI are based on hydrophilic polysulfone (PSU), hydrophobic poly(alkylene biphenyl) and intermediate poly(2,6-dimethyl-1,4-phenylene oxide) (PPO), quaternized with trimethylammonium (TMA) moieties grafted on long (LC) or short (SC) side chains. The complementary properties of these materials for the oxygen reduction reaction (ORR) in alkaline solution are studied. The direct functionalization of metal organic frameworks (Zr-MOF and Fe-MOF) with PSU-TMA moieties is also investigated to increase the processability of the electrodes and the integration of the ionomer with the catalyst, avoiding interface and delamination problems.

For membranes, the integration of Layered Double Hydroxides (LDH) with Zn/Al (containing also an Ionic Liquid)[3] or Mg/Al [4] or exfoliated LDH[5] dispersed as a filler in composite anion exchange membrane (AEM) based on PSU or PPO grafted with TMA or DABCO is investigated to increase the conductivity, chemical and hydrolytic stability in alkaline conditions. The integration of electrospun nanofibers of poly phenyl sulfone in proton conducting membranes based on sulfonated poly(ether ether ketone) (SPEEK) or sulfonated poly (phenyl sulfone) (SPPSU)[6] is explored to reduce the dimensional swelling and thus improve the hydrolytic stability of membranes.

The adopted strategies give great advantages in term of stability, catalytic activity and ion conduction by combining and increasing the synergy between materials with tuned properties.

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Luminescent Solar Concentrators for Efficient and Sustainable Use of Solar Energy

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Solar energy is a renewable source with great potential, clean and sustainable, that reduces the carbon footprint by not generating polluting emissions. Although its use requires high initial investments, it is one of the most economical energies in the long term and the only one capable of generating heat, reducing the use of solid fuels. However, the technology currently available has several technical limitations.

Luminescent solar concentrator (LSC) technology is an innovative solution that can provide greater efficiency in capturing sunlight, even in diffuse lighting conditions, allowing better use of solar energy. Its versatile design facilitates integration into windows, facades and other architectural surfaces, promoting the development of self-sufficient buildings. It also reduces costs by minimizing the amount of photovoltaic material required and improves sustainability by taking advantage of a wider spectrum of radiation without generating polluting emissions.

An LSC is transparent device with luminescent particles that absorb and re-emit light at longer wavelengths, guiding it by internal reflection to the edges, where solar cells convert it into electricity, improving photovoltaic efficiency.

In this work, a new second LSC generation will be presented, with the ability to capture a wide range of the visible-UV spectrum, covering wavelengths between 350 nm and 750 nm, and to re-emit at a longer wavelength. This luminescent system is composed by an optimal combination of organic molecules embedded in a polymeric matrix.

The final LSC is obtained by deposition of the luminescent suspension onto glass, followed by solvent removal, which allows the formation of a homogeneous and efficient coating.

As a luminescent system, several molecules capable of absorbing in the UV/visible part of the spectrum and re-emitting at longer wavelengths were selected. The goal is to capture as much of the spectrum as possible with as few luminescent species as possible, so that each absorbs a specific fraction of the electromagnetic spectrum. Together, these species will allow various wavelengths of the solar spectrum to be captured, thus optimizing the use of incident solar radiation.

In addition, the selected species should enable Förster resonance energy transfer (FRET), a non-radiative transfer process that occurs when the emission spectrum of the donor overlaps sufficiently with the excitation spectrum of the acceptor. To maximize the efficiency of the system, it is essential to find the optimal conditions that favor this interaction between the luminescent species.

Compositional Complexity and Structural Disorder as Enablers for the Circular Economy

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E5_1, Z3 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Circular Economy (CE) represents a concept concerning the production and consumption of goods which basically should reduce the amount of waste to a minimum. There is an obvious contradiction between the need for a CE and the tremendously increasing amount and complexity of consumer goods, their planned obsolescence, and the massive amount of waste due to the take-make-waste peculiarity of their production/consumption.

CE has a powerful enemy, i.e. the second law of thermodynamics, which actually prevents that closing the production loops leads to full resource efficiency. Thus, minimizing residues and losses should be considered as

important as and in addition to closing the material loops. The consequence is the stringent need to minimize the entropy increase across the various added value chains.

However, we will show in the present talk that entropy increase may not always be seen as acting against CE. Firstly, we will discuss the concept of structural and compositional disorder. Secondly, we will elaborate on the compositional complexity in materials as an effective way to consider highly heterogeneous waste streams as valuable secondary raw materials. And thirdly, we will perform a prospective discussion on preparative concepts and strategies to develop materials with maximized performance and high tolerancy for admixtures & impurities.

Vacuum Insulation Panels for Liquid Hydrogen Storage and Transportation Applications

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Vacuum Insulated Panels (VIPs) have recently become a focal point of research in various projects worldwide, particularly in the context of cryogenic insulation systems. The primary objective of employing VIPs in such applications is to reduce dependence on conventional vacuum pumps and to enhance the reliability of insulation systems by incorporating smaller vacuum elements. These smaller elements minimize the impact on overall insulation performance in the event of localized vacuum failure.

In this study, the thermal and mechanical behavior of a VIP is evaluated over a wide temperature range—from ambient conditions down to cryogenic temperatures (20 K)—using the Finite Element software Abaqus. The materials selected for the VIP prototype were chosen based on their proven performance across this temperature spectrum, as reported in recent literature. Specifically, AISI 316L stainless steel was employed for the outer envelope (foil), while K1 hollow glass bubbles were selected as the core material.

The simulations addresses the thermal performance of an assembly comprising three VIPs arranged in various configurations. Boundary conditions were applied to simulate a temperature gradient from 20 K to 300 K, representative of cryogenic operating environments. A heat flux corresponding to the 20 K side of the assembly was used as a comparative performance metric, as this flux directly correlates with the boil-off rate in practical applications.

The results obtained from these simulations will support the design of corresponding experimental setups intended to validate the numerical models. Additionally, the simulation outcomes will aid in identifying and resolving potential design challenges—such as envelope plastic deformation and non-uniform heat flux—ultimately contributing to the development of an optimized VIP configuration for cryogenic insulation applications.

Multiscale strategies for modelling the working mechanisms of triboelectric nanogenerators for drop energy harvesting

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E6_1, Z1 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

The harvesting of energy from low-frequency liquid flows is a relatively recent concept compared to the already established solar and wind energy sources, and it currently represents one of the major areas of interest in the quest to harness the potential of water as a clean and renewable energy source. In this context, triboelectric nanogenerators (TENGs) have emerged as very promising players in this field. However, despite extensive research efforts, the power output of droplet energy harvesters remains limited, primarily due to constraints in identifying materials with ideal triboelectric and wetting properties, as well as suboptimal device architectures that hinder the efficient conversion of the full kinetic energy of the incident droplets. In search for optimal solutions to this problem, the simulation of all the stages of the energy collection process is necessary, as each stage provides essential elements for the collection of energy stored in the droplets. As part of an effort involving the full development of a TENG designed to extract electrical energy from high-density droplets in a single step, in this work we have proposed a simplified model. This model is based on the conductivity of the droplet and the instantaneous electrical capacitance, which results from the high-speed contact between the droplets and the active area of the device's electrodes. This model has been implemented in finite element simulations using the COMSOL Multiphysics package. The results provide valuable information about the behavior of liquid-solid triboelectric nanogenerators and the role of the triboelectric surface pre-charging effect in shaping the temporal characteristics of the conversion event.

Mechano-Responsive Bio-Piezoelectric Nanofibers for intelligent drug delivery

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E6_1, Z1 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

Control over biodistribution and pharmacokinetics is critical for enhancing the efficacy and minimizing the side effects (vomiting, immune system suppression, organ toxicity,...) of therapeutic agents. Therefore, there is a need for on-demand drug delivery systems that precisely control release time and dosage. The electromechanical conversion characteristics of piezoelectric platforms enable them to convert external stimuli into electrical energy. However, the most common piezoelectric polymer, PVDF (poly(vinylidene fluoride)), has limitations related to non-biodegradability and fluorinated contamination. To address this need, we explored the development of active biomaterials based on poly(3-hydroxybutyric acid-co-3-hydroxyvaleric acid) (PHBV), a biodegradable and biocompatible piezoelectric polymer, for drug delivery applications by tailoring its morphology, and crystallinity. Electrospun nanofibers of PHBV were fabricated using the electrospinning technique, and different concentrations of barium titanate (BT) were added as piezoelectric ceramics to enhance piezoelectric and mechanical performance. The electrospun web was remotely activated by external mechanical source of ultrasound waves to produce electrical charges in situ and control drug release locally. The developed PHBV/BT smart nanofiber web is applicable in future biomedical fields, as well as in electronic sensors and actuators.

Energy Harvesting from Post-Consumer Plastic Waste: A Sustainable Approach to Electricity Generation

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E6_2, Z1 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

The growing accumulation of post-consumer plastic waste presents significant environmental challenges. This study explores the feasibility of using unsorted plastic waste, composed of common packaging materials such as high-density polyethylene (HDPE), polypropylene (PP), polystyrene (PS), and polyethylene terephthalate (PET), for energy harvesting applications through mechano-electric conversion. Without the need for complex re-processing or even material separation, these plastic waste compounds were directly utilized as functional layers in nanogenerators, demonstrating the ability to convert mechanical (triboelectric) and thermal (pyroelectric) stimuli into electrical energy.

In triboelectric applications, combinations of PET films with heterogeneous plastic waste compounds composed of HDPE/PP/PS/PET exhibited significant energy conversion efficiency, with peak output voltages exceeding 130 V, short-circuit current densities of 50 $\mu\text{A}/\text{cm}^2$, and charge densities of 390 nC/cm^2 . The so-called rejected recyclable plastic waste, a fraction typically sent to landfill due to its complex composition, also demonstrated promising energy conversion capabilities, achieving output voltages above 60 V in triboelectric configurations when paired with PET films. Pyroelectric measurements showed that waste plastics were capable of generating measurable voltage responses under temperature gradients, albeit at lower magnitudes compared to triboelectric effects.

As a secondary focus, the study investigated the integration of these plastic waste materials with polyvinylidene fluoride (PVDF), a polymer known for its excellent piezoelectric and triboelectric properties. The combination of immiscible plastic waste blends with PVDF resulted in a remarkable enhancement of energy conversion efficiency, achieving output voltages of up to 800 V and short-circuit current densities of 260 $\mu\text{A}/\text{cm}^2$. This hybrid approach leverages the inherent immiscibility of plastic waste to create physical domains within the polymer matrix, enhancing charge separation and energy output.

The findings of this study highlight the potential of post-consumer plastic waste as an alternative energy source and emphasize its practical applications in sustainable and cost-effective self-powered devices, such as sensors and low-power electronics. The results also provide a new perspective on the utilization of immiscible plastic waste blends, turning a recycling challenge into an opportunity for green energy solutions.

Harnessing magnetoelectric coupling at the nanoscale for advanced spintronics

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E6_1, Z1 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

Spintronic computation could potentially offer significant advantages over CMOS technology, including area and power reduction, and the ability to perform complex logic functions with non-volatile magnetic materials. However, a complete magnetic/spintronic computing system does not yet exist, necessitating a hybrid spintronic-CMOS system. A major challenge in developing such a hybrid system is the lack of scalable and energy-efficient transducers to couple electric and magnetic domains effectively.

Magnetoelectric composite materials, which combine piezoelectric and magnetostrictive films, are promising for controlling magnetization with electric fields. The magnetoelectric coupling occurs via strain: an electric field generates strain in the piezoelectric layer, which transfers to the magnetostrictive layer, creating an effective magnetic field that can rotate magnetization or generate spin waves. An inverse effect also exists, linking changes in magnetization to strain and electric fields. For microelectronic applications, these heterostructures must be miniaturized to the nanoscale. However, at these scales, strain is non-uniform, leading to complex magnetic behavior. Most studies have focused on in-plane switching of nanomagnets under high voltages.

This study demonstrates significant magnetoelectric coupling in sub-micron Ni stripes on a piezoelectric PZT layer using anisotropic magnetoresistance (AMR). Applying voltage generates strain and a magnetoelastic (ME) field in the Ni, which can be measured using AMR. The study finds a ME field in Ni as large as tens of Oe/V, consistent with simulations. Further miniaturization and material optimization could enhance this effect. The study shows a magnetization rotation of over 60° by applying voltage, with potential for further optimization.

COMSOL Multiphysics and MuMax software were used to study the mechanical and magnetic behavior of these devices. Generating charges or electric fields in thin film devices via the direct ME effect remains challenging, especially at small scales. This is crucial for spintronic applications, where conventional readout methods face limitations.

The study also investigates the direct ME effect in thin film composites of PVDF-TrFE on Ni foil. Measurements of charge accumulation on dot capacitors show that rotating Ni magnetization generates significant voltage differentials. Simulations validate these results and demonstrate scalability, with minimal variation in output voltages across different dimensions. Optimized structures and materials could achieve even higher voltage differentials, surpassing conventional detection schemes and meeting CMOS compatibility standards.

Exploring multifunctional properties of BaTiO₃ –based ceramics by addition of multi-walled carbon nanotubes

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study investigates the multifunctional properties of Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O₃ ceramics prepared using multi-walled carbon nanotubes (0 - 70 wt% CNT) as sacrificial templates to generate variable porosity levels (3% - 25%). Comprehensive analyses of dielectric, ferroelectric, pyroelectric, piezoelectric, and non-linear dielectric properties emphasized the influence of porosity on the functional properties and the possibility of exploring potential pyro/piezoelectric applications of such ceramics. Besides the dilution effect due to the porosity increase, the presence of small amounts of residual unburnt CNT, variations of pore morphology and phase interconnectivity, and the ceramic grain size reduction when increasing the CNT addition determine in a complex way the functional characteristics. All the porous ceramics are stable and can sustain the application of high fields. The pyroelectric effect is enhanced around room temperature due to the proximity of orthorhombic-tetragonal phase transformations, giving rise to high values of pyroelectric coefficients of $p \sim 21 \times 10^{-4}$ C·m⁻²·K⁻¹ and energy harvesting Figure of Merit of $Fe \sim 211$ J/m³K² for 10% CNT level. Furthermore, all Ba_{0.85}Ca_{0.15}Ti_{0.9}Zr_{0.1}O₃ ceramics present a piezoelectric energy harvesting potential for self-powered functionality. The non-linear dielectric characteristics demonstrate the advantages of introducing porosity for reducing permittivity while preserving a high tunability level for x=50% CNT addition.

Acknowledgments:

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Material design and development of Pb-free ceramics with improved piezoelectric Figure of Merits for energy harvesting applications

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E6_2, Z1 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

This study examines the influence of porosity volume fraction and morphology on the dielectric permittivity, polarization-electric field, and piezoelectric response of Pb-free ferroelectric materials by combining experimental results with a modeling approach using the Finite Element Method. The experimental investigation focused on the effects of porosity on the structural and functional (dielectric, ferroelectric, nonlinear, and piezoelectric) properties of Ba_{0.85}Ca_{0.15}Ti_{0.90}Zr_{0.10}O₃ ceramics. Microporosity levels ranging from 3% to 31 vol.% were achieved using poly(methyl methacrylate) microspheres as sacrificial templates.

Structural analysis indicated phase coexistence at room temperature, as expected for this composition. The maximum permittivity decreased with increasing porosity, from approximately 7000 (at 3 vol.% porosity) to 3500 (at 31 vol.% porosity), while the Curie temperature shifted from 47°C to 67°C with increased porosity. These changes are likely due to porosity-induced structural and internal stress modifications. An enhanced piezoelectric response was observed in Ba_{0.85}Ca_{0.15}Ti_{0.90}Zr_{0.10}O₃ ceramics with an intermediate porosity of around 18 vol.%, achieving the highest piezoelectric response of 470 pC/N and a figure of merit of 7.3 pm²/N and enhanced pyroelectric response for 15% of porosity. The optimal piezoelectric properties at this intermediate porosity level are attributed to microstructural changes (pore shape and connectivity) and possible field-induced structural modifications.

The piezoelectric energy harvesting measurements indicate the potential for using Pb-free porous ferroelectric materials in energy harvesting devices.

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Exploring the effect of phase superposition in BaTiO₃- solid solution ceramics for enhanced functional properties

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study explored the impact of phase superposition on the functional properties of BaTiO₃-based ferroelectric ceramics by substituting the B-site cation with a larger ionic radius component. BaTiO₃ powders were synthesized via a solid-state reaction method, incorporating Zr⁴⁺ (0.72 Å) to replace Ti⁴⁺ (0.605 Å) and induce structural modifications. BaZr_xTi_{1-x}O₃ (x = 0-0.06) ceramics with orthorhombic/tetragonal phases at room temperature were comparatively investigated to understand the role of phase composition for small addition of Zr on their functional (dielectric, ferroelectric, piezoelectric and tunability) properties. Concerning the values of BaTiO₃, the switching polarization, permittivity peak, tunability, and piezoelectric coefficients are changed by doping with 6 % Zr onto Ti⁴⁺ sites. The orthorhombic polymorph amount is larger in the doped ceramic and explains its higher switching polarization. These findings highlight the role of phase superposition in tuning the functional characteristics of ferroelectric ceramics and offer valuable insights for the development of advanced passive components in high-voltage industrial applications and energy harvesting devices.

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Computational analysis of inverse opal photonic crystals using the RCWA method for photocatalysis applications

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E6_2, Z1 Room (Level -3), septembre 16, 2025, 17:00 - 19:00

The development of efficient photocatalytic materials is crucial for addressing global challenges in renewable energy and environmental remediation.

One promising approach to improve the efficiency of photocatalytic materials involves the use of inverse opal (IO) photonic crystals made from these materials. Indeed, inverse opals, i.e., three-dimensional periodic porous structures, exhibit unique optical properties such as photonic band gaps and slow photon effects, which can enhance light harvesting and improve photocatalytic performance by increasing the interaction time between light and photocatalyst.

In this work, we numerically investigated the optical response (reflectance and absorptance) of inverse opal photonic crystals to incident solar light radiation using the rigorous coupled wave analysis (RCWA) method. We analyzed the influence of key structural and optical parameters (pore size, refractive index), as well as simulation parameters, including the number of computational layers, the number of plane waves, and the incidence polar and azimuth angles.

Our results show that a well-designed shift in the reflectance spectrum near the material's electronic absorption edge leads to considerable enhancement of the absorptance compared to a planar slab of the equivalent material volume. This enhancement, due to the slow photon effect, highlights the potential of the studied IO structure for applications requiring efficient solar light harvesting, such as photocatalysis.

Local vs. macroscopic dielectric and ferro/piezoelectric responses in porous BaTiO₃ ceramics determined on the basis of 3D reconstructed ceramic microstructures

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E6_2, Z1 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Porous BaTiO₃ ferroelectric ceramics with variable porosity level (i.e. with relative density between 74%-96%) are investigated by an experimental-numerical approach in order to optimise their piezoelectric harvesting response. The porous ceramics present anisotropy as derived from the deformation of sacrificial soft polymeric additives (PMMA spheres) during the pressing step [1]. 3D micro X-ray computed tomography experimental data with specific numerical procedures have been firstly used to reconstruct the ceramic 3D microstructures and to extract sample geometrical information as: pore size distribution, shape and tortuosity. These 3D microstructures have been employed as input in FEM-based models, in order to determine the local electric field and potential distributions inside the ceramic body [2]. The final aim is to evaluate the low field effective permittivity and high field ferroelectric switching $P(E)$, tunability and piezoelectric responses as a function of porosity and applied field direction. The effective permittivity is estimated by computing the total electrostatic energy of the discretized system. The polarisation-field response is calculated by using a Preisach model for describing the switching properties of the dense ceramic component under the specific local field of each element and the tunability response is computed by using a Johnson approach to describe the nonlinear dielectric response of the dense ceramic component. The resulted dielectric and ferroelectric properties derived by using this procedure are discussed in comparison with the experimentally determined ones. Piezoelectric calculations for porous ceramics are more complicated for real 3D microstructures due to the tensorial nature of this phenomenon and involve higher computational resources [3]. New approaches are currently developed for this task. The present study demonstrates the usefulness of analyses and simulations of properties at different lengthscales based on real 3D microstructures for completing the understanding of the complex relationship between composition – microstructure – local/macroscopic properties and pave the way of development of new tools for material design of porous or composite multi-materials for energy storage and harvesting.

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Design of metallic Phase Change Materials: Surface properties of liquid Al-Si-Sn alloys

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

One of the most promising technologies for efficient Thermal Energy Storage (TES) are Metallic Phase Change Materials (PCMs), characterized by superior thermal conductivity and energy storage per unit volume. Such PCMs are based on solid-liquid transitions, but their limited solutions in the liquid state may represent problem for handling. To produce materials with desired properties it is necessary to understand the relationships between the elements of a quadriade “composition-processing route-microstructure-properties” and based on it, to achieve tailored microstructure associated with a unique combination of properties. Speaking about industrial processes involving the presence of the liquid phase, the solidification is a key step to perform these processes properly. Modelling of solidification and thus, microstructural evolution is directly related to reliable thermophysical property data of metallic melts, needed as input parameters.

Direct measurements of bulk and surface properties of liquid alloys at high temperatures are often technically difficult or even impossible, and therefore, theoretical models can be used to estimate missing property values. The energetics of mixing in liquid Al–Sn, Al–Si and Si–Sn systems has been analysed through the study of the concentration dependence of various thermodynamic and surface (surface tension and surface segregation) properties in the combined framework of thermodynamics and statistical mechanical theory.

The aim of this study is to correlate the thermodynamic properties of the Al-Si-Sn system and its subsystems with their surface properties and to compare the model predicted property values to own experimental data and / or to the data available in the literature.

Adamantane plasma polymers as versatile vacuum processable triboelectric thin films for mechanical and droplet energy harvesting

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E6_1, Z1 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

Current battery technology will not be able to sustain the expected demand for small, light, and even wearable portable devices. Portable nanogenerators can harvest environmental micro-energy at the point of need, powering up low-power wireless devices. This emerging technology holds significant promise for developing disruptive, self-powered electronic systems.

Triboelectric Nanogenerators (TENG) are among the most widely adopted solutions for efficiently converting low-amplitude and low-frequency mechanical/kinetic stimuli, such as human movements, into electricity. TENGs will revolutionize on-site power for smart devices, enabling self-powered sensors. Their high versatility in device architecture and triboelectric surfaces, without requiring specific crystalline phases or stoichiometries, places them at the forefront of microscale energy harvesting. The field currently relies on fluorinated polymers over 10 μm thick mostly made via solvent-phase synthesis.

In this context, we have developed adamantane thin films as a high-performance triboelectric organic material by Remote Plasma Assisted Vacuum Deposition (RPAVD) [2-3]. Adamantane plasma polymers are advanced dielectric films developed as protective coatings for perovskite solar cells and strain-engineering of 2D nanomaterials [4-5]. In this work, we study those layers as triboelectric surfaces, capable of exhibiting both, tribopositive and tribonegative character, through simple modification of the synthesis conditions and film structure without additives or functionalisation. The ADA plasma layers—from several nanometers to several microns thickness range—are hydrophobic, non-soluble, and transparent in the UV-VIS-NIR range. RPAVD ADA films devices present voltage and current outputs as high as 88 V/cm² and 1.05 μA for a 2800 nm (tribonegative) vs. 400 nm (tribopositive) combination and maximum power density as high as 2.0 $\mu\text{W/cm}^2$. Additional examples of using RPAVD ADA films as active components in micropatterned solid-solid and top-bottom drop-TENGs will also be presented.

RPAVD provides broad control over the surface composition, topography, and crosslinking degree. The proposed synthetic method is industrially scalable and straightforwardly compatible with photolithography and surface functionalization approaches. It is also environmentally friendly, making it a reliable and competitive solution to fluorinated-free thin film triboelectric material.

Keywords: Triboelectric Nanogenerator (TENG); energy harvesting; plasma deposition; plasma polymer.

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Preparation of flexible PVDF-BT piezoelectric composite films for energy harvesting

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E6_2, Z1 Room (Level -3), septiembrie 16, 2025, 17:00 - 19:00

Energy-autonomous systems that utilize smart materials have the potential to significantly reduce fossil fuel consumption. Among these materials, those with piezoelectric properties are especially promising for integration into energy harvesting and conversion devices. Polymer-based composites with functional ceramic fillers, in particular, are attracting considerable attention due to their ability to combine the inherent flexibility and high breakdown strength (BDS) of polymers with the functional properties of embedded inorganic particles. Building on encouraging previous findings, this study presents a comparative analysis of piezoelectric materials, focusing on the mechanical, thermal, chemical, and electrical properties of flexible PVDF/BaTiO₃ composite films prepared using different techniques. We explored the impact of processing on particle dispersion and filler-matrix interactions, particularly regarding agglomeration phenomena and selective formation of PVDF polymorphs. Finally we examined how these factors influence the dielectric and piezoelectric response of the ensuing composites.

Acknowledgements: Work carried out in the framework of the National Recovery and Resilience Plan, Mission 4 funded by the European Union – NextGeneration EU and Bilateral Agreement Italy-Romania, P2-AR-CNR-2023-2025

PLLA-based piezoelectric and magnetoelectric composites for flexible energy harvesting devices

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E6_2, Z1 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Multifunctional hybrid composites are called to be the core elements of wearable electronics, electronic skin and bio-implanted devices for medical diagnosis and therapeutics, to only stand out three out of a range of application fields. They are also expected to realize autonomous sensing nodes for wireless sensor networks (WSNs). Node powering by energy harvesting from multiple sources, like mechanical vibrations or stray magnetic fields by using piezoelectric or magnetoelectric materials, is reckoned essential to avoid the cyclic replacement or recharging of batteries. A main line of research is the development of flexible polymer-matrix composites including embedded piezoelectric and magnetostrictive inorganic phases. Most works resorted to PVDF-TrFE as matrix, a fuel-based, non-biodegradable polymer with serious associated environmental concerns. Among alternatives, poly-L-lactic (PLLA) stands out because of its biobased and biodegradable character, as well as its biocompatibility.

In this context, we are investigating the suitability of bio-based thermo-polymers, like Poly-L-Lactic Acids (PLLA) and odd-numbered Polyamides (PA), as piezoelectric matrices, along with particulate BCZT piezoelectric perovskite and MZFO magnetostrictive spinel, non-toxic metal oxides, and the use of innovative approaches towards 3D-printing technologies. The control of the 3D-printing parameters is key to obtain high molecular chain orientation and crystallinity, thus allowing piezoelectric response of the matrix to be tailored. Surface functionalization of the most promising cases has been accomplished with silanes, which improved compatibility between the composite components and allowed high quality composites to be obtained. An in-depth characterization of the electrical, piezoelectric, magnetic and magnetostrictive properties is here presented, and used to discuss the piezoelectric and magnetoelectric responses. Results suggest a great potential of biobased polymeric composites for sustainable energy harvesting.

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Advancing Elastocaloric Cooling Solutions through 3D Printing of Superelastic NiTi shape memory alloy

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Elastocaloric cooling represents a promising and sustainable alternative to traditional refrigeration technologies, leveraging the reversible thermal changes in elastocaloric materials under applied mechanical stress. Shape memory alloys (SMAs), particularly NiTi alloys, exhibit exceptional elastocaloric properties driven by thermoelastic martensitic transformations. These transformations involve exothermic and endothermic phase changes between austenite and martensite phases during cyclic loading and unloading, enabling efficient heat exchange.

NiTi alloys, widely recognized for their remarkable shape memory effect (SME) and superelasticity (SE), are prime candidates for elastocaloric applications due to their excellent damping capacity, corrosion resistance, and biocompatibility. In this study, we explore the potential for advancing elastocaloric cooling systems through the additive manufacturing of NiTi using the laser powder bed fusion (LPBF) technique. LPBF enables the precise fabrication of complex geometries, which is critical for optimizing heat transfer and enhancing material performance. By manipulating the process parameters of LPBF and optimizing microstructural features, this work aims to pave the way for more efficient and scalable elastocaloric cooling solutions, contributing to the global push for sustainable refrigeration technologies.

Comprehensive microstructural characterization of the printed samples, including phase distribution, grain orientation, and defect analysis, was performed using advanced techniques such as X-ray diffraction (XRD), scanning electron microscopy (SEM), electron backscatter diffraction (EBSD), and X-ray computed tomography (CT). Subsequently, a complete thermo-mechanical analysis of the 3D-printed samples was conducted to identify key parameters for the development of elastocaloric performance. The wide range of possible sizes, shapes, and lattice structures achievable by LPBF opens new avenues for improving elastocaloric efficiency due to available deformations in tensile/compression and torsion modes. Direct adiabatic ΔT measurements mapped the elastocaloric properties and the heat transfer processes of the lattice structures. This analysis revealed critical insights into the relationship between microstructure and elastocaloric performance, highlighting the influence of LPBF processing parameters on the development of desirable textures.

Additive Manufacturing of An Sn-Based Alloy on Silicon Wafer by Laser Powder Bed Fusion for Advanced Cooling of Electronic Circuits

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

The constant growth of interest in miniaturization of power sources for electronic circuitries necessitates utilizing high-performance cooling to fulfil their thermal management requirements. Unlike conventional cooling methods that rely on heat sinks mounted on conventional thermal interface materials (TIM), which create thermal resistance and reduce heat extraction efficiency at their interfaces, we are, hereby, proposing an additive manufacturing approach using Laser Powder Bed Fusion (LPBF) to realize wafer-scale printing of an Sn-based interlayer material on which a heat sink can be fabricated. The alloy's low melting point (~ 250 °C) mitigates thermal stresses during solidification and cooling that occur in the LPBF process. The thermal conductivity of this Sn-based alloy, estimated at 39.4 ± 6.7 W/mK, surpasses those of common thermal interface materials (1-10 W/mK), making it a competitive option for heat management applications. Microstructural analysis of the printed layers on Si wafer confirms the alloy's uniformity and compatibility with silicon, proposing its effectiveness as a thermal interface material for cooling applications. By optimizing the volumetric energy density exerted during the LPBF print process, we could realize structures that are fully dense and free of cracks. The successful formation of the Sn-based alloy on Si wafer by LPBF is a stepstone for the realization of wafer-scale full additive manufacturing of heat sinks onto it.

Magneto-mechanical coupling in NiMnGaCu multicaloric alloys: functional experimental investigation under magnetic field

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E7_3, Z3 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

The Ferromagnetic Shape Memory Alloys (FeSMA) attracted increasing interest like multicaloric materials for solid state refrigeration. The most important field coupling is correspondent to magnetic and mechanical induction of thermoelastic martensitic transformation (TMT). In the present work we show for the first time an experimental investigation on NiMnCu polycrystalline alloy, in ad hoc developed experimental set up for stress strain curve in isothermal conditions under magnetic field. In this way we measured the elastocaloric and magnetocaloric effect at the same time. The entropy changes ΔS and the functional caloric parameters ΔT_{ad} vs magnetic field until 0.5 T are evaluated. The application of magnetic field seems to act like a supplementary mechanical longitudinal stress and the precise contribute of magnetic field is considered. These preliminary results are fundamental to complete understanding and modeling of coupled multicaloric phenomenon.

Development and Optimization of Polymer-Metal Composites for Superior Thermal Management

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Efficient thermal management is critical for ensuring the success and longevity of spacecraft during extended space missions. Spacecraft encounter extreme challenges such as temperature fluctuations, radiation exposure, vacuum environments, and microgravity effects, all of which impact the performance of Thermal Interface Materials (TIMs).

This study explores nanocomposites, carbon-based pastes, metal sheets, and liquid metals, with the primary goal of identifying materials with high thermal conductivity that also meet the electrical and mechanical demands of space applications. The material design emphasizes the use of green polymers and additives, supporting the shift towards more sustainable practices in commercial space exploration.

While polymers generally have low thermal conductivity, the addition of highly conductive fillers such as ceramics, carbon materials, and metals can significantly enhance their overall performance.

By adjusting the concentration of high- and low-electrical conductivity fillers, the electrical properties are precisely tuned. Metallic nanocomposites use sinterable metallic microparticles as the matrix, with added fillers. The carbon-based TIM pastes category incorporates special fillers like graphite, graphene, CNTs, and metallic AgNWs or Cu/Ag core-shell nanowires.

The results of these developed materials—nanocomposites, polymer-based TIMs, metal sheets, and liquid metals—will be presented.

Thermal Optimization for Sustainable Data Center Cooling Using Thermochemical Heat Systems

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E7_3, Z3 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

In this research, the integration of Thermochemical Materials System (TCMs) technology into data center (DC) cooling systems is evaluated as a method to improve energy efficiency by reducing electricity and water consumption, with a key focus on its impact on power usage effectiveness (PUE) and water usage effectiveness (WUE), critical metrics in data center energy efficiency. The rise of AI and machine learning has increased demand for high-power computing, leading to greater heat generation in data centers' cooling processes. While cooling temperature reach 40°C to 60°C, waste heat recovery presents a key opportunity. By capturing and repurposing waste heat, TCMs technology serves a dual purpose for heating applications, such as supporting nearby heat demands, while simultaneously enhancing cooling efficiency by reducing the load on conventional chillers. A benchmark model of data center cooling loop is developed to simulate key energy performance metrics, including electricity consumption for compressors and water usage in cooling towers. Conventional cooling systems, such as cooling towers, economizers, and mechanical chillers, are analyzed as a baseline for comparison. The integration of TCMs allows for transforming the rejected heat from DC cooling process, providing heating and cooling benefits. The results demonstrate that the proposed TCMs integration is adaptable to varying cooling water temperature requirements and significantly reduces overall electricity consumption and water usage. This integration enhances cooling performance, supports the nearby heating demands, and lowers environmental impact. This study highlights the technical feasibility and benefits of TCMs as a sustainable cooling solution, emphasizing material selection's impact on waste heat recovery efficiency. Future research should assess their techno-economic feasibility for cost-effectiveness and broader adoption in data center operations.

Novel material development for Ammonia based Thermochemical Heat valorization from Data Centers

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

With the energy consumption of data centers continuously rising and no signs of slowing down, the need to recover and utilize their low-grade waste heat becomes imperative for sustainable growth. However, the efficient valorization of this thermal energy remains a challenge due to its low temperature. In this work, framed inside the IPCEI-CIS-MISD project, we focus on the development of novel materials for ammonia-based thermochemical heat storage systems, designed to capture and upgrade waste heat from data centers for more efficient energy utilization. In order to achieve this, we through the development of hybrid heat storage and upgrade system employing multi-material 3D printing, effective thermochemical materials (TCM) and novel reactor design so that we leverage the absorption-desorption of ammonia on novel TCMs to valorize low temperature heat. The Temperature Swing Absorption (TSA) unit enables the upgrading the heat thanks to the large exothermicity of the ammonia absorption. With an efficient and sustainable use of energy in mind, a prototype of a thermochemical heat transformer will be built considering the three scopes mentioned. First, adequate TCM selection and synthesis is carried out to understand the relationship between physico-chemical properties and absorption dynamics. Then, the utilization of hierarchical supports will be explored to enhance heat and mass transfer in the system. To achieve this, temperature programmed desorption of ammonia, nitrogen-physisorption, X-ray Diffraction and X-ray Fluorescence techniques will be used to stablish chemistry-architecture-performance relationships. Overall, this study aims to demonstrate the feasibility of composites as TCMs for low-grade waste heat recovery from data-centers.

Enhancing thermochemical heat storage performance with additively manufactured aluminum alloys: A study on porous matrix design and heat transfer

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

This study focuses on incorporating aluminum alloys to enhance heat transfer due to their high thermal conductivity in addition to corrosion resistance, thereby improving thermochemical heat storage (TES) performance. Achieving high-performance TES systems requires the development of materials and processes that withstand thermal cycling and enable efficient heat transfer. TES operates by drying out hydrated salts to store energy and rehydrating them to release it. However, the inherent low thermal conductivity of these salts limits heat transfer and reduces the overall efficiency of TES systems. In this study, we address the following knowledge gap- by exploring how introducing a porous designed matrix can overcome this limitation by improving heat transfer. Specifically, we investigate the role of both the porous structure and its surface chemistry in enhancing salt-based TES performance. To this goal: (1) we will use laser powder bed fusion (LPBF) to fabricate aluminum porous matrices, leveraging its design flexibility to create tailored structures. However, 3D printing aluminum alloys via LPBF presents challenges, such as hot-cracking susceptibility due to their wide solidification range. To address this, LPBF process parameters—such as laser power, scanning speed, and hatch spacing—will be optimized. Additionally, careful metal powder handling was employed to minimize oxidation, enabling the production of defect-free materials. (2) The porous matrix will be designed to maximize surface area, allowing for the use of the maximum amount of salt, and ensuring efficient heat exchange. To evaluate performance, the thermo-mechanical properties of both the porous matrix structures and the salt-infused matrix will be investigated. Thermal conductivity will be measured using the thermal plane source method, while mechanical performance will be assessed through compression testing of the porous matrix. Overall, this study demonstrates the feasibility of additively manufactured aluminum 6xxx-series porous matrix for advanced thermal management. It emphasizes the design flexibility offered by LPBF and highlights the importance of parameter optimization in overcoming processing challenges. This work opens a pathway toward high-performance TES and heat exchanger solutions.

Kirkendall Effect guided Void Formation in PVD Manufactured Cu-Au Thin Films for low Thermal Conductivity Coatings

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E7_3, Z3 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

First observed in 1947, the Kirkendall-effect describes the mechanism of vacancy diffusion at the interface of two dissimilar materials where diffusion of some atomic species are strongly favored over the others. Thus, if these fluxes are not equal and in opposite direction, which is true for binary metallic interfaces, there must be a net flux of atoms which is matched by a flux of vacancies in the opposite direction. An important result of this effect is the accumulation of pores, also known as Kirkendall pores, near the interface of the two different materials. These pores are a result of the unbalanced atomic fluxes through the interface when the system is heated to a temperature where atomic diffusion becomes pronounced.

In many manufacturing and joining applications, the formation of Kirkendall voids is undesirable as it poses a threat to device performance, through degradation of electrical and mechanical properties. However, in 2004 the Kirkendall effect was first used to explicitly create hollow nanoparticles

with a single pore formed by the diffusion of Co and O, S or Se. The research direction of actively creating Kirkendall voids has been growing ever since. Currently, most Kirkendall voiding research is focusing on spherically or radially symmetric systems, but void formation has not yet been studied extensively in physical vapour deposition (PVD) manufactured thin film systems.

In this work, we seek to further leverage the Kirkendall effect to design porous microstructures for a better understanding of the Kirkendall voiding mechanism in thin films. This will be done by leveraging the findings of Kirkendall-void formation in simple systems such as coated nickel wires and applying it to thin films. The films will be manufactured by a PVD process to then be annealed in a rapid thermal annealing (RTA) oven under vacuum. The manufactured thin films show high porosity, where the location and size of the pores can be controlled by the sputtering process. The porosity reduces the thermal conductivity of the films making them viable options for low thermal conductivity structures or coatings in microelectronic devices.

Thermal Characterization of combined Al-Based and Sn-Based Alloys as Composite Phase Change Materials for Thermal Energy Management

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E7_2, Z3 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

The combination of aluminum-based (Al-based) and tin-based (Sn-based) alloys can be considered to produce composite phase change materials (c-PCMs) for thermal energy management and thermal energy storage characterized by peculiar combinations of high sensible and latent heat capacity at intermediate temperature together with high thermal conductivity.

This study utilizes simple models and Thermo-Calc simulations to predict and analyze the thermal properties of these alloys, including thermal conductivity, phase transition temperatures, specific heat capacity, and latent heat of fusion of the c-PCM phase. These properties are further investigated through experimental techniques such as laser flash analysis (LFA), differential scanning calorimetry (DSC), providing a comprehensive understanding of their thermal behavior.

The thermal cycling nature of thermal management material further requests to check the characterization length change of the material under repeated thermal cycles, which in the study was performed by dilatometric tests. The thermally cycled alloys offered the possibility to obtain preliminary insights on the microstructural stability of the investigated composite PCMs.

The relationship between chemical composition, microstructure, and thermal response of the alloys upon thermal cycling are analyzed, providing insights into material selection for efficient and thermally stable thermal storage/management systems.

These findings contribute to the development of advanced metallic PCMs for renewable energy and waste heat recovery applications.

Exploring the potentialities of TPMS-based composite Phase Change Materials

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E7_2, Z3 Room (Level -3), settembre 17, 2025, 14:30 - 16:30

Organic Phase Change Materials (PCMs) represent a powerful tool for thermal energy storage or thermal management purposes. Indeed, exploiting their high latent heat of fusion per unit mass and heat capacity at constant pressure, they can store/release high amount of thermal energy at constant temperature, i.e., the one of the phase transition. However, their intrinsic low thermal conductivity, severely limits their performances. For this reason, organic PCMs are usually embedded in high thermally conductive matrices, usually metallic, either ordered or disordered. In the meanwhile, additive manufacturing technologies enables the production of complex topologies, among which Triply Periodic Minimal Surfaces (TPMS). This latter definition identifies a family of structures with superior surface-to-volume ratio, ideal for exchange processes. Hence, composite PCMs (C-PCMs) are obtained from the combination of the two.

Effective thermal conductivity studies, even involving different material combinations, not only limited to organic PCMs, are numerically performed on different configurations, in order to highlight the advantages offered by TPMS over conventional lattices with the means of adimensional indexes.

C-PCMs thermal behaviour is also examined in terms of geometrical features under transient regime and a univocal methodology for establishing the triggering of the onset convection in this kind of composite is set via developing a permeability-dependent modelling.

Last but not least, the authors exploit the possibility of filling the C-PCM with different materials, having different transition temperatures and thermophysical properties. Indeed, another peculiar feature of the TPMS is to split the surrounding domain into two non-interconnected and non-interacting regions. This allows the possibility of having a multi-step temperature management, which can find application beside working system with a specific working temperature range, matching the two different PCM transition temperature.

The study successfully demonstrates at least from numerical point of view the feasibility of having such a system.

Innovative and sustainable materials for high temperature Thermal Energy Storage (TES) systems

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Renewable energy, such as solar, wind, ocean and geothermal energy, plays a crucial role in mitigating climate change and the global warming effect. It is clean and available almost everywhere to meet the growing energy demand in a sustainable way, eliminating the greenhouse gas emissions caused by the exploitation of fossil fuel reserves. Among the different renewable energy sources, the sun is the most abundant. However, the intermittency and weather-dependency of solar energy make challenging its industrial application.

Thermal Energy Storage (TES) technologies tackle this challenge, acting as a link between solar power generation and optimal load distribution. TES systems can be classified as sensible, latent, and thermochemical heat storage systems, with the sensible TES systems being the only ones that have currently commercial industrial applications. However, the commercial sensible heat storage systems struggle to supply high heat temperatures, due to limitations of the used materials' thermal and mechanical stability.

For example, the Ordinary Portland Cement-based materials and especially concrete, which are widely used in sensible solid-state TES systems, undergo thermal degradation at temperatures higher than 450 °C. However, the decarbonization of certain manufacturing processes in energy intensive industries, such as glass, metal, and cement, make essential the development of novel, for low-cost materials that can withstand higher temperatures, offering higher storage capacity to sensible TES systems.

This work aims to investigate the use of geopolymers based on Construction and Demolition Waste (CDW) as an alternative to the Ordinary Portland Cement-based materials for TES systems that will operate at temperatures higher than 700 °C.

Geopolymers are sustainable materials with very good mechanical and thermal properties and an inherent fire resistance. The development of CDW-based geopolymers was theoretically investigated in both alkaline systems, of sodium and potassium and their applicability in TES systems was experimentally evaluated. Specifically, their thermal stability at temperatures up to 800 °C was studied and basic thermal and mechanical properties, such as specific heat, thermal diffusivity and compressive strength at these temperatures, were evaluated. The experimental results of this research revealed that the developed CDW-based geopolymers are very promising materials to be applied in sensible TES systems working at high temperatures.

Interrelation between Microstructure and Thermal Conductivity of Metal-Graphene Material Systems

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E7_3, Z3 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

In this study, the relationship between microstructure and thermal conductivity of metal-graphene material systems, such as pure copper-graphene, AlSi₁₀Mg-graphene and Ti6Al4V-graphene, is examined. In these material systems, the distribution of graphene within the metal matrix influences the thermal conductivity to a large extent, introducing considerable thermal anisotropy [1]. Furthermore, the interface thermal conductance (ITC) between the metal and graphene forms a critical factor that may impact the total heat transport across. To date, thorough studies on the relationship between these factors have not yet been conducted. Hence, in this paper, we investigate the influence of the material microstructure on the thermal conductivity of metal-graphene composites comprised of metals with thermal conductivities ranging from 6.7 W/mK for Ti6Al4V to 366 W/mK for pure copper.

The addition of graphene to metals has been proposed as an efficient way to improve the thermal conductivity, as graphene exhibits a high in-plane thermal conductivity of 3,000-5,000 W/mK [2]. However, the low through-plane thermal conductivity of 5-10 W/mK of graphene, combined with its incompatibility issues with metals, makes it difficult to develop composites with superior thermal conductivity. For instance, the ITC of pure copper-graphene has been reported to be 23 MW/m²K, whereas that in polymer-graphene material systems has been demonstrated as 50-165 MW/m²K [3]. Accordingly, only rather limited thermal conductivity improvements in some metal-graphene systems have been reported [4].

In this work, we measured the thermal conductivities of pure copper-graphene, AlSi₁₀Mg-graphene, Ti6Al4V-graphene as a function of the graphene wt.%. These findings were confronted with the microstructures characterized using scanning electron microscopy and transmission electron microscopy. Moreover, the wt.% dependency of the thermal conductivity is compared with theoretical thermal models, such as effective medium approximation. The thermal model was also adopted to describe the effect of ITC on the overall thermal conductivity. Some composites form interfacial bonding layers, such as Al₄C₃ and TiC which alter the conductivity. It was observed that the thermal conductivity increases by up to 150 % in Ti6Al4V, as a result of these interface reactions. The corresponding influence of microstructural features on the resulting thermal conductivity will be discussed in the final presentation.

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Development of GrCop42/Copper-Inconel 718 multi material structure through laser powder bed fusion for heat transfer applications

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E7_1, Z3 Room (Level -3), september 17, 2025, 10:30 - 13:10

The development of multi material structures using laser powder bed fusion (LPBF) technology by combining desired thermo-mechanical properties, offers significant potential for enhancing heat transfer applications, particularly in aerospace. This study focuses on the fabrication of pure Copper-Inconel 718 (Cu-IN718) and Copper alloy-IN718 (GrCop42-IN718) multi-materials, by leveraging the high-temperature strength and thermal stability of IN718 with the great thermal conductivity of Cu and GrCop42. The integration of high-strength IN718 with high-thermal conductive Cu/GrCop42, aims to improve heat exchanging capabilities, specifically for advanced engineering applications. However, additive manufacturing of high-strength multi material interfaces remains challenging due to significant differences in their thermo-physical properties and weak bonding and defects in interface. In this study, the effects of process parameters and the consequence of materials in layers or each layer on the interface properties of the LPBF'ed Cu-IN718 and GrCop42-IN718 were analyzed, and the process parameters were optimized to reach the good metallurgical bonding interface between Cu/GrCop42 and IN718. Through this research the interface microstructure characteristics, element distribution, phases in interface, thermal conductivity, and microhardness of these multi materials were investigated. The melting behavior, mixing of IN718 and Cu/GrCop42 elements and in-situ phases in interface, and formation mechanism of multi materials in different consequence of materials were discussed. The formation of interface characteristics is primarily driven by Marangoni convection, which enhances the mixing of IN718 and Cu/GrCop42 elements, facilitates the development of a stable transition layer at the interface, and enables a seamless transition between the two metal interfaces. Compared to IN718, the Cu-IN718 and GrCop42-IN718 multi material structures exhibited significantly enhanced thermal conductivity. These advancements open up and paves the way for the additive manufacturing of multi materials in next-generation aerospace structures.

Suitability of plasma sprayed AlSi10Mg+Sn coatings for Thermal Energy Management

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E7_2, Z3 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Phase Change Materials (PCMs) are smart materials, which can store/release thermal energy at constant temperature via latent heat of transformation. Solid-liquid transformation is the most exploited one. In this view, the design of a suitable container for the managing the volume of the liquid PCM is fundamental.

In this view, the adoption of immiscible systems, made up by at least two elements which do not interact at both solid and liquid phase, demonstrates to be an added value for these purposes. Al-Sn is one of the most relevant examples. The former acts as high thermally stable matrix, whereas the second one works as active PCM. In order to function properly, the active PCM should be efficiently dispersed in the matrix, which can effectively promote confinement. A high solidification rate has to be imposed to the material when liquid for the achievement of such a microstructure.

In this view, plasma spray coating technique is tested for establishing its suitability as production process for PCM purposes. AlSi10Mg and Sn powders were employed for this work. An Al-Si-based alloy is selected since Si do not perturb the immiscible nature of the Al-Sn binary system.

Microstructural analyses, both in as-produced and heat-treated conditions, were performed on the samples in order to establish if they are able to meet or not PCM requirements for a prolonged service as thermal management coatings. Also surface roughness analysis was performed in this sense to monitor the appearance of the coating. Their cyclic thermal performances, at least for preliminary stage, are tested as well with repeated DSC. Dilatometric tests are employed for understanding the thermo-mechanical behaviour of the resulting coatings.

Plasma spray technique reveals to be a practical solution for the realization of PCM temperature management coatings.

Optimization of Heat Transfer Between Phase Change Materials and Thermal Loads Using Thermal Conductivity Enhancers

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E7_2, Z3 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

For future human space missions, ensuring crew health is paramount. Research has shown that calcium signaling, a fundamental cellular process, can be influenced by microgravity, making it crucial to investigate. Current experiments employ the fluorescent protein CaMPARI2, which irreversibly photoconverts under elevated Ca^{2+} and ultraviolet light, and require precise thermal control due to heat flux from LEDs exceeding 2.5 W/cm^2 . Because these temperatures must be kept stable without external power, phase change materials (PCMs) are used to stabilize temperature. However, PCMs have low thermal conductivity, limiting effective heat dissipation. This study addresses that challenge by investigating discrete thermal conductivity enhancers, added as separate structural elements, to improve heat transfer without reducing PCM volume.

A variety of configurations were evaluated, including aluminium foams of varying porosities, carbon foam, fibrous metal networks, and traditional fin or pin structures. These configurations were selected to optimize thermal conductivity while maximizing the proportion of PCM within the buffer, thereby preserving the overall thermal storage capacity of the system. The investigation began with preliminary experiments using a water-filled, simple setup to screen and eliminate materials that did not meet the necessary performance criteria. This phase allowed the identification of promising candidates based on their ability to rapidly conduct heat away from a simulated load.

Building on these results, the second phase involved integrating the selected enhancers into a prototype container filled with PCM. This setup more closely mimicked realistic operating conditions by incorporating a controlled thermal source and subjecting the system to regulated heating and cooling cycles. Finally, a third set of experiments was performed using a real thermal buffer assembly within a functional system, providing further insight into the operational performance and integration challenges of each enhancer type.

Results indicate that specific aluminium foams, fins, and pins significantly improve heat dissipation compared to a baseline PCM system and other structures. However, while aluminium fins offer excellent thermal transfer, they are relatively heavy, which reduces the available PCM volume and overall energy storage capacity. Additionally, achieving a reliable thermal interface between the enhancer and the container proved challenging with foams. In contrast, conical aluminium pins emerged as the optimal solution, providing comparable thermal performance while being lighter and easier to integrate, thereby preserving PCM capacity and ensuring effective thermal management.

All mission-specific requirements, including minimal mass, limited volume, and precise temperature control, were successfully met, confirming the viability of this approach for future human spaceflight applications.

Elastocaloric effect in polycrystalline NiMnTi alloys produced through suction casting and melt-spinning processes

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E7_3, Z3 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

The use of caloric materials for solid-state cooling applications presents a promising and sustainable alternative to traditional vapor compression-based refrigeration methods. In particular, elastocaloric technologies offer advantages such as compactness and simplicity of operation, reduced environmental impact and high efficiency. Among elastocaloric materials, superelastic shape memory alloys (SMAs) stand out, owing to the reversible stress-induced martensitic transformation which involves a high latent heat. NiMnTi-based alloys, in particular, show remarkable elastocaloric performance due to the large unit cell volume change during the Austenite-to-Martensite transition. In this study, two polycrystalline NiMnTi alloys were produced using two different processing routes, i.e. melt spinning and suction casting, starting from the arc melted precursor material. The effects of processing parameters and heat treatments on the thermoelastic martensitic transformation and on the alloy microstructure were investigated through calorimetric and microstructural analyses. Moreover, isothermal compression tests were performed to evaluate the superelastic behavior and the cycling stability of the produced alloys. In addition, the elastocaloric performance was evaluated in terms of adiabatic ΔT directly measured by thermocouples during quasi-adiabatic mechanical testing. The NiMnTi samples produced via suction casting demonstrated the highest elastocaloric performance, with an adiabatic ΔT reaching up to 15 °C. Lower performance was exhibited by melt spun ribbons, in which an inverse behavior was detected in tensile strain recovery measurements under applied loads. The current study contributes to expanding the fundamental knowledge on NiMnTi alloy produced by means of a cost-effective and traditional casting process in order to lay the foundations for further development of advanced processing routes, including melt-spinning and suction casting.

Bio-Waste Derived Activated Carbon for Sustainable Energy Storage Applications

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Due to escalating climate changes and energy crises, the need for alternative renewable energy sources is crucial. H₂ has emerged as a green energy carrier however, its shipment and storage are the major obstacles to its large-scale adoption. The existing hydrogen storage systems, such as geological formations, pressure tanks, and liquid hydrogen, suffer from limited capacity, low energy efficiency, high costs, and safety concerns. To address these challenges, reliable, safe, and efficient alternative materials with high gravimetric capacity are vital. Hydrogen storage in porous carbons is considered a promising technology due to the rapid rate of hydrogen adsorption-desorption, natural abundance of raw materials, and good regeneration capacity, particularly in automotive applications. Despite encouraging findings, no material currently meets the U.S. Department of Energy (DOE) target of 6.5 wt% hydrogen storage at ambient conditions. Hence, this study investigates bio-waste-derived activated carbon as a sustainable hydrogen storage material with integrated thermal management properties. Spent coffee grounds were carbonized at 350 °C, 400 °C, and 450 °C, followed by KOH activation at 800 °C under the flow of argon gas. The synthesized activated carbons were characterized using SEM, TGA, and BET surface area analysis, and their hydrogen uptake capacity was evaluated using a gravimetric sorption analyzer.

The results revealed that the activated carbons exhibited high thermal stability (retaining >80% mass at 600 °C), well-developed porosity (SEM images), and high BET surface area (up to 2728 m²/g for Arabica and 1983 m²/g for Robusta), contributing to enhanced hydrogen adsorption capacity. The hydrogen uptake at room temperature and 35 bar pressure was 0.997 mmol/g for Robusta spent coffee activated carbon. Given their high thermal resistance and adsorption efficiency, these materials hold potential for waste heat recovery, adsorption-based cooling, and hydrogen-powered thermal energy systems. This study highlights the dual role of bio-waste-derived activated carbon in hydrogen storage and thermal energy management, contributing to the development of sustainable and net-zero energy solutions.

Keywords: Hydrogen adsorption, activated carbon, spent coffee grounds, renewable energy, thermal energy management.

Hybrid foamed concrete as a porous material for thermal energy management applications.

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Environmental pollution and energy crisis are one of the biggest problems the world is facing due to industrialisation, rapid population and living standards growth. Just in the UK, heat represents almost half of the use of energy, as around 80% of domestic heat is supplied by natural gas. Under current trends towards environmental pollution, waste and the Ordinary Portland Cement's production (in >5 billion tons annually, as concrete, due to its inherent strength and durability properties, is the second most used substance on Earth after water, thus responsible for more than 7% of the CO₂ global emissions), are one of the most significant in impacting (negatively) the global climate and human wellbeing.

To reduce the building thermal energy consumption (reducing the space heating and cooling energy) and increase energy saving for civil buildings while in service. Thus, the work presented here is focused on the design and fabrication of the novel hybrid freestanding concrete (Fig.1.) based on the foam scaffolding, to be applied as a light thermal insulation material [], with unique tailored structural properties. The study included the systematic research on the single interface (bubble) by Profile Analysis Tensiometer (PAT), the stability measurements of the 3D foam dopped with Portland Cement, followed by an appropriately design gel casting protocol [], in order to achieve a low-costs, high-porosity, fire- resistance material.

Green processes using 3D waste materials- water purification in Energy sector.

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), September 17, 2025, 13:10 - 14:30

Vermiculite (VMT) is known to have excellent antibacterial and sorption properties (removal of anti-inflammatory drugs, dyes, heavy metals, bio-recalcitrant compounds, nitrogen, and phosphate compounds). Organically modified vermiculites are also well-known nanostructured adsorbents of organic compounds from water or gaseous phases, similar to organically modified smectites or bentonites. The Activated Carbon (AC) famous for extraordinary antiseptic properties and very high specific surface area, therefore, by merging the properties of AC and VMT in the foam form, we can achieve a new generation of materials that have high multielement sorption capacities and antibacterial properties, capturing contaminants and preventing the bacteria colony formation in water storages/systems for a long time. Additionally, having a very high specific area and specifically tailored opened structure, allows fast penetration and treatment of a contaminated water through the large and highly selective area derived from porous structure of a foam itself and additional porosity given by mixed AC and VMT.

The presented work highlights the advancements in the sustainable materials that can be used as filters/adsorbents actively capturing i.e. Uranium and other heavy metals, other pollutants providing antiseptic capacities of the filters with a wide industrial application such as hydrogen production, long term space missions, CO₂ capturing and waste management.

The results from this study could pave the way for the development of multifunctional building materials that not only provide structural support but also offer effective EMI shielding. Such materials could find applications in various sectors, including data centers, healthcare facilities, and critical infrastructure protection.

Advancements In Sustainable Concrete for Global Challenges

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Global warming is an important issue now a days and the major driver for this phenomenon is CO₂ emissions [1]. To tackle this issue both the thermal management system and CO₂ reduction are important tasks to develop. Moreover, due to the ageing nuclear power plants and the hazardous effect of radiation leads to the importance of having radiation shielding materials. It is important to develop novel composites that can withstand CO₂ emission under the thermal management system for radiation shielding material.

Concrete has been a widely accepted material for a variety of applications including thermal storage material, radiation shielding material, building structure materials etc. However, it has faced several challenges due to its density and weight, workability, cost, thermal insulation, maintenance and environmental impacts [2]. To tackle those issues, several researchers tried to develop novel concrete utilizing several the natural or industrial waste, fibres, minerals, nanoparticles so that it can help to reduce the CO₂ reduction to align with the net zero emission. However, there is still concern about the sustainability of those concrete and its effectiveness of the concrete, as there is still under review.

Incorporating porous structure to the concrete can be solution of the many issues towards its drawbacks. Porous structures help to reduce the weight of the structure having the larger surface area and high absorption capacity [3]. Moreover, it can be eco-friendly through utilizing the plants, soil, natural minerals which helps to reduce the CO₂ emissions to align with the net zero emissions [4].

To tackle all the concern, this research is focusing on two distinctive area. It will contribute a hollow review about the effectiveness of the novel concrete for radiation shielding material and its impact towards CO₂ reduction to maintain the net zero emissions. Moreover, this research also contributed towards developing a novel porous concrete composite utilizing the natural clay mineral to meet towards the sustainability and CO₂ reduction for radiation shielding applications.

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Shielding properties of a novel porous concrete towards Electromagnetic Interference

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Electromagnetic interference (EMI) has become a pervasive issue in our increasingly connected world, affecting both natural ecosystems and human-made electronic systems. As technology continues to advance, the need for effective EMI shielding solutions has grown more urgent. This ongoing research project aims to explore an innovative approach to EMI shielding using specially designed concrete samples, combining cost-effectiveness with potential large-scale applicability.

An important aspect of this research is its potential environmental impact. By using a concrete mixture with fewer aggregates, the production process is expected to result in lower CO₂ emissions compared to traditional concrete manufacturing. This aligns with the growing need for sustainable construction materials that can also provide advanced functionalities like EMI shielding. The effectiveness of EMI shielding is typically measured in decibels (dB), with higher values indicating better shielding performance. Previous studies have shown that concrete composites can achieve shielding effectiveness ranging from 20 to 50 dB in the X-band frequency range, depending on their composition and thickness. Our experiment aims to evaluate how the unique porous structure of our concrete samples compares to these benchmarks and how to reduce the thickness of the concrete.

The results from this study could pave the way for the development of multifunctional building materials that not only provide structural support but also offer effective EMI shielding. Such materials could find applications in various sectors, including data centers, healthcare facilities, and critical infrastructure protection.

Exploring the microstructural and electrochemical behavior of the CuMnNiSn alloy for thermomagnetic applications

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E7_2, Z3 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

The major part of the energy globally produced is lost during energy conversion, and most of it is released as heat, this waste heat can be classified into three grades: high temperature (above 650 °C), medium temperature (230–650 °C), and low temperature (below 230 °C) [1]. High and medium-grade waste heat can be readily utilized, but for low-grade waste heat, there is no effective way to recover it [1]. In this sense, developing thermomagnetic devices that use ferromagnetic materials with Curie temperatures close to room temperature may allow the recovery of low-grade waste heat [2]. In this study, the thermal, electrochemical, and microstructural behavior of the CuMnNiSn alloy was evaluated to verify its potential application in thermomagnetic devices. Material's phase composition was studied using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy dispersive X-ray spectroscopy (EDS), the electrochemical behavior in refrigeration fluids was studied by potentiodynamic polarization, and the thermal behavior was studied by differential scanning calorimetry (DSC). The microstructural characterization by XRD, SEM, and EDS indicates that the as-cast alloy presented two phases with equimolar composition, but with different space groups (Fm-3m and F-43m). The linear polarization analyses were initially evaluated using distilled water as a corrosion medium, which did not strongly affect the material's surface, with a corrosion current density of $\sim 1.6 \mu\text{A cm}^{-2}$ and a corrosion potential of $\sim -81.3 \text{ mV}$. A thermal treatment was carried out to improve the homogeneity of the alloy and verify its microstructural and electrochemical response, but the heat-treated alloy still presented two phases, with a similar corrosion behavior ($\sim 1.5 \mu\text{A cm}^{-2}$ and $\sim -68.5 \text{ mV}$). Nonetheless, preliminary results indicated that the Curie temperature of the CuMnNiSn alloy reduces from 100 °C to 60 °C after heat treatment, which is an attractive characteristic for the recovery of low-grade waste heat energy.

Metallic-Phase Change Materials casting: comparison of experimental results with theoretical consideration.

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E7_2, Z3 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Metallic Phase Change materials could offer an alternative to salt-based PCM, when higher thermal conductivity is required. Among metallic PCM, Al-Sn based alloys have received considerable interest and several methods of production were proposed, mostly based on powder processes, to obtain the desired microstructure. In the present work, several Al-Sn metallic Phase Change Materials, with different composition, were produced by induction melting and cooled by different means. The obtained cast products and their microstructures were analyzed by image analyses. Results were correlated to material properties and casting/pouring conditions, try to establish a comparison with theoretical consideration.

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Non-vanadium aqueous redox flow batteries

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E7_1, Z3 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Aqueous Redox flow batteries (ARFBs) are a promising technology for large scale energy storage system. For improving the performance and stability of the ARFBs, the determination of proper active materials is most crucial. The active materials are dissolved into supporting electrolytes, and such developed two electrolytes like anolyte and catholyte are stored in tank, determining cell voltage and maximum solubility. In turn, capacity and power density of ARFBs are decided. Vanadium has been played as the role so far. However, due to its low reserves and rapid cost fluctuation, many attempts have been made to replace it to other materials. As the alternative, iron (Fe) based complexes coordinated with different ligands are considered due to the benefits of wide redox potential window, high solubility to supporting electrolyte, low crossover rate, and relatively cheap price. In this presentation, their electrochemical properties and kinetic parameters are evaluated quantitatively to determine their optimal condition. In turn, cycle tests of ARFBs using them are implemented to measure their performance and stability. As a result, it is proved that ARFB using Fe complexes as redox active materials is viable enough to compete with vanadium RFB and lithium battery in some prospects.

Insight into He trapping mechanisms in implanted 9Cr and 14Cr ODS steel for fusion reactor applications

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E8_4, Z3 Room (Level -3), septembre 18, 2025, 17:00 - 19:00

Helium (He) accumulation and bubble/cavity formation in structural materials pose a critical challenge for ensuring the long-term stability of fusion reactor components. High-energy neutron irradiation of the structural steels results in He generation through transmutation of iron (Fe) and chromium (Cr) atoms which compromises its mechanical integrity. Few studies have shown that oxide dispersion-strengthened (ODS) steels, which are promising materials for the first wall/blanket, are able to mitigate He-induced embrittlement due to their unique microstructural features for trapping He. However, if the high density of grain boundaries and nano-oxides/matrix interfaces play a key role in the limitation of bubbles formation, the interaction between He atoms and these interfaces is not fully elucidated.

In this study, we comprehensively investigated He bubble formation and its characteristics in 9Cr and 14Cr ODS steels following He ion implantation at three different temperatures: 25°C, 400 °C, and 600 °C. Advanced microscopy techniques, including the High-Angle Annular Dark-Field (HAADF) imaging and Electron Energy-Loss Spectroscopy (EELS) in an aberration-corrected atomic resolution microscope (ARM) were employed to characterize the bubble size and its distribution, as well as the He atom density and internal pressure within bubbles at various microstructural features.

Our findings reveal significant differences between 9Cr and 14Cr ODS steels in He trapping, bubble characteristics, and its evolution with temperature. These differences are shown to be due to differences in their respective microstructural features such as grain size, oxide distribution, composition and interface characteristics (i.e. coherent or incoherent). These novel measurements provide a comprehensive understanding of the mechanisms governing He trapping and swelling.

By correlating the temperature effects on He bubble behavior with the microstructural features of ODS steels, this work advances our understanding of He-induced damage mechanisms in nuclear materials. The innovative use of EELS, involving careful isolation and analysis of He signal for quantifying He atom density and pressure within bubbles offers a valuable tool for characterizing irradiated materials. The present results instigate future research for further optimization of microstructural stability of fusion blanket steels under extreme irradiation environments.

Joining, Coating and Characterization of SiC/SiC and SiC-based cladding materials for safe Nuclear Energy Applications

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E8_1, Z2 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Silicon carbide (SiC) fiber-reinforced silicon carbide matrix composites (SiC/SiC composites) represent a cutting-edge solution for improving safety in nuclear fuel cladding technology as well as for use in advanced fusion and fission reactors. Despite their promise, challenges remain in optimizing the materials and processes for joining and coating these composites. Recent research efforts have renewed the interest in SiC preceramic polymers to address these issues.

This approach involves the use of polycarbosilane polymers enhanced with SiC nanoparticles and fibers. The process includes a series of thermal treatments: curing the material in vacuum at 200°C to establish initial structural integrity, followed by pyrolysis in an inert atmosphere at 1450°C to convert the polymer into a robust ceramic form. These steps are critical for achieving strong and durable joints.

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Thermo-mechanical, lead corrosion and thermal stability assessment of innovative Alumina Forming Austenitic Alloys for LFRs

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

The development of new generation Lead-cooled Fast Reactors (LFRs) encounters the key challenge of long-term degradation of structural materials when exposed to liquid lead (Pb). Current research identifies alumina-forming austenitic (AFA) steels as a promising material class for structural applications in LFRs. A novel range of AFA steel compositions has been determined through thermodynamic simulations to predict mechanical properties, corrosion resistance, and thermal stability. The experimental activity has been carried out by casting 0.5 kg rods then scaled-up to 80 kg ingot through VIM and VAR processes. Thermo-mechanical tests have been conducted using a Gleeble machine to identify optimum forming parameters afterwards used for the hot rolling of larger sheets. The material corrosion resistance has been assessed through Pb corrosion tests for 1000 hours at 600°C. Additionally, the thermal stability of selected compositions has been evaluated by oven ageing. Comprehensive bulk characterization techniques, including SEM, XRD, and OM, have been utilized to analyze microstructure and phase transformations. Finally, the behavior under irradiation is being studied using an advanced in-situ TEM setup with heavy ion irradiation.

Accelerated Oxidation of Stainless Steels in Heavy-Water Reactor Spent Fuel Pool Accidents

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Spent nuclear fuel bundles from heavy-water reactors are stored on racks in spent fuel pools at reactor sites after discharge to allow for radioactive decay and cooling. These cylindrical fuel bundles, containing nuclear fuel rods, are arranged in stainless steel racks in a regularly spaced pattern to facilitate effective cooling, ensure radiation shielding, and maintain organized storage. To maximize storage capacity, high-density racks are commonly employed. In the event of coolant leakage, the spent fuel may overheat, causing the surrounding water to boil and create a high-temperature steam environment. Prolonged contact with overheated spent fuel further raises the temperature of the racks, increasing the risk of oxidation. Under these conditions, 304 stainless steel, the primary material used in the racks, is prone to rapid oxidation, potentially compromising its structural integrity. This study investigates the high-temperature oxidation behavior of 304 stainless steel in these accident scenarios.

To simulate the exposure of high-temperature stainless steel to a steam-containing atmosphere, an induction heating method was employed. The stainless steel specimens were heated inside a quartz tube while water vapor, generated by heating water on a hot plate, was continuously injected into the tube. Thermogravimetric analysis (TGA) was performed on STS304 specimens (8 × 20 × 3.5 mm) at temperatures ranging from 800 to 1100 °C for 2 hours. The oxidized specimens were characterized using scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), and X-ray diffraction (XRD) to analyze their structure and composition.

The high-temperature oxidation of stainless steels in a steam-containing atmosphere was significantly more severe compared to exposure in a non-steam atmosphere. Furthermore, compared to literature data typically obtained in closed chambers containing steam, this study observed accelerated and more severe oxidation under the simulated accident conditions. SEM/EDS analysis revealed the formation of a bilayer oxide structure, with an Fe-rich outer layer and a Cr-rich inner layer. In water vapor environments, a higher proportion of iron oxide was observed, attributed to the decomposition of chromia into chromium hydroxide, which promotes the formation of iron oxide. This effect intensified at higher temperatures, leading to accelerated oxidation rates. These results demonstrate that high-temperature oxidation in water vapor, as expected during spent fuel pool coolant leakage accidents, significantly undermines the structural integrity of 304 stainless steel, highlighting its susceptibility in such scenarios.

High-Temperature Oxidation Behavior of Zirconium Alloys in Simulated Spent Fuel Pool Accident Conditions

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Spent nuclear fuel is typically stored in wet storage pools, where decay heat is dissipated, and radiation is safely contained using a coolant. Although accidents in these storage pools are rare, events like natural disasters causing coolant leaks cannot be completely ruled out. In such situations, spent fuel rods can overheat due to the inability to remove decay heat. As the coolant evaporates, the rods are exposed to a steam-rich environment, which significantly accelerates the oxidation of zirconium alloy cladding and may lead to catastrophic failures. This study focuses on understanding the high-temperature oxidation behavior of zirconium alloys under such accident-like conditions.

To mimic the self-heating effect observed in real-world accidents, an induction heater was employed. Weight changes were monitored in real-time and normalized to weight change per unit area for direct comparison with literature data. The results clearly showed that oxidation rates in a steam atmosphere were much higher than in air, emphasizing the aggressive nature of steam in promoting cladding degradation. Additionally, tests conducted in such an open environment, where self-heated high-temperature zirconium alloy was exposed to a continuous steam flow, revealed faster oxidation rates and greater weight gains compared to the previous results reported in the literature, which were often performed in closed chambers with static steam.

The oxidized samples were further examined to understand their surface morphology and chemical composition using scanning electron microscopy (SEM) and energy-dispersive spectroscopy (EDS). Phase composition was analyzed through X-ray diffraction (XRD), while cross-sectional studies highlighted variations in oxide thickness and composition at different depths. These findings shed light on the mechanisms that cause cladding failures during accident scenarios, offering valuable insights to enhance the safety and dependability of spent nuclear fuel storage systems.

Overview and status of the IFMIF-DONES Facility

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E8_3, Z3 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

The International Fusion Materials Irradiation Facility – Demo Oriented Neutron Source (IFMIF-DONES) is a research infrastructure for irradiation the materials to be used in a fusion reactor. The facility would provide a unique neutron source of energy spectrum and flux level representative of those expected for the first wall of future fusion reactors.

Materials irradiation data under such conditions are of fundamental interest for the fusion community to consolidate the fusion reactors engineering design and licensing and to validate modelling tools for materials radiation damage. The facility will be also able to address some tritium technologies related experiments.

Its Construction Phase started in 2023 in the proposed site of the Escúzar Metropolitan Park (located in the Granada 18 km southwest from Granada city).

This paper will present an overview of the implementation, engineering design and main irradiation characteristics of the facility.

Characterization of cyclic softening effect on EUROFER-97 mechanical properties through combined LCF + tensile tests

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E8_4, Z3 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

The reduced activation ferritic-martensitic (RAFM) steel X10CrWVTa9-1 (commonly referred to as EUROFER-97) represents the first candidate as structural material for the ITER Test Blanket Module (TBM) and the DEMO Breeding Blanket. As such, its full characterization and codification is essential for the reliable design of such components and the consequent successful licensing, construction and safe operation of future fusion machines. A strong effort is thus underway at European level to perform an extensive mechanical testing campaign supported by different EU labs within the EUROfusion Consortium with the goal of filling the gaps still existing in the material properties database, updating the Material File required to implement EUROFER-97 in the RCC-MRx design code for the design and manufacturing of the ITER-TBM and contributing to the data collection for the DEMO Material Properties Handbook (MPH). In particular, one of the most relevant point to address is to evaluate the applicability of the existing RCC-MRx design rules and the related allowable stresses to EUROFER-97, considering the well-known softening behaviour of such material under cyclic loading as opposed to the hardening typically associated with austenitic steels for which those design rules have been mainly established. In this context, a dedicated experimental test campaign involving different research labs has been launched in the framework of the EUROfusion Work Package Materials within the TBM subproject (WPMAT-TBM) to investigate how the EUROFER-97 tensile properties are affected by the cyclic softening of the material. In this line, several tests were performed at the mechanical testing laboratory of the ENEA Brasimone Research Centre during the years 2024-2025. The test matrix includes a set of combined tests consisting of uniaxial strain-controlled low-cycle fatigue (LCF) tests, each followed by a tensile test on the pre-fatigued specimen. The LCF tests were executed at 300°C and 550°C until the maximum number of cycles allowed by the latest (2022 Edition) RCC-MRx fatigue design curve was reached. Then, the pre-fatigued specimens were tested in tension at RT, 300°C and 550°C. Additionally, some tensile-only tests at RT, 300°C and 550°C were also carried out, as a reference, on virgin samples machined from the same plate. All the specimens were fabricated from EUROFER-97 batch 3 with transverse orientation with respect to the rolling direction. This paper provides an account of the execution of the above-mentioned tests and the main results obtained along with a brief discussion of the latter.

Qualification of Materials for Lead-cooled Fast Reactors: Testing standardization and experimental results

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

In recent decades, Lead-cooled Fast Reactors (LFRs) have gathered significant interest from the HLM (Healy Liquid Metal) scientific community. As a result, different projects were founded in Europe, US and China, with the related experimental activities carried out. However, in the occasion of the 2023 GEMMA (EC Project) conference in Bologna, two key findings were highlighted from the results presented:

- Nuclear-grade conventional structural materials, such as AISI 316 and 15-15Ti austenitic grades, exhibit good corrosion resistance in liquid lead (Pb) environments up to 450–480°C, provided optimal oxygen control is maintained.
- Experimental data show a notable degree of scatter, likely due to variations in experimental setups.

An obvious approach to address the data scattering challenge is the standardization of experimental facilities, protocols, methodology for analysis of data and their interpretation. These are prerequisites for any LFR developer intending to submit material data to the regulator for licensing reactor prototypes for low temperature operations (400 – 450°C).

In this framework, newcleo in collaboration with ENEA has commissioned a high-throughput facility to conduct an initial evaluation of nuclear grades materials of newcleo's interest (regulated in RCC-MRx code) against corrosion in lead at reactor operating conditions. The test bed is a standardized stagnant Pb cell with bubbling gas injection oxygen control system. Preliminary results on 15-15Ti AIM-1 and 316 grade under stagnant conditions are currently under characterization. In this work we will present some insights about the experimental data for nuclear qualified materials at conditions relevant for operations of a low temperature LFR; with these conditions newcleo intends to deploy to fully demonstrate this technology in an operative environment in the early 2030.

Irradiation and corrosion behavior of oxide-forming FeCrAlNi coatings deposited by HiPIMS

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Lead-cooled fast reactors are considered among the most promising Generation IV nuclear reactors, owing to their inherent safety and high-power density. Nevertheless, liquid lead causes severe degradation of conventional structural and cladding materials, mainly due to oxidation, dissolution and erosion of the steel matrix. Additionally, high-dose irradiation due to fast neutrons can further enhance corrosion, promoting the formation of defects in the material [1]. In this respect, the cladding is one of the most critical components as it faces the highest temperature and radiation fields, while containing the nuclear fuel. Therefore, proper mitigation strategies must be adopted to protect the cladding material, avoiding unwanted modification of the steel matrix properties. In this framework, surface coating technology can be considered a valuable technique. Indeed, without modifying the properties of the bulk material, the surface of any component can be ideally engineered through the deposition of a protective coating [2]. To improve the corrosion, mechanical and radiation resistance of standard nuclear-grade steels, the composition, density, morphology, adhesion, compatibility to the substrate, and self-healing capabilities of the coatings play a crucial role.

This contribution reports about the development of FeCrAlNi coatings deposited by High Power Impulse Magnetron Sputtering (HiPIMS) on steel substrates. Coatings were produced by simultaneously co-sputtering a steel and an aluminum sources. This strategy should allow to control all the aforementioned properties. The co-sputtering process enables, on the one hand, to precisely tune the amount of Al in the coating, which should promote the formation of a stable and protective oxide layer when in contact with liquid lead [3]. On the other hand, the use of a sputtering target with a composition similar to the one of the substrate should improve the compatibility between the two. Additionally, the ion rich plasma characterizing the HiPIMS process can improve growth and evolution of the coating in terms of density, morphology and adhesion [4]. The prepared samples were tested in both ion irradiation and liquid lead corrosion experiments under relevant operating conditions. The coatings were characterized in terms of morphology, microstructure and elemental distribution before and after the tests, exploiting SEM/EDX, TEM, XRD and Raman spectroscopy.

[1] X. Gong et al., Prog. Mat. Sci. 126, 100929 (2022)

[2] E. Serag et al., Surf. Coat. Tech. 441, 128542 (2022)

[3] W. Zhang et al., Surf. Coat. Tech. 462, 129477 (2023)

[4] J. T. Gudmundsson, Plasma Sources Sci. Technol. 29, 113001 (2020)

Impact of vanadium addition on the mechanical properties and irradiation resistance of FeCrAl-Y2O3-Ti ODS alloys for components of Generation IV nuclear reactors

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E8_1, Z2 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Generation IV nuclear reactors will operate at higher temperatures and under higher irradiation doses than existing Generation III and III+ reactors. Therefore, there is an urgent need to develop irradiation-resistant materials with good high-temperature properties. FeCrAl oxide dispersion strengthened (ODS) alloys possess good strength at high temperatures. The good irradiation resistance of ODS alloys is related to the nanometric oxide precipitates homogeneously distributed in the matrix that act as sinks for irradiation-induced defects, mitigating irradiation damage. Moreover, FeCrAl ODS alloys present good corrosion and oxidation resistance due to the formation of a thin protective alumina layer on the surface. Alloying elements can be added to FeCrAl ODS alloys to further improve their properties.

The aim of this study is to evaluate the impact of vanadium on the mechanical properties and irradiation resistance of FeCrAl-Y2O3-Ti-V alloys prepared by mechanical alloying and spark plasma sintering. Moreover, susceptibility to 475°C embrittlement was investigated. The properties mentioned above are crucial for the application of ODS alloys in Generation IV nuclear reactors. The microstructural investigations were performed by SEM-EDS, EBSD, and TEM. Mechanical properties were evaluated by hardness measurements, nanoindentation, and tensile test at temperatures up to 800°C. The irradiation resistance was analyzed by Fe²⁺ ion implantation up to 5 dpa at 300°C.

The conducted tensile tests show high mechanical strength, i.e., the yield strength is 893±23 MPa at room temperature and 490±8 MPa at 600°C. The elongation generally increases from approximately 12% at room temperature to more than 20% at higher temperatures. The addition of vanadium increases the strength at all tested temperatures, mostly due to promoting the formation of nanometric oxides. The FeCrAl ODS alloy with vanadium seems to be resistant to 475°C embrittlement since the alloy reveals similar ductility and strength in tensile tests before and after annealing at 475°C for 1000 h. The studied FeCrAl ODS alloys also reveal good irradiation resistance, showing only an increase of hardness by 10%. The results show promising properties of FeCrAl ODS alloys and the positive impact of vanadium on mechanical properties.

Solid-State Ionic Characterization of Oxygen and Metals in Lead Nuclear Coolant for the Development of Corrosion Resistance Materials

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The effect on climate of fossil fuel energy generation is stimulating the interest in the Lead-cooled Fast Reactors (LFRs) as carbon-free energy source. newcleo Ltd. is developing an LFR through its LFR-AS-30/200 programme. LFR technology is hindered by the Liquid Metal Corrosion (LMC) on steels: lead dissolves the alloying elements (Fe, Cr, and Ni) reducing the structural integrity and altering the coolant chemistry. Advanced steels include alloying metals (AMs) providing LMC resistance by the formation of passivating oxide layers when exposed in lead. The rational design of these starts from the thermodynamics of the AM-O-Pb systems, based on the accurate assessments of the oxygen and AMs thermochemical properties in lead, such as the solubility, the activity coefficient, and the oxide solubility products. Solid-State Ionic devices based on zirconia electrolyte – i.e. the Electrochemical Oxygen Sensors (EOSs) and Oxygen Pumps (EOPs) – are reliable for thermodynamic investigation in liquid lead-alloys. In this work we describe the development of our EOS/EOP technology and its application both on the small and pre-industrial scale. On the small-scale, combining the potentiometry with the EOS and the coulometry with the EOP, we assessed the oxygen activity coefficient and the solubility limit in the thermal range of 620-825 K, obtaining results aligned with literature. For the INNUMAT European project, we will also characterize together with ENEA the Fe-O-Fe₃O₄-Pb and the Cr-O-Cr₂O₃-Pb systems by measuring the metal elemental solubilities and the solubility product constants for the related oxides. The thermochemical data being acquired will play a key-role in the modelling of the LMC phenomena and the selection of structural materials for our LFR programme. On the pre-industrial level, we are scaling up the EOS/EOP devices to support the Oxygen Control System (OCS) on the SOLEAD facility storage tank. Specifically, we are testing the kinetics for the dissolution and linear diffusion of oxygen across a fixed section of the tank, between an injection point (gas bubbling or EOP) and a monitoring point (EOS). The results should provide an empirical model of oxygen diffusion in lead to a target surface of a material to be passivated. Moreover, we are testing the efficiency of the electrolytic oxygen removal by EOP at different oxygen contents. These studies investigate the dynamic response of a big-scale lead pool to a possible failure of the OCS, and the effects on the materials corrosion resistance when the normal operating conditions for the coolant chemistry are lost.

Plastic deformation in CrMnFeCoNi HEA: Linking 3D EBSD and Molecular Dynamics simulations

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

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High-entropy alloys (HEAs) are an emerging class of materials known for their outstanding mechanical strength, hardness, resistance to corrosion and irradiation, positioning them as promising candidates for use in extreme operating environments, such as aerospace, future fission (generation IV) and fusion power plants.

In this work, the nanomechanical response of a Cantor CrMnFeCoNi HEA is examined through nanoindentation testing and characterized using three-dimensional Electron Backscatter Diffraction (3D EBSD) reconstruction. This advanced technique allows for high-resolution mapping of geometrically necessary dislocation (GND) density and grain reference orientation deviation (GROD) angles around the indent, offering valuable insights into localized deformation characteristics and strain gradients.

Molecular dynamics (MD) simulations were used alongside experimental observations to capture atomistic-scale structural responses, showing qualitative agreement with mesoscale experimental results. The combination of 3D EBSD and MD simulations highlights the collaboration between cutting-edge experimental techniques and computational modelling, uncovering the intricate mechanisms of dislocation nucleation and evolution during nanoindentation. This study emphasizes the value of integrating multiscale approaches to enhance our understanding of deformation behaviour in HEAs.

Evolution of the microstructure of neutron irradiated RPV model steels with different content of Ni, Mn and Si

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E8_3, Z3 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Long Term Operation (LTO) of nuclear power plants is one of the ways followed to achieve the decarbonisation targets contained in the European Strategic Energy Technology Plan (SET-Plan). In this context, it is necessary to understand the mechanisms that lead to a degradation of reactor pressure vessel (RPV) steels exposed to high neutron fluences. Hence, the microstructure of several RPV model steels with different contents of Ni, Mn and Si, has been investigated before and after neutron irradiation by means of transmission electron microscopy (TEM), atom probe tomography (APT), small angle neutron scattering (SANS) and positron annihilation spectroscopy (PAS) in the frame of STRUMAT-LTO project funded by the EU [1]. The combination of all of these characterization techniques leads to a better understanding of the synergetic effect of alloying elements in the damage microstructure and to the correlation with the hardening of the studied materials as the content of Mn + Ni increases. Regarding the study by means TEM, the analysis reveals a decrease of the density of dislocation loops as the content of Mn and Ni mainly increases. In addition to that, microstructural results indicate that Mn effect seems to be more acute. On the contrary no effect in the density of dislocation loops has been noticed when the content of Si varies. According to APT and SANS results, for low and medium contents of Mn in the steel, the number density of Mn-Ni-Si nano-precipitates (MNSPs) increases as Ni content increases and for a given content of Ni the number density of clusters increases with Mn. On the contrary, Si has a low influence on cluster number density. PAS found an association between MNSPs clusters and the behavior of point defects. Finally, there is a good correlation between microstructural results and irradiation hardening of the materials.

[1] M. Kolluri, O. Martin, F. Naziris, E. D'Agata, F. Gillemot, M. Brumovsky, A. Ulbricht, J-M. Autio, O. Shugailo, A. Horvath, Structural MATerias research on parameters influencing the material properties of RPV steels for safe long-term operation of PWR NPPs, Nuclear Engineering and Design, Volume 406, 2023, 112236, ISSN 0029-5493, <https://doi.org/10.1016/j.nucengdes.2023.112236>

Durability of W/WC coating on inner surface of 316L steel Venturi tube in contact with high velocity flow of liquid Pb-Bi eutectic at 350 °C after one year of operation

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

The durability of structural materials in contact with heavy liquid metals (Pb, Pb-Bi and Pb-Li eutectics) is one of the key issues to be addressed on the way to master liquid metals as a functional media of novel nuclear and non-nuclear installations. This work presents and discusses the experimental results on the durability of W/WC coating exposed to a high velocity flow of liquid Pb-Bi eutectic.

The inner surface of a Venturi segment in the loop was made of 316L steel and coated with a W/WC layer by chemical vapor deposition (HARDIDE-T). The thickness of the coating is about 50 µm. The main purpose of this coating was to avoid the potentially severe erosion processes by the high velocity of the flowing liquid metal. The temperature of the liquid metal was 350 °C. The flow rate entering the Venturi segment of the loop was about 4.9 kg/s, which corresponds to the local maximum velocity of liquid metal at the Venturi throat of 6 m/s. The concentration of oxygen dissolved in liquid Pb-Bi was maintained at 2×10^{-7} mass%. After an one-year test, the Venturi part of the loop was segmented and examined in detail for durability of the preformed coating. The general conclusion is that the coating successfully protected the inner surface of the Venturi segment with respect to the high velocity flow of Pb-Bi eutectic. The morphological and structural features of W/WC coating are discussed based on the surface and cross-sectional metallographic studies.

Liquid metal embrittlement occurrence by lead and Pb-Bi eutectic of Face-Centered Cubic metallic alloys: austenitic steels and Complex Concentrated Alloys

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E8_2, Z3 Room (Level -3), septembre 18, 2025, 10:30 - 13:10

One of the challenges in the development of Lead Fast Reactors or Accelerator Driven Systems is the reliability of the structural materials in contact with the coolant, such as lead or the Lead-Bismuth Eutectic (LBE), and at high temperatures. In addition to damage due to irradiation, one of the major damages for the structural materials could be due to corrosion by liquid metal and, under stress (mechanical stress or stress caused by temperature fluctuations), structural materials can be susceptible to liquid metal embrittlement (LME), i.e. partial or total loss of ductility in the presence of liquid metal and therefore an earlier fracture. Because of the LME sensitivity of the Body-Centered Cubic alloys, the most ductile Face-Centered Cubic (FCC) alloys could be preferred because of their low LME sensitivity below 450 °C and despite the corrosion observed, in particular the selective dissolution of Ni and possible LME sensitivity at high temperatures (500 °C and more). The objective of the presentation is the study of the LME occurrence of different FCC metallic alloys (austenitic steels and Complex Concentrated Alloys), susceptible to be used in the presence of liquid LBE and Pb. To evaluate the LME sensitivity, Small Punch Tests were performed in air and liquid LBE and Pb saturated in oxygen at different temperatures between 200 °C and 500 °C and at different strain rates. Then, the fracture surfaces and cracking were observed by Scanning Electron Microscopy. Additional tensile tests and EDX-EBSD analysis (Energy Dispersive X-ray and Electron Backscatter Diffraction) are carried out to characterize the cracking paths in the presence of liquid metal and possible microstructure transformations. All the materials present ductile behavior and ductile fracture in air. The steels are less susceptible to LME than the studied CCAs. In case of LME occurrence, intergranular cracks were observed and selective dissolution of Ni and Mn were noted in specific conditions. Lower strain rates and higher temperatures promote LME sensitivity. The LME occurrence is discussed taking into account the microstructure, the hardness, and the composition of the alloys. The study was supported by the GEMMA and INNUMAT projects (Euratom research and training programme: respectively 2014-2018 - grant agreement No 755269, and 2021-2022 - grant agreement 101061241).

Advanced investigations to understand the damage of a Face-Centered Cubic metallic alloy in presence of liquid lead and Pb-Bi eutectic and under mechanical loading

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In presence of liquid metal, one of the major damages for the structural metallic materials could be due to corrosion by liquid metal and/or, under stress (mechanical stress or stress caused by temperature fluctuations), structural materials can be susceptible to liquid metal embrittlement (LME), i.e. partial or total loss of ductility in the presence of liquid metal and therefore an earlier fracture. These possible damages need to be investigated for the qualification of the structural metallic materials in contact with the coolant (liquid lead or the Lead-Bismuth Eutectic (LBE)) for the Lead Fast Reactors or Accelerator Driven Systems. Thus, because of the LME sensitivity of the Body-Centered Cubic alloys, the most ductile Face-Centered Cubic (FCC) alloys were preferred because of their low LME sensitivity below 450 °C and despite the corrosion observed, in particular the selective dissolution of Ni. But in recent years, cases of LME sensitivity have been observed for austenitic steels at temperatures above 450°C and for FCC Complex Concentrated Alloys (CCA) from 300 °C in the presence of liquid LBE and from 400 °C in liquid Pb. Intergranular cracks were observed and selective dissolution of Ni and Mn were noted in specific conditions. Lower strain rates and higher temperatures promote LME sensitivity. The objective of the work is the study the occurrence of damage in the presence of liquid lead, LBE, and bismuth for a FCC metallic alloy under mechanical loading and decouple purely corrosion-related aspects from those related to LME aspects by mechanical tensile testing, microscopic characterizations, and thermodynamic analysis. Tensile tests have been carried out in air and in liquid Pb, Bi, and LBE saturated with oxygen at temperatures between 300°C and 500°C, at different strain rates. After test, fracture surfaces and cross-sections of the fractured specimens have been observed using SEM (Scanning Electron Microscopy), EDX-SEM (Energy Dispersive X-ray), and SEM-EBSD (Electron Backscatter Diffraction), to analyse the effects of the liquid metal on the fracture mode, microstructure (phases and composition), and cracking. Additional TEM (Transmission Electron Microscopy) analyses have been performed to investigate the damage, especially phase transformations. Thermodynamic analyses using Thermo-Calc to understand the evolution of the material in the presence of liquid metal towards equilibrium are studied. Taking into account all these investigations, the corrosion, the corrosion induced by mechanical loading, and the liquid metal embrittlement occurrences are discussed.

Mechanical properties of neutron irradiated 316L stainless steel additively manufactured by laser powder bed fusion: effect of post-manufacturing heat treatments

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E8_1, Z2 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Rapid advancements in additive manufacturing (AM) technologies are driven by the opportunity for industries to revolutionize the global part manufacturing and supply chain landscape. They are now opening up opportunities for nuclear industry to build complex components while reducing cost, time, energy consumption and carbon footprint [1]. In that context, austenitic stainless steels are one of the main targets to be used for reactor core and primary coolant system components, since they offer a good combination of strength, ductility, and toughness, together with low sensitivity to oxidation-corrosion and superior irradiation resistance.

In this work we performed an investigation of 316L material produced by AM, Laser Powder Bed Fusion (L-PBF) process, with four heat treatment conditions: stress relief, low and high temperature solution annealing and hot isostatic pressing (HIP) [2]. Neutron irradiation experiments were performed in the material testing reactor BR2 of SCK CEN at 300 °C and with a dose up to about 4 dpa. Pre- and post-irradiation experiments were performed, including Charpy impact and tensile tests as well as the microstructural investigations based on scanning electron microscopy and transmission electron microscopy.

Despite variation between initial conditions in terms of microstructure and yield stress, neutron irradiation causes hardening in all investigated alloys, with a converging yield stress for all alloys at about 4 dpa. In all Charpy tests of 316L L-PBF samples, the increase of neutron dose caused a gradual decrease of absorbed energy: at the highest dose of about 4 dpa, the relative decrease of absorbed energy is the largest for the solution annealed at 1150 °C (SA1150) and HIP batches. An increase of irradiation induced hardening is fully correlated to the decrease of absorbed impact energy. This study does not indicate a positive impact of the HIP treatment regarding in-pile mechanical properties, since impact of the porosity difference is observed. Microstructural investigations focusing on the fracture surface properties and atomic scale defect characterization were performed allowing mutual comparison of different additive manufacturing batches and the reference material to their mechanical properties.

[1] W. E. Frazier, Metal additive manufacturing: a review J. Matls. Eng. Perform., 23 (2014) 1917-1928.

[2] M. J. Konstantinovic et al., J. Nucl. Mat. 607 (2025) 155662.

Harmonization of materials testing for LFR: R&D proposal on guidelines for corrosion tests in molten Pb/LBE

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The scattering on experimental data is an important issue for the design of nuclear systems working with innovative coolants. Indeed, the difficulty to predict the corrosion and mechanical behaviour because of the non-alignment of experimental data is reflected in the delay in the qualification path of materials in the specific environment. About that, in the frame of the past European collaborative project GEMMA, Round-Robin tests on static corrosion tests in Pb and LBE (candidate coolants for LFR systems) were performed by various European laboratories to check the alignment of the methodology and the results. The round-robin tests were performed by the partners in Pb and/or LBE using the same experimental conditions (same type of material, HLM temperature, comparable oxygen concentration, comparable surface finishing) but using their own experimental device for corrosion tests. At the end of the corrosion tests, a large scatter of data in terms of entity of corrosion was observed among the results of the various partners participating to the tests.

Currently, there are no commonly agreed standards related to the execution of corrosion tests in liquid metals such as liquid Pb alloys. Preliminary guidelines for corrosion tests and post-test analysis of specimens have been implemented a decade ago in the MATTER project and round-robin tests have been performed by laboratories in LBE. However, despite using the same device for corrosion tests and test specimens were centrally produced, the results of the tests varied significantly. For this reason, aiming at speeding up the qualification of materials, it is mandatory to identify potential reasons of the data scattering and to prepare and develop adequate guidelines/protocols and standards for the execution of the corrosion tests and the post-test analysis on the exposed specimens.

The present abstract describes an R&D project proposal focused on the alignment of the methodology and results in the corrosion practice in molten Pb/LBE. The proposal was developed in the frame of the activities of CEN Workshop 064 Phase 4 “Design and Construction Codes for Gen II to IV nuclear facilities” promoted by AFCEN. The project is organized in three main phases and tasks: 1) preliminary definition of guidelines for corrosion tests and post-test analysis of specimens; 2) execution of round-robin tests by the European laboratories to validate the guidelines and to take possible actions to mitigate the scattering; and 3) final version of the guidelines and submission of standard practices to standardization bodies.

Corrosion mitigation strategies in molten lead: coatings and advanced alloys for nuclear LFR systems

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Austenitic steels such as AISI 316L and 15-15Ti AIM1 are being considered as candidate structural materials for nuclear Lead-cooled Fast Reactors (LFRs). However, their chemical compatibility with molten lead represents a major issue due to severe corrosion effects. Non-protective oxidation and solution of steel constitutive elements are commonly observed phenomena, particularly severe in low dissolved oxygen conditions and/or at high temperatures. These limitations restrict the applicability of these materials only to specific operational conditions. In response, the nuclear materials research community is developing strategies to mitigate the corrosion damage. To address these challenges, two main solutions are being considered: 1) the use of high-resistant coatings or surface modifications deposited on the candidate structural steels, and 2) the employment of new advanced bulk alloys with intrinsic corrosion resistance.

This study focuses on assessing the chemical compatibility of ceramic alumina coatings, FeCrAl pack cementation and advanced bulk AFA (Alumina-forming Austenitic) steels when exposed to molten Pb, to be used as potential strategies against liquid metal corrosion. For the purpose, coated-steel specimens and AFA specimens were exposed to molten lead at a temperature of 550 °C for durations up to 8000 hours in the frame of H2020 GEMMA project. The exposures were performed using the experimental facility BID1 at the ENEA Brasimone, consisting in a mixed tank containing 150 liters of molten lead in which the samples were immersed. Post-test examination was performed on the exposed specimens using SEM-EDX and XRD techniques. After the exposures, it was observed that the alumina coatings and the FeCrAl pack cementation showed no evidence of corrosion and mainly conserved their structural integrity, being able to act as a corrosion barrier. AFA steels showed promising and outstanding corrosion protection features in molten lead, demonstrating to be a good candidate solution as bulk structural material in LFRs.

Correlation between creep and stress relaxation properties in a martensitic steel

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E8_4, Z3 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

The demand for longer service lives for power plants clashes with the difficulty of obtaining reliable material performance data over time.

Extrapolation over long timescales of properties determined through accelerated testing is a complex and not risk-free practice, yet sometimes it is necessary because of time consuming experimental testing. In this paper, a strategy to potentially accelerate the characterization of creep properties by performing repeated relaxation tests is suggested.

The method, applied on the martensitic high alloyed steel X20Cr13, relies on the similarity of the physical mechanism leading to mechanical stress relaxation (stress reduction under constant strain) and creep deformation (strain increase under constant stress), which is a powerful incentive to correlate the results of creep tests and stress relaxation tests (SRTs).

Simple approaches, such as assuming a power law between stress and strain rate are usually unreliable, however it is shown that after a number of repeated SRTs, the rate of the stress drop, proportional to the creep rate via the Young's modulus, decreases and eventually matches the minimum creep rates measured in conventional creep tests.

The procedure is not to be considered as a replacement of creep testing, since design codes under creep conditions require proper creep data. However, it could be used to estimate creep rates at stress values too low to be investigated in reasonable time (for example for the determination of the negligible creep regions) or to quickly check if a new batch of a material already known has consistent properties. Another possible field of application could be life assessment, a situation in which only limited portions of material are usually available, since a single relaxation test could be used instead of a set of creep tests.

Three new high alloyed AFA steels for LFRs

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

Alumina-forming austenitic (AFA) steels satisfy two key criteria for materials suitable for use in lead fast reactors. They can form in-situ alumina scales that can mitigate the corrosion attack of liquid Pb, and they have an austenitic structure that is necessary for avoiding issues with liquid metal embrittlement. Therefore, AFA steels are one of the advanced material solutions that are at time intensively discussed among the designers and developers of LFR's. Within the EU project INNUMAT KIT designed three high alloyed AFA materials targeting phase stable austenitic steels that can withstand liquid Pb at 600°C and above. The composition of the AFA alloys were optimized using thermodynamic modelling. The amount of Al was kept as low as possible in combination with the Ni and Cr content to suppress as much as possible the formation of ferritic phases, but also as high as required to foster alumina formation during exposure. The latter was based on achieving similar Al activity like for already successfully tested AFA materials.

Finally, three different steels with the following composition were manufactured at SWERIM in Sweden and hot rolled for testing: AFA-A: 15.2Cr 22Ni 2.7Al 3Mn 0.8Nb 0.2V 0.08C 0.02Y; AFA-B: 15.2Cr 24Ni 3.1Al 3Mn 0.8Nb, 0.2V, 0.08C, 0.02Y, and AFA-C: 14.5Cr, 24Ni, 3.85Al, 3Mn, 0.8Nb, 1.1W, 0.08C, 0.02Y. Nb, V and W were added for higher strength at elevated temperatures.

Following final annealing, all three alloys exhibit a fully austenitic structure, with grain sizes ranging from 50 to 100 µm. The alloys are exposed to liquid Pb with an oxygen content of 1×10^{-7} wt% at three different temperatures: 500°C, 600°C and 700°C. Each specimen is exposed on two differently prepared surfaces: one side is polished, and the other is ground. The specimens exposed at 700°C show signs of surface attack in certain areas. The presentation will provide insights into the corrosion resistance of the three high-alloyed AFA steels in liquid Pb at the three temperatures, aiming to forecast their long-term behaviour and explore ways to enhance compatibility, if necessary. Additionally, the susceptibility of the three steels to liquid metal embrittlement (LME) will be addressed taking into account the results of Small Punch Tests performed in air and in liquid Pb at different temperatures and strain rates.

Development of physics-based models for volatile fission products in minor actinide-bearing fuels for generation IV reactors

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E8_3, Z3 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Fission Generation-IV technologies aim to reduce waste generation and enhance fuel efficiency by adopting Minor Actinides (MA)-bearing fuels, which enable the transmutation of MA. In this context, Fuel Performance Codes (FPCs) are necessary to conduct safety analyses and to accelerate the qualification of MA-fuels, but their predictive capabilities must be enhanced by advanced modeling of MA-fuel thermomechanical behavior. This study develops a physics-based model for volatile fission products (FPs), such as cesium, iodine and tellurium, in MA-fuels. Volatile FPs migrate toward the outer fuel pellet, where they contribute to the formation of the Joint Oxide Gaine (JOG) that affects fuel behavior and cladding corrosion. The developed model, which comprehensively describes the production, transport, and release mechanisms of volatile FPs within the fuel, is implemented into SCIANTIX, an open-source computer code, developed at Politecnico di Milano, aimed at simulating fission gas behaviour in nuclear fuels at the meso-scale level. Once validated, the model will significantly enhance the predictive capabilities of FPCs thanks to their coupling with SCIANTIX, supporting the design and qualification of advanced nuclear fuels for next generation reactors.

On a physics-based model of HBS pores overpressurization and its effects on high burn-up fuel fragmentation

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In nuclear reactor accidents with high heating rates and/or temperatures of oxide fuel, overpressurization of gas-filled bubbles and pores can lead to fuel material rupture into fine fragments and gas release into the rod free volume. A fracture-mechanics-based model, developed and validated by the author, predicts fission gas release from micro-cracks propagating from overpressurized grain-boundary bubbles in UO_2 . This work extends the model to High Burn-up Structures (HBS), focusing on fuel fragmentation driven by overpressurized HBS pores. The extension required further investigation into stress intensification due to spherical pores and detailed knowledge of gas content, cavity size, shape, and number density. Additionally, the dependence of HBS material properties on temperature, burn-up, and low-angle grain-boundary (LAGB) accumulation were considered, based on experimental observations of UO_2 radial microstructural evolution. The extended model is integrated into SCIANTIX, an open-source computer code, developed at Politecnico di Milano, aimed at simulating fission gas behaviour in nuclear fuels at the meso-scale level. Once validated against experimental data, the model will provide a tool for predicting high burn-up fuel fragmentation (HBFF), allowing the extension of average burn-up limits of nuclear fuel and enhancing the efficiency and economic viability of nuclear power.

Microstructural characterization of advanced doped UO₂ fuels

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E8_3, Z3 Room (Level -3), septiembre 18, 2025, 14:30 - 16:30

Uranium dioxide based nuclear fuels have been widely investigated for their performance in light water reactors (LWRs). The findings of this study provide valuable insights into the impact of doping UO₂ fuel, contributing to the development of high-performance nuclear fuels with improved safety, efficiency, and durability for future reactor applications. Therefore, incorporation of various additives or dopants into UO₂ matrix has been explored to enhance its physical and chemical properties, leading to improved fuel behavior during irradiation.

Dopants serve distinct purposes in modifying fuel characteristics. Grain size growth can be achieved through the addition of Cr₂O₃, Nb₂O₅, Al₂O₃ or V₂O₅. Mechanical properties can be improved with the inclusion of ZrO₂, while Enhanced Thermal Conductivity (ETC) can be obtained by incorporating SiC, BeO, Al₂O₃ or MgO. Additionally, burnable neutron absorbers (BNA), including Gd₂O₃ and rare-earth oxides of Sm₂O₃, Dy₂O₃, Eu₂O₃, and HfO₂, play a crucial role in controlling excess reactivity in nuclear reactors.

Among the promising dopants, europium and zirconium stand out. Europium is an effective, neutron absorber, making it suitable for use as burnable neutron absorber for extended reactor cycles as Eu₂O₃ with less than 10 wt%. This approach optimizes reactor operation by mitigating the initial excess reactivity in fuel assemblies. Meanwhile, zirconium-doped UO₂ ceramic pellets exhibit outstanding performance in LWRs environments (Shippingport, with 26-38 wt% of UO₂), with greater corrosion resistance in high-temperature water or steam, stable thermal conductivity under irradiation, low neutron absorption cross-section, and reduced swelling rates compared to undoped UO₂ fuel, in addition to be a promising matrix for actinides disposal.

Understanding the microstructural properties of optimized nuclear fuel is essential for fuel design, development, qualification, manufacturing, and predicting in-reactor behavior. This research examines the influence of Eu and Zr doping on the microstructure of UO₂ fuel pellets, both capable of withstanding the demanding conditions of nuclear reactors. Pellets containing varying concentrations of Eu₂O₃ (0.02, 0.2, and 2 wt%) and ZrO₂ (20, 40 and 80 wt%) were prepared. The density, phase composition and microstructure of these ceramic samples were characterized using the Archimedes method, X-ray diffraction (XRD), Raman spectroscopy and scanning electron microscopy (SEM).

Development, Qualification and Industrialization of materials for Lead Cooled fast Reactors – The INNUMAT approach

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E8_2, Z3 Room (Level -3), septiembre 18, 2025, 10:30 - 13:10

The harsh working conditions typical of GEN IV fission reactors impose the development of NEW materials or the tailoring of REFERENCE materials to general requirements of nuclear applications and to the specific requisites of the considered technology.

Among GEN IV NPPs under development using Heavy Liquid Metals coolants, LFRs (Lead-cooled Fast Reactors) technology is one of the most promising.

To foster the R&D efforts and the industrialization of such LFR technology, the European Community launched several projects. INNUMAT project aims to develop innovative structural materials for nuclear applications and put them on track towards qualification for fission lead-cooled and molten salt fast reactors as well as fusion DEMO.

The REFERENCE materials studied within INNUMAT for LFR NPP are

- AISI 316
- HEAs
- AFA steel
- Coated 15-15Ti
- Weld Overlay

While the NEW materials are:

- FeCrAl ODS;
- Mo Alloys;
- MAXTHAL and MAX PHASES

In INNUMAT approach, the development of new materials or of referenced ones and their application at prototypical and industrial level is organized in different phases:

- High through-put development of new materials and tailoring of referenced materials for GEN IV LFR applications.
- Pre – qualification campaign performed on a wide range of materials. During these stages is advisable to use standardized tests and if not possible proceed with the implementation of interlaboratory Round Robin Testing. This methodology aims to mitigate variability stemming from measurement techniques and testing procedures by isolating the material as the sole variable. By enforcing standardized testing conditions across all participating laboratories, the generated data can achieve the desired levels of comparability, consistency, accuracy, and reliability. All mandatory requirements to obtain the recognition as a new standard and helpful to achieve the acceptance within nuclear construction codes ASME BPVC and RCC-MRx at the end of the development process.
- Complete qualification campaign performed on the candidates selected at the conclusion of pre-qualification activity. Qualification shall be performed taking in account also the materials manufacturability assessment at industrial level and the requirements for the acceptance of new materials within ASME BPVC and RCC-MRx construction codes.
- Materials industrialization process and acceptance procedure within nuclear construction codes ASME BPVC and RCC-MRx;

Scope of this presentation is to discuss the main aspects in material development approach proposed in INNUMAT project for LFR reactors, the limitations and the “grey-areas” of nuclear construction codes ASME BPV and RCC-MRx, and perspectives on future applications.

Investigating Water Radiolysis and Iron Speciation in Water-Cooled Breeding Blanket for DEMO: Implications for Corrosion Mitigation and Surface Effects

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E8_4, Z3 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

Understanding the effects of radiation on coolant chemistry is essential for ensuring the long-term integrity of structural materials in advanced nuclear fusion systems. In the framework of DEMO's Breeding Blanket (BB), exposure to neutron and gamma radiation induces water radiolysis, generating reactive species (e.g., O₂, H₂O₂, HO•) that significantly influence corrosion mechanisms and surface degradation. When additional elements, such as iron ions, are introduced into the system due to dissolution or corrosion of structural materials, their interactions with radiolytic products can significantly alter the chemical equilibria. Understanding how these species influence and are affected by radiolysis is crucial, as it directly impacts material degradation, coolant stability, and overall system performance.

To investigate these effects, we performed numerical simulations assessing the interplay between water radiolysis, iron speciation, and pH evolution in the Water Cooled Lead Lithium (WCLL) Breeding Blanket cooling circuit. The study focuses on the transformations of Fe²⁺/Fe³⁺ under irradiation and their impact on oxidation-reduction equilibria, with implications for material surface stability in operational conditions.

The results highlight that iron oxidation and hydrolysis strongly influence the local pH, leading to substantial variations that can accelerate material degradation. Additionally, the effectiveness of hydrogen addition in reducing oxidant concentrations has been shown to depend on both iron content and pH.

This study contributes to the broader effort of optimizing water chemistry for advanced nuclear applications, providing fundamental insights into the interplay between radiolysis, surface reactivity, and material degradation. A deeper understanding of these mechanisms is essential for evaluating the effects of irradiation on material surfaces, particularly in relation to corrosion processes, to enhance component longevity in nuclear environments.

2012

High velocity impact on tungsten: molecular dynamics study

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E8_4, Z3 Room (Level -3), septiembre 18, 2025, 17:00 - 19:00

We investigate high-energy collisions between tungsten (W) dust particles and tungsten plasma-facing components (PFCs) in fusion reactors. Using advanced Molecular Dynamics (MD) simulations, the study reveals significant material deformation, melting, and vaporization resulting from W projectile impacts at velocities up to 9 km/s. The results indicate that crater volume and dislocation length increase linearly with impact kinetic energy across samples containing over 350 million atoms. Our study involves the effect of impact angle, temperature and crystal orientation of the single crystal W target, with the first attempts to simulate polycrystalline target as well. The analysis of microstructural defects, such as helium bubbles and vacancies, further reveals their impact on crater formation and dislocation interactions. By integrating experimental data with simulation insights, a novel damage model was developed, significantly advancing our understanding of dust-wall interactions needed for refined predictive models to enhance the resilience of PFCs in advanced fusion reactors.

High-Entropy Zirconates as future Thermal Barrier Coatings: Resistance to Corrosion by Volcanic Ashes and Sands

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E9_1, Seminario 8 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Optimization of processes and the maximization of the usage of resources is crucial for an environmentally lower impact of technology. In this context, thermal barrier coatings (TBCs) are used in airplane turbines, to protect the metallic substrates from high temperature and harsh atmospheres. This allows operating the system at temperatures higher than the melting point of the substrate. With increasing operating temperature, the fossil fuel is combusted more completely, and the efficiency according to Carnot is maximized. The state-of-the-art TBC material yttria-stabilized zirconia is supposed to be advanced. Rare-earth high-entropy zirconates are promising new TBC materials. Therefore, their thermophysical properties need to be investigated and assessed. Additionally, TBCs also need to act as environmental barrier coating (EBC), withstanding inorganic dusts, sands or volcanic ashes that are ingested into the turbine while operation. These debris particles are mainly composed of calcia, (magnesia), alumina and silica, thus commonly called C(M)AS. The melting of these particles can lead to the infiltration of the T/EBC, and due to chemical interaction, the coating can be damaged irreversibly. The interaction of those new materials with (C(M)AS) need to be examined in order to estimate the resistance and extend of corrosion.

Our investigation of the high-entropy rare-earth zirconates $(\text{Nd}_{0.2}\text{Sm}_{0.2}\text{Gd}_{0.2}\text{Dy}_{0.2}\text{Er}_{0.2})_2\text{Zr}_2\text{O}_7$ and $(\text{Y}_{0.2}\text{Nd}_{0.2}\text{Sm}_{0.2}\text{Gd}_{0.2}\text{Dy}_{0.2})_2\text{Zr}_2\text{O}_7$ with the (C(M)AS) model compositions $\text{C}_{24}\text{A}_{17}\text{S}_{59}$ and $\text{C}_{33}\text{M}_9\text{A}_{13}\text{S}_{45}$ (values in mol%) show the formation of the apatite $\text{RE}_{14}(\text{SiO}_4)_9\text{O}_3$ and zirconia as main reaction products. The $\text{C}_{33}\text{M}_9\text{A}_{13}\text{S}_{45}$ interaction shows a faster consumption of the zirconates that are detectable via X-ray diffractometry (XRD) only after 5 min of reaction time. Zirconates are still detected after 1 h of $\text{C}_{24}\text{A}_{17}\text{S}_{59}$ interaction. For reaction with $\text{C}_{24}\text{A}_{17}\text{S}_{59}$ longer than 50 h, additionally the formation of zircon is observed, which is the result of a higher content of silicon in comparison to $\text{C}_{33}\text{M}_9\text{A}_{13}\text{S}_{45}$. Thus, in the $\text{C}_{33}\text{M}_9\text{A}_{13}\text{S}_{45}$ corrosion, all silicon is consumed for the formation of the apatite phase. Next to XRD analysis, energy dispersive electron microscopy (EDX) is used to determine the newly formed phases. With this method the non-crystalline anorthite phase $\text{CaAl}_2\text{Si}_2\text{O}_8$ is identified, which is the residue of non-reacted $\text{C}_{24}\text{A}_{17}\text{S}_{59}$ that is forming a glass upon cooling.

Infiltration experiments gain deeper insight into the solid-melt interaction and diffusion of cations during the reaction progress.

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Design and properties of novel innovative insulating materials for high-performance motors of electric vehicles

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The development of high-performance electric motors has become increasingly important owing to the paradigm shift in the energy system of mobilities from petroleum to electricity. Electric surge causes a partial discharge between the coil wires in the motors, which causes the breakdown of the insulation material on the coil. Therefore, the development of thermostable insulating materials with high electric discharge resistance is one of the key technologies for the practical application to next-generation electric devices.

We have recently developed a novel composite material, whose electric-discharge-resistant lifetime is 10 thousand times longer than conventional motor coil insulators using boehmite alumina (BA) as the filler.

A recently developed motor coils have complex geometries, which drastically improves the performance, and stability of motors, and allows downsizing of motors. However, performing insulating coating on the novel coil is difficult with the conventional varnish dipping method due to the surface tension of the solution. Electrophoretic deposition (EPD) is a technique that allows a coating without defect. Therefore, the development of polyimide (PI)/BA composite materials with EPD ability is important for high-performance electric vehicles and other electric devices.

We have developed several PI/BA hybrid EPD materials. One example of the hybrid electrodeposition materials of PI and BA was easily prepared by the reprecipitation method to give suspension whose particle size is 120 nm and the zeta potential was +38 mV. The suspension was very stable after long-time standing. The electrodeposition of the material was performed on a copper plate as a cathode by the imposed voltage from 10 V to 250 V. The thickness of the coating layer reached 63 micrometers after 10 min electrodeposition. The Coulomb efficiency, 10% weight loss temperature, and the BA content of the EPD coating were 28 mg/C, 512 °C, and 17%, respectively. The BA content of the EPD coating relatively corresponds to the original BA content in the EPD material. The breakdown voltage was more than 6.6 kV, which was obtained by measuring leakage current increasing the implying voltage by 500 V/s at AC 50 Hz.

The molecular design and properties of other PI/BA EPD materials are also discussed.

Computational design of new electrolytes for supercapacitors

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
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One of the key challenges in developing safe and efficient batteries and supercapacitors lies in designing electrolytes with a broad electrochemical stability window. Achieving this requires a combination of experimental synthesis, characterization, and theoretical modelling. Accurate prediction of the electrochemical stability of new electrolytes is essential to accelerate the optimization of electrochemical energy storage systems. Although conceptually straightforward, determining the electrochemical stability window (ESW) of ionic liquid-based electrolytes is a computationally intensive and complex task. Various quantum theory approaches exist, each differing in accuracy and computational cost. The simplest method, albeit the least precise, involves correlating the ESW to the energy difference between the HOMO (Highest Occupied Molecular Orbit) and the LUMO (Lowest Unoccupied Molecular Orbital) [1]. A more advanced technique calculates the energy difference between ions and their oxidized/reduced forms, considering both vertical and adiabatic transitions. This approach can also account for implicit solvent effects and zero-point energy, though it still has limitations [1]. Another approach factors in a surrounding shell of counter-ions for the ion under study, addressing long-range electrostatic effects while using an implicit solvent model [2]. However, this method requires arbitrary decisions about the number of counter-ions included and does not accurately simulate Coulombic interactions between them. We propose a novel method to estimate ion energies using a multiscale QM/MM approach. In this framework, the ion of interest is treated using an accurate quantum mechanical method, while the surrounding counter-ions are modelled with a semiempirical approximation. Counter-ion distributions are derived from geometries generated by classical molecular dynamics simulations, with long-range electrostatics addressed through an implicit solvation model. By integrating the accuracy of quantum mechanics with the efficiency of molecular mechanics, this approach enables more precise and computationally practical predictions of the ESW for ionic liquid-based electrolytes. Our model was successfully validated ionic liquids based on the TFSI⁻ anion and the PYR13⁺, PYR14⁺ and EMIM⁺ cations.

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Optimizing press-fit diodes reliability through manufacturing process modifications

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The reliability of press-fit diodes in power electronic applications is a challenge due to the multicomponent nature of these devices, because the high currents that leads to high temperatures during operation induce thermomechanical stresses at the interfaces. To assure long lifetimes and small failure rates, the design of the diode as a well as a robust manufacturing process is essential. In this work, we show how the changes in the manufacturing process to increase the robustness of the device determine the quality of the diodes. Heating processes were modelled and measured by thermography to determine the influence of the solder thickness and uniformity in the thermal behavior of the devices, so they can bear high currents to reach temperatures in the order of 250°C in the epoxy region, which is the hottest part of the diode. A further improvement of the behavior was obtained by the proper choice of an epoxy with a limited expansion. It eventually reduces the stress and strain effects at the interfaces, preventing the breakdown of the diodes even at continuous currents as high as 40 A.

Titanium Production Through Carbon Free Methods - The UAT Process

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E9_1, Seminario 8 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Reducing the reliance on carbothermic reduction of metal ores is a key challenge facing the metallurgical industry in the modern age. Carbothermic reduction processes emit greenhouse gases and often other harmful chemicals. To help overcome this issue, UAT has developed and patented a scalable metallothermic reduction route for the production of titanium. The process presented here consists of two major steps: 1) metallothermic reduction of a Ti bearing ore to form a metal phase and a slag phase and 2) electrorefining of the extracted metal to form a high purity titanium “wool” product. The UAT method produces no direct greenhouse gases, outperforms existing processes in energy requirements, and functions using a wide variety of ore types. Furthermore, alloys such as Ti-64 and TiAl_x can be produced directly without the implementation of an alloying stage. The resulting wool can be ground into powder, directly pressed and sintered without the aid of a binder, or used as a feedstock for other melting processes. In this presentation, we will review the thermodynamic basis of the extraction step, as well as some details of the electrorefining step, discuss the various types of ores that can be used, and review a variety of alloy compositions that can be directly synthesized with UAT’s two-step process.

Sustainable Synthesis of High-Performance Lithium Nickel Manganese Oxide Cathodes: A Study of Mn-Based Precursors and Calcination Effects

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E9_1, Seminario 8 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Lithium-ion Batteries (LIB) have been in the center of research interest in recent years due to the growing demand for efficient energy storage across diverse applications. From small consumer electronics such as smartphones to large-scale implementations in electric vehicles (EVs), buses and e-bikes, LIBs play a crucial role in modern energy solutions. Additionally, their integration into grid-level storage systems, particularly in conjunction with photovoltaic (PV) and wind energy, is expanding rapidly.

One of the most critical components of LIBs, both in terms of cost and efficiency, is the cathode. Among the various cathode materials studied, lithium cobalt oxides (LCO), derived materials such as nickel-rich layered oxides ($\text{LiNi}_x\text{Co}_y\text{Mn}_{1-x-y}\text{O}_2$) and lithium-rich layered oxides, and high-capacity organic cathodes have been extensively explored. In particular, lithium manganese oxides (LMO) and lithium nickel manganese oxides (LNMO) have attracted significant attention due to their high working voltage ($\sim 4.7\text{V}$), favorable theoretical capacity ($\sim 147\text{ mAh g}^{-1}$), and cost-effectiveness.

This study focuses on the development of high-performance LNMO cathode materials with a targeted stoichiometric composition of $\text{Li}_1\text{Ni}_{0.5}\text{Mn}_{1.5}\text{O}_4$ (LNMO). Two different Mn-based precursors were investigated: (i) calix-flashed calcined and quench-cooled Mn_xO_y micron-sized powder and (ii) MnO_2 synthesized in NTNU via the HAlMan process. The HAlMan process is a novel method that enables the production of MnO_2 during the process from readily available, low-cost raw materials, reducing dependency on conventional mining and refining methods. By utilizing this approach production costs can be optimized while aligning with green chemistry principles, contributing to the development of environmentally friendly cathode materials for next-generation lithium-ion batteries.

Both precursor materials were subjected to calcination at 800°C to achieve the desired spinel structure, ensuring optimal electrochemical performance. A comparative analysis was conducted to assess the impact of precursor selection on the structural, morphological, and electrochemical properties of the synthesized LNMO. Additionally, the influence of varying calcination conditions was explored. X-ray diffraction (XRD) confirmed the formation of a well-ordered spinel phase, while scanning electron microscopy (SEM) provided insight into structural and morphological information depending on the precursor selection.

Electrochemical characterisation, including galvanostatic charge-discharge cycling and electrochemical impedance spectroscopy (EIS), provided valuable insights into capacity retention, rate performance, and ionic conductivity. The findings highlight the advantages of using calix-flashed calcined Mn_xO_y and HAlMan-processed MnO_2 as a sustainable and cost-effective alternative Mn source for LNMO synthesis over commercially available Mn_xO_y sources, reinforcing their potential for next-generation lithium-ion batteries.

Development of new equations for unsaturated infiltration.

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E9_1, Seminario 8 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Infiltration processes are widely used in the manufacture of composite materials, but today it is still a challenge to find equations that accurately describe the process. The equation that governs them (Navier-Stokes equation) has not yet been solved. Therefore, there are different approaches that describe the process more or less faithfully. First of all, we must define whether the process is reactive or not. In the case of reactive infiltration, it is the chemistry that governs the process, as has just been clearly demonstrated [1], a fact of great relevance since in transport there are two fundamental parts that are manufactured using this technique.

If there is no chemical reaction, there are two main approaches to describe the process, if we ignore the simplest one, which is Darcy's law [2], such as Richard's law and the modification of Darcy's law for unsaturated liquids where we can use the Brooks and Corey approximation [3] or others [4].

In this work, a new approximation is shown based on the description of fluid dynamics in non-cylindrical pores of liquids that do not wet the solid and the effect of saturation. Another very different case is when the liquid wets, and under certain conditions the flow of fluids can occur through what has been called creeping liquids.

The equations developed have been used to describe the infiltration process of liquid Al alloys, in porous media mainly of porous SiC preforms, and to a lesser extent of Al₂O₃, TiC, graphite [4-6]

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Composite materials obtained by reactive infiltration: The Si-Ti-C system

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Within the aeronautical industry, one of the most advanced materials used is the SiC/Ti composite material, where the reinforcement is SiC fibers obtained by CVD, among other parts, which have been used in the manufacture of turbine blades. Therefore, the Si-Ti-C system is of vital importance in this industry [1].

In this work, another view of the Si-Ti-C system is shown, but in this case for the manufacture of SiC/TiSi₂ composite materials by reactive infiltration [2-4]. These materials have the advantage over SiC/SiC obtained by reactive infiltration in that at high temperatures, as occurs with the SiC/MoSi₂ system, there is a ductile-brittle transition that makes them viable competitors as a complement to SiC/SiC in jet engines, where they have achieved an improvement in energy efficiency of 5%.

In this research, both the infiltration process of different Si-Ti alloys and the optimization process are presented. The infiltration kinetics and the thermomechanical properties of all the materials obtained have been analyzed. The mechanical properties have been analyzed both at room temperature and at 900° C. These materials show an increase in bending strength of 25% compared to their counterpart obtained by Si infiltration at room temperature, and have shown greater creep resistance.

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Sustainable Aviation Fuels from CO₂ and H₂: Additive Manufacturing-Enabled Catalyst Systems

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E9_1, Seminario 8 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The transportation sector, like many others, faces the critical challenge of reducing fossil fuel consumption and minimizing carbon dioxide (CO₂) emissions—a concern that is particularly acute in aviation, which accounts for approximately 2–3% of global CO₂ output. In response, innovative methodologies are required for the production of renewable synthetic fuels from CO₂ and green hydrogen (H₂).

This study introduces a Power-to-X technology designed to convert CO₂ and H₂ into sustainable fuels and high-value chemicals—such as synthetic kerosene for aviation—alongside other valuable products, all under comparatively mild reaction conditions. The process commences with the electrochemical reduction of CO₂ to carbon monoxide (CO), followed by the dehydration of primary alcohols and subsequent chemocatalytic reactions that synthesize long-chain hydrocarbons via biomimetic strategies.

The presentation will detail the process design with particular emphasis on integrating additive manufacturing techniques to fabricate catalytic systems exhibiting hierarchical porosity distribution. These advanced structures facilitate enhanced mass transport and improved overall process efficiency. By obviating the need for multiple upgrading steps and enabling operation under milder conditions through a hybrid catalyst integration system, the proposed concept markedly enhances the energy efficiency of fuel production, yielding higher outputs compared to conventional methods.

This advancement holds a potential for decarbonizing the aviation industry by providing a sustainable alternative to fossil-derived jet fuels, thereby reducing the sector's carbon footprint and contributing to the achievement of global climate objectives.

3D in vitro skin model as broadly available and comprehensive platform for antibacterial therapies

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F1_2, Z2 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Background:

The global rise of skin infections, exacerbated by antibiotic-resistant bacteria, is nowadays a great challenge to healthcare. Traditional treatments are increasingly losing their potential, leading to severe impacts on patient quality of life and survival rates. Consequently, many efforts are made to develop innovative antibacterial therapies. To test this new strategies, conventional methods, such as 2D cell culture and planktonic bacteria culture, often fail to replicate the complexity of infection environments, highlighting the potential of 3D in vitro skin models as a superior alternative.

Methods:

The initial focus of the study has been the development of a 3D in vitro skin model. The dermis compartment was biofabricated by embedding human fibroblasts in a gelatin methacryloyl matrix, with human keratinocytes seeded on top the dermis to form the epidermis. The models were cultured for 31 days in an air-liquid interface configuration. The model demonstrated robust barrier formation and extracellular matrix remodelling. A 3 mm biopsy puncher was used to simulate controlled wounding, followed by inoculation of *Staphylococcus aureus* (Gram-positive) or *Escherichia coli* (Gram-negative) to mimic infection. Antibiotic treatment was applied after 24 hours. The samples were subsequently analysed for bacterial survival and skin model responses.

Results:

Results were remarkable: differences between wounded and unwounded samples underlined the barrier effect: indeed, the bacterial proliferation was lower in unwounded samples, for both bacterial strains, meaning that the developed epidermis was able to partially stop the bacterial proliferation. Moreover, the 3D skin model was able to react to both wound and infection in a complete and complex way in terms of extracellular matrix deposition and remodeling, inflammatory response, antimicrobial peptides production and change in cellular behaviors, from epithelial to mesenchymal and from fibroblasts to myofibroblasts. Another important outcome was the change in skin response during infection, showing the ability of both bacteria, in different ways, to impair the model immune response. Also, the antibiotic interacted with the model, modulating some markers, giving some evidences of the release of endotoxins with *Escherichia coli* death.

Conclusions:

In conclusion the developed 3D in vitro skin model has the potential to become a future landmark as platform for infection investigation and novel therapies testing. Indeed, it demonstrated to be able to behave in a complex and complete way despite being easily producible and low cost. These properties

put it in a prominent position for future standardization of platforms to test antibacterial therapies and strategies.

ADDITIVE MANUFACTURING OF BIOABSORBABLE CONTINUOUS WIRE-REINFORCED COMPOSITES FOR TISSUE ENGINEERING

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F1_3, Z2 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Additive Manufacturing (AM) has emerged as a transformative approach in biomedical research, offering significant advantages for addressing bone defects, where the fabrication of highly complex and patient-specific structures is essential. Bone tissue presents unique challenges for scaffold development due to its microstructural complexity and variation in mechanical properties. Effective 3D-printed scaffolds should replicate these characteristics while incorporating bioabsorbable materials to support bone healing. Unlike permanent implants, which remain in the body as foreign materials after and may require second surgeries for removal due to inflammatory responses, bioabsorbable implants gradually degrade and are absorbed in the human body. As a result, after degradation, only the natural tissue remains. On the other hand, composite materials are considered a promising option for bone scaffolds, as they combine the benefits of both polymers and metals. However, achieving polymer-based composites with mechanical properties that effectively mimic both cortical and trabecular bone remains a significant challenge, particularly for cortical bone, where higher mechanical demands must be met. Among AM techniques, Fused Filament Fabrication (FFF) is the most suitable for this purpose, as it allows the processing of a broader range of materials than other 3D printing methods, including continuous wire-reinforced composites. The integration of continuous wire reinforcement enables greater implant customisation by adjusting wire orientation in each layer to optimise the mechanical properties according to application and patient needs. This approach provides an optimal solution for enhancing the mechanical performance of polymer-based scaffolds used in bone regeneration. However, despite its potential, limited research has been conducted on the manufacturing of 3D-printed continuous wire-reinforced materials, with only a single study exploring biocompatible and bioabsorbable materials for tissue engineering.

The aim of this work is to manufacture and characterise bioabsorbable wire-reinforced polymers as a potential solution for the healing of bone defects. The first step involves a feasibility study in which polymer matrix composite laminates, reinforced with large diameter (300 μm) continuous metallic wires, will be manufactured using different wire orientations. For the first time, multidirectional wire-reinforced materials will be produced by FFF. Once the manufacturing method is validated, composite laminates of polylactic acid (PLA) and magnesium wires will be fabricated and analysed. Mechanical characterisation and degradation studies will be conducted to ensure that the laminate design accounts for progressive materials degradation without compromising structural integrity, thereby aligning with the regeneration time of native tissue. Finally, biological characterisation will be carried out through in vitro testing.

Gelatin Methacryloyl as an effective alternative to conventional matrices for patient-derived 3D models of metastatic colorectal cancer (mCRC).

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F1_2, Z2 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Gelatin Methacryloyl (GelMA) is a biomaterial that has gained increasing attention in biomedical research in recent years due to its remarkable tunability and biocompatibility properties. As a semi-synthetic hydrogel derived from gelatin and functionalized with methacrylic anhydride, its features can be easily modified through variations in concentration and crosslinking degree, allowing for the creation of highly customizable matrices for 3D models¹.

Colorectal cancer is the third leading cause of cancer-related deaths worldwide and the 5-year relative overall survival for metastatic patients remains poor. This study introduces a tunable matrix based on GelMA for enhancing 3D models of patient-derived metastatic colorectal cancer (mCRC). Traditional 2D cell cultures inadequately replicate the complex tumor microenvironment, limiting the accuracy of preclinical drug testing and cancer research. The developed GelMA-based matrix aims to overcome these limitations by providing a more physiologically relevant scaffold that mimics the extracellular matrix of mCRC.

The study has been carried out with five patient-derived mCRC organoids from the XENTURION platform shared by Prof. L. Trusolino². All the organoids derived from liver metastatic, heavily mutated and resistant CRC tumor and showed the same transcriptional profile and sensibility to drugs of original tumor. The GelMA-based matrix was synthesized and optimized through in vitro 3D proliferation essays, for mechanical properties and biocompatibility, supporting realistic cell morphology, proliferation, and invasion behaviors. Two different types of GelMA sources (porcine type A and bovine type B) have been tested and three different concentrations for each one. Methacrylation level and GelMA concentration dictate pore size and matrix stiffness, impacting cell behavior. Different GelMA-based matrix morphology was analyzed via SEM, stiffness assessed through rheology, and methacrylation degree quantified using the Fluoraldehyde quantitative assay (OPA assay).

In vitro assays demonstrated that the GelMA A-based matrix is comparable to existing 3D culture systems in maintaining essential cellular functions and interactions. Two-week 3D cultures in the GelMA A-based matrix showed that patient-derived mCRC organoids proliferated and organized into typical tube-like structures, displaying good interactions and high viability upon confocal analysis and MTT assay.

The next steps will involve performing long-term 3D cultures in the GelMA matrix and subsequently confirming the tight similarity in the transcriptional profile and drug response of the patient-derived mCRC organoids. Ultimately, the aim is to propose our matrix as a valid alternative to conventional ones (Matrigel, BME), leveraging GelMA's superior tunability, mechanical stability, greater batch-to-batch consistency, biological versatility and low cost of self-lab-production^{3 4}.

Advanced composite nano-structured bioactive scaffolds for bone tissue engineering

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F1_2, Z2 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

The treatment of large bone defects is currently one of the major challenges in clinical orthopedics, as defects resulting from musculoskeletal tumors, infections, or trauma are unable to heal spontaneously, even with adequate medical care. The development of novel macro-porous bioactive composite nano-structured materials for treatment of large bone defects and human hard tissue regeneration is the main focus of this research, aiming to enable controlled volume, improve osseointegration and promote the formation of new bone tissue. In the first step multi-ion doped nano-structured meso-porous calcium hydroxyapatite (nHAp) was synthesized hydrothermally and multi-ion doped nano-structured meso-porous bioactive glasses (nBAG) was synthesized using micro-emulsion sol-gel method. In the second step, biodegradable scaffolds based on a poly(methacrylic acid)/gelatin interpenetrating network (IPN) were developed using 3D-printing and free radical polymerization. The effects of inorganic nano-particles on the microstructure, biodegradability, swelling behavior, mechanical properties, and biological performance of composite scaffolds were investigated. Magnesium, strontium, copper, and zinc therapeutic cations, used as dopants during the synthesis of rod-like nHAp and spherical nBAG particles, were successfully incorporated into the crystalline and amorphous structures, respectively. In both cases, biocompatible particles with the desired morphology and meso-porosity were obtained. The resulting composite hydrogels, based on poly(methacrylic acid) and gelatin IPN, exhibited a uniform microstructure and appropriate macro-porosity and biocompatibility. The biodegradability and porosity of the 3D-printed composite hydrogels were further controlled by the formation of a polymeric coating on the scaffold surface. The swelling behavior, biodegradability and mechanical properties in large quantities depend on the percentage of incorporated nHAp and nBAG bioactive particles. Both the 3D-printed and free radical polymerized scaffolds also showed potential for the controlled release of antibiotic and anticancer drugs. Due to their superior physico-chemical, mechanical, and biological properties, the obtained bioactive materials exhibited significant potential for applications in biomedicine, and bone tissue engineering.

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Macrophage Immune Response to a Skin-Mimicking Biocompatible Matrix: A Functional Insight

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F1_2, Z2 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

3D biological models able to reproduce the physiology and the behavior of human tissues/organs are the focus of the newest groundbreaking research, enabling the scientific advancement of personalized medicine while simultaneously adhering to the principle of the 3Rs. Among the key features necessary to achieve a physiological and functional 3D model, there is the ability to replicate an immune response after stimuli. During the immune response, the immune system recognizes substances or microorganisms, for the purpose of defending against exogenous factors. The immune response, as the inflammation, implies the ability to recruit immune cells, as lymphocytes, granulocytes, monocytes, macrophages and others, in the damaged site of the skin, activating biological cascades of signals which matures the inflammatory response. Reproduce the complete and complex response to pathogens of in vitro immune system, considering both resident and circulating, is almost unexplored in literature for 3D skin model.

In this contest, a particular focus can be put on the behavior of monocytes and macrophages, which play a crucial role in the pro- and anti-inflammation processes, within the biological 3D skin model previously developed in our lab. This 3D model is composed by the epidermis and dermis layers, which are constitute respectively by human keratinocytes and human fibroblasts. Fibroblast are embedded in gelatin methacryloyl (GelMA) to obtain a three-dimensional structure with cell-embedded. The ability to act as a barrier was verified.

The research here presented directs its attention to the differentiation and polarization processes of monocytes and macrophages. They were cultured within the gelatin methacryloyl matrix in different radio and concentration. The differentiation process, as well as signaling processes between cells of the same type and between monocytes and macrophages, were extensively analyzed by fluorescence microscopy, digital PCR, colorimetric analysis.

Further analysis were conducted to unveil details on the interaction between macrophages, monocytes and other immune cells, as healthy lymphocytes, when embedded in gelatin methacryloyl.

The incorporation of immune cells, into the existing epidermis-dermis skin model creates a more advanced and physiologically relevant platform for drug and therapy screening. This innovation will greatly improve the model's functionality, providing a dynamic system for studying skin-related immune reactions. By closely mimicking the interactions between skin tissues and the immune system, this model will serve as a valuable tool for investigating disease mechanisms and therapeutic responses.

Advanced Hydrogel Bioinks composed of Natural Nanofibers and Polysaccharides for 3D Bioprinting applications

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F1_3, Z2 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

The advent of 3D bioprinting has revolutionized fields such as tissue engineering and drug development, by enabling the biofabrication of 3D cell-laden constructs that mimic native tissues architecture. This innovative technology relies on the layer-by-layer deposition of ‘bioinks’ (cell-laden biomaterials) under computer-controlled conditions to create functional biological tissue analogues. Polysaccharide-based hydrogels are widely employed as bioink matrices due to their favorable rheological properties, ease of crosslinking, structural similarity to the extracellular matrix, and inherent biocompatibility. However, achieving a precise control over their mechanical and rheological properties remains a challenge. One promising approach to address these limitations is the incorporation of nanostructured additives, which can enhance the performance of hydrogel-based bioinks.

In this communication, we explore the use of natural nanofibers, such as protein amyloid nanofibrils and nanofibrillated cellulose, into polysaccharide-based hydrogel bioinks composed of alginate [1], pectin [2], gellan gum [3], cellulose [4], FucoPol [5], and carrageenan. These biobased nanofibers, characterized by their high aspect ratio, mechanical robustness, thermal stability, and biocompatibility, demonstrate significant potential for the development of nanocomposite bioinks with enhanced rheological properties and printability. The incorporation of these nanofibers results in 3D bioprinted constructs with superior mechanical integrity and improved biological performance, paving the way for advanced biofabrication strategies in regenerative medicine and other biomedical applications.

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Improving Fatigue Resistance in Organic-Inorganic PCL-Based Melt Electrowritten Scaffolds for Biomedical Applications

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F1_1, Z2 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

Biological structures such as coral, tree, enamel and fish bone demonstrate exceptional fatigue resistance, allowing them to withstand repetitive mechanical loading over prolonged periods without experiencing structural failure or degradation [1]. Understanding the fatigue behavior of engineered biomaterials is crucial to ensuring their durability and long-term functionality under dynamic mechanical forces inspired by these biological structures [2]. Consequently, anti-fatigue properties have become a significant focus in biomedical engineering, given their critical role in the design of implants, scaffolds, and prosthetics [2,3].

The objective of this study was to develop fatigue-resistant organic-inorganic structures using melt electrowriting (MEW) technology. MEW is a solvent-free additive manufacturing technique that employs electrohydrodynamics to fabricate micron-scale fiber struts with a highly ordered pore architecture and interconnected porous networks [4,5]. Initially, highly ordered MEW scaffolds were fabricated using polycaprolactone (PCL), a gold-standard thermoplastic polyester for MEW applications [6]. In the present study, the scaffolds were designed with varying fiber orientations, including 0-90°, 0-60°, 0-45°, and 0-30°, to evaluate the influence of architecture on mechanical and fatigue performance. On the other hand, to enhance the surface properties of the PCL-MEW scaffolds, an alkaline surface treatment was performed, followed by the coating of the scaffolds with gelatin (GEL) solutions loaded with mesoporous bioactive glass nanoparticles (MBGNs). Scanning electron microscopy (SEM) analysis revealed bead-free and uniformly deposited layers by layer PCL-MEW scaffolds, as well as the successful coating of GEL or MBGNs-loaded GEL on their surfaces. Additionally, Fourier transform infrared (FTIR) spectroscopy further confirmed the presence of PCL, GEL, and MBGNs in the coated scaffolds. Furthermore, preliminary quasi-static nanoindentation tests conducted on strips of the neat PCL-MEW scaffolds revealed a reduced elastic modulus of 1.1 GPa and a hardness of 70 MPa. These findings suggest that integrating organic and inorganic components into MEW scaffolds offers a promising strategy for enhancing fatigue resistance under various loading conditions. This approach highlights the potential of MEW technology in developing advanced biomaterials for biomedical applications.

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Keywords: melt electrowriting, organic-inorganic structure, fatigue properties

Fabrication and Optimization of GelMA Hydroxyapatite Scaffolds for 3D Printing via Digital Light Processing

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F1_4, Z2 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Advancements in digital light processing (DLP) technology for 3D printing of polymer-ceramic photocurable resins are driving innovation in medicine and tissue engineering. This approach allows for the fabrication of highly precise, biocompatible scaffolds tailored for tissue regeneration. The development of sustainable photocurable resins derived from natural and biodegradable components offers a safer alternative to conventional epoxy and acrylate-based materials, reducing both toxicity and environmental impact. These next-generation materials enhance biocompatibility, optimize structural integrity, and contribute to more efficient and personalized solutions for bone and cartilage tissue repair.

In this study, a biocompatible photocurable polymer-ceramic composite was formulated using gelatin-methacrylate (GelMA) and hydroxyapatite (HA) nanoparticles (~300 nm average size). GelMA was synthesized in water at different pHs, and its degree of functionalization (DoF) was analyzed using nuclear magnetic resonance (NMR) spectroscopy. The photocurable resin was prepared by dissolving GelMA in water, followed by the addition of a photoinitiator and HA nanoparticles. To optimize the 3D printing process, curing depth experiments were conducted by adjusting LED power and exposure time. Rheological analysis was performed to evaluate viscosity and investigate how variations in GelMA/water ratio and HA content influence the resin's flow behavior during printing. FTIR analysis was conducted to evaluate the degree of conversion and the efficiency of photopolymerization. Additionally, FESEM analysis was performed to investigate the internal microstructure, including the dispersion of HA within the GelMA matrix, pore morphology, and overall homogeneity of the composite scaffolds.

NMR analysis revealed that GelMA synthesized at pH 10 achieved the DoF, that is 92%. The enhanced DoF at pH 10 improved crosslinking efficiency during photopolymerization, as assessed with FTIR analysis, leading to stronger and more stable samples with superior mechanical properties and controlled degradation.

Printability tests indicated that a GelMA concentration of 30 w/v% provided the best printing performance. Compositions with HA content ranging from 15% to 55% were printed to evaluate the balance between printability and mechanical performance. After printing, samples were freeze-dried and their physical, mechanical and morphological properties were evaluated. FESEM micrographs revealed a not homogenous dispersion of the ceramic filler inside the matrix and new tests are ongoing to overcome this drawback. Moreover, HA addition affected samples porosity, leading to a more homogenous pores distribution with less interconnected pores. On the other side, as expected, density increased by increasing HA content. Finally, preliminary mechanical tests confirmed the benefits of HA addition on the GelMA/HA scaffolds compressive strength.

Volumetric 3D Printing toward 3D printing complex structures for biomedical application

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), settembre 15, 2025, 13:15 - 14:30

Vat polymerization processes, which are based on the photopolymerization of a photocurable resin, in the last few years have broadened their application field from industries, research, healthcare and everyday life [1].

These technologies enable high-resolution prototyping and fabrication but are limited by slow layer-by-layer printing and the need for support structures for complex geometries.

For these reasons, new technologies have emerged in the recent years, also known as Volumetric 3D Printing (VP), to overcome these limitations. They are a light-mediated based on photopolymerization process and on a layer less approach which directly polymerizing a defined resin volume, enabling printing of complex, low-defect 3D objects within seconds and without support structure. Among all, Xolography is brand-new VP technologies that we recently buy in our lab. This is a VP technology where the curing processes is mediated by a photoswitchable photoinitiators, also known as dual-color photoinitiators, added to the resin which are activated by a first wavelength, while absorption of the second wavelength induce a local photopolymerization. Thus, polymerization only occurs at the intersection of lights of the two wavelengths.

Herein we present the development of water-based formulations and all the characterization to assess the suitability of them for the Xolography processes. [2,3]

For this work, Poly (ethylene glycole) Diacrylate (PEGDA) with different molecular weight was employed as photoactive monomer. Indeed, PEGDA is reported to be widely used for the fabrication of hydrogel thanks to its good solubility in water and biocompatibility and, in addition, it allows to obtain complex functional 3D structures.

The proposed approach enables the possibility to obtain 3D complex structures within minute which can be

further functionalize for biomedical application, for example, as bioelectronic interface by inducing a conductive phase exploiting an interfacial polymerization [3].

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Polysaccharides chemical modification for biomedical additive manufacturing

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F1_3, Z2 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Polysaccharides are carbohydrate-based biomaterials that are extensively used in the biomedical field. Their unique chemical structures are critical in determining their bioactivity exploited in a wide range of applications. However, some limitations may potentially hinder their use. In this context, many approaches have been studied to incorporate additional functional groups, cross-link the macromolecular structure, and vary the physico-chemical properties of the polysaccharides [1].

In this contribution, the application of computer-aided wet-spinning [2] was investigated to process different polysaccharide hydrogels into 3D scaffolds exploitable for tissue engineering: i) hyaluronic acid and chitosan polyelectrolyte complex scaffolds chemically cross-linked with poly(methyl vinyl ether-alt-maleic acid) (PMVEMA) [3] and ii) carboxymethyl chitosan scaffolds ionotropically crosslinked with Zn²⁺ and grafted with collagen [4].

The polyelectrolyte complex formation, cross-linking, and chemical functionalization were studied by infrared spectroscopy, nuclear magnetic resonance, thermogravimetric analysis, mass spectrometry, and differential scanning calorimetry. Furthermore, it was established that cross-linking processes were effective in improving the stability of hydrogels in physiological environment. Zn²⁺ crosslinking endowed the scaffolds with strong antimicrobial activity against E.coli and S.aureus. The in vitro cytocompatibility of both types of hydrogels was assessed using the Balb/3T3 clone A31 murine embryonic fibroblast cell line. The results indicated that the PMVEMA cross-linking and the collagen grafting enhanced cell biocompatibility and colonization within the scaffolds, as well as the wound healing process. This demonstrates that these hydrogels are suitable for long-term cell culture experiments and wound dressings for skin regeneration.

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Cell-Derived Extracellular Matrices for 3D in vitro Tumor Models for Breast Cancer Research

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F1_2, Z2 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Decellularized Extracellular matrices are new scaffolds for bioengineering of 3D tumor-ECM in vitro models. The tunable composition, properties, and structure of Cell-derived Matrices (CDMs) make them versatile and easy to use by using desired cell types. Moreover, ECM composition can be modulated with the use of specific cells, or stimulants such as macromolecular crowding (MMC) or biomolecules. The aim of this work is to develop fibroblast CDMs from human dermal fibroblasts (hDFs) at 2D and from bone marrow human mesenchymal stem cells (BM-hMSCs)/Human Adipose-derived stem cells (hAMSCs) at 3D on PLA microparticles to assess their potential to bioprint cancer models for drug screening.

In this study, we generated CDMs from hDFs at 2D culture and CDMs from bone marrow human mesenchymal stem cells (BM-hMSCs)/Human Adipose-derived stem cells (hAMSCs) on Poly Lactic acid (PLA) derived microparticles (MPs) using several stimulants, and decellularized by chemical methods. MPs were generated by jet break-up method, and their size distribution was calculated by ImageJ whereas their porosity was imaged under SEM.

The ECM production before and after decellularization was evaluated by BCA, hydroxyproline, qRT-PCR, immunofluorescence and mass spectrometry. Then, CDM was methacrylated (CDM-MA) to prepare CDM Hydrogels. Hydrogels Young modulus were determined. Methacrylation of CDM was verified by ¹H-NMR and porous structure of them was determined by SEM. After hydrogels characterization, bioinks were prepared by mixing MCF7 cells with CDM-MA and GelMA, and tumoroids were bioprinted. Cell-laden hydrogels were cultured for 14 days. Cell viability and morphology was evaluated by confocal microscopy. Moreover, the doxorubicin resistance of the cell-laden hydrogels was determined by Alamar Blue. Based on our results, HDF are able to deposit a CDM that closely recreates the tumor ECM. MCF-7 cells formed spheroids in CDM hydrogels and they were alive after culturing 14 days with a high resistance to doxorubicin. Mixing GelMA with CDM increased young moduli of hydrogels to recreate the tumor stiffness and enables the bioprinting of cancer models. Altogether, these findings suggest that CDM-based bioinks and hydrogels could be a powerful biomaterial to develop more physiological relevant cancer models.

Smart polymer materials based on fiber spinning and additive manufacturing

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F1_1, Z2 Room (Level -3), septiembre 15, 2025, 9:20 - 10:20

Polymer fibers are a unique type of material that combines a high aspect ratio, large surface area, and a high degree of orientation of polymer chains, allowing them to be used in a wide variety of applications, the most well-known of which is reinforcement.

However, the fibers are difficult to handle due to their length, making them difficult to combine with additive manufacturing. Various fiber spinning approaches, including electrospinning and electrowriting, have been used as an additive manufacturing method or in combination with additive manufacturing of smart structures. Despite the advantages of these fiber spinning methods, they have limitations. For example, programmable fiber deposition using electrospinning is challenging. Although electrospinning allows programmable fiber deposition, this method is slow, and the deposited fibers lack one of their main advantages, the orientation of the polymer chains, making them less effective for reinforcement. We have recently developed a fundamentally new fiber spinning method that allows for fast and programmed fiber deposition of fibers with oriented chains and can be easily combined with additive manufacturing. This and other fiber spinning methods combined with additive manufacturing open new perspectives for the fabrication of smart biomimetic structures, such as for tissue engineering.

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3D Bioprinted Cell-Laden Gel for Autologous Chondrocyte Implantation (ACI) Procedures

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F1_3, Z2 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Autologous chondrocyte implantation (ACI) is a surgical approach designed to repair cartilage defects in joints by using the patient's chondrocytes. These cells are harvested, cultured in vitro, and then implanted into the defect site, typically secured beneath a membrane to ensure they remain in place. For example, matrix-assisted chondrocyte implantation (MACI) involves encapsulating the chondrocytes within a membrane before implantation. This study explores the potential enhancement of MACI through the Reactive Jet Impingement (REJI) bioprinting technique. Utilizing the Chondro-Gide commercial product, the REJI bioprinting system was employed to print gels loaded with chondrocyte cells directly onto the surface of Chondro-Gide patches. This approach ensures that the bioprinted cell-laden gel features well-defined and consistent cell densities. Here we report on evaluating the use of REJI bioprinting utilising an in vitro ACI model.

The REJI bioprinting technique was utilized to print chondrocytes derived from the Y201 stem cell line within a collagen-alginate-fibrinogen (CAF) hydrogel. The gels were printed onto the surface of Chondro-Gide patches at two distinct cell densities: 5 million cells per mL and 25 million cells per mL of gel. Over 14 days, the expression of functional genes, extracellular matrix (ECM) formation, and mechanical properties were monitored. Quantitative and qualitative analyses were conducted through assays to assess cell viability, DNA quantification, gene expression (ACAN, COL2A1, COL1A1, and SOX9), immunocytochemistry, and immunohistochemistry. The morphology of the CAF hydrogels was also examined using scanning electron microscopy (SEM).

The REJI system successfully printed CAF hydrogels with low and high cell densities onto Chondro-Gide patches. Immunocytochemistry, immunohistochemistry, and SEM results demonstrated an increase in the production of collagen type II, glycosaminoglycans (GAGs), and ECM-like matrix components over the culturing period, with higher production rates observed in high-density CAF gels compared to low-density ones. These findings suggest that the phenotype and cell-cell interactions were preserved. Live/Dead assays confirmed the cytocompatibility of the CAF gels from the early stages of culturing. DNA quantification indicated that high-density chondrocytes encapsulated in CAF gels remained viable for 14 days.

The REJI bioprinting system effectively prints and maintains Y201-derived chondrocytes, facilitating the production of matrix proteins when cultured in vitro. High-density CAF gels exhibited enhanced production of collagen type II and ECM-like matrix, suggesting that a high cell density in a biomimetic gel formulation on Chondro-Gide may offer an improved approach to MACI for regenerating articular cartilage tissue.

Reactive jet impingement bioprinting with fibre, metal and ceramic substrates for enhanced composite cell cultures

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F1_4, Z2 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Reactive jet impingement (ReJI) is a bioprinting technique developed at Newcastle University which allows cell filled hydrogels to be printed onto a wide range of biomaterial substrates.

The process works through the generation of two droplet streams, one a polymer solution, and the other a solution which initiates crosslinking of the polymer solution to create a hydrogel. The droplet streams are directed to collide in a “V” configuration at which point the crosslinking reaction occurs and a hydrogel droplet is created which falls to the substrate. If cells are suspended in either the polymer solution or the crosslinking solution or both, then the cells are ultimately encapsulated in the hydrogel droplets and cell filled gel droplets are produced. Through using microvalves with the capability to produce droplets at a high frequency and using hydrogel systems which provide for rapid cross-linking reactions a high throughput bioprinting system can be produced.

A valuable aspect of this approach to printing cells is that because the solutions are dispensed from the micro-valves when they are suspended in low viscosity solutions no significant shear stresses are generated in the flow. The reaction which creates the high viscosity gel happens after the solutions have been jetted, and this means that hydrogels can be created which contain a high concentration of cells without affecting viability. The high concentration has advantages in terms of the bioactivity seen within gels: cell-cell and cell-extracellular matrix interactions are closer to those seen in native tissues which means that the behaviour of the in vitro cultures is more representative of real tissues.

This presentation will show how the ReJI bioprinting process can be used with fibre, metal and ceramic substrates to create composite structures for regenerative medicine or in vitro modelling. Collagen, alginate and fibrin bio-inks have been used to print a range of cell types onto calcium-alginate and polycaprolactone fibre substrates to produce smart wound dressings and cardiac models, and onto metal and ceramic substrates to biologically enhance musculoskeletal implants immediately prior to implantation. The produced cell cultures have been evaluated for cell viability and function to demonstrate the value of the bioprinting approach in promoting the development of bioactive composites.

3D constructs enhanced with nano(bio)materials for functional regeneration of both hard and soft tissues.

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F1_2, Z2 Room (Level -3), settembre 15, 2025, 10:50 - 13:10

Advanced clinical devices should not only serve as biocompatible support for tissue regeneration but also actively engage with host tissues to promote rapid and functional healing of both soft and hard tissues. Novel and personalized approaches are particularly needed when the intrinsic regenerative efficacy of tissue is impaired or delayed due to the patient's clinical context, the regenerative capability of the injured tissue, and/or the occurrence of concomitant complications.

To address this challenging perspective, advanced fabrication technologies like 3D printing and electrospinning have been extensively utilized in current literature to process both natural and synthetic functional polymers, creating biomimetic scaffolds for various clinical applications.

The potential and versatility of these constructs are further enhanced when combined with (bio)active and stimuli-responsive nanomaterials, enabling additional functionalities, such as the spatiotemporally controlled release of therapeutic agents and bio-specificity.

This contribution aims to showcase recent studies, primarily conducted within collaborative EU-funded projects, focused on designing and validating novel solutions to prevent adverse remodeling in bone, skin, and cardiac tissues. Composite 3D scaffolds and flexible nanofibrous membranes have been fabricated using 3D printing and electrospinning, employing a variety of engineered formulations. These formulations include both naturally derived polymers (e.g., collagen, chitosan) and synthetic polymers (e.g., PCL, PVDF), combined with nanomaterials such as bioactive mesoporous glasses (MBGs), mesoporous silica nanoparticles (MSNs) loaded with drugs, nano-hydroxyapatites, and superparamagnetic iron oxide nanoparticles. Additionally, surface functionalization with biomolecules or coatings that respond to endogenous or exogenous stimuli can expand the range of functionalities and modulate the release properties according to the targeted clinical specifications.

Focusing specifically on bone tissue engineering, collagen-based formulations enriched with nano-hydroxyapatite or MBG, were optimized with special attention to rheological properties and the inorganic/organic ratio to enable 3D printability or electrospinning. The inclusion of superparamagnetic nanoparticles was also explored to create stimuli-responsive membranes that promote cell differentiation through mechanotransduction mechanisms.

In the field of cardiac tissue regeneration, the focus will be on recent achievements in designing an electrospun piezoelectric patch enriched with ultrasound-responsive MSNs for in situ, on-demand release of anti-inflammatory and anti-fibrotic agents after myocardial infarction (MI). To achieve this, MSNs were grafted with sodium alginate and cross-linked with CaCl₂ to exploit the reversibility of coordination bonds between Ca²⁺ and COO⁻ groups of SA.

Furthermore, the final constructs have undergone extensive physicochemical characterization and in vitro/in vivo assessments, providing essential data on biocompatibility and the efficacy of the proposed clinical solutions.

Bilayer electrospun membrane enabling the stimulation of angiogenesis in advanced 3D skin model

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The skin, the largest multifunctional organ of the human body, acts as a protective barrier against physical, chemical and biological factors from the external environment, and is responsible for maintaining homeostasis, adjusting the temperature and hydration of tissues. The performance of the skin is a vital function, and any damage has a detrimental impact and requires an effective treatment. However, the market offers a limited number of medical treatments, and the availability of new therapies is slowed down by the difficult advancement from pre-clinical testing to clinical trials. To overcome this issue is imperative to transition from the conventional 2D cell culture and animal models to 3D in vitro models. These 3D in vitro models have the capacity to replicate the organization and physiological function of the natural tissue, are more cost-effective and manageable than animal models. Nevertheless, the development of 3D in vitro skin models presents significant challenges due to the complexity and heterogeneity of real skin, including vascularization, immune interactions and prolonged healing processes. Among these challenges, the formation of an organised vascular network is essential to maintain homeostasis and the pathogenesis of the engineered tissue. The purpose of the present work is to stimulate angiogenesis and the vascularization within a pre-existing dermis-epidermis 3D in vitro skin model¹ can be used as a platform for drug screening.

To achieve this objective, electrospinning (ESP) technology has been exploited to fabricate a fibrous structure comprising two overlapping layers, designed to facilitate the formation of endothelial tissue and the sprouting of vessels through various morphological stimuli of cells. The first layer features an oriented pattern, while the second layer has a random pattern. These different architectures are achieved by using different types of fibre collectors (rotating and plate collectors, respectively) during the electrospinning process. The targeted ESP formulations combine natural functional polymers, including collagen and gelatin, which promote cell adhesion, and synthetic polymers, such as polycaprolactone to provide mechanical support. The fibrous structures are intended to release a range of angiogenic factors, such as VEGF and EGF, to promote angiogenesis and sprouting of blood vessels through the skin model. The release of these factors over time will be modulated by several strategies, including the incorporation of degradable polymeric (i.e. polylactic-co-glycolic acid) particles and/or mesoporous silica particles, as well as the direct anchoring to the fibre surface.

¹S. Villata et al. 2024 ACS Appl. Mater. Interfaces

Advanced biofabrication technologies to design in vitro central nervous system models

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F1_4, Z2 Room (Level -3), settembre 15, 2025, 17:00 - 19:00

Introduction/Objectives

The recovery of central nervous system functions after injuries remains an unmet clinical need as neurodegeneration involves a cascade of biological events leading to neuronal damage and loss of tissue functionality, whose full comprehension is still not achieved.

Advancements in the creation of engineered 3D in vitro models of nervous tissue provide new opportunities in the understanding of these mechanisms, due to the ability of these models to mimic the neural microenvironment with greater physiological relevance than traditional 2D culture systems. Here we combine additive manufacturing technologies and biomimetic bioinks to develop a 3D neural construct, intended for the in vitro modeling of nervous tissue in physiological and pathological conditions.

Methods

Gelatin Methacryloyl and Thiolated Hyaluronic Acid were mixed to produce bioinks for a motor neuron cell line (NSC-34) and a neural stem cell line (NE-4C) encapsulation. The cell-loaded hydrogels were printed on a polycaprolactone (PCL) oriented microfibrillar structure, fabricated by melt electrowriting technique. The obtained constructs were cultivated for up to 21 days to achieve cell maturation towards astrocytes and neurons. Then, a traumatic event was mimicked by mechanical and chemical insults to recreate a spinal cord injured model in vitro.

Results

The optimization of photo-crosslinkable Gelatin methacryloyl (GelMA) and Hyaluronic acid-based hydrogels was carried out to successfully bioprint neural stem cells (NSCs) without affecting cell viability and behavior. According to the results, the 3D bioprinted scaffold effectively supported the growth and proliferation of encapsulated NSCs, providing an ideal microenvironment for their differentiation into mature neurons and astrocytes. Moreover, the inclusion of an anisotropic pattern was shown to direct neuronal cell elongation according to a preferential orientation, thus enhancing the establishment of a mature and interconnected neural network. Lastly, the efficacy of this system in modeling neuronal injury was assessed by reproducing nervous tissue trauma in vitro.

Conclusions

Overall, it was demonstrated that the combined use of biomimetic hydrogels and organized 3D structures can significantly foster neural cell maturation in vitro, thus offering new opportunities for the creation of functional engineered tissue analogs.

Acknowledgments

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Biofabrication of a piezoelectric cardiac patch for the regeneration of the infarcted heart tissue

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F1_4, Z2 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Heart failure post-myocardial infarction (MI) is among the leading causes of mortality worldwide, primarily due to the limited regenerative capacity of myocardial tissue. The Horizon Europe REBORN project aims to develop an implantable multifunctional fibrous patch able to promote the regeneration of ischemic tissue and restore the physiological cardiac functionality. To this aim, a drug-loaded piezoelectric patch, biofabricated by electrospinning (ESP) was developed. The patch is designed to promote cardiomyocyte activity thanks to the aligned fibres, electromechanical coupling, and the release of anti-inflammatory and anti-fibrotic agents, as well as cardiomyocyte proliferative agents to control biological events after MI.

Polyvinylidene fluoride (PVDF) formulations for ESP were prepared using a safe solvent mixture combining acetone and dimethyl sulfoxide. Aligned nanofibers (diameter of 200-300 nm) were produced using a rotating collector, and ESP parameters optimized, up to a pilot scale using a system with 15 needles. The optimized process enabled the attainment of high PVDF crystallinity (about 48%) and maximized the piezoactive β phase content (above 90%). Low-pressure oxygen plasma was used to modify the hydrophobicity of PVDF to a super hydrophilic-like behavior, improving biocompatibility and reducing inflammatory response, as observed in in vivo test on infarcted mice seven days after implantation. Drug loading in the fibrous patch was achieved by electrospinning hybrid formulations incorporating nanocarriers (e.g., mesoporous silica loaded with both anti-inflammatory and antifibrotic drugs), as well as by solubilizing the drug directly into these formulations. The patch also incorporates nanoparticles able to promote cardiomyocyte proliferation. The electrospun patch was characterized in terms of piezoelectrical and mechanical properties, obtaining good piezoelectric response due to the high amount of β phase ($d_{33} = -6.3$ pm/V) and suitable mechanical properties ($E = 65 \pm 12$ MPa; $\sigma_R = 11 \pm 2$ MPa). Cytotoxicity assays were performed using human cardiomyocytes and fibroblasts, and preliminary suturing in vivo tests were performed using mouse and pig models of MI. The patch can be easily handled and manipulated and was sutured to infarcted heart tissue in a pig model, withstanding pulling, stretching and needle passage without rupture. The patch delivery to the epicardium was proven using tools already available for transdiaphragmatic pericardial approach (e.g., integrated in electroanatomic mapping catheters). In summary, a low-toxicity ESP process was used to biofabricate a piezoelectric patch with suitable properties for being sutured on the infarcted heart tissue with low inflammatory response. The patch design was successfully optimized to enable the in situ release of anti-inflammatory, antifibrotic, and cardiomyocyte proliferative agents.

Novel biomaterial ink formulations and approaches for in situ bioprinting and regeneration of colorectal mucosa and submucosa

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F1_2, Z2 Room (Level -3), septiembre 15, 2025, 10:50 - 13:10

Two million individuals in the European Union suffer from colorectal diseases, which account for several pathologies that affect the mucosa and submucosa layers of the anus, rectum, and colon. Among these pathologies, familial adenomatous polyposis (FAP) and ulcerative colitis (UC) could benefit from the removal of the intestinal mucosa and submucosa. Currently, when their removal is necessary, patients undergo a proctocolectomy (i.e., surgical removal of the rectum and all or part of the colon) with a subsequent ileal pouch that preserves the patient's continence but is often burdened by significant complications.

In this context, the EU project "TENTACLE" aims to develop a radically new strategy for the surgical treatment of UC and FAP by means of an innovative in situ 4D bioprinting suite to fabricate shape-morphing, layered bioconstructs directly inside the patient's rectum/colon. The unique formulation of the bioconstructs will promote the regeneration of colorectal mucosa and submucosa and will enable tissue regeneration also by delivering antibiotics and antifibrotic molecules. In addition, the mucosa layer will possess a shape-morphing capability, triggered by humidity, that will induce the creation of crypts on its surface, aiming to replicate the natural colorectal ones.

The TENTACLE in situ 4D bioprinting suite will include a novel colonoscopic bioprinter that will be mounted on commercial colonoscopes and will feature an extrusion-based bioprinting unit, a valvejet printhead, and a photocrosslinking apparatus.

Regarding the composite formulations used to print the layered bioconstructs, these will be based on two novel bioink formulations containing patients' cells and sharing a matrix based on photocrosslinkable gelatin and thiolated polysaccharides. These bioinks will be ad hoc enriched with engineered micro- and nano-carriers incorporating antibiotic and antifibrotic agents in the form of spray-dried micro- and nanoparticles and/or cyclodextrins.

The TENTACLE approach, in situ bioprinting suite, and composite bioink formulations will be validated ex vivo and in vivo in small rodents and swine models, thus paving the way for translating the approach, the bioprinting suite and the bioink formulations toward the clinics.

Overall, the TENTACLE project will introduce a minimally invasive alternative to proctocolectomy and is expected to positively impact the quality of life of patients affected by FAP and UC.

Bioprinting and electrophysiological evaluation of a 3D cardiomyocyte culture

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F1_3, Z2 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Cardiotoxicity has been the major reason for drug withdrawal from clinical trials. New in vitro cardiac models which appropriately reflect human physiology are required. Contractile functions of in vitro cardiac models are essential measurement in assessing cardiac physiology and responses to pharmacological interventions. In our study, we use reactive jet impingement (ReJI) bioprinting to fabricate a 3D cardiac cell model and measure electrophysiology through a high-density multi-electrode array (HD-MEA) system.

ReJI bioprinting uses two different valves to jet out the gel precursor bioink composed of collagen, alginate and fibrinogen (CAF) to react in mid-air with the crosslinker bioink of thrombin, calcium chloride and HL-1 cells, depositing on the substrate as 3D cell-laden hydrogel construct with cell density of 5×10^6 cells/ml. This work assessed the cell viability, morphology, expression of cardiac-specific biomarkers (myosin and desmin) and gene expression (anti-natriuretic peptide and connexin43).

To assess the contractile functions of the 3D in vitro model, HL-1 cells were cultured in 2D MEA chips as controls, while the 3D gel carrying HL-1 cells was bioprinted directly onto the 3D MEA chips. Both chips have 4096 electrodes with a pitch of 60µm. The 3D chip has the electrodes on pillars while the 2D has the electrodes embedded on plane surface, with each electrode able to record the electrical signals generated from HL-1's spontaneous contraction as field potential. The field potential in 2D samples began from approximately 0.7 mV with regular waveform on day 1 to 1.4 mV on day 3 and declined to 0.8 mV with an inconsistent waveform on day 7. The 3D gel samples instead had a field potential of 0.7mV with consistent waveform from day 1 to increased field potential of 1.8mV and well-defined waveform on day 7. We further assessed the pharmacological responses by exposing the HL-1 cardiac cell to the β -adrenoceptor agonist isoproterenol and selective hERG potassium channel blocker E-4031 separately, demonstrated increased and reduced beat rate respectively, suggesting CAF gel encapsulated cells can responds to drug applied externally.

This provides an improved cardiac tissue in vitro model, and the processing techniques allow for the development of more complex in vitro models, involving co-culture of different cardiac cell types, to study tissue function, response to drugs, and the testing of new devices for tissue regeneration.

Multiscale Perfusable Cardiac Tissue Model Using Electrospun PCL Fibres and a Bioprinted Cardiac Co-Culture

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F1_4, Z2 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Developing physiologically relevant in vitro cardiac models is essential for improving drug testing and advancing regenerative medicine. Here, we present a novel approach for reconstructing functional cardiac tissue using a perfusion-based system integrating electrospun polycaprolactone (PCL) fibre scaffolds and bioprinted cardiac co-cultures. The engineered constructs incorporate a high-density cell-laden hydrogel composed of collagen, alginate, and fibrinogen (CAF) to support cardiac myocytes and fibroblasts, forming a biomimetic microenvironment.

Using the Reactive Jet Impingement (ReJI) bioprinting technique, human cardiac myocytes and fibroblasts (5 million cells/mL) were precisely deposited within CAF hydrogel onto PCL fibres, forming an integrated cardiac construct (5 mm diameter, 20 mm length). These constructs were maintained in a custom-designed 3D-printed perfusion system, where an optimized flow rate of 5 mL/min using a peristaltic pump was applied to induce physiological pulsatile flow. After an initial static culture period, samples were divided into static and perfusion culture groups and maintained for an additional seven days. The perfusion system was designed with controlled media exchange through inlet and outlet channels, along with a drainage system to prevent leakage.

Cell viability, proliferation, morphology, and functional marker expression were analysed at key time points for static culture and perfusion culture using fluorescence microscopy, proliferation assays, immunocytochemistry, and gene expression analysis. Results demonstrated that perfusion culture enhanced cellular organization, proliferation, and enhanced cardiomyogenic marker expression, suggesting improved maturation and function compared to static culture.

This study highlights the potential of multiscale scaffold integration with controlled perfusion for constructing physiologically relevant cardiac tissue. The approach offers a robust platform for preclinical drug testing, disease modelling, and cardiovascular tissue engineering applications, reducing reliance on animal models and enhancing the translational relevance of in vitro studies.

Coaxial Electrospinning of an Anisotropic Piezoelectric PVDF-based patch for Modulated Drug Delivery in Myocardial Infarction Therapy

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F1_4, Z2 Room (Level -3), septiembre 15, 2025, 17:00 - 19:00

Myocardial infarction (MI), among cardiovascular diseases, is currently one of the leading causes of mortality worldwide. After an ischemic event, incorrect remodelling of myocardium occurs, with the formation of a non-functional fibrotic tissue. Current therapeutic strategies, including reperfusion and pharmaceuticals, do not consent tissue regeneration, postponing the progression of the disease, possibly until heart failure. In this context, the Horizon Europe REBORN project aims to develop a drug loaded, nanofibrous patch which enables post-MI tissue regeneration by integrating piezoelectric activity for electro-mechanical coupling with the surrounding tissue, alongside with in situ modulated drug delivery of anti-inflammatory, antifibrotic and pro-regenerative molecules. Electrospinning (ESP) has been selected for its ability to manufacture aligned nanofibrous scaffolds that replicate the anisotropic microstructure of physiological myocardium, as well as for its versatility. In fact, when ESP is used in its coaxial configuration (coax_ESP), it is possible to modulate the drug loading within the fibres, along the radial distance, thereby impacting the diffusion-driven release mechanisms. In this research, coax_ESP in combination with a rotating drum collector was used to fabricate a piezoelectric polyvinylidene fluoride (PVDF) patch, enabling a modulated co-delivery of Ibuprofen (IBU) and Pirfenidone (PIRF), and showing anisotropic mechanical features. PVDF is a fluoropolymer known for its excellent biocompatibility, mechanical durability, and piezoelectric features, which depend on its β -phase content. When PVDF is processed by ESP, it is possible to induce high β -phase recrystallization, thus increasing its piezoelectric activity. PVDF-based polymeric solutions were used for both the core and shell, to preserve ESP-induced piezoelectricity and mechanical features. IBU and PIRF at the concentration of 1% w/v were incorporated into the shell and core solutions respectively to enhance the anti-inflammatory release, while providing a slower and sustained release of the antifibrotic agent. The therapeutic windows of IBU and PIRF were defined by assessing drug concentrations' effects on inflammation and fibrosis markers in macrophages and cardiac fibroblasts. Computational analysis performed on SEM images confirmed the production of highly aligned nanofibers, with a dimension of approximately 300 nm. The characteristic β -phase behaviour along with the proper drugs incorporation were confirmed by XRD and FTIR. Additionally, DSC analysis showed an overall crystallinity of around 45%. Piezoelectricity of the patch was confirmed by piezoelectric coefficient calculation derived from butterfly-shaped hysteresis curve ($d_{33} \sim 10$ pm/V). The drug release kinetics, assessed by HPLC, highlighted the effectiveness of the coax-ESP in modulating the release of IBU and PIRF within their therapeutic windows.

Spray-dried polymeric carriers for in-situ mucosal and submucosal regeneration in colorectal disease

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Colorectal diseases accounts for more than 2.2 million deaths in Europe. Among these, familial adenomatous polyposis and ulcerative colitis are two severe conditions, with the former potentially leading to the development of colorectal carcinoma, while the latter showing limited response to pharmacological treatments over time. When surgical intervention is required, proctocolectomy (i.e. the complete removal of both the colon and rectum) or its restorative variant are typically performed, compromising patients' quality of life. In this context, minimally invasive removal of damaged mucosal and submucosal tissues and subsequent regeneration by innovative multi-functional engineered biomaterials has the potential to obviate the need for highly invasive surgery. Over the past few decades, drug loaded micro-, and nano-carriers based on synthetic and natural polymers gained increasing interest in the field of regenerative medicine, due to their excellent bioactivity, drug protection effect from environmental degradation and tuneable release kinetics. Their incorporation within an in-situ injectable hydrogel formulation mimicking mucosal and submucosal extracellular matrixes can synergistically promote the physiological tissue restoration while modulating the local delivery of the pharmaceuticals. In this research, chitosan (CHIT) and poly-lactic-co-glycolic (PLGA) based delivery systems were synthesized as micro- and nano-carriers using the spray-drying technique. Specifically, CHIT particles were loaded with neomycin (NEO) to provide a prompt, in situ, broad-spectrum antibiotic effect, while PLGA particles were loaded with pirfenidone (PIRF) to inhibit tissue fibrosis. CHIT was selected for its antioxidant, anti-inflammatory, and antimicrobial properties, which can be further enhanced by the short-term controlled release of NEO. Conversely, PLGA is a versatile and biodegradable polyester used for medium-term drug release systems (i.e., one to two weeks) of hydrophobic drugs. The optimization of the spray-drying process was conducted by testing different sets of parameters, including inlet and outlet temperatures, pump flow rate, and aspiration power, with the aim of achieving a single-step synthesis process for both the materials. Different polymer/drug ratios and molecular weights were evaluated and the resulting particles features, such as morphology, dimension and crystallinity versus amorphous features of the drugs were assessed. Cumulative drug release kinetics, evaluated by HPLC, were further tuned in their therapeutic windows by tailoring sodium-tripolyphosphate ionic reticulation and lactate/glycolate ratios respectively for CHIT- and PLGA-based carriers. To better mimic colorectal environment, release tests were conducted both in saline medium (TRIS-HCl) and in simulated intestinal fluid (SIF). Further tests on carriers' homogeneous incorporation in the in-situ injectable hydrogel will be assessed to ensure a reproducible drug release.

A Functional AM approach for Biofabricating Micro-Optofluidic Devices for Medical Non-invasive Diagnosis-related Bioapplications

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F1_3, Z2 Room (Level -3), septiembre 15, 2025, 14:30 - 16:30

Micro-optofluidic (MoF) devices, integrating microfluidics and optical sensing, offer significant advantages for medical diagnostics (Achille et al. 2021, Basiri et al. 2021, Bahmaee et al. 2020). They enable real-time, label-free detection with high sensitivity while requiring minimal sample volumes (Fiorini et al. 2005, Wu et al. 2023). Their potential for portable applications makes them promising tools for non-invasive disease monitoring across various medical fields.

In this study, a MoF device was designed, fabricated, and characterized for potential medical non-invasive diagnostic applications. It was manufactured using a functional Additive Manufacturing (AM) approach to ensure suitable optical properties, surface chemistry, and biocompatibility. A biocompatible and transparent 3D-printable resin was selected, and the device was realized using the P μ STL ultra-high-resolution 3D-printing technique.

The primary function of the MoF device is two-phase flow process monitoring through optical detection based on optical absorption phenomenon (Cairone et al. 2016). Its performance was evaluated by studying slug-flow and cell concentration monitoring. The investigated slug-flow process was composed by air and water. Slug-flow monitoring is essential in several physiological and pathological conditions, including respiratory, cardiovascular, renal, and neurological medicine (Selsby et al. 1990, Leerson et al. 2023, Mohsen et al. 2021). For instance, in respiratory medicine, slug-flow monitoring aid in assessing mucus clearance in chronic obstructive pulmonary disease. In cardiovascular care, it helps detect emboli in dialysis and extracorporeal membrane oxygenation, while in intravenous therapy, it ensures precise drug infusion. The device was also tested for cell concentration monitoring by analyzing a two-phase mixture of *Saccharomyces cerevisiae* cells suspended PBS at different concentrations. Accurate cell concentration measurement is crucial for diagnosing various medical conditions (Laszlo et al. 2014, Hassan et al. 2015, Lehnert et al. 2024). In oncology, label-free MoF devices can detect circulating tumor cells (CTCs) in blood for early cancer detection. In hematology, they assist in determining red and white blood cell counts to diagnose anemia and infections. In nephrology they involve urine analysis to detect kidney diseases through cellular debris and infection markers.

An extensive experimental campaign was conducted under various conditions, testing different laser power levels $P \in \{1;3;5\}$ mW, flow rate $FR \in \{0.1;0.2;0.3\}$ mL/min, and cell concentrations $C \in \{0;10^6;10^7;10^8\}$ in 10 mL of PBS. A Design of Experiments approach was used to determine optimal operating conditions for robust device performance. The results confirmed the MoF device's capability to effectively monitor slug-flow ($R^2 \in \{76.94\%;98.27\%\}$) and differentiate between different cell concentrations ($R^2=98.74\%$), demonstrating its potential for future medical diagnostics.

Functional Coatings with Macroscale Nanocontainers: Innovation or Redundant Complexity

Ph.D. Swathi Naidu Vakamulla Raghu¹, Ph.D. Adam Patalas, Prof Manuela Sonja Killian

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

ABSTRACT: Metal-oxide (MO) surfaces have successfully been modified to elicit specific responses attributed to either structural variations and/or chemical functionality. Structural modification of a bulk surface is achieved by exploiting the combined effects of top-down and bottom approaches during electrochemical anodization (EA). Imparting nanoscale geometries has reportedly improved biointegration as a result of structural similarities to corresponding biological environments namely, the extracellular matrix.[1] Additionally, an influence on surface reactivity due to chemical variations has also been observed.[2] In this context, nanostructured bulk surfaces are highly relevant as hybrid materials. This work investigates their ability to elicit multi-functional responses. Herein, nanocontainers are fabricated via EA and deposited onto ceramic implant discs.[3] These nanostructures can further be modified via facile application of self-assembled monolayers (SAM) to subsequently seal or 'cap' the nanotube mouths[4] making them ideal for triggered release applications in the biomedical field. Such bulk surfaces modified with nanotubes may be used to store drugs or therapeutics that can selectively release under appropriate conditions as this hybrid assembly can readily transform static bulk surfaces to those capable of dynamic elution from the overlying nanotubular reservoirs. The hybrid material was thoroughly characterized using scanning electron microscopy (SEM), ToF-SIMS, water contact angle measurements (WCA) etc. These nanocontainers would be capable of facilitating 'smart' developmental strategies towards controlled multi-drug release models that can even elicit sequential release of drugs to limit clotting, inhibit infection and ultimately promote healing.

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Solvothermal production of a piezoelectric layer on titanium implant materials

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F2_1, Andalucía I Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Demographic changes and advancing technologies have led to an increase in surgical procedures and the growing use of implants, particularly in dental and orthopedic applications, where titanium is predominantly used. Despite the numerous advantages of titanium, postoperative complications such as implant loosening and inflammation remain prevalent. To address these issues, surface modifications are required to enhance properties like osteointegration and the suppression of inflammatory reactions. Biomimetic development concepts, e.g. the interaction of tissue with piezoelectric surfaces, are very promising to be adopted. [1] This study focuses on developing a piezoelectric coating of barium titanate (BaTiO_3) on fabricated titanium implants.

Barium titanate, with its comparatively high piezoelectric charge constant of 200 pC/N, exhibits a pronounced ability to generate (bio-) electrical signals under mechanical stimuli, promoting metabolic activity, facilitating structural remodeling and growth. [2] In the study, the synthesis of barium titanate involves anodic oxidation of titanium to form a titanium oxide layer, followed by a two-step solvothermal process to convert the oxide into.

Intensive research have focused on the first step on transformation. The thickness, morphology and density should be adjusted so that ductile, adhering and tetragonal BaTiO_3 is produced, which is necessary to realize the piezoelectric reactions. For this purpose, anodic oxidation is investigated by varying the electrolytes, the voltage (20 – 100 V) and the oxidation time (5 minutes – 3 hours). Electrolytes used include sulfuric acid, sodium sulfate, a phosphate buffer and ammonium tetrafluoroborate. Resulting titanium oxide layers were analyzed via scanning electron microscopy (SEM) and X-ray diffraction (XRD) to assess their structure and phase composition.

Results indicate a positive correlation between oxidation duration and voltage (up to 80 V) and the thickness of the titanium oxide layer. The majority of electrolytes produced stable oxide layers with flower-like oxide structures emerging from the base layer. Only ammonium tetrafluoroborate generated tubular and spherical crystalline structures. Regardless of the morphology, anatase titanium oxide layers were formed in almost all experiments, except for one experiment using sodium sulfate, which produced rutile titanium oxide.

Future experiments will assess the ability of these titanium oxide layers to facilitate a optimized formation of barium titanate with the piezoelectric properties of the coating.

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Tailored-magnetic nanoparticles for theranostics in osteosarcoma

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Superparamagnetic iron oxide nanoparticles (SPIONs) have gained significant attention in cancer diagnosis and therapy due to their nanoscale dimensions, surface functionalization capabilities, and responsiveness to external magnetic fields. These properties make SPIONs ideal candidates for theranostic applications (1). While some SPIONs are commercially available as imaging contrast agents, only two have been approved for cancer treatment, and none have been specifically investigated for osteosarcoma therapy.

In this study, we explored suitable functionalization strategies of SPIONs using different ligands and coatings, including cyclodextrins (CDs), amino acids, silica, and polyacrylic acid (PAA). A comprehensive physicochemical and magnetic characterization was conducted to assess and compare their properties. Our studies pointed out that water-soluble MagnetoCyclodextrins (SPIONs-CD) exhibited excellent reproducibility, monodispersity, biocompatibility, and stability in water, PBS, cell culture media, and blood plasma for at least 24 hours and they were exploited as multifunctional drug delivery systems for osteosarcoma. Different drugs were included in SPIONs-CD (i.e., Salinomycin, Doxorubicin). Cellular behavior and cell/material interactions were assessed in vitro using various cellular models, including U2-OS osteosarcoma cell line, hFOB cells, bone marrow-derived mesenchymal stem cells (BM-MSCs), MDA-MB-231 human breast cancer cells.

Moreover, functionalization of SPIONs with 3-aminopropyltriethoxysilane (APTES) or PAA produced uniform, spherical nanosized particles armed with amine or carboxylic groups suitable for further decoration with ligands for radiolabeling (i.e., DOTA, DFO).

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Controlling release kinetics from nanotube drug containers - modulated diameters, capped and multi-molecule filled nanotubes

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The integration of drug delivery coatings in orthopaedic applications is attracting interest due to its potential to improve the success rate of implant systems. Several published reports have focused on the aspect of controlled drug release to aid in the optimization of drug delivery. Herein, we report on a novel and simple approach to extending drug release time and limiting the undesirable burst release from zirconia nanotubes (ZrNT) via structural modification.[1] The latter involves fabricating a double-layered structure with a modulated diameter and is achieved via voltage adjustment during electrochemical anodization. The drug loading and release studies from the structurally modified ZrNTs, characterized via SEM and ToF-SIMS were monitored using UV-Visible spectroscopy and compared with their homogeneously thick equivalents. We report a significant reduction in the initial burst release phenomenon using this modification and other complementary strategies investigating release inhibition systems,[2] resulting in an overall improvement in release performance. Capping and/or multi-molecule modification of the nanocontainers allows to render the drug release smart and responsive to external triggers. These simple modifications of ZrNT successfully enhance drug release performance, allow for flexibility in designing drug delivery coatings for specific implant challenges,[3] and offer new insights into alternate biomaterials based on metal-oxide nanostructures.

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Acknowledgements

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Characterization of Oxidized Alginate-Gelatin Nanocomposite Hydrogels Incorporating MXene Nanosheets for 3D Bioprinting

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Hydrogels are highly promising materials for tissue engineering applications due to their high water content and ability to fabricate individualized three-dimensional (3D) scaffolds. To further enhance their functionality, hydrogels can be combined with conductive materials, creating electrically conductive hydrogels (ECHs) that can mimic the electrical microenvironment of bone tissue. Such properties can promote osteoblast attachment, proliferation, and differentiation, ultimately driving bone tissue regeneration.

In this study, an oxidized alginate-gelatin (ADA-GEL) hydrogel was modified with MXene, an electrically conductive and osteogenic two-dimensional (2D) nanomaterial, to produce degradable and 3D printable nanocomposite hydrogels. We comprehensively investigated the influence of MXene concentration on the hydrogels' morphology, mechanical and electrical properties, 3D printability as well as swelling and degradation behavior. Additionally, cell-material interactions were evaluated in both 2D and 3D cell culture models using MG-63 osteoblast-like cells.

The results demonstrated that the hydrogel properties could be tailored by adjusting the MXene concentration, allowing the creation of a library of ADA-GEL-MXene nanocomposite hydrogels. Scanning electron microscopy and micro-CT imaging were performed to detect the MXene particles embedded in the hydrogel matrix. While the mechanical properties remained consistent across different hydrogel formulations, the electrical conductivity increased with higher MXene loading. Furthermore, all formulations supported 3D printing of grid-like scaffolds up to 10 layers. Moreover, the incorporation of MXene nanosheets improved the osteogenic differentiation compared to the pristine hydrogel, as evidenced by alkaline phosphatase staining. However, a critical MXene concentration threshold was identified above which cell behavior was compromised.

In conclusion, optimizing the MXene concentration is crucial to balancing mechanical strength, electrical conductivity, and biocompatibility. Nevertheless, the developed ADA-GEL-MXene hydrogels show great potential for 3D bioprinting and bone tissue engineering, with the additional possibility of applying electrical stimulation in future studies to enhance bone regeneration.

Magnetoelectric, bio-hybrid nanointerfaces as enablers of wireless tissue stimulation and drug management

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Magnetoelectric nanoparticles (MENPs) are capable of generating highly localized electricity if stimulated with a relatively low-intensity magnetic fields (H). MENPs are core-shell structures with an inner magnetostrictive phase and an outer piezoelectric shell, whose electrical output can be efficiently modulated via their composition, geometrical features, and interface area. Such multi-functional nanostructures have recently attracted a great interest in biomedicine, exhibiting at room temperature the so-called “magnetoelectric” (ME) effect, which is a linear coupling between an external H (in the mT range, human safe) and a generated, highly localized electric field (E, in the order of 105 V/m). Moreover, thanks to the possibility of either functionalizing their surface with bioactive molecules or encapsulating them in soft matrices, these unique nanostructures can be exploited for the fabrication of a plethora of biomedical devices for wireless, spatially-selective tissue stimulation and controlled drug delivery. In the study herein presented, CoFe₂O₄ –BaTiO₃ spherical MENPs were embedded within soft, biocompatible polymeric matrices, to develop flexible and functional biointerfaces. By adopting a holistic computational framework, a multi-physics, finite-elements model was established to (i) assess the effects of different materials-related parameters (i.e., MENPs volume fraction, polymeric matrix electrical properties) onto the electrical output of the bio-hybrid nanointerface, and to (ii) predict the optimal device configuration that could potentially interact with a biological surrounding.

MENPs' ability to release active drugs upon proper stimulation with external H has been recently experimentally demonstrated. By acting as nano-sources of E, MENPs can actively regulate their molecular interactions with loaded cargos and cells nearby. One of the hypotheses at the basis of this phenomenon lies on two subsequent steps: (1) the local E generated under a static H leads to a temporary dielectric breakdown of the cell membrane and particle penetration (nanoelectroporation); (2) under alternating H, a modulated dipole moment at the MENP outer shell is considered responsible for weakening the electrostatics bonds between particles and drugs. Based on these premises, we used our computational model to define the operational ranges, in terms of static and alternating magnetic fields, to maximize MENPs' nanoelectroporation and drug delivery performances. ME nanointerfaces surely represent powerful tools to develop alternative, cutting-edge therapeutic strategies. Within this framework, our studies not only are providing material-based recipes for an optimal MENPs-system fabrication, but are also contributing to gain thorough insights on the MENPs functioning at the interface with a biological surrounding, to effectively attain their bioresponsive capabilities.

Hydrogels based on natural polymers for the magneto-mechanical stimulation of cells

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F2_1, Andalucía I Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The development of 3D cell scaffolds utilizing magnetic-responsive materials represents a significant advancement in addressing persistent challenges in Tissue Engineering [1, 2]. This approach enables the creation of structured materials that can be simultaneously manipulated by external magnetic fields, providing non-invasive control over both the mechanical properties and biological behavior of the scaffolds.

In this study, we introduce a novel class of magnetoactive, biocompatible hydrogels synthesized by incorporating biopolymers (such as polysaccharides and proteins), magnetic microparticles, and living cells into a colloidal suspension. These hydrogels function as an effective artificial extracellular matrix that supports and promotes cellular growth, proliferation, and differentiation. To achieve controlled patterning of the scaffold's microstructure, a triaxial magnetic field [3] is applied during gelation, organizing the magnetic particles into microstructures within the hydrogel matrix. Non-stationary magnetic fields are then used to remotely activate and manipulate these microstructures over time, offering dynamic control over the cellular microenvironment.

To analyze the hydrogels' response to magnetic stimulation, we integrate advanced techniques such as videomicroscopy and confocal rheometry with the triaxial magnetic field generator. These methods allow for real-time, in-depth observation of the hydrogel's behavior under magneto-mechanical forces. The results demonstrate that magneto-mechanical stimulation induces significant changes in the internal microstructure of the hydrogels, leading to localized deformations. These deformations are shown to influence key cellular processes, including migration, proliferation, and differentiation. Additionally, ongoing investigations are focused on understanding how these mechanical deformations affect cellular biochemical and morphological changes.

This innovative approach offers important insights into the interaction between cells and magnetoactive materials, providing a pathway for optimizing their use in biomedical applications. This work enhances our understanding of how mechanical and magnetic stimuli can influence cellular behavior, paving the way for the next generation of Tissue Engineering solutions. Furthermore, the precision and control enabled by the triaxial magnetic field technique establish it as a valuable tool for microrheological characterization, facilitating the analysis of hydrogel mechanical properties at the microscale in ways previously not achievable.

Acknowledgements:

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Magnetic Nanostructured Complex with DFO for Dual Imaging Applications

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

The development of a smart system for theranostics represents a promising approach to personalised cancer treatment. The research presented here focuses on the design of a material for diagnostics, integrating magnetic resonance imaging (MRI) and positron emission tomography (PET), with the potential for future functionalisation toward therapeutic applications.

In particular, the successful synthesis and functionalisation of Fe₃O₄ nanoparticles with polyacrylic acid (PAA) via an optimised co-precipitation method was achieved, followed by the conjugation of deferoxamine (DFO) through coupling chemistry. FTIR analysis confirmed successful synthesis and modification by covalent linkage, while SEM revealed spherical Fe₃O₄/PAA/DFO nanoparticles with a size of 28 ± 8 nm. DLS and ζ-potential measurements confirmed the material's stability over 30 days at pH 7.4.

The potential of the Fe₃O₄/PAA/DFO complex as an MRI contrast agent was demonstrated through a linear correlation between T1, T2, and T2* relaxation times and magnetic DFO complex concentrations ranging from 1-50 µg/mL, with relaxation times of 5.0 ± 0.4, 444 ± 60, and 4233 ± 646 mg/mL·s, respectively, confirming the potential for diagnostics. Furthermore, preliminary ⁶⁸Ga labelling demonstrated successful incorporation, as confirmed by instant thin-layer chromatography, indicating efficient radiolabelling for PET imaging.

To further evaluate the potential of Fe₃O₄/PAA/DFO magnetic nanostructure as a dual imaging agent, biological evaluation on BM-MSCs, U2OS, and 143B cell lines will be performed. Further modifications, such as functionalisation with Pt-based anticancer drugs, could enhance its theranostic potential, enabling both diagnosis and targeted therapy within a single system.

Microfluidic Synthesis of Targeted Lipid-Coated ZnO Nanoparticles for Advanced Cancer Immunotherapy

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Cancer immunotherapy has revolutionized oncology by improving long-term clinical responses and survival rates. However, it often fails due to immune evasion mechanisms, high costs and complex manufacturing processes. Cellular reprogramming offers new strategies to differentiate any cell type. Moreover, cells can be differentiated in situ bypassing the pluripotent state and enabling in vivo reprogramming. Small molecules (SMs) can boost the efficiency of traditional transcription factor-mediated reprogramming or even enable their substitution. Proper selective delivery of these SMs is crucial and nanotechnologies play a pivotal role in this context. In fact, SMs can be either encapsulated in liposome or absorbed on solid nanoparticles, enhancing both in vitro and in vivo efficacy while improving the selectivity of the delivery by exploiting targeting moieties such as monoclonal antibodies or peptides. Liposomes and lipid-coated nanoparticles can be both used as efficient tumor-targeted drug carrier. Our lipid-coated ZnO nanoparticles have the advantages of high drug adsorption capacity, enhanced stability, and biocompatibility when lipid-coated, bringing an advancement to the conventional drug-loaded liposomes. We employed a herringbone microfluidic chip to produce these NPs in a standardized, consistent, scalable, and high-throughput manner. Notably, this is a pioneering application of a microfluidic system for creating hybrid inorganic/organic L-ZnO NPs. To achieve specific tumor targeting, we incorporated ligands for EGFR receptors into the lipid coating. Characterization of these nonconstruct and their biocompatibility has been evaluated through different human and mouse in vitro models before assessing their internalization capabilities. The biocompatibility of both liposomes and L-ZnO NPs is significantly increased in in vitro experiments, in particular compared to pristine ZnO NPs. The use of a microfluidic chip ensures high reproducibility in the preparation process of these nanoparticles, resulting in consistent size, shape, and surface characteristics, and is successfully employed in the production of lipid coated inorganic nanoparticles. The incorporation of EGFR-targeting ligands into the lipid coating enables effective functionalization of the NPs which present enhanced specificity and efficacy of tumor targeting. Lipid-coated ZnO nanoparticles (L-ZnO NPs), synthesized via microfluidic chip, demonstrate superior biocompatibility, stability, and drug adsorption compared to bare ZnO nanoparticles. This method ensures reproducible and scalable production, suitable for clinical applications. Incorporation of EGFR-targeting ligands enhances tumor-specific drug delivery efficacy, showcasing potential for precise delivery in both therapeutic and cellular reprogramming contexts.

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Stimuli-responsive, drug-loaded nanoconstruct for multiple myeloma treatment: therapy and diagnosis

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), settembre 17, 2025, 13:10 - 14:30

Despite the progress made in the last few years, the development of effective tools against severe pathologies such as tumors is proving to be extremely challenging. While advancements in nanomedicine towards cancer treatment have exhibited that the use of nanocrystals (NCs) can be truly promising, potential drawbacks related to their utilization, such as the non-specific uptake of these materials in healthy organs and their potential immunogenicity, are still scarcely considered. This work aims to develop an innovative theranostic nanoconstruct based on lipid-coated, iron-doped zinc oxide nanocrystals (ZnO-Fe NCs), whose properties have revealed huge potential for in vitro and in vivo applications, focusing on the treatment of multiple myeloma, a tumor for which relapses and disease progressions are common among affected patients. The nanoconstruct therapeutic potential is due to its biocompatibility and the possibility to be remotely activated by ultrasound stimulation in order to ensure targeted drug release, while, for diagnostic purposes, it can be tested as contrast agent under ultrasound stimulation (i.e. echography).

To this aim, ZnO-Fe NCs were first synthesized and functionalized, before being coated with a shell composed of a mix of synthetic lipids, PEG and cholesterol. To further enhance the therapeutic capabilities of the nanotool, Carfilzomib (which is a commonly used drug for multiple myeloma treatment) was added into the lipidic shell. The obtained nanoconstruct was then deeply characterized, with particular focus on the diagnostic potential of the NCs as echographic contrast agent. Furthermore, to assess its therapeutic capabilities, it was administered to two different multiple myeloma cell lines to assess its intrinsic cytotoxicity (with and without the drug embedded into the shell) and when stimulated with ultrasounds, aiming at a sonodynamic treatment. Measurements performed through Electron Paramagnetic Resonance spectroscopy demonstrated indeed the generation of reactive oxygen species (ROS) derived from the ultrasonic stimulation of the nanoconstruct.

Preliminary in vitro results indicate that this innovative nanoconstruct can be an exceptionally interesting starting point for the treatment of multiple myeloma, since its therapeutic capabilities can be greatly enhanced by tailored adjustments, such as the functionalization of the lipidic shell for targeting purposes. Furthermore, echographic measurements demonstrated that the obtained nanoconstruct can be exploited not only as a therapeutic, but also as an extremely effective diagnostic tool.

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New insights into the molecular organization of fluorescent nanovesicle-based bioimaging probes from Molecular Dynamics simulations

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Fluorescent organic nanoparticles (FONs) are emerging as biocompatible nanostructured platforms for biomedical applications due to their high tunability in terms of functionality and optical properties [1]. Among different nanocarriers, quatsomes are unilamellar nanovesicles formed by the self-assembly of quaternary ammonium surfactants and cholesterol, which have been shown to be highly homogeneous in size and morphology over years [2,3].

Quatosome nanovesicles containing fluorescent molecules have shown outstanding photostability and high brightness due to the confinement of a large number of dye molecules in a small space [4]. In previous studies,

the loading of a carbocyanine pair in the membrane gave rise to the FRET effect in a nanosized domain for the first time achieving high FRET efficiency (up to 85%) [5,6]. However, the development of ultrabright formulations often remains a challenge due to the presence of aggregation-induced quenching at high fluorophore loadings.

In this work, all-atomic molecular dynamic simulations have been carried out to simulate a quatosome bilayer patch in the presence of different dyes. The main goal is to perform an in-depth structural analysis of the molecular organization in the membrane bilayer and provide insight into the inter-molecular interactions and aggregation states of embedded fluorophores. The new insight gained will guide the design and optimization of new bioimaging probes.

Next-Gen Radioprotection: Thermo-Sensitive Hydrogels for Localized Amifostine Release

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F2_1, Andalucía I Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Amifostine is the only FDA-approved pharmacological agent for the treatment of radiation-induced damage in head and neck tumoral malignancies; however, its clinical application is constrained by the absence of an efficient delivery system. Most conventional systemic administration routes have demonstrated suboptimal concentration in the interested site and rapid clearance of Amifostine. With the increasing incidence of cancer leading to a rise in radiation-based therapies, our objective is to mitigate its adverse effects by employing an adjuvant platform designed to improve the state of art of anti-tumoral clinical strategies.

We have developed a multimodal platform to support a localized and controlled release of the radioprotective agent within the X-ray-irradiated region, aiming to modulate the non-therapeutic effects triggered by the treatment. The thermo-responsive polymer pNIPAM was conjugated with hyaluronic acid to form an injectable, thermo-sensitive hydrogel preloaded with nanoparticles that encapsulate and regulate the kinetic release of Amifostine. FTIR and H-NMR analyses confirmed the synthesis of HA/pNIPMA polymer, temperature sweep characterization performed via rheological analyses confirmed

sol-gel transition at body temperature. Hydrogel's application is intended for local injection, thus exerting its therapeutic benefits specifically at the site of radiation exposure.

The healing approach is based on the in-situ delivery of the radioprotective agent in a therapeutic concentration. Amifostine is encapsulated within PLGA nanoparticles, which were synthesized via a double emulsion technique, achieving an encapsulation efficiency of 86% and a complete release of the cargo over 24 hours.

In order to mimic the tumoral micro-environment and the diseased tissue, we have generated a spheroidal 3D model based on oral mucosa tumor cell line (Cal27), human dermal fibroblasts (HDF) and human microvascular endothelial cells (HMEC). The spheroids are cultured in ultra-low attachment plates and then embedded in collagen to resemble the extracellular matrix. Amifostine's ROS scavenging properties and clinical efficacy in 3D model have been characterized after irradiation using an X-ray irradiator simulating the radiation dose, 2Gy to 20Gy in single or multiple dose regimes, to which cancer patients are subjected during radiotherapy sessions.

In conclusion, our work focuses on enhancing the current application of Amifostine as a radioprotective agent during radiotherapy sessions. The platform we are developing is designed to optimize a safe release while promoting localized therapeutic effects, minimizing the drug's off-target tissue accumulation.

A dual light and magnetic responsive mesoporous silica nanosystem for cancer therapy

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Superparamagnetic iron oxide nanoparticles (SPIONs) have the capability to generate an intrinsic magnetic field in the presence of an external magnetic field (MF) and this magnetic response persists only as long as the external MF is applied. In addition, these nanosystems can be magnetically guided and focused to the desired location, which is an advantage for clinical purposes. In terms of biomedical applications this property allows for real time non-invasive follow-up treatments. Furthermore, SPIONs have excellent biocompatibility, chemical stability, low production cost, ease of surface functionalization, easy elimination via metabolism and renal excretion. Therefore, SPIONs have been widely studied for multiple biomedical applications such as magnetic resonance imaging (MRI), hyperthermia therapy, targeted drug delivery and recently bone tissue engineering. Furthermore, there has been remarkable breakthrough in the current research on osteogenesis mediated by iron oxide nanoparticles.

On the other hand, photodynamic therapy (PDT) has emerged as a promising alternative, using photosensitizers that, upon light activation, generate reactive oxygen species to induce cell death in targeted tissues. We have recently designed a novel third-generation rhodium-based nanophotosensitizer (RhNPs-MSNs-Tf) incorporating Rh nanoparticles (RhNPs) into the structure of mesoporous silica nanoparticles (MSNs) functionalized with transferrin (Tf) for active targeting of tumor cells. The use of MSNs improves the vehiculation of the near infrared responsive RhNPs in physiological media. After physicochemical characterization, the RhNPs-MSNs-Tf system demonstrated significant singlet oxygen generation upon near-infrared (NIR) irradiation, confirming its ability to induce PDT. Its photodynamic efficacy and cytotoxicity was also proved using an in vitro model, a mass spectrometry-based untargeted metabolomics and the in vivo chicken chorioallantoic membrane model.

In this study, we have first obtained SPIONs via a thermal decomposition method and transferred them to aqueous media via ligand interchange with dimercaptosuccinic acid. Then, the external surface of the rhodium-based nanophotosensitizer (RhNPs-MSNs-Tf) has been decorated with the SPIONs via covalent attachment to the transferrin protein. Hence, both photodynamic and magnetic guidance properties are integrated into a single nanocomposite to obtain a more efficient cancer therapy.

Neuroprotective profile of carbosilane dendrimers as nanocarriers of Memantine against Alzheimer's disease

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F2_2, Andalucía I Room (Level +1), septiembre 18, 2025, 10:30 - 13:10

Nowadays, the prevalence of neurodegenerative diseases (ND) has increased, yet the etiology of these pathologies remains unknown. ¹ Moreover, the harm done of these neurological disorders could be associated to multiple factors occurring simultaneously (i.e., excitotoxicity, misfolded proteins that forms toxic aggregates, oxidative stress, neuroinflammation...). In the field of nanotechnology, dendrimers have been widely explored for disease-modifying treatments, including Alzheimer's disease (AD). These nanoplatforms are well-defined and ramified structures of polymeric nature that provide multivalency and, furthermore, their intrinsic properties could lead them as perfect candidates for drug delivery systems. ²

In this sense, we have demonstrated in previous studies that carbosilane-based dendrimers with ammonium-peripheric groups have the ability to cross the blood-brain barrier and prevent amyloid fibrils from misfolding in diabetes II and Alzheimer's mice model, one of the main toxic effect that leads the neurodegeneration process. ³, ⁴ Based on these results, our research focused on

functionalizing these systems with Memantine, an uncompetitive glutamatergic N-methyl-D-aspartate (NMDA) receptor antagonist. Our interest in this molecule relies on its capacity to reduce excitotoxicity without inferring with other factors implicated in NMDA activation. ⁵ Thus, combining the inherent capacities of dendrimers with Memantine properties, we could achieve structures with an antiamyloidogenic profile. ⁶

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Thymol-Zinc Combinations for the Prevention of Biofilm Formation on 3D Printed Polysaccharide-based Scaffolds

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F3_1, Andalucía II Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The rise of bacterial infections linked to biofilm formation on biological and material surfaces is a major concern. Developing medical devices that combine antibiofilm and antimicrobial activity with wound healing properties offers a promising strategy for preventing soft tissue and musculoskeletal infections. However, non-antibiotic alternatives are preferred due to antimicrobial resistance, and using non-drug, Generally Recognized As Safe (GRAS) substances can simplify regulatory approval, classifying the device as a medical product rather than a medicine. Additionally, there is increasing interest in using biodegradable polymers for sustainable scaffolds to minimize environmental impact.

This study aimed to develop 3D-printed medical devices based on xanthan gum (XG) and guar gum (GG) to reduce biofilm formation, produce antimicrobial effects, and support wound healing. For the design, we considered that hydroxypropyl- β -cyclodextrin (HP β CD) could enhance the scaffolds' ability to host antimicrobial essential oils like thymol, while XG could hold divalent metal ions like Zn²⁺ to provide complementary mechanisms for biofilm prevention. The approach included: i) obtaining and characterizing HP β CD-thymol complexes, ii) loading HP β CD-thymol and free thymol into an optimized ink, iii) incorporating Zn²⁺ into the 3D-printed scaffolds, and evaluating antimicrobial activity through microcalorimetric techniques and biofilm cell viability tests. The antimicrobial properties of the scaffolds against *Staphylococcus aureus*, *Pseudomonas aeruginosa*, and *Staphylococcus epidermidis* were evaluated both by CFU counting and by real-time monitoring of metabolic heat using isothermal microcalorimetry. Calorimetric techniques, although still incipiently applied in the field of the regenerative medicine, may provide more precise, direct and robust information on the performance of the scaffolds minimizing risks of bias associated to subsequent handling and steps of traditional microbiological techniques. The biocompatibility of the scaffolds was assessed using hemolysis and cell viability tests, while angiogenic and tissue integration properties were evaluated in an in ovo CAM model [1].

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Laser Surface Texturing of Titanium-Based Implant Alloys

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Titanium alloys are widely used as implant materials, due to their excellent biocompatibility, and good mechanical and corrosion properties. Titanium implants primarily serve as mechanical support, and are bio-inert, lacking antibacterial properties. Bacterial infections are a major cause of implant failure and surgical revisions. Therefore, the focus of research is on infection prevention, which has made infection prevention a key focus of research. The challenge lies in modifying the implant surface to enhance antibacterial properties without affecting the bulk material.

The aim of this study is to examine the impact of laser surface alloying of Ti6Al4V alloy with copper on the microstructure, phase transformations, hardness, mechanical, corrosion, and antibacterial properties of the material. Thermodynamic modeling was performed using Thermo-Calc software based on CALPHAD method, and phase stability in equilibrium conditions was determined. Surface microstructure and distribution of Ti₂Cu phase were analyzed by Optical Microscopy and Scanning Electron Microscopy (SEM), equipped with an energy dispersive X-ray spectroscopy (EDS) detector. Identification of phases was carried out by X-ray Diffraction analysis (XRD), while phase transformations were detected by Differential Scanning Calorimetry (DSC). A correlation between laser beam optimization and hardness, corrosion, and antibacterial effectiveness was established.

Metal Ion-Enhanced Titanium Abutments for Optimized Soft Tissue Attachment

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F3_2, Andalucía II Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Peri-implantitis, a condition characterized by gingival inflammation and bone loss, affects over 50% of patients and represents a significant challenge in oral health. Titanium (Ti) and its alloys, widely used in dental implants, exhibit excellent mechanical properties and biocompatibility. However, their biological inertness results in weak adhesion between human gingival fibroblasts (HGFs) and implant abutments, compromising the gingival seal and facilitating bacterial infiltration. To enhance biological performance, this study explores the functionalization of anodized Ti surfaces with metal ions (Mg^{2+} , Mn^{2+} , Zn^{2+} , Zr^{4+} , Sr^{2+} , and Cu^{2+}) to improve HGF adhesion and modulate bacterial colonization.

Ti6Al4V discs were anodized and subsequently treated with metal chloride solutions, followed by heat treatment and washing. Surface characterization was performed using SEM/EDX, contact angle measurements, and ICP analysis to determine ion presence and release. In vitro HGF assays evaluated cell adhesion, migration, proliferation, and collagen secretion, while immunoassays assessed gene expression of immune markers. Proteomic analyses identified adsorbed proteins, and antimicrobial tests were conducted using *Streptococcus gordonii*.

Results indicated that all ions, except Cu^{2+} , enhanced HGF adhesion. Mn^{2+} , Zr^{4+} , and Sr^{2+} significantly increased cell projection and proliferation, while Zr^{4+} and Sr^{2+} promoted collagen secretion. Ion-treated surfaces exhibited immunomodulatory effects and altered protein adsorption profiles. However, bacterial colonization remained unchanged.

In conclusion, the functionalization of Ti surfaces with Sr^{2+} , Zr^{4+} and Mn^{2+} demonstrates promising potential to improve gingival integration of dental abutments. While bacterial adhesion was not significantly reduced, the enhanced cellular response suggests these modifications may contribute to better clinical outcomes by reinforcing the peri-implant soft tissue seal.

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Dendritic zeolites as drug delivery systems to face antimicrobial resistance

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F3_1, Andalucía II Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Antimicrobial resistance (AMR), occurring when bacteria become unresponsive to traditional treatments, is recognized as a significant global health emergency. This situation makes it imperative to seek new therapies.¹

Zeolites are crystalline microporous aluminosilicates that could serve as promising drug delivery systems for antimicrobial drugs due to their properties such as regular porosity, ion exchange capacity, and high surface area. However, the microporous nature of conventional zeolites with pores of less than 1 nm, limits their encapsulation capacity.² Recently, a dendritic ZSM-5 zeolite (MFI structure), featuring radially oriented and branched nanounits and highly interconnected pore channels that create trimodal porosity (micro, meso, and macro-pores), was reported by some of us.³ This material displays remarkable adsorption and catalytic properties showing the potential to overcome the limitations of conventional zeolites due to its improved accessibility.

Dendritic zeolites have not yet been explored as drug delivery systems. Aluminum, a primary component of zeolites, has been associated with potential neurotoxicity, embryotoxicity, and carcinogenic effects.⁴ By substituting aluminum with safer heteroatoms, such as gallium, in the zeolitic framework, we can reduce toxicity and introduce new functionalities, given that gallium has proven antibacterial ability, among others.⁵

Herein we propose a combined therapy based on a dendritic gallium containing zeolite (Ga-MFI) loaded with a broad-spectrum antibiotic (i.e. amikacin) within its porosity. The dendritic zeolites were prepared using a modified procedure based on a previous work.³ Following their synthesis, the dendritic nanoarchitecture was confirmed, along with its small nanometric size (209 ± 39 nm). The biocompatibility of the nanomaterial was assessed in HL60 cells exhibiting cell viability higher than 99% even at high concentrations (1 mg/mL). Then, amikacin was encapsulated within the meso/macro-pores by an incipient wetness impregnation method, reaching important loadings of 28 ± 6 wt.%.

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Functionalization with an Amino Acid and Silver of Titanium Surfaces for Balancing Cytocompatibility and Infection Control

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F3_2, Andalucía II Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Orthopedic and dental implants must fulfil two primary functions: to ensure effective osseointegration, even in the case of poor host bone quality and to reduce the risk of infections. The first function is almost met by current surface treatments of titanium and titanium alloys, which are widely used for bone implants.

Concerning the second function, existing implant surfaces remain significantly inadequate.

A bacteriostatic and antibiofilm action would be sufficient for bone implants, as the primary goal is to prevent the need for implant removal due to biofilm formation. A second surgery is highly invasive and carries a significant risk of further infections and localized bone resorption. Conversely, a strong antibacterial effect could compromise the cytocompatibility of the implant. The combined action of local bacteriostatic surfaces coupled with the systemic assumption of antibiotics in the first days after implantation, could be a good strategy to avoid the risk of biofilm formation on bone implants guaranteeing a fast osseointegration process.

In the case of titanium and its alloys surface functionalization with silver ions or nanoparticles has been extensively studied to impart antibacterial properties to bone implants. However, this strategy presents challenges in balancing surface cytocompatibility with antibacterial efficacy, mainly if nanoparticles are formed. Additionally, recent reports indicate the emergence of bacterial strains resistant to silver.

We investigated the antibacterial properties and cytotoxicity of Ti6Al4V functionalized with silver using a cysteine-silver solution. To optimize the surface for functionalization, the alloy underwent a previously established chemical treatment. Characterization was carried out through Field-Emission Scanning Electron Microscopy (FESEM), zeta potential titration curves, release testing, and X-ray Photoelectron Spectroscopy (XPS) analysis. Antibacterial assessments included inhibition halo tests with *S. epidermidis* and biofilm formation assays with *S. aureus*. Additionally, direct cell cultures with human mesenchymal stem cells (hMSCs) and a co-culture model of bacteria and hMSCs were conducted. The findings revealed that silver ions (Ag^+) were predominant on the functionalized surface (58%), while a significant proportion of Ag-S chemical bonds (22%) was also detected, with minimal presence of metallic silver nanoparticles. hMSCs exhibited proper adhesion and alignment, and the functionalized surface demonstrated the ability to maintain cell viability in a co-culture of bacteria and hMSCs. These results confirm the effectiveness of cysteine as a linker for silver functionalization on Ti6Al4V, achieving a balance between cytocompatibility and bacteriostatic properties. The role of cysteine in preventing the development of resistance by bacteria will also be discussed.

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Engineering exosome-functionalized electrospun fibres: a new strategy for modulating cellular responses in soft tissue

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F3_1, Andalucía II Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The surface of polymer nanofibers is typically highly hydrophobic, as described by the Wenzel and Cassie-Baxter models. This hydrophobicity reduces protein adsorption and cell adhesion. However, appropriate surface modifications can enable the incorporation of bioactive compounds, such as exosomes. Its small membrane vesicles of endocytic origin secreted by most animal and plant cells with sizes ranging from 50 nm to 150 nm. This structure are capable of inducing tissue regeneration by delivering growth factors, proteins, microRNAs, messenger RNAs, noncoding RNAs, and lipids. Altering the surface morphology of nanofibers to modulate their biological activity represents a novel strategy for regulating immune and cellular responses in vivo. In this context, nanofibers serve as carriers for exosomes, a subclass of extracellular vesicles that play a crucial role in intercellular communication. Once released, exosomes deliver bioactive molecules that regenerate tissues, guarantee homeostasis and accelerate soft tissue regeneration.

In this study, we used plant exosomes from marigold (*Calendula officinalis* L.), which were introduced onto electrofibres made from a biocompatible polimer – polylactide (PLA). The surface of the fibres was chemically modified by ammoniolysis - to increase its chemical activity. Deposition of exosomes on the surface was carried out by electrospray. The fibre membranes were then examined from microstructural (SEM), structural (FTIR-DRIFT), and physicochemical perspectives. The biocompatibility of non-woven membranes with exosomes and membranes with added exosoams was tested by determining the viability and cytotoxicity of RAW 274.3 macrophage cells after 3 and 7 days of their contact matrix surface. Membrane modification with exosomes has been shown to significantly affect the secretion of anti-inflammatory interleukins and stimulate collagen secretion.

Membrane modification with exosomes has been shown to significantly influence the secretion of anti-inflammatory interleukins and stimulate collagen secretion.

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Surface modification of bioactive glasses through plasma technology to impart antiadhesive properties

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F3_2, Andalucía II Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Bioactive glasses are widely investigated and used in the field of bone tissue regeneration. However, their surface, if not appropriately modified, can be quickly colonized by bacterial strains, with subsequent formation of biofilm, detachment and development of infections in the surrounding tissues.

This work focuses on the surface modification of two glass compositions (SBA2 and S53P4) via non-thermal atmospheric pressure plasma treatments to impart antimicrobial properties, avoiding the use of antibiotics or antimicrobial agents. This technique allows to provide tailored surface characteristics by adjusting parameters such as process gas and reactor conditions. The glasses were produced using the melt and quenching technique, the melt was cast into a mold to obtain a bar, subsequently cut into slices which were polished to level out the surface. Samples were activated using He/O₂ or He/N₂ plasma and subsequently coated with polymer coatings (e.g. siloxanes) to impart antiadhesive properties. Plasma-treated glasses were characterized in terms of morphology and composition using Field Emission Scanning Electron Microscopy (FE-SEM) with energy dispersive spectroscopy (EDS) and Fourier Transform InfraRed (FTIR) spectroscopy, surface properties by optical laser confocal microscopy, Water Contact Angle (WCA) and zeta potential measurements. Moreover, in vitro bioactivity tests in simulated body fluid and bacterial assays were carried out to evaluate the surface ability to reduce bacteria adhesion.

The obtained results evidence that the plasma-treated samples show a modified topography, roughness and wettability, and different functional groups, useful for inhibiting bacterial adhesion. The bioactivity of the glasses is maintained even after depositions or plasma treatments and finally, a significant reduction of multidrug-resistant *Staphylococcus aureus* is observed on the surfaces of the two treated glasses. Therefore, the non-thermal atmospheric pressure plasma treatment represents a promising technique for developing bone regeneration devices able to promote osseointegration and decrease infection development.

Functional starch/porphyrin-based materials for wound healing

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F3_1, Andalucía II Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Effective wound care is crucial for preventing infections and promoting skin regeneration. However, both conventional and modern wound dressings often have limitations, such as inadequate exudate absorption, poor moisture balance, and difficulty in removal, which can delay healing and increase the risk of secondary infections. These challenges highlight the urgent need for innovative materials to enhance wound management. Polysaccharides, due to their biocompatibility, have been emerged as promising candidates for developing advanced wound dressings. On the other hand, porphyrin derivatives, known for their photosensitizing properties and ability to eliminate pathogenic microorganisms, offer a novel approach to antimicrobial wound care.

In this study, functional starch-based films doped with a porphyrin–triphenylphosphonium derivative were developed using the solvent casting method. Comprehensive characterization of the films was performed, including mechanical, physicochemical, and biological evaluations, to assess their suitability for wound healing applications. The incorporation of porphyrins conferred a yellowish color while maintaining transparency, and increasing water uptake, stretchability, and photosensitizing activity. By integrating antimicrobial photodynamic therapy into a polysaccharide-based platform, these innovative dressings have the potential to reduce infection risks and contribute to the advancement of more effective and sustainable wound care solutions.

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3D-printed PEEK with Antimicrobial and Bioactive Coatings Using Vacuum Arc Plasma Deposition

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F3_2, Andalucía II Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The integration of additive manufacturing (AM) in biomedical engineering has revolutionized the fabrication of medical implants, particularly using polyetheretherketone (PEEK), a high-performance polymer with excellent mechanical strength, biocompatibility, and radiolucency. However, the clinical application of PEEK implants remains challenged by the need for enhanced antimicrobial properties and improved osseointegration. This study presents a novel hybrid manufacturing approach that combines Fused Filament Fabrication (FFF) 3D printing with in-situ vacuum arc plasma deposition to generate antimicrobial and bioactive thin-film coatings on PEEK implants. This hybrid method paves the way for new personalized, infection-resistant, and osseointegrative implants, particularly in orthopedic and spinal applications where infection control and simultaneous tissue integration are of critical importance.

The study investigates the application of this manufacturing method to produce different metal and metal oxide coatings on 3D-printed PEEK in a single-step fabrication. The tested coatings include silver (Ag), copper (Cu), and zinc (Zn), for their antimicrobial potential, and titanium dioxide (TiO₂) due to its osseointegrative potential. Surface characterization using a laser scanning microscope (LSM) reveals that thin film coating generated by this method maintains the surface structure of its substrate and only minimally alters its surface roughness. The surface wettability is highly increased by TiO₂ coating. Cross-cut tests confirm strong adhesion of the thin film coatings to the PEEK substrate. Results from bacterial adhesion assays show that zinc, among the tested coatings, exhibits the highest antimicrobial efficacy against *Staphylococcus aureus*, with a significant reduction in bacterial counts at a minimum coating thickness of 20 nm. Additionally, TiO₂ coating confirmed its role in enhancing the osteoblast adhesion and proliferation, thus being a suitable candidate for improving PEEK bioactivity. Further, a TiO₂/Zn composite coating demonstrates a strong combination of antimicrobial protection and osteogenic support, suggesting its potential for reducing post-surgical infections while promoting bone integration.

Future research will focus on optimizing Zn release kinetics to balance antimicrobial activity and biocompatibility, thus preparing the clinical applicability of these kind of novel 3D-printed PEEK implants for infection prevention.

Surface Design of Faceted Oxide Particles: Boosting Antimicrobial Properties

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F3_1, Andalucía II Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The rise of antibiotic-resistant bacteria poses a significant threat to healthcare, environmental health, and sustainability. Developing selective antimicrobial materials that effectively combat infections while remaining safe for mammalian cells is a critical priority. Metal oxide nanoparticles (MOs), including copper oxides (CuO and Cu₂O) and titanium oxide (TiO₂), are promising candidates for their non-specific multiple mechanisms of antimicrobial action against a broad spectrum of bacterial species, including some important multidrug-resistant bacteria.

This study aims to synthesize MOs with highly controlled morphologies and structures to optimize their surface chemical characteristics and boost antimicrobial effects. MOs surface characteristics and size were deeply characterized in both dry and wet environments with a suite of physico-chemical techniques. Moreover, the mechanisms of MOs antimicrobial activity, including the capacity to generate reactive oxygen species (ROS) and ion release in biomimicking fluids were explored. The antimicrobial activity of the most promising MOs was assessed towards Gram-positive (*Staphylococcus aureus*) and Gram-negative (*Escherichia coli*) bacteria and their cytocompatibility was assessed towards model cellular membranes (red blood cells).

Cu₂O and TiO₂ nanoparticles with well-defined crystallographic facets were successfully synthesized, achieving precise morphological control. In situ formation of core-shell Cu₂O/CuO heterostructures via mild heating of cubic Cu₂O nanoparticles enhanced Cu₂O stability. Notably, Cu₂O exhibited a stronger bactericidal effect than CuO due to its oxidation state and electron transfer ability, copper ion release, and ROS generation due to the Fenton reaction. Furthermore, hemolytic assays confirmed the cytocompatibility of the material with mammalian cells, underscoring its potential for antimicrobial applications. Further studies will elucidate faceted-mediated TiO₂ antimicrobial mechanisms and probe doping with nitrogen and carbon compounds to enhance bactericidal activity. These findings provide new insights into the role of metal oxide surfaces in antimicrobial efficacy and present a promising strategy for developing next-generation antimicrobial agents.

Development of a novel antibiotic-doped calcium-phosphate cement for bone infection treatment

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F3_2, Andalucía II Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

This study aims to develop a degradable and biocompatible calcium phosphate cement (CPC) loaded with gentamicin and vancomycin for the local treatment of a broad spectrum of strains causing osteomyelitis.

The two antibiotics were incorporated, either individually or in combination, into the solid phase of the Graftys® Quickset (GQS) injectable cement.

The impact of their incorporation on the physicochemical properties of the cement was examined, the antibiotics release was evaluated, and the biocompatibility was validated in vitro. The antibacterial properties were characterized for different bacterial strains including Gram + and – bacteria, *S. aureus*, *S. epidermidis*, *Pseudomonas aeruginosa* and antibiotic-resistant strains, such as MRSA or MRSE, either in planktonic or biofilm state.

The incorporation of antibiotics did not result in any significant alterations of the intrinsic properties of the GQS cement. Apart from an extended setting time, which remained in an acceptable range for the clinician, mechanical strength, porosity, injectability are not altered. These results are confirmed by an XRD study which confirms that there is no direct interaction between the antibiotics and the cement during hardening.

The loaded cement enabled the rapid release of very high concentrations of antibiotics locally around 10 to 100 times the minimum inhibitory concentrations for the organism in presence, without exerting any cytotoxic effects on human osteoblasts but with a strong and wide antibacterial effect on various bacteria grown as planktonic or as a biofilm.

Altogether, these data indicate that this new version of the GQS cement loaded with gentamicin and vancomycin represents a very attractive local treatment of osteomyelitis.

An innovative heparinization strategy for blood-contacting biomaterials: Alternating current electrophoretic deposition for enhanced hemocompatibility and antibacterial properties

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F3_2, Andalucía II Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Titanium alloys (aTi) are widely used in orthopedic and dental implants due to their excellent mechanical strength, corrosion resistance, and biocompatibility. Recently, their application has expanded to blood-contacting devices (BCDs) such as stents, heart valves, and grafts, but aTi-based BCDs often face challenges in interacting with biological tissues, leading to the risk of thrombosis and infection. To address these limitations, we present an innovative surface modification technique using alternating current electrophoretic deposition (AC-EPD) to coat bare aTi substrates with heparin (HEP). This method provides a rapid, cost-effective, single-step process that overcomes the shortcomings of existing approaches. aTi heparinized substrates (aTi-HEP) exhibit a significant improvement in hemocompatibility, achieving an 80% reduction in protein adhesion, an effect that persists for seven days. In addition, aTi-HEP effectively prevents platelet adhesion and reduces the rate of hemolysis by 50%, highlighting the improved blood compatibility. In addition, aTi-HEP improves fibroblast cell viability by 30%, indicating superior biocompatibility. Improved antibacterial performance was also observed, with reductions in *S. epidermidis*, *S. aureus*, and *E. coli* colonization of 36%, 43%, and 25%, respectively. In conclusion, the AC-EPD heparinization method provides a simplified, efficient, and cost-effective strategy for aTi substrate modification, paving the way for safer and more effective BCDs. This approach has significant potential to improve patient outcomes by minimizing complications associated with thrombosis and infection.

Innovative PLA Nanocomposites with MWCNTs and MWCNTs-COOH for Printed Electronics (PE)

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F4_1, Z2 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Printed electronics (PE) have a wide range of potential applications in sensors. Currently, the substrates used for PE are typically made from fossil-based materials, with poly(ethylene terephthalate) (PET) being a common example. PLA, known for its eco-friendly nature, is gaining attention in the electronics industry due to its unique characteristics, such as high tensile strength, Young's modulus, non-toxic properties, and its recyclability and compostability. PLA offers a more sustainable alternative to traditional polymers, requiring 68% fewer greenhouse gases and 65% less energy to produce compared to fossil-based polymers. The primary objective of this work is to develop PLA-based nanocomposites as alternative substrates to replace PET in printed electronics. However, PLA has some limitations, including brittleness and a low crystallization rate. To address these issues, our team has proposed PLA nanocomposites incorporating MWCNTs and MWCNTs-COOH, which offer improved mechanical and physicochemical properties. The functionalized nanomaterial enhances compatibility with the polymer matrix, leading to better mechanical performance. Additionally, a series of plasticized samples were prepared to improve the elongation of the nanocomposite substrates, and the electrical conductivity of the samples was also evaluated.

In this study, PLA nanocomposites with varying amounts of MWCNTs and MWCNTs-COOH were prepared using a solvent casting method to create masterbatches, followed by melt mixing with a Haake–Buchler twin-screw co-rotating melt mixer. Compression-molded PLA-based nanocomposite samples were then created to assess the impact of the nanomaterials on their physicochemical and mechanical properties. The addition of the fillers did not alter the melting or glass transition temperatures of PLA, but it significantly improved the crystallization temperature from the melt. The incorporation of nanomaterials enhanced both the tensile strength and Young's modulus, while the elongation was increased in the plasticized samples. To further analyze the surface properties, adhesion tests were performed using different inks on both the PLA-based substrates and the commercial PET substrate commonly used in printed electronics.

Acknowledgements

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ENHANCING THE SENSITIVITY AND REPRODUCIBILITY OF GRAPHENE FIELD-EFFECT TRANSISTOR BIOSENSORS FOR PRECISE LABEL-FREE SARS-COV-2 DETECTION THROUGH OPTIMIZED SURFACE BIOFUNCTIONALIZATION

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F4_2, Z2 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

Since the COVID-19 pandemic, the necessity for a widespread, rapid and highly sensitive diagnostic tool has become a reality in the society. The incorporation of new detection devices, such as biosensors, that overcome the general drawbacks of the gold standard technologies is a necessity. At this point, the employment of two-dimensional nanomaterials, especially graphene, into point-of-care biomedical devices stands as a pioneering approach poised to transform diagnostic landscape. Despite the improvements in development of these type of biosensors, the relation between their surface functionalization and sensing response remains ambiguous. Owing to this statement, we have performed deep research combining a careful sensor design and fabrication and a precise surface modification of these biosensors to demonstrate how this could be crucial in enhancing their sensing performance. Particularly, we have biofunctionalized graphene field-effect transistor (GFET) sensors by surface modification with different biochemical reactions to promote either random/heterogeneous or oriented/homogeneous immobilization of anti-SARS-CoV-2 spike protein antibody. Both approaches were thoroughly analysed by in-silico simulations, physicochemical and biochemical techniques and electrical characterization. Then, sensing capacity of SARS-CoV-2 virus simulated clinical samples was further evaluated. Remarkably, the oriented GFET modification approach exhibited significantly reproducibility and responsiveness, surpassing the detection sensitivity of conventional non-oriented GFET by over twofold, without the need for sample preparation and providing rapid results. Beyond the immediate application of this advancement in COVID-19 diagnostics and future pandemic awareness, these results address unexplored mechanistic aspects of 2D nanomaterial-based biosensors, emphasizing the crucial role of biofunctionalization in improving diagnostic performance.

Keywords: Graphene Field effect transistor, biosensor, oriented immobilization, two-dimensional materials, nanobiotechnology, antibody

Reference: Lozano-Chamizo L, Márquez C, Marciello M, Galdon JC, de la Fuente-Zapico E, Martinez-Mazón P, Gonzalez-Rumayor V, Filice M, Gamiz F. High enhancement of sensitivity and reproducibility in label-free SARS-CoV-2 detection with graphene field-effect transistor sensors through precise surface biofunctionalization control. *Biosens Bioelectron.* 2024, 250,116040.

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Novel nano- and submicron carriers with controlled high enzyme loading for electrochemical sensing

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F4_3, Z2 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Enzymes are widely used in biosensing due to their high specificity for target molecule detection. Enzyme-based electrochemical biosensors offer several advantages, including high selectivity, rapid response, ease of use, compatibility with opaque solutions, and potential for miniaturization, making them suitable for portable and cost-effective devices. However, conventional enzyme-based sensors face several challenges, such as low immobilization density, difficulties in quantifying and controlling enzyme loading, reduced activity on electrode surfaces, and the risk of denaturation or deactivation during storage and use.

Here, we present a novel solution by fabricating a high-sensitivity enzymatic electrochemical biosensor using solid particles functionalized with grafted polymer brushes and a precisely quantified amount of immobilized enzyme. The enzymes were immobilized via physical absorption into polyelectrolyte brushes grafted from carriers. This pre-immobilization approach enables precise control over enzyme quantity and activity before deposition onto the electrode. The immobilized enzymes exhibited high loading density and activity and demonstrated long-term stability with minimal activity loss during storage.

As a proof of concept, we tested this system using laccase as the enzyme and hydroquinone as the substrate. The results showed a remarkable enhancement in enzymatic activity—at least 75 times higher than that of enzymes stored in buffer under optimal conditions. The sensor achieved the highest sensitivity reported in the literature for this enzyme-substrate pair, with a maximum response of 0.8 A·M⁻¹ for a 4 mm in diameter electrode. The lowest detection limit, determined via chronoamperometry, was 0.28 μM.

Additionally, we elucidate the mechanism of enzyme-polymer interactions, and the electrode kinetics involved in the redox processes. This work provides a reliable and efficient platform for enzymatic biosensing, offering enhanced sensitivity, stability, and precise enzyme control, which are critical for real-world biosensor applications.

Laser-induced graphene on synthesized polyimides

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

In recent years, laser-induced graphene (LIG) has attracted significant attention due to its excellent physicochemical properties and potential applications in wearable and flexible electronics. This method of graphene production offers a simple, fast as well as cost-effective approach compared to traditional techniques, making it highly suitable for various technological applications. Polyimides are among the most compounds commonly used as substrates for laser-induced graphene formation on polymers. However, most studies have focused on commercially available polyimides, while research involving the prior synthesis of polyimides remains limited. Inducing graphene on synthesized polyimides offers the possibility of tuning the biocompatibility of the substrate, as well as its' structural, chemical, and physical properties, which is of paramount importance for optimizing material quality for applications.

In this study, graphene has been laser-induced on synthesized polyimides. Different polyimide resins were synthesized using N-[3-(2,5-dioxo-2,5-dihydro-1H-pyrrol-1-yl)phenyl]acetamide and the following compounds with terminal amino groups: urea, 4-[(4-aminophenyl)sulfonyl]aniline, 1,2-diaminoethane, 1,6-hexamethylenediamine, at high temperature by polymerization in the melt. The resulting polyimides were characterized using various physicochemical techniques. Additionally, after the successful preparation of laser-induced graphene, the mechanical and electrical properties of the material were investigated to evaluate its potential application in wearable sensors. The following characterization methods were performed: Raman spectroscopy, Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy with energy dispersive X-ray spectroscopy (SEM-EDS), X-ray diffraction (XRD), cytotoxicity and mechanical testing. The results provide valuable insights into the relationship between polyimide structure and the efficiency of laser-induced graphene formation, highlighting the potential of these materials for future technological advancements.

This research was supported by the Science Fund of the Republic of Serbia, #4950, Polymer/graphene heterostructures for physiological sensors – Polygraph.

SERS based biosensing: leveraging the ex-vivo potential of a plasmonic sensor for the classification and prediction of cancer patterns

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F4_1, Z2 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Surface-enhanced Raman scattering (SERS) spectroscopy is a technique that allows to enhance the intrinsic, though weak but also extremely precise, fingerprint Raman signal obtained from molecules of interest. SERS has shown increased potential for the detection of analytes in unusual small concentrations, down to the single-molecule range [1] being, at the same time, characterized by an extremely high multiplexing ability surpassing the conventional and widely applied fluorescence techniques [2]. SERS extensively demonstrated its application at the proof-of-concept level in cancer, however it still lacks clinical demonstration because of reproducibility and stability.

In this work a plasmonic nanosensor composed by gold nanostars (GNS; plasmonic material) embedded in a porous hydrogel (biocompatible matrix) is proposed to detect and differentiate the specific SERS signals associated to the biological fingerprint carried within the plasma from prostate cancer (PCa) and benign hyperplasia (BPH) patients, as well as healthy donors (n=120).

Prior to the trial of the sensor, an optimization of the biosensor was performed in clinically relevant conditions. GNS sterilization was optimized for their safe contact with biological specimens. The hybrid material was optically and morphologically characterized with UV-Vis-NIR spectrometry, scanning and transmission electron microscopy (SEM and TEM), and Raman spectroscopy. To evaluate the SERS efficiency of the sensor different Raman reporters, biological surrogate's samples and viability/degradation tests were performed.

To test the suitability of the sensor on clinically relevant settings, the latter will be incubated within the plasma from patient's cohort already mentioned. The classification of the clinical samples based on their SERS profiles will be accomplished by using machine learning (ML) algorithms.

A comparison between ML applied to SERS profiles coming only from the plasma or from the plasma in contact with the sensor was performed to understand the plasmonic sensor's relevance in the performance of this nouvelle approach as a less invasive, more sensitive, and standardized cancer diagnosis tool. Discrimination results in mice plasma showed promising performance, rated up to 92% on Area Under the Curve (AUC) values, and also showed the sensor's relevance by the values of AUC up to 94% obtained for cell supernatants measured in contact with the sensor against AUC up to 61% for cell supernatants alone.

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Tuning the chiroptical response of discrete gold nanoparticles

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F4_3, Z2 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Chirality is a molecule or structure property that is present in our daily life, and it can be from nano (conformation of small molecules) to macro (our hands or the shape of galaxies). Generally, enantiomers show similar physical properties, however, normally they have opposite optical properties, depending on how they are rotating the plane of polarization of an incident beam light.

When an electromagnetic beam interacts with plasmonic nanoparticles, this generates a localized surface plasmon resonance (LSPR) with highly intense electromagnetic field at nanoparticles surface. Coupling the LSPR of achiral structures with chiral molecules, it is possible to increase and modify the chiroptical response of the hybrid nanomaterial. Chiral plasmonic nanostructures have been developed by assembly achiral plasmonic nanoparticles into chiral configurations by using chiral templates or chiral molecules [1]. Recently, plasmonic nanoparticles with an intrinsic chirality have been achieved [2,3].

In this context, we have developed one step synthesis of chiral-plasmonic nanoparticles by using achiral gold nanorods as seeds. We have studied the chirality evolution by HR-TEM as well as the chiral efficiency. Likewise, depending on the seed used, we are able to control and tune the CD response of the new chiral nanoparticles. Thanks to the layer by layer technique we have deposited on a glass substrate different layers of chiral nanoparticles and the chiroptical response have been evaluated. Moreover, taking advantage of the CD better efficiency than the LSPR, we have used the chiral substrates to develop a more efficient system to measure the refractive index sensitivity.

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Wearable Heart Rate Sensors Based on Laser-Induced Graphene on Alginate and Novel Polyurethanes

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F4_2, Z2 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

The rapid expansion of wearable sensor technology has raised concerns about electronic waste and environmental sustainability. Traditional wearable sensors are often made from non-degradable materials, contributing to long-term pollution and disposal challenges. As the demand for wearable health monitoring devices grows, it is essential to develop biodegradable alternatives that maintain high performance while minimizing environmental impact. In this study, we present two biodegradable substrates for wearable sensors: a naturally derived cross-linked sodium alginate (CL-SA) film and a novel synthetic polyurethane based on α,ω -dihydroxy-poly(ϵ -caprolactone)-b-poly(dimethylsiloxane)-b-poly(ϵ -caprolactone) (PCL-b-PDMS-b-PCL).

The alginate film was synthesized by dissolving sodium alginate in distilled water, followed by crosslinking with Ca^{2+} ions. Laser-induced graphene (LIG) was produced on CL-SA substrates via direct laser induction. For the polyurethane-based substrate, we synthesized a polymer network using PCL-b-PDMS-b-PCL, 4,4'-methylenediphenyl diisocyanate, and hydroxy-functional hyperbranched polyester through a two-step polymerization. Polyurethanes with soft segment contents of 40, 50, and 60 wt% were prepared for subsequent integration with LIG.

To assess the potential of both materials for wearable sensor applications, we performed an extensive physicochemical analysis of synthesized substrates and LIG samples on each substrate. Raman spectroscopy, scanning electron microscopy with energy-dispersive X-ray spectroscopy, X-ray diffraction, transmission electron microscopy, and Fourier-transform infrared spectroscopy were used to examine the structure and composition of the prepared materials. The analysis revealed that while CL-SA provides a biodegradable platform, the polyurethane-based network offers superior flexibility, making it more suitable for wearable applications. Given its enhanced flexibility, we selected the polyurethane-based LIG sensors for real-time heart rate monitoring. Utilizing the piezoresistive properties of LIG, we recorded heartbeat signals by connecting the sensors to a pulse simulator and a measuring device. Voltage changes were measured over time in constant current mode, demonstrating the sensor's ability to detect subtle physiological signals with high sensitivity.

These results highlight the potential of integrating LIG with biocompatible and biodegradable substrates for sustainable, high-performance wearable sensors. By combining biocompatibility, flexibility, and precise physiological detection, this work paves the way for eco-friendly, next-generation health monitoring technologies.

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Enhanced Electrochemical Sensing of Doxorubicin Using a Polymer Nanocomposite-Modified Screen-Printed Carbon Electrode

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Advancements in electrochemical sensor design continuously refine surface kinetics, leading to enhanced analytical performance, greater reliability, and broader application potential. Among various sensor platforms, screen-printed electrodes (SPEs) have gained significant attention for sensitive drug detection due to their adaptability for surface modifications. The integration of carbon nanomaterials, noble metals, and polymers has substantially improved electroanalytical performance, leveraging their unique chemical and physical properties to enhance electrode reactivity.

This study presents the development of a novel electrochemical sensor based on a polymer-modified carbon SPE for the detection of doxorubicin (DOX) at low clinical concentrations. The sensor's unique modification involves a nanocomposite of reduced graphene oxide decorated with gold nanoparticles, embedded within a Nafion matrix — a configuration not previously reported in the literature for DOX detection. The synthesized material was characterized using FTIR, Raman spectroscopy, XRD, and SEM.

Electrochemical analysis via cyclic voltammetry demonstrated precise quantification of DOX, exhibiting a linear concentration range of 1.5 to 22.1 μM and an improved detection limit of 9.263 μM , compared to 16.676 μM for the unmodified SPE. The developed sensor also exhibited an enhanced sensitivity of 0.272 $\mu\text{A}/\mu\text{M}$, significantly higher than the bare electrode's 0.152 $\mu\text{A}/\mu\text{M}$. Additionally, its high surface area, efficient functionalization, and rapid response highlight its potential for practical applications in anticancer drug monitoring.

Optimization of Liquid-Gate Graphene Field-Effect Transistors for Enhanced Sensing Reliability and Portable Characterization

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F4_2, Z2 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

Graphene has attracted considerable attention across a wide range of applications due to its exceptional properties, which include high electrical conductivity, mechanical strength, chemical stability, sensitivity, and a large surface-to-volume ratio. These characteristics make graphene particularly useful in the development of novel electronic and sensor devices. Graphene field-effect transistors (GFETs), especially when integrated with a liquid gate, offer a versatile platform for detecting various molecules and ions in biological samples, making them highly promising for biosensing applications. However, the liquid gate and the formation of the electric double layer, both of which are essential for the sensing mechanism, introduce significant variability in the detection process. This variability can impact the accuracy and reproducibility of measurements, making it crucial to address these challenges for more reliable performance in practical applications.

This study focuses on optimizing the fabrication and lithography processes of liquid-gate devices to minimize variability and enhance device reliability. To achieve this, we employ a wafer-scale process with planar devices, eliminating the need for external gate probes. By using this approach, we ensure more consistent results across large-scale device arrays. Additionally, we enhance the standard lithographic process by incorporating a sacrificial layer to protect the graphene during fabrication, preventing damage and improving the overall quality of the devices.

Hundreds of devices have been characterized both morphologically and electrically to assess and refine the layout design and lithographic techniques, leading to a reduction in device variability. Characterization efforts include extensive morphological imaging (SEM, AFM, XPS and Raman) and electrical performance analysis, as well as detailed low-frequency noise measurements and interface state density determination, which provide critical insights into device behavior. Moreover, we introduce a printed circuit board (PCB) as a key innovation to facilitate electrical characterization outside of laboratory environments. The PCB enables the measurement of device performance in real-world, portable settings, offering greater flexibility and practical applicability in biosensing scenarios.

Looking ahead, the next phase of this research will focus on the functionalization of graphene to enable the detection of specific biological molecules. This step will involve tailoring the surface properties of graphene to enhance its selectivity and sensitivity for target analytes, making it a more effective tool for biosensing applications.

Microbial production of silver nanoparticles: characterization and applications

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F4_3, Z2 Room (Level -3), septiembre 16, 2025, 17:00 - 19:00

Silver nanoparticles (AgNPs) are highly valued for their distinctive physical and chemical properties, enabling applications in diverse fields such as antimicrobial coatings for medical devices, water purification systems, and biosensors for electronics and bioimaging. Conventional physical and chemical synthesis methods often pose environmental concerns, generating significant amounts of byproducts. This has driven a growing interest in sustainable alternatives, particularly microbial-based approaches. In this context, bacteria from extreme environments have shown great promise, as their adaptability to harsh conditions allows nanoparticle synthesis under a broad range of parameters.

In this study, AgNPs were biosynthesized using the cell-free secretomes of various thermophilic microorganisms from our collection. The synthesis process was monitored via UV-Vis spectrophotometry, while the nanoparticles were characterized using transmission electron microscopy, Fourier transform infrared spectroscopy, and dynamic light scattering with zeta potential analysis. Additionally, their catalytic and conductive properties were evaluated demonstrating their potential for several applications. These results highlight extremophilic microorganisms as valuable biological resources for the sustainable production of nanomaterials, reinforcing their role in advancing eco-friendly biotechnological processes.

Engineering Fluorescence Resonant Energy Transfer (FRET) via plasmonic systems for ultra-sensitive biosensing

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F4_2, Z2 Room (Level -3), settembre 16, 2025, 14:30 - 16:30

Fluorescence Resonant Energy Transfer in the Förster regime is a widely studied photodynamic process based on a non-radiative dipole-dipole interaction between an excited donor molecule and a ground-state acceptor molecule [1]. Due to its strong dependence on the distance and relative orientation of the interacting dipoles, as well as the electromagnetic properties of the surrounding environment, FRET has emerged as a powerful tool for biosensing applications. While FRET inhibition can be achieved by increasing the donor-acceptor distance, its enhancement can be realized through interaction with resonant photonic environments, such as plasmonic structures or optical cavities [2].

This project explores the electromagnetic interaction between multi-resonant plasmonic systems and a biological FRET platform. By tailoring plasmonic resonances to match the absorption and/or emission spectra of the donor-acceptor pair (DAP), we aim to selectively modulate the acceptor fluorescence, enabling precise control over FRET efficiency [3]. Beyond fundamental insights into energy transfer mechanisms, this approach holds great potential for developing highly sensitive biosensors. Compared to conventional sensing platforms, plasmon-assisted FRET offers superior specificity, rapid response, and the ability to detect biomarkers at ultralow concentrations, making it a promising candidate for next-generation diagnostic tools.

In this initial phase, we focused on a model biological system consisting of an engineered *E. coli* strain expressing a fusion protein composed of a cyan fluorescent donor (eCFP) and a yellow fluorescent acceptor (eYFP), connected by an amino acid linker of variable length (CLY#, Cyan-Linked-Yellow, where # indicates the linker distance). Furthermore, this work investigates the electromagnetic interaction between a biological FRET system and simple plasmonic structures, such as gold nanoparticles with a diameter of 50 nm. This well-defined system provides an ideal testbed for investigating and optimizing the interplay between FRET and plasmonic nanostructures, paving the way for advanced biosensing strategies with enhanced performance.

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SERS-based platform for mutation analysis in acute myeloid leukemia

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F4_1, Z2 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Acute myeloid leukemia (AML) is the most common form of acute leukemia in adults and is frequently associated with poor outcomes to conventional therapies in the most affected population [1]. After treatment with chemotherapy, even patients that clinically achieve complete remission can relapse through the persistence of minimal residual disease (MRD). Current diagnostic tools are not enough for early detection of MRD [2]. An accurate and early diagnosis of MRD would allow the application of appropriate therapy, improving the prognosis of patients. Surface-enhanced Raman scattering (SERS) spectroscopy has remarkably flourished in the recent years and demonstrated to be powerful tool for detection of specific markers, and for diagnosis [3,4]. The main goal of this work is to create a non-invasive diagnostic tool for the early detection of specific mutations in AML disease. For this purpose we designed, fabricated, tested and optimised a SERS sensor for efficient and fast detection of AML mutations, without any pre-amplification. Thus, some substrates were developed using an innovative strategy where gold nanostars were grown in situ. Afterwards, immobilisation of molecular beacons was performed and the performance of the substrates was tested using synthetic targets. This will promote a multiplex and quantitative detection of specific AML mutations in blasts isolated from patient samples, enabling the application of personalised therapy and consequently improving the prognosis of patients.

Microfluidic based LC sensor and antennas with tuned performances using liquid conductors

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This study explores the feasibility of constructing LC resonant circuits and antennas using liquid-based media within microfluidic channels. A hybrid fabrication approach combining stereolithography (SLA) 3D printing and xurography was employed to develop these microstructures. The microfluidic channels, printed using Elegoo Standard White resin, were designed for liquid capacitors and sealed with a PVC top layer embedded with aluminum conductive tape to enable capacitance measurements. The capacitor structure exhibited capacitive properties, with channel dimensions of 0.7 mm in width and depth and an active area of 18 × 21 mm. The process of design and fabrication of the following electronics components is presented: capacitor, inductor, LC sensor and antenna. The inductor is designed as square inductor with 5 turns, whereas capacitor as interdigitated electrode system with 13 fingers. Combining of this L and C components, LC sensor is created. In the microfluidic channel, the liquid (ionic) conductor is injected (liquid with electrolytes - Powerade). The quantity of injected ionic conductors can adjust the value of inductance or capacitance and as a consequence the resonant frequency can be tuned. Using impedance analyser, the electrical parameters: inductance, capacitance, impedance and phase angle are measured. For the antenna, xurography was solely used, employing a PVC foil substrate. A conductive loop made from aluminum tape formed the inductive component. A cutter plotter was used to cut the microfluidic channels in the PVC foils in the middle, and again PVC foil at the top with the inlet for the liquid conductor. These layers are laminated using hot laminator under pressure to obtain compact structure. The liquid was introduced into the antenna using a syringe to ensure precise and controlled insertion into the designed channels. Final antenna dimensions were 91 x 40 mm. The antenna's performance was evaluated using a vector network analyzer to determine S-parameters. Compatibility of LC sensor and antenna and their inductive coupling for wireless sensing applications was determined.

High-Sensitivity Graphene Liquid-Gate Transistors for Next-Generation Biosensing Applications

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F4_2, Z2 Room (Level -3), septiembre 16, 2025, 14:30 - 16:30

The escalating global threat of antimicrobial resistance (AMR) demands innovative solutions for rapid and precise diagnostics. Current detection techniques are often slow, costly, and impractical for real-time applications, exacerbating the misuse of antibiotics and accelerating the emergence of drug-resistant pathogens. In this context, graphene field-effect transistors (GFETs) have emerged as promising biosensing platforms due to their extraordinary sensitivity, high carrier mobility, intrinsic low-noise properties, ease of use, and low cost.

This work presents a systematic optimization of graphene liquid-gate transistors tailored for biosensing applications, enabling the detection of proteins, glucose, viral particles (e.g., SARS-CoV-2, HPV), and cancer biomarkers (melanoma, colorectal cancer). The proposed fabrication process includes graphene transfer onto SiO₂/Si substrates, microelectronic-based fabrication, passivation strategies, and biofunctionalization with linker molecules and antibodies, ensuring selective and reliable analyte detection.

The biosensing mechanism is based on the modulation of the GFET's electrical output characteristics, which shift proportionally to the charge and concentration of target biomolecules. Experimental validation demonstrates a clear and linear response for low-to-medium analyte concentrations, confirming the potential of GFETs as highly sensitive diagnostic tools. However, challenges related to device variability and signal reproducibility remain, necessitating deeper insights into the role of surface functionalization.

To address these limitations, we leverage nanometric structural characterization and TCAD simulations to explain the experimentally observed behavior of liquid-gated GFET biosensors. The simulation results, which model liquid-gated GFET biosensors while accounting for antibody distribution effects, reveal a quantifiable shift in the sensor's I-V characteristics, demonstrating strong agreement with experimental findings. However, non-uniform antibody adsorption introduces variability in the measured current, underscoring the need for precise surface engineering strategies.

Our findings underscore the transformative potential of graphene-based biosensors in next-generation point-of-care diagnostics, offering a fast, cost-effective, and scalable solution for real-time disease detection. Future work will focus on enhancing reproducibility through advanced biofunctionalization techniques and integrating microfluidic architectures to further refine sensor performance.

SERS-on-a-chip as an excellent tool for the One Health approach of AMR monitoring

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F4_1, Z2 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

One Health approach in the EU Commission recognizes that the health of humans, animals, and the wider environment are inherently linked and interdependent. It is particularly essential for antimicrobial resistance (AMR) because resistant organisms can spread quickly through healthcare facilities, animals, food and the environment, making treating certain infections more challenging, and increasing the risk of disease spread, severe illness and death. Expanded monitoring of antibiotics and pathogens, adopting the One Health approach, can help better understand the effectiveness of actions to reduce antibiotic use and take a more holistic and systemic course of action to control AMR.

Surface-enhanced Raman scattering (SERS) in combination with microfluidic technology, provides very sensitive detection of molecular species even in the single-molecule regime. On the one hand, SERS measurements can now be carried out in nanoliter volume in an automatic and reproducible manner; on the other hand, SERS offers to microfluidic devices an ultra-fast detection in small volumes. Implementing SERS-on-a-chip in environmental and biosciences is becoming very popular as it provides significant information about the studied system even directly from complex environments such as seawater, biological fluids, living tissues, and cells. This talk will focus on demonstrating SERS-on-a-chip configuration's ability to monitor antibiotics and pathogens.

Electrically Controlled Molecular Motions Tracked by Graphene-Enhanced Fluorescence Lifetime Microscopy

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F4_1, Z2 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Graphene's near-field effects, when combined with fluorescence measurements, offer a powerful approach for observing molecular-scale distances in aqueous environments [Gaudreau 2013; Adao 2019]. Here, we demonstrate the application of this technique to track on-demand molecular motions induced by the electric gating of a graphene-based device. Using 3D origami DNA architectures tethered to graphene via molecular linkers, we applied a back gate voltage through gold contacts, enabling operation in two distinct voltage regimes [Azevedo 2024]. The resulting molecular responses were tracked with high precision using fluorescence lifetime measurements.

We successfully observed molecular motions linked to the flexibility of the molecular binding unit, transitioning between open and compact conformations. Furthermore, leveraging recent advancements in fluorescence wide-field TIRF microscopy, which allows for simultaneous tracking of multiple molecular emitters with millisecond-range temporal resolution [Soares 2024], we created molecular machines with a highly sensitive fluorescence-based readout system. In particular, we used fluorophore-labeled DNA hairpins to detect their unfolding kinetics during the hybridization reaction with fully and partially complementary DNA sequences containing a 10-mismatch nucleotide region located at the 5', 3' ends and in the middle of the DNA single strand. The average unfolding times were estimated to be between 0.21 and 0.29 seconds for the fully complementary, top, and bottom mismatch strands and notably longer for the middle mismatch strand in a range between 0.42 and 0.51 seconds. Moreover, based on fluorescence lifetime measurements, the axial nanometer-scale distances of the attached dyes reveal significant differences. The dye was 10 nm above the graphene surface in the middle mismatch DNA strand, while the fully complementary, top, and bottom mismatch strands showed distances of around 12 nm. Our approach paves the way for future applications in nanotechnology and molecular sensing.

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Cancer Diagnostics Reimagined: Applying Novel Biosensing Techniques in Clinical Research

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F4_1, Z2 Room (Level -3), septiembre 16, 2025, 10:30 - 13:10

Advancements in biosensing technologies have the potential to revolutionize cancer diagnostics and patient monitoring by surpassing the limitations of conventional analytical methods. However, many of these innovations remain confined to research laboratories and fail to translate into clinical practice. This gap often arises from a lack of coordination between technical and clinical research, leading to the development of tools that do not fully address clinical needs.

Embedding the development of new biosensing tools within a hospital setting provides a unique opportunity to align technological innovation with real-world medical applications. Direct collaboration with clinicians, clinical laboratories, and patients facilitates the iterative refinement of these technologies, ensuring their relevance and usability in patient care.

This presentation will explore efforts at the Laboratory of Nanomedicine at Istituti Clinici Scientifici Maugeri, a research hospital in Italy, to adapt two advanced biosensing approaches—Single Molecule Array (SiMoA) and Raman spectroscopy—for clinical oncology applications. SiMoA's ultra-sensitive detection capabilities enable the profiling of cancer-derived extracellular vesicles directly from the blood of breast cancer patients, offering novel insights into disease progression. Raman spectroscopy, meanwhile, is emerging as a powerful tool for cancer diagnostics, with applications in both tissue analysis for surgical margin detection and liquid biopsy for profiling circulating tumor cells.

Thanks to the close collaboration between researchers and medical professionals, we focus on the adaptation of the novel sensing strategies to move beyond theoretical breakthroughs. This talk will thus highlight our ongoing journey to bridge the gap between material science and clinical application, ultimately pursuing how to enhance diagnostic precision and informing therapeutic decision-making in oncology.

Advanced Nanoindentation Approaches to Assess the Mechanical Behavior of Dental Composites

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F5_2, Seminario 6 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Nowadays dental composites are mainly reinforced with quartz particles, often called conventional, and polymerized in layers or in bulk-fill mode. A modern approach is to reinforce the composite with short optical fibres (SFRC). The optical fibres can enhance the polymerization process and improve mechanical behaviour.

In this study we tested 5 groups of dental composites, where the samples were standardized in a 5x5x5 mm geometry. In total n=18 samples were produced, the groups were the following: group 1: (control) conventional layered composite in 2+2+1 mm, group 2: layered SFRC in 2+2+1 mm, group 3: bulk-fill SFRC, group 4: bulk-fill conventional, group 5: layered in 2+2 SFRC and 1 mm conventional. After the polymerization the hardness of samples were measured with the nanoindentation technique both on the top, side and bottom along with creep measurement on the top. After the measurements the samples were stored in water for 30 days and finally the mechanical behaviour and parameters were measured once again. During the 30 days the water absorption of each sample were measured.

The conventional bulk-fill dental composite (group 4) showed significantly lower mean hardness ($p < 0.001$). The SFRC did not show statistically significant difference in the hardness. Bulk-fill SFRC and conventional showed significant difference in the mean elastic modulus ($p = 0.005$). The creep behaviour showed a significant difference as well, especially the time behaviour parameters (retarded modulus and viscosity in the standard linear model). The water absorption showed significant difference between the groups, the SFRC bulk-fill showed a significant less mean water absorption. The groups also showed a linear correlation between the water absorption and time passing ($p < 0.001$, $r = 0.71-0.85$).

The SFRC samples showed similar hardness while the bulk-fill conventional composite had less hardness.

Combining In Ovo Testing and MicroCT Imaging to Assess Tissue Integration and Angiogenesis in Porous Scaffolds

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Preclinical in vivo studies are widely used to evaluate the compatibility and performance of a wide range of materials for biomedical applications, but ethical concerns and challenges in translating animal data to humans have spurred the search for animal-free alternatives. The FDA Modernization Act 2.0 has accelerated this shift by promoting the 3Rs principles and supporting the development of innovative methods for medical device and pharmaceutical approval [1].

This study explores the use of the chorioallantoic membrane (CAM) of fertilized hen eggs as a promising alternative for evaluating the blood compatibility, angiogenesis, and tissue integration of a wide range of biomaterials, from contact lenses to bone scaffolds. The in ovo CAM test is cost-effective, reliable, and reproducible, and is not considered an animal experiment under Directive 2010/63/EU until embryonic day (ED) 17, as the chick embryo does not experience pain before ED 14. Visual monitoring of the CAM allows for the classification of biomaterials based on their potential ocular irritation (since the CAM resembles the conjunctiva) [2] and their ability to promote or inhibit microcapillary development around and over the scaffolds [3].

Additionally, this work aimed to combine in ovo testing with microcomputed tomography (microCT) imaging to provide precise, non-destructive, 3D visualization of tissue integration within porous materials. Bone scaffolds and wound dressings were tested on fertilized eggs within the timeframe when the experiment is not considered an animal experiment. After incubation, the CAMs were fixed, stained, and imaged with microCT to assess blood vessel formation and tissue integration. The method enabled accurate quantification of tissue ingrowth and vessel formation across various biomaterials [4]. Bone scaffolds with open porosity showed extensive vascularization and integration with the CAM, while wound dressings did not integrate, indicating that they can be safely removed without disrupting the underlying tissue. In conclusion, this combination of in ovo testing and microCT imaging offers a promising animal-free alternative for evaluating biomaterials in tissue engineering applications.

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Protein adsorption on biomaterials for tissue integration: a predictive way and a surface modification strategy

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F5_1, Seminario 1 + 2 Room (Level +1), settembre 16, 2025, 14:30 - 16:30

Protein adsorption is the first step in the integration of an implanted biomaterial with tissues. It sequentially leads to clot formation, the inflammatory cascade, the osseointegration process, and/or soft tissue adhesion. Biofilm formation is also influenced by the protein layer adsorbed on the implant surface.

Surface characteristics, such as topography and morphology (at the micro- and nanoscale) or surface chemistry (exposure of functional groups, wettability, and charge), can affect the overall amount of adsorbed proteins and the surface selectivity for specific proteins. Therefore, a detailed study of protein adsorption is an interesting approach to predicting the outcome of an implantable biomaterial and guiding its design. Protein pre-adsorption can also be used as a surface modification strategy to direct the biological response of a surface toward a specific target.

Nevertheless, the study of protein adsorption has, so far, been underestimated in biomaterial characterization protocols. This is partly due to the complexity of this type of characterization, which, however, can be addressed through the use of more recently developed techniques.

The development of a detailed characterization protocol for protein adsorption is also relevant for minimizing the use of animals in experimentation.

A characterization protocol will be presented to provide insights into a surface's potential selectivity for proteins, the surface coverage by the protein adsorbed layer, the chemical interaction between the surface and proteins, and possible changes in the tertiary structure of the adsorbed proteins. As an example, modified titanium surfaces will be analyzed.

It will be demonstrated how certain surfaces can selectively promote the adsorption of fibrinogen over albumin or fibronectin, or how they can adsorb these proteins in different configurations. Additionally, correlations between this behavior and specific surface properties will be presented.

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Self-Healing polysaccharide-based hydrogel as three-dimensional carrier for tissue repair

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F5_1, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Self-healing hydrogels are a crucial tool in tissue engineering, offering the advantage of autonomous repair (i.e. self-repair), which minimizes the need for extensive intervention and makes them ideal for developing functional implants with minimal disruption to surrounding tissues [1]. The biocompatibility of these materials is essential, making the use of natural polysaccharides, abundant in the extracellular matrix, highly beneficial. These hydrogels are typically synthesized using dynamic covalent bonds, enabling them to self-heal under physiological conditions. Additionally, the incorporation of inorganic components, such as magnetic particles, allows for external control over the material's behavior [2].

A key advantage of using these hydrogels as cell carriers is their ability to prevent cell loss during injection, as they shield cells from the shearing forces encountered in the injection process [3]. This property makes them particularly suitable for applications in cell-based therapies and tissue regeneration.

This study focuses on the development of biomimetic self-healing hydrogels synthesized via dynamic imine cross-links formed through a Schiff reaction between amino and aldehyde groups of functionalized polysaccharides. The resulting hydrogel exhibits self-repair capabilities, restoring its structural integrity after being injected through needles under physiological conditions. To study the mechanical properties of these hydrogels before and after the extrusion, rheological characterization is conducted using a torsional rheometer under various conditions, assessing viscoelastic behaviour, self-healing efficiency, and mechanical tunability. Additionally, the incorporation of carbonyl iron microparticles is explored to evaluate the impact of external magnetic fields on hydrogel structure and mechanical performance. Furthermore, cellular behaviour is analyzed through morphological characterization and biocompatibility assays to assess the hydrogel's interaction with cultured cells.

The results highlight the versatility of self-healing hydrogels as biomaterials for tissue engineering, offering a tunable mechanical response, adaptability, responsiveness to dynamic environmental stimuli, and significant potential as cell carriers.

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A Microfluidic Model to Evaluate the Proangiogenic Effects of Biomaterials

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F5_2, Seminario 6 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Vascularization is critical for the successful integration of biomedical implants, as a sufficient blood supply is essential for their functionality. To promote revascularization, various strategies have been explored, including the incorporation of angiogenic factors. However, these approaches are hindered by challenges such as the limited stability of the factors and their high production costs. As an alternative, optimizing the physicochemical properties of biomaterials to stimulate vascularization has been actively investigated.

Current models used to assess implant vascularization exhibit significant limitations, including the difficulty in isolating the effects of individual material parameters. Furthermore, traditional assays often fail to accurately replicate in vivo conditions. Microfluidic platforms have emerged as a promising solution, providing precise control over the cellular microenvironment, mimicking physiological conditions, and enabling more efficient and cost-effective studies.

In this work, we introduce a 3D model utilizing microfluidic technology that addresses the limitations of traditional methods, providing a more biomimetic tissue environment. This platform allows for the evaluation of how bioactive biomaterials, releasing signaling molecules like ions or proteins, modulate angiogenesis. The model was validated through computational simulations and experiments assessing cell migration [1].

This compact microphysiological platform enables the investigation of interactions between biomaterials and endothelial cells to evaluate their capacity to promote vascularization. Its application could accelerate preclinical testing of biomaterials and enhance the understanding of the mechanisms underlying vascular formation, addressing the shortcomings of traditional models. This innovation provides a reliable and efficient alternative for tissue regeneration research and the development of novel biomaterials.

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Bone-on-a-chip with biomimetic scaffolds

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Bone tissue engineering (BTE) is a promising option in the face of the growing incidence of bone diseases that require transplants. BTE uses a scaffold of a biomaterial that mimics bone tissue, but in static conditions we do not achieve the dynamism that exists in vivo.

Microfluidic devices can facilitate the development of conditions that closely emulate the in vivo environment by allowing fluidic control of oxygen and nutrient supply and controlled application of mechanical stimulation.

The convergence of biomaterials, stem cells and microfluidics has enabled the fabrication of devices Organ-on-a-Chip (OoC) that replicate the real microenvironment of a tissue or organ. OoCs allow different physical or chemical stimuli to be applied to the tissue that recreate cellular physiology, offering greater control of the cellular microenvironment.

The material selected for the manufacture of these devices, in addition to being biocompatible, must have the appropriate physical and mechanical properties to match the mechanical characteristics of the target organ, which is essential when mimicking bone.

B5Tec has a flow controller designed and developed by the company that allows the flow rate to be controlled with great precision. This has been used to develop a Bone-on-a-chip prototype together with the UCM research group.

We used 3D titanium scaffolds that were encapsulated in resin bases with a PDMS cap. All materials of the prototype and flow controller were found to be biocompatible. We performed a culture of pre-osteoblastic cells, in differentiation medium, observing that in different dynamic conditions we have cell proliferation and that intermittent flow increases osteoblastic differentiation. With this result we performed a co-culture with intermittent flow of preosteoblasts and macrophages, observing that there was proliferation of both cell types and again increased osteoblastic differentiation.

These results are novel and promising for achieving a situation of dynamic tissue growth in the laboratory, which would represent a significant advance in the simulation of the complex bone microenvironment. It should be noted that in the future they could be implantable in vivo, since we use biocompatible materials, and they could be developed with a focus on personalized medicine, based on the patient's own cells.

The new technology offers additional advantages such as real-time monitoring in a highly automated way, reducing costs and reallocating the costs necessary for experiments and allowing a large number of reproducible tests to be carried out in a short time and with reliable results, thus reducing research times.

Photocrosslinked 3D Foamed Scaffolds Based on GELMA/HEMA copolymers and MBGs: Potential Application in Bone Tissue Engineering

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The treatment of bone defects represents one of the great challenges of orthopedic surgery, with autografting standing out as the best option to address this problem. Therefore, one of the great challenges in the field of Tissue Engineering (TI) is the development of structures that fulfill the same functions as an autograft, but without the limitations that these entail. In this context, bioactive mesoporous glasses (MBG) in the SiO₂-CaO-P₂O₅ system present great potential in the field of TI for bone regeneration, as they offer a large specific surface area and high porosity. To increase the regenerative capacity of the materials, the incorporation of Sr²⁺ and Zn²⁺ or Sr²⁺ and Mn²⁺ ions has been studied. In this project, the in vitro regenerative properties of three-dimensional GelMA-HEMA/MBG hybrid scaffolds have been investigated by 3D printing.

On the one hand, mesoporous bioactive glasses (MBG) have been synthesized in the system 85 SiO₂-10 CaO- 5 P₂O₅, doped on one hand with 4% ZnO and 2.5% SrO and on the other hand 1% MnO and 2.5% SrO and undoped. On the other hand, a biocompatible copolymer of gelatin with a degree of methacrylation of 95% and 2-hydroxyethylmethacrylate (GelMA-HEMA) has been synthesized. Both MBG and GelMA-HEMA copolymer have been blended to obtain bioinks for robocasting with MBG, processable for the fabrication of three-dimensional meso-macroporous scaffolds. Scaffolds exhibiting hierarchical porosity: mesopores (around 4 nm), macropores (1-600 µm) and big channels (1000 µm), were prepared.

The maximum swelling of a maximum of 250 wt% of the scaffolds in PBS and alfa-MEM in a few hours indicates their capacity to adsorb nutrients necessary for cell development, and to adapt to the bone defect in which they are implanted. These scaffolds, in addition to their demonstrated cytocompatibility, offer good structural morphology and interconnected porosity, resulting in adequate cell development. In cellular assays, it has been demonstrated that scaffolds with teriparatide-loaded MBGs stand out in cell differentiation and mineralization assays compared to unloaded scaffolds. Scaffolds with strontium- and zinc-doped MBGs show the best proliferation, as well as differentiation above scaffolds with strontium- and manganese-doped MBGs. Furthermore, an improvement in the osteogenic properties of the scaffolds when loaded with teriparatide has been observed, due to the synergy between the inherent properties of the MBGs, therapeutic ions and the effects of the osteogenesis agent.

Omics technologies to identify key biochemical pathways involved in the antitumor activity of a mesoporous silica nanosystem containing selenium nanoparticles

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Breast cancer is the most commonly diagnosed cancer in women, primarily affecting those aged 50 and older. Among its various subtypes, the Luminal A estrogen receptor-positive (ER+) tumor is the most prevalent and has the best prognosis, as it can be treated with chemotherapy and hormonal therapy. However, these treatments involve significant challenges due to the high concentrations currently required, leading to drug resistance and severe side effects. Therefore, new therapies capable of selectively targeting cancer cells while sparing healthy tissues are still urgently needed.

In response to this need, this study proposes a novel nanosystem that combines two antitumor agents: selenium nanoparticles (SeNPs), known for their chemotherapeutic properties, and tamoxifen (TMX), a drug commonly used to treat hormone-responsive breast tumors. Both agents are compressed within a single nanosystem composed of mesoporous silica nanoparticles (MSNs), with transferrin (Tf) anchored to the surface. This functionalization enhances the selectivity of the system (MSNs-TMX-Tf-SeNPs) towards cancer cells that overexpress transferrin receptors (TfR).

Following the synthesis and physicochemical characterization of the nanosystem, functional characterization was performed to evaluate its efficacy in an in-vitro model using T47D breast cancer cells (Luminal A subtype). Furthermore, omics technologies were employed to identify the key biochemical pathways involved in the antitumor activity of this novel nanosystem.

The results demonstrated a significant antitumor effect, primarily inducing senescence and, to a lesser extent, late apoptosis, likely attributed to TMX activity. Moreover, two critical mitochondrial metabolic pathways were found to be disrupted: the tricarboxylic acid (TCA) cycle and one-carbon metabolism, specifically the folate cycle. Additionally, damage to the endoplasmic reticulum was observed, associated with alterations in the biosynthesis of monounsaturated fatty acids and cholesterol. These disruptions ultimately led to hypoxia and oxidative stress, triggering autophagy and cell death.

Biofunctional magnetic scaffolds that enhance osteogenic differentiation of mesenchymal stem cells through mechanotransduction

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Magnetic composite biomaterials have garnered significant attention in bone tissue engineering (BTE), as dynamic magnetic fields have been shown to modulate the proliferation and differentiation of various cell types. The aim of this manuscript is the fabrication of biofunctional magnetic scaffolds combining Fused Deposition Modeling (FDM) and thermal Drop-On-Demand (DoD) inkjet printing. The 3D scaffolds were initially fabricated from thermoplastic polymers, including poly-L-lactic acid, polycaprolactone, and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) by FDM and subsequently super paramagnetic iron oxide nanoparticles were incorporated via DoD. The obtained results demonstrated the precision and versatility of the fabrication technique, as well as the scaffolds' stability under physiological conditions and their magnetic capability. Biological evaluation with human bone marrow mesenchymal stem cells confirmed the scaffolds' biocompatibility and enhanced osteogenic potential under the application of a magnetic field, which activated mechanotransduction processes. These findings indicate that the developed 3D magnetic biofunctional scaffolds hold great promise as a tool for advanced and personalized bone regeneration therapies.

Multifunctional copper-containing mesoporous glass nanoparticles for wound healing in bone infection treatment

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F5_2, Seminario 6 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The prevalence of chronic wounds in bone infections is a key factor to take into account since they hinder the regeneration of the damaged tissue. This situation leads to a continuous proinflammatory state and a decrease in the level of stem cells. Although the management of these wounds focuses on applying passive protective barriers that keep the wound environment away from external agents, often infections cannot be prevented, leading to ischemia and necrosis.

This research work reports the design and development of innovative nanosystems based on biocompatible and multicomponent radial mesoporous glass nanoparticles (RNPs), in the SiO₂-CaO-P₂O₅ system, for wound healing in bone infection treatment. The combination of the antibiotic rifampicin (RIF) and reparative metal ions (Cu²⁺) in a unique nanosystem, allows the incorporation of antimicrobial and regenerative agents to combat wound healing, infection and promote bone regeneration.

Rifampicin-loaded radial mesoporous glass nanoparticles in the SiO₂-CaO-P₂O₅ system (RNPs) containing Cu²⁺ in the outer shell were synthesized by a simple and versatile method. RNPs were externally functionalized with a third-generation polypropylene dendrimer (PPI-G3), which allows the complexation of metal ions through its tertiary amines and, moreover, favors bacterial internalization via its protonated primary amines. The nanosystem promoted fast wound closure (98.1%), high biocompatibility (>70%) and a great capacity for migration and invasion. The versatility of the nanosystem obeys its capacity to load any antibiotic and its ability to complex any therapeutic metal ion according to clinical needs. These results envision the possible development of personalized therapies for wound healing in bone infection treatments.

Impact of synthesis method, coating, and functionalisation on the cellular internalisation and efficacy of superparamagnetic iron oxide nanoparticles for bone tissue engineering

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F5_2, Seminario 6 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Superparamagnetic iron oxide nanoparticles (SPIONs) have emerged as versatile tools in a variety of biomedical applications, including bone tissue engineering. Their ability to induce specific cellular responses and facilitate bone regeneration makes them promising candidates for bone repair therapies [1]. In turn, the method of synthesis of SPIONs influences the structural and magnetic properties of the nanoparticles, which affects their efficacy in biomedical applications [2]. In addition, the size, coating and functionalisation of SPIONs are determining factors in their interaction with cells. Smaller nanoparticles may facilitate greater cellular internalisation, but may also present toxicity risks. On the other hand, specific coatings and functionalisations can enhance biocompatibility and direct cellular activity [3]. Therefore, in this work SPIONs have been synthesised by different methods: i) thermal decomposition of an organometallic precursor, ii) flame spray pyrolysis and iii) polyol-mediated liquid phase thermal decomposition. The SPIONs were then coated with dimercaptosuccinic acid or citric acid depending on the synthesis method, functionalised with an RGD peptide for targeting to cellular integrins and extensively characterised. Subsequently, a comparative internalisation study of SPIONs was carried out. For this purpose, bone marrow-derived human mesenchymal stem cells (hBM-MSCs) were used and flow cytometry assays with different endocytosis inhibitors, transmission electron microscopy, iron quantification and cytocompatibility analysis were performed. The results showed different internalisation dependent on SPION type, dose, coating and functionalisation, as well as different endocytosis mechanisms involved in nanoparticle uptake. In addition, different cellular localisation was observed depending on the time of study. These results are crucial to evaluate their role in different biomedical applications such as bone tissue engineering through mechanotransduction processes.

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Enhanced osteogenic differentiation and extracellular matrix formation by mechanically stimulated electroactive scaffolds

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F5_2, Seminario 6 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Background

Mechanical stimulation applied on cell-loaded scaffolds in in vitro cultures recapitulates the physiological bone tissue and effects the osteogenesis. Poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS) is a electrically conductive polymer that responds to mechanical stimulation producing an electrical signal that promotes the osteogenic differentiation of pre-osteoblastic cells by opening the voltage-gated calcium channels. The aim of this study was to examine the biological behavior of pre-osteoblastic cells when seeded onto electroactive PEDOT:PSS-containing scaffolds applying uniaxial compression as mechanical stimulation relevant to physiological body movements.

Methodology

PEDOT (0.15 % w/v and 0.10 % w/v) was combined with 5 % w/v poly(vinyl alcohol) (PVA) and 5 % w/v gelatin, casted into wells, freeze dried and crosslinked. The scaffolds were physicochemically, mechanically and biologically characterized. Scaffolds seeded with pre-osteoblastic cells were subjected to uniaxial compression by means of a bioreactor with a frequency of 1 Hz and a strain of 10% for 1 h every day for 21 days. The loading parameters resemble the in vivo loading situation. Cell viability and morphology of the pre-osteoblastic cells seeded onto the scaffolds was determined. The alkaline phosphatase (ALP) activity, the collagen and calcium production were quantified. Determination of the calcium and phosphorous mineralization through atomic-resolution mapping and Energy Dispersive Spectroscopy (EDS) was carried out, as well as X-ray diffraction (XRD) analysis, aiming to detect biomineralized matrix.

Results

Elastic moduli ranged between 1 and 5 MPa. The degradation rates indicate a mass loss of 15% after 21 days. Scanning electron microscopy images displayed strong adhesion of well-spread cells, while the cell viability increased over time. The ALP activity at days 3 and 7 was significantly higher in the dynamic culture compared to the static one. Increased collagen and calcium secretion validate osteogenic response and extracellular matrix formation. Moreover, EDS and XRD analysis revealed the presence of bone-like apatite formation on scaffold surfaces after 21 days.

Conclusion

The results indicate that the PEDOT:PSS/PVA/gelatin scaffolds support the adhesion, proliferation, and osteogenic differentiation of the pre-osteoblastic cells under mechanical stimulation. Furthermore, the development of a comprehensive 3D mechano-active model establishes an innovative platform for studying osteogenesis under conditions closely resembling the body natural state. This approach contributes to advancing in vitro evaluation but also significantly reduces the need for in vivo experimentation.

Dynamic stimulation using uniaxial compression promotes the osteogenic and anti-osteoclastogenic responses of cellular co-cultures within composite scaffolds

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Introduction

The dynamic bone tissue undergoes continuous remodeling through lifetime regulated by different cell types, bone forming osteoblasts and bone resorbing osteoclasts. Mechanical stimulation applied on bone tissue can shift the balance between these two cell populations [1]. In this study, the application of uniaxial compression in a three dimensional (3D) co-culture comprising human bone marrow mesenchymal stem cells (hBM-MSCs) and human peripheral blood mononuclear cells (hPBMCs) was established and validated [2]. The two cell populations were seeded onto 3D scaffolds produced by fused deposition modeling. The scaffolds composition was 90/5/5 %wt of poly-L-lactic acid, polycaprolactone and poly(3-hydroxybutyrate-co-3-hydroxyvalerate) substituted with 2.5% wt strontium-nano-hydroxyapatite.

Methodology

hBM-MSCs (7x10⁴ cells/scaffold) were seeded and cultured under static and dynamic culture conditions for 13 days, followed by the addition of hPBMCs (50x10⁴ cells/scaffold) and application of mechanical stimulation every other day for 25 min at a frequency of 1 Hz and a strain at 8% of the scaffold side (400 µm of displacement). Cell proliferation and morphology were monitored via a reduction-based cell viability assay, scanning electron microscopy (SEM) and confocal microscopy. Measurements of the alkaline phosphatase (ALP) and tartrate acid phosphatase (TRAP) activity were conducted to determine the effect of the scaffolds on the osteogenesis and osteoclastogenesis. Quantitative polymerase chain reaction was applied to quantify gene expression changes of osteogenesis-related markers (osteonectin, osteoprotegerin and osteocalcin), and osteoclastogenesis-related markers (TRAP, dendritic cell-specific transmembrane protein and nuclear factor of activated T cells 1).

Results

The cell viability assessment displays excellent biocompatibility, while SEM and confocal microscopy images display well-spread cells. After 14 and 28 days, the ALP activity is higher in the dynamic co-culture compared to the static one and the corresponding hBM-MSCs mono-culture. The TRAP activity results showed a significantly lower TRAP activity in the dynamic co-culture than in the static co-culture and the hPBMCs mono-culture after 14 days. Gene expression of osteogenesis related markers was significantly higher in the dynamic co-culture than in the static and mono-cultures of hBM-MSCs.

Conclusions

The results confirm that the mechanical stimulation enhanced the osteogenesis and suppressed the osteoclastogenesis in an in vitro cell co-culture of hBM-MSCs and hPBMCs due to the communication of the two cell populations compared to the monocultures and the static co-cultures.

Bioprinted bioactive complex constructs under mechanical stimulation promote vascularized bone formation

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F5_1, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Background

Osteogenesis and angiogenesis are coupled in a spatiotemporal and inter-dependent manner during bone regeneration. A complex 3D bioprinted model was biofabricated as a holistic vascularized bone model, comprising (i) an outer zone from a photocrosslinkable hydrogel with electrically conductive properties aiming to enhance osteogenesis under dynamic conditions, and (ii) an inner zone including a vascular-like tubular structure from a biofunctional nanocomposite hydrogel to induce angiogenesis. The objective is to bioengineer a complex 3D bioprinted vascularized bone model and evaluate the synergistic interactions of the functional bioinks in dynamic cell cultures.

Methods

The angiogenic matrix was prepared by dispersing gellan gum in a laponite suspension. Wharton's jelly mesenchymal stem cells (WJ-MSCs) were incorporated in the nanocomposite forming a bioink functionalized with platelet-rich plasma (PRP). The osteogenic matrix was prepared from a blend of poly(3,4-ethylenedioxythiophene) polystyrene sulfonate (PEDOT:PSS), polyvinyl alcohol, gelatin and polyethylene glycol diacrylate combined with bone marrow mesenchymal stem cells (BM-MSCs). Biofabrication of vascularized bone model was achieved through 3D bioprinting. For dynamic cultures, mechanical stimulation (1 Hz, 10% strain, 1 h) was applied daily for 28 days. Biocompatibility study included Live/Dead assay and evaluation of ECM formation. Angiogenic and osteogenic differentiation were examined through immunofluorescent staining, determination of VEGF/BMP-2 secretion by ELISA, gene expression via quantitative polymerase chain reaction (qPCR), ALP staining, calcium and collagen quantification. Subcutaneous implantation of the constructs was performed for two weeks.

Results

Bioinks maintained over 90% cell viability from day 1 to day 9, and were positive for all ECM markers. At day 28, qPCR analysis demonstrated that in dynamic conditions the complex model exhibited significantly increased expression of TIE1, Ang1, VEGFA, and VEGFR2, indicating an elevated angiogenic potential. Moreover, a significant increase in key osteogenic markers, including BGLAP, SPARC, OPG, and RUNX2 was observed, highlighting the enhanced osteogenic potential of the biofabricated constructs under dynamic culture conditions. Quantification by ELISA demonstrated that the complex model in dynamic conditions consistently yielded higher VEGF concentrations (313 pg/ml). Similarly, BMP-2 release in composite dynamic setups peaked at 28 ng highlighting the pronounced impact of dynamic culturing on enhancing BMP-2 release. Immunostaining at 2 and 4 weeks confirmed positive osteogenesis in biofabricated constructs from day 14, with dynamic conditions, notably with PEDOT:PSS, showing enhanced effects, suggesting the activation of mechanotransduction pathway.

Conclusions

The data support the hypothesis that paracrine signals from both angiogenic and osteogenic pathways, particularly under dynamic culture conditions, contribute to accelerated osteogenesis.

Agarose as a tissue mimic for porcine kidney at the macro and micro-length scale

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F5_1, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Agarose exhibits mechanical properties that are adjustable and have been widely used in tissue engineering [1-6]. Agarose is a linear polysaccharide that is extracted from marine red algae, containing D-galactose and 3,6-anhydro-L-galactose [5,6]. This study aimed to find an appropriate agarose concentration that matches the mechanical characteristics of pig kidney at the micro length scale and compare these to macro-scale properties. For all agarose samples and porcine kidneys, the shear storage modulus and loss modulus were measured at the micro-length scale using nanoindentation measurements with a 100 μm diameter probe, ranging from 10 Hz to 110 Hz. Measurements at the macro-length scale were carried out with a rheometer from 0.1 Hz to a maximum of 9.5 Hz at a shear strain amplitude of 0.1% and fit to a fractional derivative mechanical model. The storage modulus at the micro-length scale was higher by factor of 1.2 to 70 than the storage modulus at macro-length scale in kidney samples and agarose (depending on agarose concentration), which is linked to gel and tissue microstructure. An agarose concentration of 1.2% best fitted the kidney tissue properties at the macro and micro-length scales.

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Hybrid Polymeric Biomaterials for Tissue Engineering: Electrospun Fiber-Reinforced Hydrogels

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F6_2, Z4 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Electrospun fibers and hydrogels have distinct but complementary roles in tissue engineering, offering a combination of mechanical support, topographical guidance, and a biomimetic 3D microenvironment. Electrospun fibers enhance mechanical stability and provide anisotropic structural cues, while hydrogels emulate the extracellular matrix, fostering cell proliferation and differentiation. By integrating these materials, hybrid scaffolds can achieve advanced functionalities tailored to diverse tissue engineering applications.

This study presents the development of composite scaffolds that leverage the synergy of electrospun fibers and hydrogels. Two approaches were explored: first, fragmented and surface-modified polycaprolactone (PCL) electrospun fibers were incorporated into hyaluronic acid (HA) hydrogels to improve cell adhesion, proliferation, and extracellular matrix production. The hybrid scaffold demonstrated enhanced mechanical properties and cytocompatibility, supporting fibroblast function in soft tissue engineering applications. Second, aligned PCL fibers embedded within gelatin methacryloyl (GelMA) hydrogels were designed to promote muscle cell differentiation. The aligned fiber structure significantly improved scaffold strength and facilitated cell alignment, resulting in enhanced muscle tissue formation.

Additionally, magnetic particles were integrated into electrospun fibers to enable precise alignment within hydrogels using external magnetic fields. This innovation introduces a new dimension of structural control, enabling the formation of anisotropic scaffolds that replicate the native organization of complex tissues. The magnetic alignment of fibers within the hydrogel matrix enhances both the mechanical properties and the directional guidance of cellular behaviors, paving the way for novel approaches to tissue regeneration.

The findings highlight the versatility of electrospun fiber-reinforced hydrogels and their potential to address challenges in soft and musculoskeletal tissue engineering by offering tunable mechanical properties, topographical guidance, and spatial organization. These hybrid biomaterials represent a promising platform for the development of next-generation scaffolds tailored to the needs of regenerative medicine.

Bio-Based NIPU Nanoemulsion Sponges for Sustained Drug Delivery in Topical Wound Delivery

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

The growing demand for greener and more sustainable polymeric materials has significantly driven the interest of scientific research in recent decades. In this context, non-isocyanate polyurethanes (NIPUs) have emerged as a promising alternative to conventional polyurethanes (PUs), which rely on toxic isocyanates and petroleum-derived precursors. NIPUs are synthesized via non-isocyanate pathways, most commonly through the reaction of cyclic carbonates with amines, forming urethane linkages without the use of hazardous monomers. This approach not only reduces toxicity but also aligns with the principles of green chemistry by utilizing bio-based raw materials, offering reduced environmental impact, lower carbon footprints, and enhanced safety in production and application.

In the present study, polymer sponges based on novel bio-based non-isocyanate polyurethanes (NIPUs) deriving from bio-based di-acids (adipic, succinic, azelaic, and malonic), 1,6-hexamethylenediamine, and glycerol carbonate via a polyaddition reaction which were developed for the topical wound administration of chloramphenicol (CHL), a broad-spectrum antibiotic. The NIPUs were synthesized via a polyaddition reaction using bio-based di-acids (adipic, succinic, azelaic, and malonic), 1,6-hexamethylenediamine, and glycerol carbonate. The sponges were designed to provide a biocompatible and environmentally friendly platform for sustained drug release in wound treatment. Infrared spectroscopy (FTIR) confirmed the formation of urethane linkages, while scanning electron microscopy (SEM) verified the porous morphology suitable for drug loading and controlled release. Swelling behavior studies demonstrated the sponges' ability to retain moisture, promoting an optimal wound-healing environment. Enzymatic hydrolysis tests revealed a degradation profile compatible with biomedical applications, ensuring a balance between stability and bioresorption. The developed NIPU-based sponges present a promising alternative for sustainable and efficient drug delivery in topical wound care.

Synthesis of eugenol derived biobased polymers as Green alternative to plastics

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The chemical industry has traditionally relied on crude oil and gas as feedstocks. However, this heavy reliance on fossil resources is increasingly at risk due to anticipated shortages and price volatility. Moreover, global warming driven by CO₂ emissions and growing environmental concerns have prompted Industry and Academia to explore and develop new, sustainable, and safer chemical processes. In recent decades, Green Chemistry has emerged as a promising approach for synthesizing polymers addressing the drawbacks of traditional fossil resource dependence of conventional synthetic methods. Thus, Green Chemistry aims to create materials that are “benign by design”, focusing on the importance of sustainable feedstocks and minimizing their harm to ecosystems. Therefore, the development of biobased polymers has increased significantly, because of their low toxicity and price, renewability, sustainability, and biodegradability. For that, aromatic green raw materials are studied. Eugenol, extracted from clove oil or cinnamon extract, or even through the depolymerization of lignin, offers different functionalities in its structure that allow easy modifications and make it a versatile precursor for polymeric materials. In addition, the synthesis of polymers should go in accordance with the concepts of circular economy, prioritizing recyclability from the beginning to provide a sustainable solution for plastic waste and for preserving monomeric units across multiple recycling cycles.

Nowadays, polymer industry uses polyols and polyisocyanates to synthesize polyurethanes (PUs), since they are incredibly versatile due to their diverse structures and properties. However, polyurethanes have been ranked among the 50 most hazardous polymers due to the respiratory sensitizing and carcinogenic properties of diisocyanates, as well as the toxicity of phosgene used in their production. Hence, non-isocyanate polyurethanes (NIPUs) represent a promising alternative to traditional polyurethanes, with significant environmental and health benefits. In fact, a carbamate monomer easily obtained from eugenol has been employed as starting material to the synthesis of a series of NIPUs via transurethanization reaction carried out in the absence of solvent. The focus of this work is the characterization of those new biobased NIPUs in order to understand structure–property relationships, fundamental for processing and real-world applications. The resulting polymers were structurally characterized by Nuclear Magnetic Resonance (NMR) and Fourier Transform Infrared spectroscopy (FT-IR), while their thermal properties were determined through Thermal Gravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC). Lastly, Gel Permeation Chromatography (GPC) was used to determine molecular weight and polydispersity. Furthermore, NIPUs research and innovation continue to drive this field towards a more sustainable future.

Synergistic effects of arginine and tannic acid on chitosan matrices: A green approach for hemostatic sponge development

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F6_3, Z4 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

This study presents the development of a novel multifunctional hydrogel biocomposite sponge designed to address the complexities of wound healing, including rapid hemostasis, infection prevention, and tissue regeneration. Recognizing the limitations of conventional wound dressings that lack multifunctionality, this study introduces a 3D chitosan/tannic acid (CS/TA) hydrogel. After testing three chitosan/tannic acid (CS/TA) ratios, CS/TA-1 (1:0.16), CS/TA-2 (1:0.25), and CS/TA-3 (1:0.34), the most effective formulation, CS/TA-2, was enhanced with sodium alginate (SA) and arginine (Arg) for optimal performance. Arginine, with its unique guanidinium functional group, acted as a green crosslinker, enhancing the sponge's mechanical strength, hemostatic efficiency, and biocompatibility while promoting cellular interactions. Its inclusion significantly amplified antioxidant activity (>90%), mitigating oxidative stress and contributing to enhanced therapeutic outcomes. Ionic crosslinking and freeze-drying created a porous, absorbent sponge with high water retention and compression resilience. SEM confirmed the sponge's interconnected porosity, enabling cell infiltration and nutrient exchange. Blood Clotting Index (BCI) assessments demonstrated the hemostatic effectiveness of CS/TA/SA/Arg-3, with 25% BCI at 5 minutes and 20% at 15 minutes, along with excellent hemocompatibility, achieving a 2.08% hemolysis rate. These results suggest the hydrogel sponge's potential for effective wound management in emergencies and clinical applications.

Numerical analysis for a PEGDA microfluidic-device featuring a Y-shape for hydrogel microspheres synthesis

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F6_3, Z4 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

The microfluidics devices offer remarkable flexibility, integration capability, improved precision and efficient raw materials use. Implementation of different channel sizes and geometries is key to generate monodisperse droplets. The microfluidics operation relies on the viscous forces interplay, capillary forces, nozzle diameter, surface tension between the dispersed and continuous phases. Polyethylene glycol diacrylate (PEGDA) is a polymeric material used in tissue engineering and biomedical applications due to its biocompatibility and ability to form three-dimensional networks through photopolymerization. In this study a numerical analysis was performed in order to find the ideal conditions for the PEGDA hydrogel microspheres formation by using different flow rates featuring a Y-microfluidic device by considering a prepolymer PEGDA hydrogel solution as the dispersed phase and mineral oil as the continuous one. As a result, the numerical analysis shows that the small-size microspheres diameter (200 to 600 μm) is inversely proportional to the flow rate increase for the continuous phase while the dispersed-phase flow rate is kept constant. On the other hand, by decreasing the continuous flow rate, it does not generate the microsphere due to it agglomerates the dispersed phase. In contrast, the increment on the continuous flow rate allow to form ovals due to the drift that present the dispersed phase. The application milestone is focused on drug delivery such as in cancer treatments in order to improve the efficiency and reduce the side effects such as cytotoxic ones. By having the smaller the particle, the most efficient it can be.

Engineering bacterial nanocellulose membranes for skin applications

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

The growing concerns with sustainability and safety are driving the design of biomedical devices and other therapeutic systems towards innovative biobased solutions. For example, the use of natural polymers as an alternative to conventional synthetic counterparts is gaining increasing interest, due to the inherent biocompatibility and biodegradable nature of the former. Bacterial nanocellulose (BNC) is a highly pure nanocellulose produced by some aerobic bacteria (e.g., bacteria from the *Komagataeibacter* genus) in the form of hydrogel-like membranes with an intricate porous 3D nanostructure and very high water content (>98%). The capacity of BNC membranes to be easily impregnated with aqueous solutions, together with its notable mechanical properties and biocompatibility, allows the use of BNC for the delivery of different drugs and bioactive compounds, in the form of patches, membranes, skin care/cosmetic products and other systems for biomedical applications.

In this communication we will dive into recent works of our research group on the use BNC for the topical/transdermal delivery of anti-inflammatory (i.e., diclofenac¹) and antiviral drugs (viz. acyclovir²), but also of bioactive plant extracts³, hyaluronic acid⁴ and dexpanthenol⁵, highlighting the thorough characterization of the BNC-based materials, including their biocompatibility and drug-delivery performance.

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Bacterial nanocellulose membranes containing flavonoid-based metal complexes with potential for wound healing

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Wounds, especially deep, chronic and infected wounds, often infected by multidrug-resistant bacteria, represent an increasing burden worldwide. An ideal wound dressing material should be biocompatible, malleable and non-adherent, capable of absorbing exudates while hydrating the wound site, and possess biological functionalities that support the wound healing process, such as antioxidant and antibacterial activities [1]. Bacterial nanocellulose (BNC), a singular nanocellulose substrate produced by non-pathogenic bacteria, is increasingly used as a wound dressing due to its nanofibrillar three-dimensional structure, which provides ideal conditions for wound healing, in combination with its biocompatibility, good gas permeability and ability to incorporate bioactive compounds [2]. An example of bioactive compounds that can be incorporated into BNC membranes are flavonoid-based metal complexes, which can exhibit 3D structures, mechanisms of action that cannot be achieved with organic molecules alone, and even enhanced biological activities due to the synergistic combination between the ligands and the metal ion [3,4].

In this context, the aim of this work was to develop innovative wound dressings composed of BNC membranes loaded with flavonoid-based metal complexes. For this purpose, two novel coordination compounds, namely zinc(II) complexes incorporating quercetin or morin and the N-donor ligand 1,10-phenanthroline, were synthesized in the presence of the BNC membranes. The resulting materials were characterized by X-ray diffraction, infrared spectroscopy, thermogravimetric analysis and SEM/EDS analysis, and evaluated regarding their mechanical properties as well as their antioxidant and antibacterial activities. The incorporation of the flavonoid-based metal complexes improved the healing ability of BNC by impart it with biological properties that boost the wound healing process.

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Additive Manufacturing and Optimization of Magnetoactive Polymer Composites Based on Cobalt Iron Oxide

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F6_2, Z4 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

The advancement of Additive Manufacturing (AM) techniques has facilitated the fabrication of multifunctional smart materials, pushing the boundaries of 3D printing into the realm of 4D printing. 4D printing structures can undergo controlled, time-dependent transformations in response to external stimuli. Stereolithography (SLA), an additive manufacturing technique, utilizes photopolymerisation to enable the fabrication of structures with high resolution and remarkable efficiency, making it a suitable platform for the fabrication of responsive materials. This study focuses on the synthesis of novel magnetoactive polymer composites (MAPCs) tailored for 3D printing via SLA and their potential use in biomedical applications. Magnetoactive polymer composites (MAPCs) are a class of smart materials consisting of two major constituents, a non-magnetic matrix and magnetic fillers. These composites exhibit tunable mechanical properties, including elasticity, damping, form, and shape, when subjected to an external magnetic field enabling remote actuation and deformation without direct physical contact. . The MAPCs synthesised in this study are composed of cobalt iron oxide (CoFe_2O_4) nanoparticles at varying concentrations within a biocompatible photopolymer resin, enhancing the magnetic responsiveness of the polymer. Cobalt iron oxide, a ferrimagnetic material with high coercivity and notable magnetostrictive properties, is particularly well-suited for applications requiring remote actuation and magnetic control. Following synthesis, the composites were optimised to ensure their suitability for SLA-based 3D printing by adjusting and refining processing parameters to achieve optimal printability and structural integrity. After 3D printing and optimisation, mechanical testing was conducted to identify the ideal combination that resulted in the best mechanical performance. The synthesised MAPCs were further characterised to assess their chemical, thermal properties. This study works on advances in the development of stimuli-responsive biomaterials with potential applications in remote actuation and implantable devices. The ability to fabricate these dynamic structures through SLA represents a significant step toward the development of advanced, multifunctional biomaterials with transformative potential in medicine and engineering.

Keywords: Smart Materials, Additive Manufacturing, Cobalt Iron Oxide, Polymer, Stereolithography, Magnetoactive polymer composites, 4D printing, Implantable devices, Stimuli-Responsive

Olive oil waste as basis for polyurethane coatings

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Despite the recent burgeoning interest for biobased materials, plant oils have been studied for more than 20 years as building blocks in a wide range of synthetic routes. Demanding policies from EU government and increasingly requests from overall society is forcing to an overtaking to fossil-based products, marked by a detrimental large footprint.

Vegetable oils are mainly constituted by a mixture of triglycerides, which are three long fatty acids with some double bonds intercalated in the aliphatic chains, which varies depending on the source. These double bonds are considered reactive sites as well as other routes are based on breaking of the chains and consequently extraction of derived esters.

Polyurethane (PU) is a crucial polymer in our daily life. Discovered in the 80s, it has become one of the most versatile groups of polymers used. One of the main reasons is the variety of properties which depends on the sort of synthesized PU that goes from rigid foam, flexible foam, coating, elastomers, adhesives and sealants. Some industries are already facing the challenge to substitute some of the components. One of the biggest dares is to meet the requirements and accomplish those properties compared to fossil-based PU.

As far as we know, only a sort of PU foam has been recently partially obtained from olive oil. In this work, non-competition with food principle is kept and only a material considered as a waste derived from milling industry has been used. Thus, the first objective aims at the valorisation of a waste product such as earth residue generated during the refining process in the milling. In a unitary transformation process, this waste material can represent an amount larger than 1000 tons per day. An analysis of fatty acid composition and physicochemical properties was carried out with different solvents.

In a second step of this approach, the extracted sample was converted into the ester in order to homogeneously react with diethanolamine and obtain the necessary amount of hydroxyl groups which is the ground of the customized amide-polyol. Later, the polyol synthesized is used for a straightforward PU coating formulation with an NCO ratio ranging between 1.5 and 2.5.

NMR, FTIR and DSC characterization of the polyols has been performed to confirm the chemical synthesis. Specific tests of the coatings such as adhesive, anti-corrosion and hydrophobicity index have been analysed to find out its properties.

Bioactive release profile of electrospun alginate nanofibers loaded with nitric oxide

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Nitric oxide (NO) is a radical gas produced by the human body to maintain homeostasis serving as a biological mediator and chemical transmitter. It is necessary in vascular muscle relaxation, neurotransmission, and response to infection. Due to its physiological role, its light, diffusible nature, NO is also delivered exogenously through NO-donors for applications in wound healing, oncology and neurology¹.

Its therapeutic potential depends on precise control and calibration of NO release. However, current mechanisms are spontaneous and influenced by factors such as scaffold type, concentration, and environment. Monitoring NO kinetics, localization, and dosage remains challenging without advanced techniques².

Gas sensors offer high sensitivity, but are unsuitable for liquid biological environments. Widely used methods like the Griess assay lack real-time monitoring and exhibit high variability. Techniques such as electrochemical sensors, chemiluminescence and high-performance liquid chromatography are effective but prone to interference, costly and impractical for frequent biological assays³.

A promising colorimetric approach involves the oxidative reaction between NO and oxyhemoglobin, shifting absorption bands to serve as a quantitative NO indicator. This method is sensitive, straightforward, and cost-effective. However, it is limited to spectrophotometric measurements of hemoglobin solutions, restricting sample volume, monitoring duration, and parallel assays. Compared to the Griess Assay, the hemoglobin assay has a similar limit of detection ($\sim 1 \mu\text{M}$) but higher repeatability.

To address these limitations, we developed a high-throughput protocol automating 24-hour monitoring and enabling parallel analysis of 96 samples. This system supports diverse formats and was designed for NO release detection from solid hydrogel matrices. Reducing the sample volume improves the LOD by enhancing sensitivity through better concentration dynamics and signal detection. This innovation provides thorough NO release monitoring, advancing smart-releasing materials for therapeutic applications.

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Dissolvable pullulan microneedles for transdermal lidocaine delivery

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Local anesthetics, such as lidocaine, play a crucial role in various medical procedures, ensuring pain reduction and minimal discomfort for patients. However, administration of these local anesthetics often brings some discomfort or pain in the case of hypodermal injections and may be hindered by a slow skin diffusion when using creams and ointments. In the past years, microneedles (MNs) gained relevance as innovative drug administration systems that can overcome the barrier of the stratum corneum and administer a drug in a swift and minimally invasive way.¹

Herein, dissolvable lidocaine-loaded pullulan microneedles (PL-Lid MNs) were produced through micromolding and characterized to evaluate their potential for the non-invasive administration of anesthetics. The produced MNs displayed sufficient mechanical strength, enduring up to 1.5 N per needle without breakage. The ability to overcome the stratum corneum was confirmed by insertion in a parafilm skin model, reaching a depth up to 381 μm , and further validated by insertion in excised human abdominal skin where the MNs successfully reached the dermis. The dissolution of these MNs was evaluated in an agarose hydrogel model and showed complete dissolution of the MN tips after 10 min. The dissolution profile of lidocaine in PBS showed a release of 79% after 10 mins. The safety of the developed MNs was evaluated against three skin cell lines (HaCaT, 3T3, and RAW 264.7) by the resazurin assay, with all showcasing cell viabilities over 80% upon contact with the MNs. Additionally, the effect of the released lidocaine was studied on a sensory neuron cell line using fluorescence microscopy, showing that the lidocaine released from PL-Lid MNs had a similar effect in dorsal root ganglion (DRG) neurons as an in situ delivery of a lidocaine solution (14 mM). Moreover, we were able to elucidate how fast the released lidocaine provoked a response in neuronal cells through real-time fluorescence imaging by confocal microscopy. In sum, our results demonstrate the Pullulan MNs are an efficient system for the administration of lidocaine, with a low on-set time (<10 mins) owing to its swift dissolution and consequent drug release, contrasting the conventional methods for local anesthetic administration.

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Development of a hydrogel composed of alginate and lysozyme amyloid nanofibrils for the administration of a novel chemotherapeutic chrysin-based metallodrug

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Flavonoid-based metallodrugs have emerged as promising chemotherapeutic drugs [1]. In particular, chrysin has been shown to induce apoptosis and inhibit cancer cell growth and proliferation through cytotoxic effects [2,3]. In this work, we successfully synthesized and structurally characterized a Cu(II)-chrysin-based metallodrug with potent cytotoxicity against human melanoma (A375) and human hepatocarcinoma (HepG2) cell lines. The compound exhibited IC₅₀ values of $1.29 \pm 0.04 \mu\text{M}$ for A375 and $1.93 \pm 0.08 \mu\text{M}$ for HepG2 cell lines. Furthermore, cell cycle studies revealed an increased percentage of cells in the G2/M phase, suggesting cell cycle arrest in both cancer cell lines. This promising chemotherapeutic candidate was then incorporated into a nanocomposite hydrogel, composed of alginate and lysozyme nanofibrils, that was fully characterized in terms of its optical, electric, thermal and mechanical properties. In vitro release studies were also performed under homeostatic and non-homeostatic conditions. Finally, the antioxidant activity and the cytotoxicity of the loaded hydrogel were accessed in A375 and HepG2 cells to evaluate its antitumoral potential.

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Predicting Printability of Bio-inks by Capillary Rheology

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F6_3, Z4 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Background and purpose:

Extrusion-based 3D bioprinting offers a promising avenue for the fabrication of near-physiological tissue models but faces technical challenge in reliability and reproducibility. Hydrogel printability is commonly assessed by rotational rheology (RR), which does not capture the flow profile of extrusion process, resulting in poor reliability and predictability of the assessment, while visual assessment of filament morphological features is commonly performed after the bioprinting. The lack of reliable methodologies for hydrogel extrusion affects material design, bio-ink development, cell viability, and print quality, limiting the translatability of RR results to real-life extrusion of these materials. We hypothesize that faithful assessment of printability requires understanding the phenomena affecting bio-inks in the reservoir and the nozzle during the extrusion process. To this end, we employ principles of capillary rheology (CR), which characterizes material deformation and flow through capillaries, for quantitative assessment of bio-ink printability.

Methods:

We developed a CR system which enables real-time quantification of in situ bio-ink properties in a printing-like setup. For these experiments, we selected model bio-inks based on Pluronic F-127 and gelatin methacrylate (GelMA).

Results and conclusions:

Our results show a considerable discrepancy in key printability-related properties such as viscosity and shear-thinning with CR compared to RR. Besides shear-thinning behavior, CR reveals nuanced flow dynamics throughout the extrusion process, which reflect material-dependent changes in extrusion uniformity. Effects of material properties such as viscoelasticity, compressibility, and temperature sensitivity are reflected on CR data. Moreover, the integrated temperature sensors in CR show a dramatic temperature gradient throughout the bio-ink from the syringe to the capillary end, which significantly affects bio-ink behavior. These discrepancies suggest that RR cannot faithfully predict the material flow behavior under capillary extrusion, leading to inaccurate assessment when translating to extrusion process. All in all, CR provides accurate and more information on extrudability of hydrogels and pinpoints extrusion-dependent phenomena in each stage of printing course which cannot be captured with RR.

Our ongoing work aim to correlate CR and visual data for quantitative printability assessment by analyzing extrusion instabilities and uniformity to find the best pattern to optimize the bioprinting process.

First-Principles Insights into the Enhanced Catalytic Activity of Mg-Doped Prussian Blue for Hydrogen Peroxide Decomposition

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F6_1, Z4 Room (Level -3), septiembre 17, 2025, 10:30 - 13:10

Reactive oxygen species (ROS) play a dual role in biological systems, acting as essential signaling molecules under physiological conditions while causing oxidative stress when overproduced. While controlled ROS levels are crucial for cellular communication, immune defense, and tissue repair, excessive ROS can disrupt homeostasis, damage biomolecules, and contribute to chronic diseases such as cardiovascular disorders, neurodegenerative conditions, and cancer. As a result, regulating ROS levels has become a key focus in the development of therapeutic strategies.

Nanozymes, a class of nanomaterials with enzyme-like catalytic properties, have emerged as promising candidates for mitigating oxidative stress. By mimicking natural antioxidant enzymes like superoxide dismutase (SOD), catalase, and peroxidase, nanozymes efficiently neutralize ROS, converting reactive species such as superoxide radicals (O_2^-) and hydrogen peroxide (H_2O_2) into less harmful molecules. Among various nanozymes, including those based on gold, manganese, cerium, and iron (Fe)-based materials stand out due to their intrinsic SOD-mimetic properties. However, challenges such as structural instability, potential cytotoxicity, and limited biocompatibility at therapeutic doses hinder their clinical translation. Recent studies have begun exploring the environment-specific catalytic behavior and long-term toxicity of Fe-based nanozymes, particularly Prussian Blue.

In this study, we investigate the dissociation of H_2O_2 on Prussian Blue and its modified structures using first-principles simulations. To determine the dissociation pathways of H_2O_2 , we consider all possible interfaces of Prussian Blue. Our analysis explores key electronic properties, including work function, d-band center, and H–H bond stretching, to elucidate their roles in H_2O_2 activation. Bader charge analysis further reveals electron redistribution between the support material and adsorbed H_2O_2 . Additionally, employing the Computational Hydrogen Electrode (CHE) method, we incorporate solvent effects to enhance the accuracy of our findings.

Furthermore, we examine the impact of magnesium (Mg) doping in Prussian Blue, which leads to the formation of Prussian White. Depending on Mg concentration, the charge state of Fe and doping sites of Mg are altered, significantly influencing catalytic activity. Notably, Mg incorporation reduces the H_2O_2 dissociation energy barrier by 38%, demonstrating its potential to enhance catalytic efficiency. Our collaborative work with experimental researchers aims to optimize Prussian Blue nanozyme structures for improved ROS regulation and biomedical applications.

Dielectric Properties of Chitosan-Based Bionanocomposites

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F6_3, Z4 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Chitosan, a versatile biopolymer derived from chitin, has garnered significant attention due to its exceptional properties, including biocompatibility, biodegradability, and antimicrobial activity [1]. This study investigates the impact of chemical modifications and the incorporation of organic and inorganic fillers on the dielectric properties of chitosan-based bionanocomposites. Understanding these properties is crucial for developing advanced materials for applications in energy storage devices, sensors, and biomedical engineering [2,3].

Using Electrical Impedance Spectroscopy (EIS) and Fourier Transform Infrared Spectroscopy (FTIR), we systematically examined the relationship between the chemical structure of chitosan and its electrical behavior. The results revealed that neutralization process and the introduction of chitin nanofibers and barium titanate nanoparticles significantly influenced the capacitive component of the dielectric response mainly in the capacitive behavior. However, the resistive component of the chitosan films exhibited minimal changes upon these modifications. These findings provide valuable insights into the factors that rule the dielectric properties of chitosan-based materials, helping in the development of novel bionanocomposites with tailored electrical characteristics for diverse applications.

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Tubular polyester-based electrospun constructs with anti-adhesive and anti-inflammatory potential to repair ruptured deep flexor tendons

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F6_2, Z4 Room (Level -3), septiembre 17, 2025, 14:30 - 16:30

Tendons connecting muscle to bone, provide strength and stability, withstand tension and release stored energy. Current treatment methods of hand tendon traumas have shortcomings, including insufficient mechanical strength, possible adhesion reactions with surrounding tissue and inflammation issues.

The current research aims to counter both mechanical and biological problems. To achieve this, a reinforced, tubular polyester-based construct has been electrospun, composed of: an inner electrospun polyester layer containing an anti-inflammatory component (Naproxen), a middle reinforcement layer with braided monofilament and an outer electrospun polyester layer containing an anti-adhesion component (hyaluronic acid, HA). As polymer material, an acrylate-endcapped urethane-based poly(ϵ -caprolactone) precursor (AUP) has been used and benchmarked against commercially available poly(ϵ -caprolactone) (PCL).

After proving the success of the synthesis (¹H-NMR), the materials with the bioactive compounds were electrospun on tubular collectors. PCL clearly led to thicker fibers ($8.77 \pm 1.88 \mu\text{m}$) than the AUP/PCL blend ($4.30 \pm 0.41 \mu\text{m}$). The constructs remained stable for > 9 weeks, the period lesioned tendons need to pass to advanced healing [1].

In vitro assays showed that incorporation of bio-active components was successful and not-cytotoxic for human fibroblasts. These tests also indicated that HA induced a burst release in PCL constructs, while a prolonged release was observed in the stronger and denser network of AUP/PCL. Introduction of the intermediate braided monofilament layer, between the electrospun layers led to strengths of $8.56 \pm 1.92 \text{ MPa}$ as shown by ex vivo sheep tendon tensile tests [2]. The final constructs have also been used in an in vivo study on 40 rabbits [3]. A comparison was made between tubular, medicated electrospun polymers with/without reinforcement, a tubular braid as such and a modified Kessler suture as a control. Histologically, an excellent repair was observed at the tendon site with significantly different adhesion pattern depending on the applied technique.

These multilayered electrospun constructs represent a very promising mechanical and biological solution to repair deep flexor tendons. In on-going follow-up research, the potential of poly(L-lactic acid)-PCL triblock-copolymers is being explored to control biodegradability and improve the mechanical strength without the need of a braided intermediate layer.

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The versatile role of tannic acid as green crosslinker and bioactive compound in the development of Gellan Gum-based hydrogels for in situ cartilage repair

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The articular cartilage regeneration is a central focus of scientific research due to its limited capacity for self-repair following trauma or disease. This limitation arises from the absence of blood vessels, nerve structures, and a low cell population. Despite the promising prospects, a persistent challenge in this area is the lack of sufficient functional integration between engineered and natural tissues [1]. In this study, an innovative hydrogel based on a blend of two Gellan gums (GG) with different acyl content, cross-linked with Tannic acid (TA) and magnesium ions has been proposed as biomaterial for cartilage tissue engineering. Considering the poor mechanical properties of GG, the use of TA as new green cross-linker represents a promising strategy since, in addition to its crosslinking action, it displays also bioactive properties, due to its anti-inflammatory and ROS scavenging capacities [2,3]. Chemical-physical characterization by FTIR-ATR, XPS, SS-NMR, DSC, SEM, weight loss, water-uptake and rheological tests was carried out to ascertain the interactions involved in the hydrogels cross-linked structure. Cytocompatibility, chondrogenic and anti-inflammatory evaluation were tested on Human mesenchymal stromal cells (hMSC), demonstrating that GG/TA hydrogels support the immunomodulatory role and confirming the ability of TA to ameliorate LPS-induced inflammation. Along with its anti-inflammatory properties, TA exhibited also strong antibacterial activity, which is crucial for materials used in cartilage regeneration. The obtained cross-linked hydrogels showed mechanical and rheological performances that made them ideal systems for damaged cartilage repair. In summary, this research highlights the possibility of exploiting the multiple advantages deriving from the use of this natural polyphenol in the development of a natural hydrogel for application in cartilage tissue engineering.

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Synthesis of P3HB/Chitosan Blends with Enhanced Properties for Biomedical Applications

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F6_3, Z4 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Poly(3-hydroxybutyrate) (P3HB) is a biopolymer from the polyhydroxyalkanoate family, naturally synthesized by bacteria as a storage form of carbon and energy.¹ Despite the limitations posed by its high crystallinity and production costs,² holds substantial potential due to its appealing properties. Among them, exhibits piezoelectric behaviour, rendering it promising for biomedical uses by providing mechanical or electrical stimuli via piezoelectric effects.³

To address some production constraints, the ring-opening polymerization (ROP) of rac- β -butyrolactone (BBL) using metal catalysts has facilitated the synthesis of tailored P3HB.⁴ Aluminum-based catalysts, in particular, offer advantages due to aluminum's abundance and cost-effectiveness,⁵ and they have demonstrated strong ROP activity.^{6,7}

On the other hand, chitosan (CS), a natural biopolymer, has gained considerable attention in tissue engineering and regeneration over recent years due to its advantages, including biocompatibility and antimicrobial properties.⁸ Additionally, it has demonstrated piezoelectric properties, due to its non-centrosymmetric crystalline structure.⁹ However, its limited mechanical strength has hindered its application.

This study aims to combine the strengths of both P3HB and chitosan to create a material with improved mechanical properties for biomedical applications. To address this, we employ an aluminum complex with phenoxyimine ligands to produce atactic P3HB with varying molecular weights via the catalytic ROP of (BBL). These biopolymers, along with chitosan, were used as additives in blends with high-molecular-weight bacterial P3HB to enhance the material's functionality. The blends were processed via both solvent casting and electrospinning techniques, and a morphological, thermal, and piezoelectric analyses were conducted, allowing a comparative study of their structure and properties providing insights into their suitability for applications. Furthermore, a comparative biological study with fibroblast cells assessed the biocompatibility of each blend type, highlighting the influence of processing methods on cellular interaction.

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Synthesis and characterization of electrospun fibers based on piezoelectric bioplastics

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F6_3, Z4 Room (Level -3), septiembre 17, 2025, 17:00 - 19:00

Nowadays the production of electricity from renewable and wasted resources is an important challenge. A green way to produce electrical energy can be the recovering and conversion of wasted mechanical energy such as vibration, kinetic energy, or deformation energy, in electricity. This process is called mechanical energy harvesting. Piezoelectric materials could be applied to build piezoelectric energy harvesters (PEHs) as promising independent renewable power sources for low-power electronic devices such as wireless sensors, portable devices, stretchable electronics, and medical implants (biosensor) [1-2].

In this context, green piezoelectric bioplastics such as poly-L-lactic acid (PLLA), polyhydroxybutyrate (PHB) and their copolymers could represent an interesting alternative that have benefits regarding carbon footprint, thus decreasing the environmental impact of PEHs devices. However, the practical application of bioplastics is limited because its piezoelectric constant is much lower than those of ceramic piezoelectric materials, PVDF and its copolymers [3]. Thus, to find new strategies and pathway for the large-scale production and processing of green bioplastics with improved piezoelectric properties is a challenge.

This communication will focus on the design of new bioplastics with improved piezoelectric properties for energy harvesting applications offering innovative potential industrial solutions. Different strategies to develop and boost piezoelectric properties of different biobased systems will be showed such as the catalytic synthesis of PLLA and its copolymers with controlled structure and biobased additives for bacterial PHB. Emphasis will be placed on the polymeric architecture as well as on the processing method to activate the piezoelectric properties. In fact, optically active polymers can be polarized by mechanical drawing avoiding the application of high electrical fields. The morphology, thermal, electric, and piezoelectric properties of the different bioplastics will be also presented in this communication.

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Mn-Doped Ti Coatings for Dental Implants: Effects on HO β differentiation, Immune Modulation, and Protein Binding

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F7_2, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 10:30 - 13:10

Titanium (Ti) is a widely used material for dental implants due to its mechanical strength and biocompatibility. However, its bioinert nature limits osseointegration, posing challenges for long-term implant success. To address this issue, silica-based bioactive coatings have been developed using sol-gel techniques, enhancing implant stability and supporting the incorporation of bioactive molecules. Manganese (Mn), an essential element for bone metabolism, has been investigated for its role in promoting osteogenesis and maintaining osteoblast-osteoclast balance. This study evaluates the effect of Mn-doped silica coatings on Ti implants, focusing on physicochemical properties, biocompatibility, immune response, and proteomic interactions.

The Mn-doped coatings were synthesized via sol-gel and applied to Ti surfaces with varying Mn concentrations. Their structural and chemical properties were characterized using Fourier-transform infrared spectroscopy (FTIR) and surface wettability analyses. Biological characterization included cytotoxicity assays, osteoblast proliferation, osteogenic differentiation (ALP activity, osteogenic gene expression), and immune response evaluation in macrophages via cytokine quantification and gene expression analysis. Additionally, protein adsorption from human serum was assessed using nano-LC-MS/MS to determine the impact of Mn doping on protein interactions.

Results demonstrated that the sol-gel coatings fully covered the Ti surface without Mn accumulation. FTIR confirmed Si-O-Si bond formation, and Mn addition slightly increased hydrophobicity without altering surface roughness. Controlled Mn²⁺ release was observed over 56 days, reducing degradation rates. In vitro studies showed no cytotoxicity, consistent osteoblast proliferation, and enhanced expression of osteogenic markers, including COL1, BMP2, RANKL, and OCN, particularly in Mn-doped samples at 14 days. Immune response analysis revealed increased expression of pro-inflammatory markers (TNF- α , IFN- γ) in higher Mn concentrations, while lower Mn levels favored the expression of anti-inflammatory cytokines (IL-10, TGF- β). Proteomic analysis indicated enhanced affinity for proteins involved in immune response and its regulation (e.g., SLPI, immunoglobulins, SAA1), cell adhesion (CADH1, CADH5), and osseointegration (FETUA, FETUB), suggesting a positive effect on implant integration.

In conclusion, Mn-doped sol-gel coatings on Ti surfaces demonstrated promising biological responses, including improved osteogenic differentiation, controlled Mn²⁺ release, and favorable protein adsorption patterns. These coatings enhanced cell adhesion and immune modulation, potentially contributing to better osseointegration. The findings align with existing literature and highlight Mn-doped coatings as a viable strategy to improve the performance of dental implants. Future studies should explore long-term in vivo effects and clinical applications to validate these findings further.

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Development and characterisation of geopolymer and Mg doped hydroxyapatite-based coatings on Ti6Al4V substrate for orthopaedic applications

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F7_2, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 10:30 - 13:10

Titanium and its alloys are widely used as biomaterials in orthopaedic procedures, due to their optimal mechanical strength, corrosion resistance, and biocompatibility [1]. However, the clinical success of titanium implants is often hindered by poor osteointegration and microbial adhesion, leading to implant failure and high morbidity, thereby increasing healthcare costs. To overcome these drawbacks, surface modification techniques, such as coating with bioactive and antibacterial materials, have been proposed to enhance osteointegration while decrease peri-implant inflammation.

This study focuses on the development of novel coatings for titanium (Ti6Al4V alloy) aimed at improving osteointegration and providing antibacterial properties. The developed coatings are composed of magnesium-modified hydroxyapatite and chitosan particles (MgHA_CH) [2], and/or geopolymers [3], and mimic the structure and composition of natural bone, allowing for better integration and faster healing of the implant. Specifically, chitosan, a natural polysaccharide, and geopolymer, an inorganic materials, were selected for their ability to prevent bacterial colonization on the implant surface while doped hydroxyapatite was chosen for its potential to stimulate bone growth and mineralization. The coatings were applied to titanium substrates using two different techniques: electrophoretic deposition [4] and dip coating [3].

In the former case an optimization process was carried out to maximize the deposition performance and the impact of different deposition parameters including current density, deposition time and composition of the deposition solution was investigated. The coatings were thoroughly analyzed to evaluate their morphology, microstructure and chemical composition by means of scanning electron microscopy combined with energy dispersive X-ray diffraction (SEM-EDXS), and Fourier-transform infrared spectroscopy (FTIR). In addition, biological in vitro tests, including osteoblast-like cell proliferation and viability tests and antibacterial assays, were conducted to assess the biocompatibility and antimicrobial features of the coated materials.

The coated materials display good morphological characteristics and support cell adhesion, proliferation and spreading while exhibit antibacterial activity against clinically relevant bacteria, including both gram positive and gram negative strands, making them a promising solution for addressing critical challenges in the clinic.

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Modification of microemulsion-assisted sol–gel method to control the composition of multi-ion-doped mesoporous bioactive glass particles

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F7_1, Picasso Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

The microemulsion-assisted sol–gel method, combined with a cationic surfactant, is widely used to synthesize spherical mesoporous bioactive SiO₂–CaO glass particles (MBGs), which have various biomedical applications owing to their biocompatibility, bioactivity and mesoporous structure with surface properties suitable for drug loading. The biological properties of MBGs can be tailored by optimizing the calcium content, as calcium plays a critical role in MBGs bioactivity and pro-osteogenic properties. Additionally, incorporating an optimal quantity of so-called therapeutic ions promotes specific biological responses upon release, such as: osteogenic (Mg²⁺ and Sr²⁺), angiogenic (Cu²⁺ and Mg²⁺) and antimicrobial (Cu²⁺ and Zn²⁺) effects. Previous investigations have shown that the incorporation of high amounts (>20 mol%) of calcium, as well as strontium, into highly dispersed MBGs is challenging, resulting in a significant discrepancy between the nominal and actual composition. The problem stems from the synthesis process itself, as insufficient amounts of the ions are adsorbed on the surface of the silica particles, which initially form within oil droplets in water.

The aim of this study was to optimize or modify microemulsion-assisted sol–gel synthesis to better control the content of Ca, Mg, Sr, Cu and Zn in multi-ion-doped spherical MBGs. The main parameter varied was the pH value, specifically the ammonia content, which influences hydrolysis and condensation rates of tetraethyl orthosilicate (the silica precursor), as well as ions adsorption. The synthesis modification involved impregnating pure silica particles with ions after synthesis rather than relying on adsorption during the synthesis. The morphology and chemical composition of MBGs were analyzed by FESEM and EDS analysis, while an MTT assay was performed on mouse bone marrow-derived stem cells (mBMSCs) to assess in vitro biocompatibility. The specific surface area was determined by BET method. The results indicate that pH variations slightly influence MBGs size and composition. Furthermore, ions whose hydroxides are poorly soluble (Cu, Zn, Mg) were found to bind much better to silica than ions whose hydroxides are more soluble (Ca, Sr). The synthesis modification demonstrated a much greater potential for controlling the composition of MBGs compared to pH adjustments.

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CNC-manufacturing versus ceramic injection moulding for ATZ shoulder resurfacing

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F7_2, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 10:30 - 13:10

Alumina and YTZP ceramics have been established in joint endoprosthetics since the 1970s and 1980s. Zirconia rich dispersion ceramics made of alumina and YTZP are known for high strength, high fracture toughness and low wear rates for decades too. Thus, alumina toughened zirconia (ATZ) material was introduced to the endoprosthetics market in 2007. New efforts have been made to use the ATZ for production of shoulder resurfacing implants. CNC-technology will be compared with ceramic injection moulding.

This paper summarizes the designer's elaboration for the respective manufacturing technology, challenges of the two manufacturing processes and economic aspects. Product development began with formulation of clinical needs and material requirements for ATZ on basis of standards (ISO 13356, ISO 6474-2).

The first investigation results for material samples (both technologies) and CNC manufacturing of a ceramic shoulder resurfacing implant are shown. A debinding process and the thermal treatment - sintering and HIP - were carried out. High purity and the removal of any porosity are mandatory. The whole process was accompanied by the determination of properties such as green density, microstructure, investigation of chemical composition, density after sintering and HIPing and investigation of the phase composition.

Furthermore, suitable injection moulding technology was developed, based on the design and construction of a moulding tool and the choice of a commercial ATZ feedstock. A homogeneous microstructure and phase distribution in material samples could be achieved. The first sample parts were investigated according to their size accuracy.

First results for CNC-technology are shown. Green parts with densities $\geq 2,75\text{g/cm}^3$ and sinter densities $\geq 5,4\text{ g/cm}^3$ were prepared. The chemical analysis met requirements. By adjusting the thermal process, the microstructure could be adjusted so that grain sizes for Al_2O_3 and for YTZP met the requirements of standards. A homogeneous microstructure and phase distribution in material samples could be achieved. First shoulder implants made of ATZ ceramic were successfully realized with CNC-technology.

The results were obtained within the project CIMEOS (funded by Thueringer Aufbaubank, Joint project 1000449: FKZ: 2023 VFE 0008).

Alternative sintering process of biomaterials for prostheses: microstructural control using electromagnetic field

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

As the healthcare sector develops new technologies to prolong life, people tend to live longer, so the wear on specific organs becomes increasingly common. Hip fractures are often one of the causes of the deterioration in people's life quality when the population exceeds the average age of 80. Only in Spain, 48,000 surgeries were performed for hip fractures between 2017 and 2021.

The search for materials that replace bone tissue and that present high compatibility with the human body is a field that has been widely explored in recent years. This research aims to develop materials with better mechanical properties that prolong the useful life of prostheses, decrease the frequency of interventions, improve the people's quality of life, and use less energy consumption for their production.

The (Y, Ce) ATZ composite was selected for microwave sintering to study the effect of electric field sintering on the evolution of the microstructure as a function of temperature and time. Mechanical properties like conventional sintering temperature were obtained with 200 °C less and a dwell time of 15 min, as well as excellent behaviour against low-temperature degradation after 80 h at 120 °C and 1.7 bar. Developing stable biomaterials with enhanced mechanical properties is a priority to improve the quality of life and reduce the resources associated with surgical interventions and the production of parts.

- Keywords: Biomaterials; Prostheses; ATZ; Low-temperature sintering

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SYNTHESIS AND CHARACTERIZATION OF ALGINATE HYDROGELS CONTAINING 58S BIOACTIVE GLASS AND SILVER NANOPARTICLES

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The 58S bioactive glass, composed of 60% SiO₂, 36% CaO, and 4% P₂O₅ (mol%), is widely recognized in tissue engineering for its bioactivity when interacting with biological systems. This study aimed to integrate sol-gel synthesized 58S bioactive glass particles into alginate hydrogels—a biocompatible material—to develop inks with optimal rheological properties for 3D printing. Additionally, we investigated the impact of incorporating varying concentrations of 58S (ranging from 15 to 35 vol%) on the rheological behavior of alginate hydrogel-based inks containing 1.5 to 5 wt.% of additives, including Halloysite clay (plasticizer), Dolapix CE 64 (deflocculant), and PVA (binder). The hydrogel inks were homogenized using a laboratory mixer (IKA RW 20) at 300 rpm for 20 min before rheological characterization to assess their printability. Flow curves were determined using a rotational rheometer (Haake Viscotester iQ), while an oscillatory rheometer (Anton Paar MCR 92) was employed to evaluate yield strength and viscoelastic behavior. All inks exhibited pseudoplastic behavior, with the 25 vol.% formulation identified as the most suitable for fabricating scaffolds for biomedical applications. These scaffolds retained their shape and were subsequently impregnated by immersion with silver nanoparticles synthesized via laser ablation.

Enhancing Patient Comfort in Cranioplasty: Coated Titanium Implants for Better Thermal Regulation

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F7_2, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 10:30 - 13:10

Cranioplasty is a surgical procedure used to reconstruct skull defects resulting from trauma, congenital anomalies, infections, or tumor resection. The procedure aims to restore cranial integrity, protect the brain, and improve functional and aesthetic outcomes. However, cranioplasty presents significant challenges due to the skull's complex morphology and the need for biocompatible, durable, and mechanically stable materials.

Recent advancements in imaging and manufacturing technologies have enabled the development of patient-specific implants, offering enhanced precision and improving clinical results. Among the materials used for cranial implants, titanium remains a common choice due to its strength, biocompatibility, and corrosion resistance. However, its high thermal conductivity can cause patient discomfort, particularly in response to temperature fluctuations. To address this issue, this study explores the enhancement of 3D-printed titanium cranial implants by applying polyether ether ketone (PEEK) and hydroxyapatite (HA) coatings using Atmospheric Plasma Spray. The coatings aim to mitigate the thermal conductivity of titanium while preserving its mechanical integrity. The research evaluates coating quality and thermal properties across different thickness levels to determine their effectiveness in improving patient comfort.

Results indicate that both PEEK and HA coatings successfully reduce the implant's thermal conductivity, with the degree of improvement related to coating thickness. The findings highlight the potential of these coatings to optimize implant performance, presenting a promising approach to enhancing long-term outcomes in cranioplasty. By integrating advanced coating techniques, this study contributes to developing cranial implants that address functionality and patient comfort.

Mesoporous silica nanoparticles carrying an iron chelator for the treatment of iron overload diseases. Proof of concept.

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F7_1, Picasso Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Iron is a trace element essential for cellular metabolism, but it is toxic when present in excess. Hereditary hemochromatosis is a primary iron overload disease. Other disorders have a secondary iron overload due to frequent blood transfusions. The common form of iron removal therapy is periodic bleeding, but this is not feasible for β -thalassemia, and the alternative is the use of iron chelating agents, such as deferoxamine (DFO), deferiprone and deferasirox. These treatments are effective but suboptimal, either in their effectiveness in depleting iron from the liver, or in their safety due to side effects. During the last decades, notable achievements have been obtained in the field of nanotechnology for biomedical applications.

Aiming to create a safer and more effective way to administer iron chelators, we have designed mesoporous silica nanoparticles (MSNP ~200 nm in diameter) to which DFO has been covalently linked (MSNP-DFO). We have performed in vitro studies in human hepatocellular carcinoma HepG2 cells with MSNP-DFO, and in vivo studies are being performed in a murine model of hemochromatosis.

In vitro studies show that cultured HepG2 uptake MSNP, without loss of cell viability at any of the concentrations tested (50-500 μ g/ml) at 24-72 hours of treatment. Nevertheless, when incubated with MSNP-DFO there is a decrease in HepG2 viability, especially at higher concentrations and longer treatments, similar to what is observed with DFO at equivalent concentrations (10-100 μ M), indicating that the chelating capacity of MSNP-DFO is similar to that of DFO. Certainly, 72-hour treatments with MSNP-DFO or DFO decrease cell viability, but when treatments are removed after 24 hours and cells are kept in fresh medium for an additional 48 hours, DFO-treated cells do not lose as much viability as MSNP-DFO-treated cells, suggesting that MSNP-DFO retains its chelating capacity for longer. Furthermore, HepG2 cells have been iron overloaded with 100 μ M ferric ammonium citrate for 18 hours, and then treated with MSNP-DFO (200 and 400 μ g/ml) or equivalent doses of DFO (40 and 80 μ M) for 24 and 72 hours. Measuring intracellular iron levels show that DFO loses its chelating capacity over time, while MSNP-DFO retains its chelating capacity for at least 72 h.

The results obtained so far suggest that these MSNP-DFO could constitute a valuable strategy to improve the efficiency of the chelator, and that they could be considered as a future treatment of iron overload disorders.

Design, synthesis and optimization of ion-doped mesoporous bioactive glass nanoparticles with large pore size: A promising platform in bone tissue regeneration

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F7_1, Picasso Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Nanotechnology is in full swing in the field of medicine. Researchers are developing nanoparticles both for the diagnosis of diseases through biosensor devices and for the treatment of pathologies through the controlled release of therapeutic ions and biomolecules.

Here, we show a facile synthetic approach based in the sol-gel method in the presence of structure directing agents to fabricate monodisperse mesoporous bioactive glass nanoparticles with large radial pores (LP-RMBGs) adapting the recipe of Liang et al. 2015. Nanospheres were synthesized using cetyltrimethylammonium bromide (CTAB), as a template agent, and trimethylamine (TEA) as a hydrolysis catalyst. The reagents tetraethylorthosilicate (TEOS), triethyl phosphate (TEP), calcium nitrate tetrahydrate ($\text{Ca}(\text{NO}_3)_2 \cdot 4\text{H}_2\text{O}$) and $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ were used as the silicon, phosphorus, calcium and zinc sources, respectively. These reagents were sequentially added under magnetic stirring to an aqueous solution of CTAB and TEA at 30 min intervals, and allowed to react overnight. LP-MBGs Nominal compositions of 79.5-SiO₂-18CaO-2.5P₂O₅, 79.5-SiO₂-18CaO-2.5ZnO and 79.5-SiO₂-15.6CaO-2.5P₂O₅. The resulting nanoparticles suspension were centrifuged and washed twice with absolute ethanol and twice with milli-Q water at 11,000 rpm for 12 minutes. Then, the solid was collected and allowed to dry at 60°C in the oven for 24 h. Finally, the organic matter was extracted by calcination at 600°C for 4 hours with a ramp up of 1°C/min and a ramp down of 10°C/min.

The study of different concentrations of CTAB, TEA, temperature and stirring, the homogeneous size of the LP-RMBGs as well as the expansion of their pore size have been controlled. The effects of the presence of ZnO and P₂O₅ precursors on the porosity, surface area and size of the nanoparticles were also investigated. Among the different kinds of nanoparticles, large pore radial mesoporous bioactive glasses have become the subject matter due to their excellent textural and morphological features, as well as their ability to include therapeutic ions into their composition.

With these nanospheres combined therapies for bone tissue regeneration are envisioned. These nanosystems would allow for releasing therapeutic ions and co-deliver nucleic acids and other bio macromolecules hosted in the large pores. These nanoparticles can be administrated by intraosseous injection or incorporated into 3D-scaffolds to promote osteogenesis and osteogenesis in the management of bone pathologies.

Liang et al. Materials Letters, 148 (2015) 45

Arcos et al. Acta Biomaterialia 1 (2022) 501.

Sánchez-Salcedo et al. Acta Biomaterialia 166 (2023) 655.

Key words: nanotechnology, radial mesoporous bioactive glasses nanoparticles, large pores, therapeutic ions release, biomacromolecules delivery.

Mucolytic and antibiotic combination therapy through silica-based nanocarriers to eradicate *Escherichia coli* biofilms

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F7_1, Picasso Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Escherichia coli (*E. coli*) is one of the species most frequently involved in biofilm-associated infections. Biofilms hinder the penetration of conventional antibiotics, making them highly resistant to these drugs and rendering their treatment and eradication of biofilms extremely difficult.

Herein, we designed a novel, easy-to-synthesize and versatile biocompatible nanosystem to eradicate mature *E. coli* biofilms by using a unique nanoplatform based on mesoporous silica nanocarriers to co-deliver a mucolytic agent, N-acetylcysteine (AC), and an antibiotic, levofloxacin (LVX), as combination therapy. We demonstrate that, through a relatively simple synthetic approach, enhanced antibacterial efficacy is achieved by improving the penetration of the antibiotic LVX into the biofilm through the mucopolysaccharide matrix disruptive action of the mucolytic AC. The strengths of this basic research are based on the precise design and exhaustive characterization of the developed nanomaterials, together with the in-depth evaluation of the in vitro disrupting effect on mature *E. coli* biofilms. The great versatility of MSNs allows loading the different antimicrobial agents into well-defined compartments of these nanocarriers. For this purpose, LVX was loaded into the mesopores of MSNs and then coated with a gelatin layer containing AC alone or a mixture of AC and LVX. In this way, the antibiotic levofloxacin was loaded into the mesoporous silica structure, while N-acetylcysteine, as a mucolytic agent, was embedded in the outer gelatin layer. The sequential co-delivery of antimicrobial agents from the compartmented nanocarrier allows the release of N-acetylcysteine at the earliest stage, followed by the sustained release of levofloxacin. The aim was to achieve a sequential delivery of the different antimicrobial agents placed in the different compartments. A thorough characterization of the developed nanosystems was carried out and the kinetics of molecular release from the different compartments were determined.

Moreover, the antimicrobial effect of these nanosystems against mature *E. coli* biofilms was valued in vitro by confocal laser scanning microscopy and biofilm viability assays. The release behavior produces an enhanced antimicrobial effect, allowing for approximately 99.8% reduction of mature *E. coli* biofilm. Furthermore, preliminary biocompatibility studies were performed with preosteoblastic cells showing good biocompatibility and no changes in the different phases of the cell cycle after treatment with the nanosystem.

Photothermal and immunomodulatory AIE decorated 3D printed mesoporous bioactive glass/HA scaffolds for infected bone defect repair

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F7_2, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 10:30 - 13:10

Repairing bone defects infected by bacteria remains a major clinical challenge, primarily due to the complications caused by bacterial infection and the inflammatory microenvironment. To address this, there is an urgent need for novel bioactive materials that can overcome these issues. Mesoporous bioactive glass nanoparticles (MBGNs) are promising materials for bone regeneration. They form strong chemical bonds with host bone and release bioactive ions, such as Si^{4+} and Ca^{2+} , that promote osteogenesis and angiogenesis during degradation. Furthermore, MBGs can be modified through ion doping, allowing for enhancing their biological performance, such as antibacterial activity. However, incorporating antibacterial elements like Ag and Cu into MBGNs may cause cytotoxicity, and their effectiveness against biofilms remains limited [1][2]. In contrast, aggregation-induced emission (AIE) nanoparticles exhibit unique photothermal properties that are particularly effective in combating biofilm-related infections. These nanoparticles generate enhanced fluorescence and heat upon aggregation, which not only supports antibacterial activity but also ensures minimal cytotoxicity by activating their antimicrobial properties only under light irradiation [3].

In this study, we fabricated a 3D-printed hydroxyapatite (HA)/Ce-MBGN scaffold and modified its surface with AIE nanoparticles. We investigated the effects of AIE modification on the scaffold's morphology, physicochemical, and biological properties. The results showed that AIE modification significantly enhanced the scaffold's photothermal properties without altering its morphology or mineralization ability. AIE-modified scaffolds exhibited potent antibacterial activity, effectively eliminating drug-resistant *Staphylococcus aureus* bacteria biofilm. Additionally, the presence of Ce-MBGNs in the scaffold improved its antioxidant properties, promoted M2 macrophage polarization, and created a regenerative immune microenvironment conducive to tissue regeneration. The scaffold also continuously released Si and Ca ions, which stimulated the osteogenic differentiation of bone marrow stromal cells (BMSCs). In vivo studies demonstrated that the modified scaffold exhibited superior antibacterial and bone regeneration. This research highlights the potential of combining AIE nanoparticles and MBGNs in the design of advanced bioactive materials for treating infected bone defects.

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Acknowledgements

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Enhancing Bone Regeneration: Macro-porous Metallic Scaffolds Functionalized with SHED-Derived EVs

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F7_2, Manuel de Falla Auditorium (Level +1), septiembre 18, 2025, 10:30 - 13:10

The repair of large bone defects remains a significant challenge in regenerative medicine. While metallic scaffolds provide excellent mechanical stability, they often lack the osteoinductivity required for effective bone regeneration. In this study, we investigated the osteogenic potential of a 3D-printed Ti6Al4V scaffold functionalized with ceramic coatings and extracellular vesicles (EVs) derived from stem cells of human exfoliated deciduous teeth (SHED cells) embedded in a collagen hydrogel.

Ti6Al4V scaffolds were coated with graded silicate glasses and hydroxyapatite (HAP) powder doped with silver. The coatings exhibited strong antibacterial activity, with over 98% reduction in *S. aureus* and *E. coli* cell numbers. Cytocompatibility tests on SHED cells demonstrated a higher metabolic rate of SHED cells on coated scaffolds compared to uncoated Ti surfaces, while apoptosis/necrosis rates remained below 5% across all samples. SHED cells seeded directly on coated scaffolds exhibited improved attachment and proliferation compared to those on uncoated surfaces. These results indicate that the coated scaffolds combine both strong antibacterial properties and high cytocompatibility.

To introduce osteoinductive properties, EVs were extracted from SHED-conditioned media via differential ultracentrifugation. Characterization of the isolated EVs confirmed the presence of tetraspanin markers CD9, CD63, and CD81 using direct stochastic optical reconstruction microscopy (dSTORM), while their morphology and size distribution were verified by transmission electron microscopy (TEM) and nanoparticle tracking analysis (NTA). To ensure controlled release within the microporous scaffold, EVs were encapsulated in a 0.4% collagen hydrogel. Fluorescence-based NTA analysis demonstrated that approximately 50% of EVs were gradually released within the first three weeks. The osteogenic potential of EV-loaded scaffolds was assessed by qRT-PCR analysis of SHED cells cultured on the material. After 10 days of treatment, significant upregulation of RUNX-2 and BMP-2 gene expression indicated the pro-osteogenic effects of the SHED-EV-enriched scaffold.

These findings suggest integrating SHED-derived EVs within a functionalized Ti scaffold is a promising strategy for enhancing bone regeneration in large defects.

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Dual pH-responsive and shrinkable Mesoporous Silica Nanoparticles for Pancreatic Ductal Adenocarcinoma

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F7_1, Picasso Room (Level -2), septiembre 17, 2025, 17:00 - 19:00

Pancreatic ductal adenocarcinoma (PDAC) is the most prevalent form of pancreatic cancer (PanCa), accounting for 95% of cases and ranking as the third deadliest cancer in 2023.¹ Despite advances in oncology, PDAC remains highly lethal due to its dense desmoplastic stroma and complex tumour microenvironment (TME), which hinder the penetration and efficacy of conventional drugs and nanocarriers. Numerous drug delivery systems (DDS) have been explored as potential strategies to improve PDAC therapeutic efficacy.² However, significant challenges remain, particularly, the internalization of the DDSs into the tumor and the rapid immune clearance of the nanocarriers from the bloodstream, which drastically reduces their accumulation at the tumor site, resulting in less than 5% reaching the target cells.³

To improve the efficiency of the present treatments, our group have developed a dual pH-sensitive, shrinkable DDS based on mesoporous silica nanoparticles (MSNs) for combination chemotherapy against PDAC cells. To do so, MSNs are loaded with a gemcitabine-camptothecin conjugate and coated with a poly(β amino ester) polymer via a novel dual-sensitive linker. The incorporation of an electrostatic albumin corona further improves the stability of the system at physiological conditions, while endowing the system with an active targeting to the TME. This design allows for controlled stepwise disassembly under acidic conditions corresponding to the ECM and lysosomal environments and presents significantly reduced uptake in macrophage cultures. The high initial hydrodynamic size of the carrier would permit the retention within the TME via the EPR effect, strengthened by the albumin-mediated targeting. Upon exposure to the mildly acidic ECM, partial degradation of the coating enables size reduction, facilitating tumour penetration to PanCa cells. Furthermore, the biological activity of the nanoparticles was evaluated in advanced 3D culture models, designed to closely mimic the TME of PDAC.

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Corrosion behavior of Zn-1Mg and Zn-1Mg-1Ag (wt. %) alloys in simulated physiological environments

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F8_2, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Zinc (Zn) is a biodegradable metal with controlled degradation, unlike iron (Fe) which degrades slowly with long-term retention of its corrosion products and unlike magnesium (Mg) which corrodes rapidly, producing harmful hydrogen gas. Zn is known as an essential nutrient for physiological functions in the human body with intermediate potential vs SHE (-0.76 V) comparing to Fe (-0.44 V) and Mg (-2.73 V). These factors make Zn a promising biocompatible material for biomedical applications that can extend to diverse domains such as in cardiovascular stents, orthopedic scaffolds and wound closure devices [1], [2].

The main goal of this work was to analyze the corrosive behavior of cast Zn alloys:

Zn-1Mg and Zn-1Mg-1Ag (wt. %) and describe the role of silver (Ag) addition on the degradation performance. To approach this, immersion tests were performed using various solutions simulating physiological conditions such as: hanks' balanced salt solution (HBSS), Dulbecco's modified eagle medium (DMEM) and Dulbecco's modified eagle medium with the addition of 10% fetal bovine serum (FBS) during 7 days under cell culture conditions according to ASTM G1-03 [3]. During immersion, pH, osmolality and corrosion rate were analyzed. Surface degradation was examined using scanning electron microscopy (SEM) and optical profilometry. As per results of this work, both, Zn-1Mg and Zn-1Mg-1Ag provided stable pH and osmolality values, also its corrosion rate and surface damage match the biomedical applications requirements. The addition of Ag produced an earlier but uniform surface damage maintaining acceptable pH, osmolality and corrosion rate values.

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Corrosion and tribocorrosion behaviour of β -type Ti-Nb alloy produced by laser powder bed fusion & isothermal aging for implant applications

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F8_2, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Laser powder bed fusion (LPBF) has become a key technology in medical engineering for creating patient-specific titanium-based implants with tailored microstructures and optimized mechanical properties. LPBF-produced β -type Ti-Nb alloys outperform their conventionally manufactured counterparts due to their unique microstructures and localized control over mechanical properties, enabling customization for specific bone load requirements. However, load-bearing implants remain susceptible to tribocorrosion caused by motion in body fluids.

This study addresses the corrosion and tribocorrosion behavior of LPBF-produced and subsequently age-hardened β -type Ti-42Nb alloys, comparing them to conventional Ti-6Al-4V ELI. Tribocorrosion performance was evaluated under open-circuit potential (OCP) and anodic polarization (0.6 V vs. Ag|AgCl) in phosphate-buffered saline (PBS) using a pin-on-disk tribometer. Results revealed no significant differences in the corrosion behavior of LPBF Ti-42Nb alloy states in PBS, suggesting that strong passivation characteristics outweigh microstructural variations. Age-hardened alloys produced by LPBF exhibited lower wear resistance compared to the reference alloy under both OCP and anodic polarization conditions (0.6 V vs. Ag|AgCl). Despite their high hardness, the age-hardened alloys experienced greater total volume loss and wear depth. This difference is attributed to the presence of hard and brittle precipitates. The rapid detachment of ω precipitates in Ti-42Nb (LPBF-300 °C, 30 h) and α'' precipitates in Ti-42Nb (LPBF-450 °C, 30 h) results in a non-uniform hardness distribution, ultimately reducing tribocorrosion performance.

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Towards partly degradable implants made from titanium and magnesium

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F8_1, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Medical implants consisting of a degradable and a permanent part offer the opportunity to develop novel therapies and improved implant functionality. In particular, the combination of permanent titanium (Ti) and degradable magnesium (Mg) alloys as hybrid implant materials could be beneficial. Ti is a well-known excellent implant material due to the high strength and biocompatibility, while Mg has mechanical properties similar to bone, degrades in the body and stimulates several biological functions, for example bone formation. Thus, the aim of this study is to get synergy in the interaction between these strongly different metals transforming Ti into tissue stimulative material and supports Mg by load bearing application.

There are some challenges of Ti-Mg implants to overcome: (i) because of metal physical reasons the connection between Mg and Ti as key point of hybrid implant production is not trivial, (ii) due to electrochemical interaction the connection with Ti can change the degradation behaviour of the Mg part and (iii) hydrogen formed during degradation can deteriorate the mechanical properties of the Ti part. However, preliminary studies to solve these obstacles showed that Mg and Ti can be joined by a powder metallurgical sintering approach, enabling also additive manufacturing. Hydrogen evolution experiments, chemical composition determination, electron microscopy, X-ray diffraction and mechanical tests were applied for the characterisation of the hybrid Ti-Mg implant system [1].

The results point out the demand for coating of the implant surface to decrease rapid degradation of Mg which can be achieved by plasma electrolyte oxidation coating [2]. Hydrogen released due to Mg degradation ingresses into the Ti part and could lead to embrittlement if not properly controlled. By well determined hydrogen adsorption, there are hints that the biocompatibility of Ti can even be improved.

In sum, the results of the presented investigations will be used for further development of hybrid Mg-Ti implants facilitating the simultaneous application of completely different properties. Furthermore, the possibility to change the shape of the implant during application could be additional aspect with new field of patients' treatment.

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Dealloying as a facile process to improve cytocompatibility and antibacterial activity of biocompatible Ti-based amorphous alloys

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F8_2, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Implant infections and related biofilm formation are a major concern whenever implantable medical devices are considered. Since there is currently no standard treatment for implant-associated infections and antibiotic treatments are ineffective for biofilms, the best approach is to focus on the inhibition of both bacterial adhesion and biofilm formation by acting on the implant material itself. If metals are considered, Ti-based amorphous alloys are gaining importance as biocompatible materials due to the possibility i) to adapt the composition with the exclusive use of biocompatible elements and ii) to reduce the mismatch in Young's modulus between the bone and the implant material. Moreover, their biocompatibility and antibacterial activity can be improved by exploiting the dealloying process that is related to the dissolution of less noble elements from an amorphous phase enabling the surface diffusion of the noble adatoms that reorganise on the surface by forming ligaments and pores. Dealloying is an effective and simple process adapt to change both composition and morphology of the surface of the Ti-based amorphous alloys, so hindering the bacterial adhesion and the consequent biofilm formation.

In this work, two Ti-based amorphous alloys (Ti₄₇Cu₃₈Fe_{2.5}Zr_{7.5}Sn₂Si₁Ag₂; Ti₄₀Cu₄₀Zr₁₁Fe₃Sn₃Ag₃) were considered and different dealloying strategies were adopted to design the surface composition and morphology: both electrochemical and chemical dealloying was performed and different electrolyte (basic and acid) were considered. In general, mixed Ti/Zr oxides were formed with thickness ranging from tens up to hundreds of nanometres with variable morphologies. The oxide layers were studied by means of different techniques: field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS). Moreover, wettability, cytocompatibility and bacterial adhesion studies demonstrated the effectiveness of the dealloying process with the improve of the cytocompatibility and antibacterial activity.

A key point in the design of Ti based alloys are the modified surfaces to which an optimised biocompatibility is associated. Therefore, the dealloying mechanism was studied in detail in order to enable a connection between morphology and composition of the dealloyed layer and dealloying parameters used to antibacterial activity. The early stage of the dealloying process was evaluated by the calculated vacancy formation energy that described the tendency of one element to be easier released from the surface against another. Moreover, ab initio calculations evaluate characteristic XPS energy shifts between metals and oxides enlighten the role of surfaces and oxidation while the valence electron density reveals bonding features.

Developing antibacterial surfaces on Titanium based biocompatible alloys using low voltage Plasma Electrolytic Oxidation

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Modifying titanium implants' surfaces to introduce nano- and micro-scale patterning is a promising way to hinder bacterial adhesion and, thus minimize the biofilm formation and implant-related infections. β -Titanium alloys are well known for their inherent biocompatibility but there is still necessity to enhance their antibacterial properties, as most of the research that is being carried out is focused on cp-Ti or Ti6Al4V [1]. In this work we focus on two β -Ti-based alloys, Ti-24Nb-4Zr-8Sn (%wt) and Ti-45Nb (%wt), which are both free from any cytotoxic elements. The alloys were prepared by arc-melting under argon atmosphere followed by a heat treatment at 1000°C for 24 hours to ensure homogenization of the alloy composition and phases. Micro-porous and nano-textured surfaces were created through low voltage Plasma Electrolytic Oxidation (PEO), with a maximum voltage of 308V, a value relatively low when compared with the current literature [2]. The electrolyte used for the PEO treatment contained calcium acetate hydrate ($\text{Ca}(\text{CH}_3\text{COO})_2 \times \text{H}_2\text{O}$), sodium dihydrogen phosphate anhydride (NaH_2PO_4) and potassium hydroxide (KOH), aiming to form hydroxyapatite (Hap) on the coatings. The antibacterial properties of the Hap-containing coatings were improved by incorporating Ga, Zn and Ag ions within the coatings and by soaking the samples in Iodine baths as a second treatment. The surfaces were characterized by Scanning Electron Microscopy (SEM), revealing in all cases a homogeneous oxide layer that is well adhering to the substrates, and Grazing Incidence X-Ray Diffraction (GIXRD) confirmed the presence of anatase, rutile and Hap on the surfaces. Their corrosion behaviours were assessed by performing Potentiodynamic Polarization tests (PDP) and Electrochemical Impedance Spectroscopy tests (EIS) using Simulated Body Fluid (SBF) as the electrolyte, at 37°C. In addition, Hemolysis Assays (HA) and Radical Oxygen Species (ROS) measurements were carried out to evaluate the hemo- and biocompatibility of the surfaces. These results are promising for creating orthopaedic implant surfaces that simultaneously promote cell adhesion and prevent bacteria adhesion on the surface.

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PM Ti- 5 vol.% TiB₂ COMPOSITES PREPARED VIA GREEN AND COST EFFECTIVE TECHNOLOGIES FOR DENTAL IMPLANTS

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Titanium is also one of the most biocompatible metals with medical applications in prostheses, orthopaedic and dental implants, and surgical instruments. Ti belongs onto the EU list of critical raw materials and its products are significantly more expensive than steels. In aerospace industry typically 82% of the titanium became scrap metal before final goods are produced. To reduce titanium production and manufacturing costs, powder metallurgy as a near-net-shape manufacturing technology is developing for more than four decades.

After Russia's invasion of Ukraine, REPowerEU Plan is implemented to phase out Russian fossil fuel imports. Titanium production requires very high energy inputs/has large CO₂ footprint in comparison with the most used materials. Therefore, in this study, Ti - 5 vol.% TiB₂ composites were prepared from the mixture of Ti and TiB₂ powders using spark plasma sintering (SPS) technology at IMN, Gliwice, Poland and pressure less solar sintering at PSA, Almería, Spain.

The SEM and XRD analyses indicate that TiB₂ is unstable at 950 – 1300°C and transforms onto TiB whiskers: In the case of microstructures after SPS, the TiB whiskers are very difficult to observe - Kroll's etching was necessary to observe them. They are significantly thinner and smaller in comparison to solar sintered TiB whiskers. Porosity of prepared composite is in the range of 6 – 16 % for solar sintered samples. SPS samples possesses porosity below 0.1 %. Vickers hardness of prepared composite is in the range of 200-327 MHV0.5 for solar sintered samples and 358 ± 28 MHV0.5 for SPS samples. Pin-on disk measurements were performed on SPS sample against alumina. Measured coefficient of friction was 0.5378 ± 0.0246 against alumina and observed wear of 0.0436 g.

Research works on laser surface treatment and evaluation of suitability of prepared composites for dental implants are currently undergoing.

This research was mainly financed by VEGA project: Laser surface modification of Ti –TiB₂ biocomposites prepared by powder metallurgy process in order to increase their osseointegration (2/0054/23). Partial financial support by of the SFERA-III project (Grant Agreement No 823802) is also acknowledged.

Resorbable Mg-0.4Zn strands for bone fixation: pilot in vivo tests on minipigs

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Magnesium alloys are a promising material for resorbable bone support implants, particularly in cases where biodegradable fixation can eliminate the need for secondary surgeries. Among Mg-based implants, thin wires and strands show potential for applications such as sternal fixation and reconstructive hand surgeries. However, several challenges remain, including excessive hydrogen generation, concerns about the long-term safety of certain alloying elements, localized corrosion, and defects such as MgO particles in thin wires, which can lead to premature and unpredictable failures. This presentation focuses on polymer-coated extruded Mg-0.4Zn wires with a diameter of 300 µm and the strands produced from them, their surface modifications, and key findings from a pilot in vivo study using a minipig model. The study evaluates the in vitro degradation and mechanical property changes of these strands, the in vivo tissue responses to the implants, and hydrogen production near the sternum, partially fixed with Mg-0.4Zn strands.

Additive manufacturing and post-processing of a beta-type Ti-Nb alloy with tailored mechanical biofunctionality for load-bearing bone implants

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Current requirements for load-bearing bone implants are patient-specific designs and new materials for improved mechanical functionality and biological compatibility. Additive manufacturing technologies such as Laser Powder Bed Fusion (LPBF) facilitate the near-net shape production of metallic bone implants. As a non-equilibrium technique, LPBF can also generate defined microstructural states, thereby yielding unique mechanical performances. This is specifically promising for metastable alloys such as beta-type Ti alloys which combine the benefits of low elastic moduli and composition of biocompatible constituents. On the example of the metastable Ti-42Nb alloy we demonstrate how LPBF processing and post heat treatments can lead to required low stiffness in combination with high hardness and strengths.

For beta-phase Ti-42Nb, the control of LPBF parameters can lead to a strong anisotropy in the stiffness of bulk specimens. By using a non-standard top hat laser source, a unique microstructure with strong <001> texture parallel to the building direction (BD) was generated. Tensile tests along selected loading directions revealed a strong mechanical anisotropy with the lowest Young's modulus of 44 GPa parallel to BD.

Suitable post heat treatment strategies for LPBF-produced Ti-42Nb cause substantial materials strengthening effects. Heat treatments within the alpha+beta phase range at 723 K for different durations led to increasing fractions of the metastable orthorhombic alpha''iso phase, acting as an intermediate to the stable alpha phase. The beta grain boundaries are primary sites for early alpha''iso precipitation. Micromechanical analysis by means of nanoindentation (at a constant strain rate) was used for assessing the impact of time-dependent microstructural changes on the evolution of reduced modulus (E_{ru}) and hardness (H) values. Tensile tests demonstrated significant strength enhancements through treatments up to 108 ks compared to the as-built state, i.e. a yield strength of up to 1060 MPa and ultimate tensile strength of up to 1125 MPa, thereby reaching the performance level of clinical benchmark materials such as Ti-6Al-4V.

Further, LPBF is a powerful technology for the fabrication of metallic scaffolds with low structural stiffness. On the example of Ti-42Nb scaffolds, designed as triply periodic minimal surfaces (TPMS), the successful transfer of those post heat treatment strategies for microstructure modification leading to scaffold strengthening will be shown.

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Enhancing Magnesium Alloy Biocorrosion Resistance with Additivated Geopolymer Coatings

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F8_2, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

Magnesium-based bioresorbable materials have emerged as promising candidates for bone regeneration applications due to their bone-like elastic modulus and osseointegrative capabilities. However, their bioresorption rate is closely linked to their corrosion behavior, which, if excessive, can negatively impact surrounding biological tissues. The presence of chlorides—prevalent in bodily fluids—can induce severe corrosion, leading to a rapid loss of mechanical integrity before the bone tissue has fully regenerated. Additionally, the fast dissolution of magnesium and its alloys can produce byproducts, such as hydroxides and hydrogen bubbles, which may accumulate in tissues.

This study explores the development of coatings composed of a geopolymer matrix with biocompatible fillers such as glucomannan, sodium alginate, or hydroxyapatite nanoparticles to regulate the corrosion rate of magnesium in simulated biological environments. The microporous nature of these coatings allows controlled electrolyte penetration, preventing a complete barrier effect while maintaining corrosion rates within acceptable limits.

The coatings were applied using a dip-coating technique and characterized through SEM/EDXS analysis to examine their morphology and chemical composition. To evaluate their performance, coated samples were immersed in saline, phosphate-buffered saline (PBS), and Hanks' Balanced Salt Solution (HBSS), closely resembling biological conditions.

Corrosion behavior was assessed by electrochemical analyses—including open-circuit potential measurements, potentiodynamic polarization tests, and electrochemical impedance spectroscopy (EIS)—to compare the response of coated and uncoated samples in the tested solutions.

Surface functionalization of titanium foams for controlled tetracycline release using a hydrogel-based delivery system

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F8_4, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Titanium is widely used for bone tissue replacement due to its ability to mimic the properties of natural bone, including biocompatibility, corrosion resistance, and a favorable elastic modulus. Despite these advantages, its bioinert nature can hinder rapid osseointegration and increase the risk of implant failure. Moreover, titanium implants are often recognised as foreign materials and for this reason after surgical intervention, pharmacological treatment is required to mitigate inflammation and prevent local infections that could lead to implant rejection. Unfortunately, conventional drug administration methods are often inefficient, leading to undesired side effects, such as toxicity or suboptimal delivery.

To address these challenges, this study presents a novel approach using type A gelatin-based hydrogel as a long-acting drug delivery system which is infiltrated into the porous structure of the surface-modified titanium foams to provide a sustained and local drug release, improving the success of the bone replacement and patient compliance.

Specifically, titanium foams with a nominal porosity of 60 vol.% were developed using the space-holder technique and consequently modified through conventional thermal oxidation in static air and acid etching using sulfuric acid to modulate the drug release kinetics. The results shown that the acid-etched surface reduced the release rate of the drug (tetracycline) due to the increased surface roughness, whereas the hydrophilic rutile TiO₂ layer formed by thermal oxidation accelerated the tetracycline release.

This research highlights the potential of combining hydrogel systems with surface-modified titanium foams for controlled drug release, offering an innovative solution for localized treatment in bone tissue replacement surgeries.

Future studies are also being focused on optimizing the control of drug release by modifying hydrogel to enhance its thermal stability and mechanical properties as well as further surface functionalization of titanium foams using techniques such as pore surface anodization to tailor the drug release kinetic according to the therapeutic needs.

In-vitro corrosion tests of Zn and Mg-based wires for biomedical applications

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Magnesium alloys with Zn addition are promising biodegradable materials for bone fixation implants. However, their corrosion behavior must be optimized to ensure a controlled degradation rate and sufficient mechanical strength. Another key challenge is controlling hydrogen release during corrosion, which is linked to surface quality and material purity. In this study, in vitro tests were performed in DMEM at 37 °C to investigate the corrosion kinetics of Mg-Zn alloy wires (Mg, Mg-0.3Zn, Mg-0.4Zn, wt.%). These wires were braided into strands, and the amount of released hydrogen gas in DMEM was measured. Temperature and pH were continuously monitored, and corrosion products were analyzed using SEM and EDS. The addition of zinc resulted in a more controlled corrosion rate compared to pure magnesium while maintaining adequate mechanical integrity. The results provide insights into corrosion behavior and the role of Zn alloying, contributing to the optimization of biodegradable materials for medical applications.

Adjustable degradation rates for additively manufactured implants made of Zn and Mg

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F8_2, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 10:30 - 13:10

The potential of degradable implants lies in the health promise of avoiding revision surgeries. Initially, implants are intended to replace the supporting function of lost bone substance and initially should dissolve very slowly, after which they can dissolve quickly and as complete as possible. In recent years, laser powder bed fusion has become increasingly established as an additive manufacturing process for the production of targeted structures and porosities and porous metallic scaffold structures as well as smooth and continuous surfaces, which can promote cell proliferation [Hein21]. Further and more detailed structural features were created using electrochemical processes. This method shows their potential particularly in the case of complicatedly shaped surfaces, similarly. Moreover, these structures have aroused great research interest for biomaterial applications, as they allow continuous grading of their geometry [Rein20]. And so, biomorphic geometries with excellent mechanical properties and suitable load distributions are expected. Although, they should also have a controllable dissolution rate, which could be adapted to the mechanical requirements of the implant site.

In this presentation, the degradation behaviour of differently produced magnesia and zinc samples is presented. The samples have been produced either by laser powder bed fusion or rolling technology and in some cases have been provided with an artificial oxide layer. Using spectroscopic and gravimetric methods, the degradation rates are determined and the relationship between morphology, microstructure and degradation behaviour is presented. Electrochemical impedance spectroscopy is used to discuss the degradation activities in front of the interface over time. Dependencies and correlations between degradation rate and morphology, microstructure and alloy composition controlled by additive manufacturing and electrochemical methods are mapped and discussed.

Overall, these initial degradation studies of bulk and trace elements should help to enable targeted control of the degradation behaviour of additively manufactured, porous structures made of pure zinc or magnesium in the future. The work should lead to a deeper understanding of the corrosive degradation behaviour of these materials. Initial experiments are also presented below, in which important mechanical properties were correlated with different functionally graded structures.

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Laser powder bed fusion of nitinol for medical applications: Superelasticity under tensile stress

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F8_4, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

By developing laser powder bed fusion (LPBF) of nitinol, new design freedoms and enhanced functionality of future implants can be unlocked. However, challenges associated with LPBF, such as residual stresses, porosity, and microstructural variations, must be addressed to ensure the production of high-quality and reliable medical devices. Further, vaporization of nickel [1] and oxidation of titanium [2] are two important phenomena during the LPBF-process, which influence locally and globally the Ni-Ti ratio and thus significantly impact the thermomechanical properties.

This study investigates the influence of key SLM process parameters (e.g. laser power, scan speed, hatch spacing) on the microstructure and mechanical properties of LPBF-processed nitinol after specific heat treatments. A comprehensive approach along the process chain is employed, encompassing powder characterization, process monitoring and analysis at multiple steps along the post-processing chain. The latter comprises carrier gas hot extraction for oxygen content, micrographs for qualitative and quantitative evaluation of porosity, differential scanning calorimetry to determine phase transition temperatures and tensile tests at body temperature to characterize the superelasticity.

Key findings include the identification of a process window for achieving nearly full dense, crack-free parts. The phase transition temperatures can be adjusted within a temperature interval of 20 °C in the solution annealed state by means of LPBF parameter variation. Subsequent heat treatments allow to set the austenite finish temperature to the desired temperatures up to 40 °C. The heat-treated material shows superelasticity under tensile load, recovering deformations up to 6 % with a residual elongation below 0.2 % for the first cycle. Plateau stresses differ depending on LPBF process parameters and post processing but can be tuned towards 400 MPa to 500 MPa, typical values for conventionally produced semi-finished NiTi products.

These findings provide valuable insights into the optimization of the LPBF process to produce high-quality, reliable nitinol implants with fine-tuned performance. The results of this study will guide the development of additively manufactured nitinol components with superelastic properties and contribute to robust process control strategies. This will enable the utilization of the unique functional properties of nitinol in new medical applications.

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Enhancing Properties of Zinc-Based Biodegradable Alloys for Biomedical Applications via Powder Metallurgy

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Biodegradable metals have garnered significant attention in biomedical research as temporary substitutes or fixation devices for damaged body tissues. Among these, zinc alloys are particularly promising for applications such as stents and screws due to their excellent biocompatibility and favorable corrosion properties compared to other metals like magnesium and iron. However, to meet the stringent requirements of biomedical applications, these materials must exhibit enhanced mechanical properties. Therefore, optimizing the composition and processing methods of zinc alloys is crucial for developing effective biodegradable devices in biomedical engineering.

In our research, we focused on the preparation of binary and ternary zinc alloys with copper and manganese, starting from pure powders. We employed a combination of mechanical alloying (MA), spark plasma sintering (SPS), and extrusion. Optimization of preparation parameters led to the formation of fine-grained, homogeneous microstructures with intermetallic phases, resulting in improved mechanical properties.

This study examines the effects of powder metallurgy preparation on the mechanical and corrosion properties of selected alloys. Our results demonstrated a significant impact of MA parameters on the fineness and chemical composition of Zn-2Cu and Zn-1Cu-1Mn (wt.%) powders. The compacted samples, processed through SPS and extrusion, exhibited fine microstructures with grain sizes in hundreds of nanometers, intermetallic phases such as CuZn₅, and oxide nanoparticles from the original surface of the powder particles. These structural changes played a crucial role in hindering dislocation motion, thereby enhancing the strength of the material and influencing its behavior during corrosion testing. We observed increased hardness, an improvement in ultimate tensile strength from 109 MPa for pure zinc to 180 MPa for the ternary alloy, and the formation of a partial corrosion barrier during testing in a simulated physiological environment.

Our findings underscore the potential of this powder metallurgy approach in enhancing the mechanical and corrosion properties of zinc-based biodegradable alloys, thereby advancing their applicability in biomedical devices. "This research was supported by the Czech Science Foundation (GACR), project number 25-16144S, and by the grant of Specific University Research A1_FCHT_2025_011."

Challenges in evaluating the interface between resorbable magnesium materials and bone tissue

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In biomedicine, significant attention is given to biodegradable metals. Among the most promising candidates are Mg-based materials, as Mg²⁺ cations and Mg corrosion products are well tolerated by the body and naturally degraded through metabolic processes. The biomedical application of these materials could be particularly beneficial for paediatric patients due to their dynamic growth.

The aim of this study was to describe the degradation of Mg-3Y (<3.5 wt% yttrium) and Mg-4Y-4Li (4.0 wt% yttrium, 4.0 wt% lithium) alloys in a real bone environment and their interaction with bone tissue. Mg-based implants were inserted into the condyle of an adult Wistar rat (male, >480 g). Samples were extracted after 8, 12, and 24 weeks of healing, fixed in 4% formaldehyde, and subjected to micro-CT analysis and histopathological examination.

Micro-CT allows for non-destructive 3D evaluation of samples. However, due to the similar X-ray density of the examined Mg-based materials and bone tissue, distinguishing between them in micro-CT imaging is challenging. This distinction becomes increasingly difficult as the magnesium material degrades and bone regeneration progresses. This work focuses especially on the challenges of micro-CT analysis at the interface between Mg materials and bone tissue.

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The influence of the surface pre-treatments on the chitosan/bioglass coatings deposited on the titanium substrate

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F8_4, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

In biomedicine, the surface of implants plays an important role in osteointegration processes as it is a place of first contact with the human body. It can influence the acceptance of the implant and the occurrence of inflammations. Due to that, studies on the surface of biomaterials have great importance nowadays. One of the methods to improve biocompatibility is the deposition of different coatings on the substrate material. Among them are the electrophoretically deposited chitosan/bioactive glass coatings. Due to their beneficial properties as: high corrosion resistance, bioactivity, and biocompatibility, they show great potential in biomedical applications. The limitation of these coatings is their relatively low adhesion to the substrate. It can be improved through the change of parameters of the deposition process or on the way of surface pre-treatments. However, the additional modifications can influence the topography of the coating, which can also impact the biological response. In this study, we investigate the morphology and topography of the chitosan/bioglass coating electrophoretically deposited on the pre-treated titanium substrate, as well as the influence of the conducted processes on the adhesion of the coatings.

Enhancing the Mechanical Properties of Zn-Based Biodegradable Alloys Through Harmonic Structure Design

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In recent years, zinc alloys have been increasingly investigated as promising biodegradable materials for medical applications, especially in orthopaedics and cardiovascular surgery. Due to their biodegradability and good biocompatibility zinc alloys appear to be an attractive alternative to biodegradable magnesium or iron alloys. Potential applications of these materials include the manufacture of screws and nails for fracture fixation, as well as stents that can be inserted into narrowed blood vessels and other tubular organs to hold them open.

Despite their advantages, zinc alloys have some disadvantages, including poor mechanical properties, particularly low strength and limited ductility. This limits their practical applicability in challenging biomechanical conditions. Therefore, ways to improve these properties without adversely affecting the biocompatibility of the material are being intensively sought. One promising approach to achieve these goals is the creation of a harmonic structure characterised by a combination of soft cores and a hard ultra-fine-grained 3D skeleton. This approach allows for synergistic increases in both strength and ductility, which is key to the successful application of the material in medicine.

This work focuses on the study of Zn-based alloys with a harmonic structure. Advanced powder metallurgy methods, specifically mechanical milling and subsequent plasma sintering, were used to prepare alloys with controlled microstructure. Detailed analysis of the microstructure was complemented by an investigation of mechanical properties to understand the relationship between the microstructure and the resulting material characteristics. After sintering, the alloy contained oxide shells that negatively affected the mechanical properties of the material. During the extrusion process, these were broken, which led to a significant improvement of the structure in terms of efficiency of the processes enabling the synergy of the different domains of the material to be realised. As a result, the alloy achieved a tensile strength above 300 MPa and a ductility of approximately 13 %. This knowledge will allow further optimisation of the properties of these alloys for biomedical applications, which could contribute to the development of a new generation of biodegradable implants.

This research was funded by the Czech Science Foundation (project No. 25-16144S).

Exploring the deformation mechanisms and degradation in Mg10Gd using acoustic emission and in situ SR μ CT

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F8_3, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The research of biodegradable bone implant materials based on Mg has been increasing in recent years. In comparison to traditional implant materials, Mg has the advantage of being biodegradable, eliminating the need of an implant removal. Additionally, it has comparable mechanical properties to bone, providing support to the healing bone. Nevertheless, the degradation is complex and not yet fully understood since many factors influence the process. Next to commonly investigated factors like the chemical environment, also mechanical loads play a role in the degradation process. Since the mechanical deformation of a material is influenced by its microstructure, the internally occurring deformation mechanisms in as-cast and T4 heat-treated Mg10Gd were investigated using standard tensile tests with simultaneously recording the acoustic emission signal. The results show an increase in twin formation for the as-cast material which has only a negligible effect on the overall deformation. However, varying the strain rate showed an opposite effect for heat-treated and as-cast materials, indicating a major influence of the microstructure on the deformation process. Using these information, additional experiments were conducted to include the degradation process in the analysis. Here, in situ synchrotron radiation based micro computed tomography (SR μ CT) was used to combine imaging techniques and acoustic emission to quantify the degradation process while simultaneously following the damage evolution in the material. In the experiment, heat-treated and extruded Mg10Gd was deformed in a tensile test while being immersed in simulated body fluid (SBF) having similar ionic concentrations to human blood to model near-physiological conditions. By applying in situ SR μ CT, the degradation and deformation can be investigated during the deformation until the specimen failure. This investigation showed that under degradation conditions the mechanical failure is drastically faster. Additionally, the deformation showed significant differences between experiments in air and SBF, indicating differences in the deformation mechanisms. One reason for this is the occurrence of stress-corrosion cracking at low strain rates. The results clearly indicate that the interplay between degradation and deformation needs to be investigated further to enhance the understanding of degradation processes in future biodegradable bone implant materials.

Phase-Field Modeling of Magnesium Alloy Degradation for Biomedical Applications

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Biodegradable metals hold tremendous potential in the field of biomaterials, offering a solution to mitigate post-operative complications associated with permanent implants. However, enabling their commercial adoption requires a comprehensive understanding of the degradation mechanisms of these materials.

Pitting corrosion, for instance, is a critical challenge in the application of magnesium-based alloys for biomedical purposes, particularly for degradable implants. This localized form of corrosion can jeopardize the structural integrity of devices, undermining their mechanical reliability and effectiveness.

Computational models have emerged as powerful tools to support and enhance traditional in vitro studies, offering efficient methods to investigate corrosion phenomena. Among the various computational approaches developed for simulating magnesium-based alloys corrosion, phase-field (PF) models stand out for their versatility, making them a promising alternative.

Here we aim to use PF simulations to investigate the degradation of magnesium alloys used in biomedical applications. The initial approach starts with a simple model that considers uniform degradation; subsequently, the model is refined to account for the phenomenon of localized corrosion (pitting). The methodology employs an implicit description of the metal-electrolyte interface, represented by a smooth phase-field function, and a stochastic variation of interface mobility to capture the inherent randomness in pitting initiation and propagation. Our analysis focuses on the role of key parameters influencing corrosion dynamics, such as the interface thickness and the distribution of interface kinetic coefficients. Additionally, we explore the transition from uniform to localized corrosion regimes and their implications for the degradation rate and mechanical stability.

We expect this work to ultimately provide a comprehensive framework for understanding and predicting the degradation behavior of magnesium-based alloys in physiological environments, advancing the application of biodegradable materials in biomedical devices.

Processing of Ti-10Nb-10Ta alloy foams via powder metallurgy with solar sintering

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Titanium alloys with niobium and tantalum are promising materials for biomedical applications due to their excellent biocompatibility, corrosion resistance, and adaptable mechanical properties. In this study, open-cell Ti-10Nb-10Ta foams with 50 and 60 vol.% of porosity were manufactured using the space-holder powder metallurgy technique, employing NaCl as a pore-forming agent. The novelty of this study was the one step sintering and nitriding of ternary titanium alloy foams using a low-cost Fresnel lens as solar concentrator.

The experimental procedure included powder mixing and compaction with the space-holder, followed by the space-holder dissolution in water and finally solar treatment under N₂-5%H₂ atmosphere to achieve optimal sintering components. Thermal analysis revealed that an exothermic reaction occurred in the range of 470-520 °C, attributed to the formation of titanium nitride (TiN). Additionally, solar heating activates the solid-state diffusion process during sintering, optimized at 1200 °C, which requires much less time than using electric furnaces (15-30 min vs. several hours).

Microstructural characterization confirmed the presence of TiN in the surface of the components, effective metallurgical bonding between powder particles, and homogeneous porosity distribution which fits with the designed parameters. These results demonstrate that the application of solar thermal cycle enables the production of high-quality titanium alloy foams with optimized microstructure, promoting high pore interconnectivity, and the formation of a TiN surface layer that enhances hardness without compromising structural integrity.

All the manufactured foams exhibit an optimal pore size (200–600 µm) that could promote cell growth, rounded cubic pore morphology, preventing stress concentrations, and interconnected porosity network that could facilitate the circulation of bodily fluids, making them particularly suitable for bone implants. This study confirms that the combination of space-holder and solar concentrated energy technologies is an efficient and sustainable methodology for producing titanium alloy foams.

Combinatorial Development of Mo-Ag Thin Films for Antibacterial Coatings: High-Throughput Synthesis, Characterization, and Performance Evaluation

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F8_4, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

High-throughput methodologies, particularly thin film combinatorial approaches, are transforming materials discovery by enabling rapid and systematic exploration of vast compositional spaces. Among these, physical vapor deposition (PVD) magnetron co-sputtering has emerged as a powerful tool, allowing precise control over compositional gradients and microstructures. This study focuses on the development of molybdenum-silver (Mo-Ag) alloys as antibacterial coatings for biomedical applications. Silver (Ag) is widely recognized for its antibacterial properties, but its uncontrolled ion release can lead to cytotoxic effects. Molybdenum (Mo), in contrast, provides high mechanical stability and controlled degradation. By combining these elements, we aim to develop coatings that balance antibacterial efficacy, biocompatibility, and structural stability, with a regulated ion release profile to minimize toxicity.

Mo-Ag thin films were synthesized using PVD magnetron co-sputtering, followed by heat treatment to relieve residual stresses and modify phase composition. Chemical and phase analysis confirmed the incorporation of Ag within the Mo matrix, while microstructural characterization using scanning electron microscopy (SEM) and transmission electron microscopy (TEM) provided insights into grain structure and morphology. Nanoindentation tests assessed the mechanical properties, particularly hardness and elastic modulus.

To evaluate degradation behavior, corrosion testing was conducted in Hank's solution, simulating physiological conditions. The results showed that Mo-Ag coatings exhibit a controlled corrosion rate, which was further analyzed through ion release measurements to establish a correlation between degradation kinetics and elemental dissolution. The cytocompatibility of these coatings was evaluated using both direct and indirect in vitro assays, confirming an acceptable level of biocompatibility. Additionally, antibacterial activity was assessed through in vitro tests, demonstrating bacterial suppression.

This study demonstrates that Mo-Ag is a promising system for antibacterial implant coatings. The developed high-throughput synthesis and characterization workflow proved to be an efficient approach for discovering new materials for biomedical applications. Future integration with CALPHAD modeling and machine learning-based predictions would further enhance the efficiency of materials discovery by guiding experimental efforts toward optimized compositions.

Additive manufacturing of metallic bioresorbable stents

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F8_1, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Customizable, bioresorbable cardiovascular stents utilizing additive manufacturing (AM) offer a transformative approach to heart health, directly addressing two of the most critical needs in modern medical devices: personalization and non-permanence within the body. Currently, only metallic materials can fully meet the stringent demands of cardiovascular stents, with strut size that minimizes its impact on the blood flow. Through 3D printing with metals, stents can be tailored to each patient's unique vascular anatomy, ensuring a customized fit that enhances effectiveness while having the required resistance.

Most current implants are permanent, and in some health problems, once the tissue or organ is healed, they become superfluous as happens to cardiovascular stents. Bioresorbable stents would gradually dissolve as the artery heals, reducing the long-term risks of permanent implants such as chronic inflammation and restenosis, while supporting the body's natural healing process. The most considered bioresorbable materials that can be additively manufactured are based on Mg and Fe, and they provide the mechanical strength required for arterial support while fully degradable over time.

Laser Powder Bed Fusion (LPBF) technology is the metal AM technology that provides the best resolution and detail, and it has been used to manufacture stents and stent-like structures with Mg (WE43) and FeMn (Fe20Mn0.5C) alloys. The freedom of design that LPBF provides has been used to optimize the performance of the stents, and conventional and auxetic designs have been used.

Also, to meet the stringent roughness requirements of cardiovascular stents, the surface of the 3D printed stents has been modified to reduce the intrinsic roughness of the LPBF process and to modulate the degradation rate and its interaction with the biological environment. In the case of the Mg-based stents, a sol-gel silica coating has been deposited to assimilate their corrosion rate to the conventional healing times of cardiovascular arteries.

The microstructure and roughness of stents have been evaluated. Also, tensile and compression mechanical tests have been applied to stents and structures with a central part with a stent-like structure but with clamps compatible with standard universal testing machines. The results obtained match those obtained from mechanical simulations.

Therefore, it has been proven that LPBF is a valuable tool for manufacturing bioresorbable stents and testing structures that cannot be fabricated with other techniques.

Optimizing the mechanical properties of Ti-6Al-4V alloy produced by selective laser melting for biomedical use

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F8_3, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

This study investigates the potential of a Selective Laser Melting (SLM) Ti-6Al-4V alloy, specifically in relation to orthopedic implants. SLM is an additive manufacturing process that offers several benefits for creating customized medical devices. These structures help reduce the alloy's elastic modules, reduction of stress shielding that can occur in conventional implant materials. To improve the mechanical properties and microstructure of the Ti-6Al-4V alloy produced by SLM, the effects of a hot isostatic pressing (HIP) treatment at temperatures ranging from 850 °C to 950 °C are examined. HIP is known to reduce internal porosity and promote phase transformation in titanium alloys, affecting overall performance. Key findings from the research include:

1. Phase transformation: HIP treatment results in transformation of α' -martensite to a more stable α (Ti) and β (Ti) two-phase microstructure.
2. Reduction in internal porosity: Using HIP significantly reduces internal porosities in SLM-produced samples, improving their structural integrity.
3. Mechanical properties: While HIP increases ductility, it also reduces tensile strength. This compromise is typical of many materials that undergo post-treatment, in which improved formability is achieved at a cost of strength.
4. Potential for biomedical applications: Overall, the combination of SLM and HIP post-treatment results in Ti-6Al-4V alloys that are more suitable for use in biomedical applications, especially orthopedic implants, due to their improved mechanical properties and reduced internal defects.

This research highlights the promising potential of SLM and HIP post-processed Ti-6Al-4V alloys for use in medical devices, offering a tailor-made, bio-inert solution with optimized mechanical properties for orthopedic applications.

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New generation of porous composites titanium/ Hap biomaterials.

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Modern societies are faced with an increasing demand for orthopedic implants, which is challenging both medicine and materials engineering. The dynamic growth of the implant market is driven by the need to develop biomaterials with improved durability and biocompatibility. This thesis focuses on improving the properties of titanium alloy (Ti6Al4V) based surgical implants to extend their lifetime and improve their functionality. The primary research hypothesis is that the combination of titanium alloys with hydroxyapatite (HAp) and the laser texturing (LST) of the surface of the samples can result in a biomaterial with exceptional mechanical and biological properties. Hydroxyapatite, as the main mineral component of bone, enhances the bioactivity and osteointegration of the implant, while the use of laser surface treatment allows the microstructure and topography of the material to be precisely modified. The porous structure encourages the penetration of cells, resulting in rapid osteointegration, and moreover offers the possibility of applying drugs and antibiotics directly to the implant, which also speeds up recovery. The implant surface is further structured by laser to increase the specific surface area.

The research of the present work is comprehensive, as it includes the development of a method to obtain the aforementioned composites for accurate physico-chemical analysis. The powder metallurgy manufacturing process consisted of several steps, starting with the preparation and obtaining of powder compositions in different proportions, followed by isostatic cold pressing and then sintering. The characterization of the obtained materials was carried out using different analytical techniques such as Fourier transform infrared spectroscopy (FT-IR), optical microscopy and X-ray diffraction analysis. The research focuses on the analysis of the tribological and biological properties of the newly developed Ti/HAp/LST composite. Microstructural characterization and biocompatibility tests in an environment simulating biological conditions were performed. The XTT tests carried out confirmed the lack of toxicity of the resulting composites both before and after laser structuring. The results show significant improvements in properties and bioactivity, suggesting that the proposed material could find application in modern orthopedic implants. The development of a new generation of Ti/HAp/LST composite biomaterials represents a step forward in surgical implant technology, offering a solution with improved functionality, greater durability and higher biocompatibility. The authors gratefully acknowledge financial support of the project “New Generation of

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Laser Textured and Bioactive Ti/HAp/MXene Biomaterials

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Nowadays, abnormalities affecting the skeletal system are an increasingly common problem. This is related to the phenomenon of an aging population, as well as the occurrence of various accidents that cause bone damage. It is often required to implement an implant, which must meet the appropriate requirements to be used in a living organism. Such a material must meet a number of requirements, i.e. biocompatibility and bioactivity. For this reason, metallic implants are increasingly being abandoned, and alternative ceramic-metallic composites are being introduced. Ceramics, i.e. hydroxyapatite, thanks to their structure resembling natural bone, contribute to the regeneration of bone tissue and introduce bioactivity into the system. On the other hand, metals, in this case titanium alloy Ti-6Al-4V, provide adequate mechanical properties. Bone implants, especially of the hip joint, are exposed to constant stress and friction, which contribute to implant wear and often revision due to inflammation. An additional element that will benefit implant longevity is laser texturing, which can affect bioactivity by creating a well-defined and controlled surface roughness. This will allow, among other things, the growth of cells in appropriate areas, which will contribute to bone regeneration. Another way to improve the tribological properties of Ti/HAp composites is to implement MXene coating. These relatively new 2D materials have been identified as solid lubricants and compounds that form beneficial tribophilms. Moreover, they have been noted for their potential due to their large surface area, drug-loading ability, and biocompatibility and non-toxicity to the living organism.

The biomaterials were prepared by using the powder metallurgy method and then selecting appropriate sintering conditions. At the initial stage, the percentages of hydroxyapatite, porophore and titanium in the powder mixtures were determined, which were then compressed using the cold method and the samples prepared in this way were sintered. The next step was to perform laser surface texturing (LST) to improve friction and anti-wear properties. A layer of MXenes was also implemented as a lubricant that can improve friction and wear.

The performed physicochemical and structural analysis of the obtained composites showed the potential of the designed material for use in bone tissue regeneration.

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Mg-Fe nanocomposites overcome the strength-corrosion dilemma of Mg-based materials

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F8_3, Seminario 4 + 5 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The low strength and poor corrosion resistance of magnesium (Mg) has prevented its use for load-bearing bone fracture fixations. Core of this limitation is Mg's low solubility for most elements combined with its low electrochemical potential. This favors precipitation of secondary phases (i.e., micro-galvanic elements) but also excludes Mg-based composites (highly active galvanic couples), both of which would allow to improve strength significantly. Alternative concepts for high-strength yet slowly degrading Mg-based materials thus need to be developed. Here, we present promising results, indicating that the detrimental effects of galvanic corrosion might be overcome by manipulating the composite architecture at the nanoscale. Using nanostructured Mg-Fe composites – so far thought an incompatible materials combination – we find that a reduction of the phase spacing significantly slows down Mg-corrosion rates, achieving even the ultra-low corrosion rates of ultra-high purity Mg. However, in contrast to UHP Mg, the nanoscale composite spacing allows for strength levels from 500 MPa up to 1 GPa. We discuss possible mechanisms enabling this advanced material performance and outline indications for future applications based on the enormous extension of the property space for Mg-based materials.

How to involve students – and citizens - in strategic developments in materials science: the case study of a “court for the future generations”

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G_1, Seminario 7 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The “court for the future generations” is an original format of event developed by the French media “Usbek & Rica”. In a scenarized way, real witnesses, or experts, testifying in the interest of the future generations, are questioned by a “fake” court composed of an attorney, a prosecutor and the president of the court. The jury, ultimately ruling, is picked by a lottery system in the audience. Tens of such events have already been organized in France, to explore topics of concern for current and future generations. For its relevance to communicate with a large audience (civil society, students, professionals), and the possibility to address, in a short time and in a light and humoristic manner, many facets of the addressed question, this format has been selected to organize an event around the future of materials science for scientists, students and civil society (40%, 40% and 20% of an audience of about 350 people, respectively). The question selected was “should we keep inventing materials?”.

Indeed, orientations in materials development, as in many other scientific fields, have been mostly following decisions and fundings decided by governmental institutions, industries, and of course researchers. However, they obey not only scientific and financial principles, but also, among others, ethical and ecological ones. Recently, materials are at the forefront of ecological concerns: although increased recycling and circularity is called for, research seems to remain focused on overcoming its own limits by continuously inventing always-more-complex materials for specific applications, consuming more energy, away from circularity. Is this race for high-tech materials a requirement to build tomorrow’s society, or should we now focus on sobriety? Should we keep inventing materials? To answer this questions, 4 witnesses from the industry (head of SafranTech), academia (Professor at UC Louvain), and specialists in the history of materials science (Emeritus professor) and in its future (SciFi writer), were invited. Many topics, including the motivations behind materials developments, future trends, and suggestions for increased democracy in strategic choices were covered. The debate was carried on by two PhD students in the role of the attorney and the prosecutor.

In this presentation, the context and the format “court for the future generations” will be presented, before to discuss this specific event: the witnesses, the court, the arguments, including all the preparation steps. At last, the practical organization will be rationalized, to end with the dissemination and the future steps of this project.

A Team-Based Framework for First-Year Materials Physics Education

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Traditional materials science curricula often prioritize abstract theory over early engagement with applied design challenges. However, recent studies have explored innovative approaches to teaching introductory materials science courses, emphasizing active learning and real-world applications. Project-based learning (PBL) has been implemented in first-year engineering curricula, integrating multidisciplinary projects with traditional lecture content [1]. These projects enable students to apply theoretical concepts to practical challenges and connect abstract concepts with real-world engineering decisions.

This study presents a pedagogical model for first-year undergraduate materials physics that integrates active, team-based learning with real-world material selection tasks. Over a half-semester project, student teams analyze applications (e.g., biodegradable packaging, lightweight automotive components) through iterative research, experimental data analysis, and ethical evaluation. The framework employs a structured problem-solving approach, developing through problem identification, experimental validation, and teams' presentations. This phased method fosters critical thinking, teamwork, and effective technical communication.

Key innovations include integrating ethical design principles through case studies on global challenges like material shortage, encouraging participants to balance performance with societal impacts. Failure-driven learning is integrated via reflective reports, promoting resilience and iterative improvement. Authentic assessments, such as peer evaluations and stakeholder pitches, replicate real-world accountability.

Data from pre/post surveys indicate that most students improved their ability to connect theoretical concepts with practical constraints, alongside developing stronger collaboration skills. Performance in material selection tasks, assessed through rubric-based grading, also showed notable improvement. This framework illustrates that early exposure to open-ended, ethics-driven design projects strengthens foundational materials science knowledge and enhances professional readiness.

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Embedding Responsible Research and Innovation in a doctoral training programme

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G_1, Seminario 7 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Here we present the integration of Responsible Research and Innovation (RRI) training into a UK-based Centre for Doctoral Training, addressing the growing need for research and researchers that anticipate and respond to societal challenges. Exposure to a wider knowledge base complementing their technical skills encourages early career researchers to engage with broader dimensions of their work, incorporating communication, sustainability, legal, ethical, and other issues around equality, diversity and inclusion.

We show that, from the student perspective, there is no strong need for any previous explicit exposure to theories of interdisciplinarity. As such, we posit that effective RRI training in this vein can be adapted and embedded successfully in other related programmes. Access to quality RRI training across the UK and internationally is variable, and so this work addresses this gap.

The course design emphasises active learning and critical engagement across disciplines, providing students with the means to navigate complex research landscapes responsibly. It puts student agency and authentic learning front and centre, both of crucial importance when looking to engender a sense of responsibility in strongly society-linked subjects such as materials science and engineering.

This emphasis on student agency and authentic learning is demonstrated in the assessment portfolio, particularly in the inclusion of an innovative student-led citizens' assembly. The experience equips students with skills unachievable in traditional doctoral education.

This engagement of doctoral students with RRI training is having a broader impact on research practices across the university, demonstrating first- and second-order effects both on researchers of the future and the institutions within which they work.

All claims above are evidenced by results gathered in a student survey and via semi-structured interviews with students and staff involved with the wider Centre for Doctoral Training.

How to connect materials education with cutting-edge product development on the university level by enriching classroom knowledge with extracurricular engineering projects

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G_1, Seminario 7 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

International student competitions enable engineering students to improve their technical expertise significantly and to gain a lot of hands-on practise. By tackling such complex real-world problems students gain quasi-work experience and get to apply the theoretical knowledge they acquired in university courses. This is very important in materials education, because the physical test of the products design and its materials properties will exhibit problems and solutions that can hardly be taught in regular course modules.

One example of such a competition is the Formula Student, which was already established some decades ago. Participating teams design, construct, and fabricate single-seater formula-style race cars. They compete against teams from other universities around the world at international events. Aside from competing on the racetrack (dynamic disciplines), students also participate in so-called static disciplines that aim at evaluating the design process, their understanding of cost and manufacturing, and business skills. It is therefore a perfect interdisciplinary project to embed materials science into a high-performance product development.

In this contribution, we present a teaching approach that connects intracurricular and extracurricular elements to significantly enhance learning outcomes. We show how theoretical course knowledge can be augmented to reach the level of cutting-edge product development with the best choice of materials and manufacturing methods in a bottom-up student-driven learning environment. Key prerequisites to do so, such as the incorporation of companies, will be discussed as well as typical obstacles that occur in our teaching approach. Additionally, we use product examples to explain in detail which steps of the learning process are triggered and how (peer) docents can systematically guide student learners through it. These examples consist e.g. of 3D-printed weight-optimized and function-integrated uprights and gearbox parts that are subjected to high loads. In summary, we demonstrate how students can increase their materials skills significantly by taking part in extracurricular activities such as Formula Student and how this approach can be transferred to similar tasks in engineering education.

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Bringing Cutting-Edge Research to the Lecture Room: Material Acceleration Platforms for Applied University Students

Prof. Dorottya Kriechbaumer¹

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G_1, Seminario 7 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

This paper presents a practical example of how an introduction to Material Acceleration Platforms (MAPs) and other advanced, high-throughput, automated research tools can be effectively integrated into applied university education for master's students from diverse academic backgrounds. The concept will be demonstrated as a sub-module of a "Heterogeneous Catalysis" course, with a focus on the synthesis, characterization, and design of catalysts. The audience consists of an interdisciplinary group of students with backgrounds in chemical engineering, mechanical engineering, materials science, and computational modeling.

A detailed approach will be presented on how advanced materials research tools, such as MAPs and other automated solutions, are incorporated into a module traditionally focused on legacy lab tools. The goal is to combine both conventional methods and cutting-edge techniques within the same curriculum, ensuring that students are exposed to a broad spectrum of solutions, from foundational to advanced, providing a well-rounded education early in their academic careers. A proposed structure for a lecture series and laboratory practice will be outlined, allowing students to apply theoretical knowledge in real-world contexts and gain practical experience in accelerating catalyst synthesis, characterization, and design. These strategies are intended to foster interdisciplinary knowledge integration, preparing students for the multifaceted challenges of modern materials science and engineering.

Additionally, the presentation will introduce active teaching methods that align with the learning objectives, such as flipped classrooms, collaborative problem-solving sessions, and virtual lab simulations. Concrete example exercises and best practices will be shared, with a focus on engaging students and continuously monitoring their progress. Insights from the project "Time Efficiency: Implementing Flipped Learning to Activate Students" in the "Heterogeneous Catalysis" module will be presented.

The paper will also address the challenges and opportunities of integrating advanced tools into graduate education, particularly in an interdisciplinary context. Feedback from students participating in this interdisciplinary pilot program will be shared, along with suggestions for improvement and insights into how students from different academic fields engage with these methods. Practical recommendations for educators wishing to incorporate similar approaches into their courses will be provided, emphasizing the importance of adapting to the diverse learning needs of students from various disciplines.

Use of Parametric Models and Data in Scenario Based Approach for Materials Education and Professional Training

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Modelling at different scales (e.g. Density Functional Theory (DFT), Molecular Dynamics (MD) Simulation and Numerical Modelling) plays an important role in engineering R&D and materials education. The framework of Industry 5.0 requires the workforces with enhanced data-competence, interdisciplinary knowledge and skills, particularly, in materials. Parametric modelling is a powerful tool for many different engineering disciplines from traditional mechanical engineering, manufacturing to medical engineering, for which materials education is a key pivoting knowledge block. The use of parametric tools allows the users to analyse and visualise detailed data for complex materials, as well as evaluating different scenarios, which is important for both materials education and professional training. It can also produce comprehensive data for training and development of complex interdisciplinary knowledge. Data-led framework, equipped with education focused parametric study tools, will help opening new opportunities in establishing user focused framework in materials education and training with optimum impact beyond the traditional direct experience-based research and education approaches.

In this paper, the use of parametric modelling and data system for training and learning development of complex material systems are presented through three cases in different technical areas: modelling and testing of welded structures and precipitations (materials and manufacturing); foot orthotics with a particular focus on biomechanics (medical engineering) and complex porous structures and application (energy sectors). In each case, the use of parametric modelling linked with DFT modelling, MD Simulation and numerical modelling is presented. The key functions and framework of parametric models to empower the end users is analysed. Different approaches for identifying the factor of significance and use of key knowledge blocks are shown in this work. In addition, the key issues in designing parametric studies and material data system for integrated research and education development over different disciplines is comparatively studied and discussed.

(# we have asked for a Poster presentation in the review, can be converted into a presentation if required)

Innovative Learning in Materials Engineering: A Hands-on Approach to Material Design and Characterization

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G_2, Seminario 7 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

This study presents a novel educational project for first-year Materials Engineering students, designed to enhance their understanding of material design and characterization through hands-on experience. Unlike traditional coursework, students were challenged to create a material from scratch, optimize its properties, and document the process scientifically.

The project included four key phases: (1) selecting and designing the material according to the desired properties, (2) synthesis and processing, (3) characterization using laboratory techniques, and (4) documentation in the format of a scientific journal submission. Additionally, the students presented their materials at a simulated investor fair, where they defended their innovations to the audience.

This experiential approach enhances critical thinking, teamwork, and problem-solving skills. Although this project-based learning process requires that both teachers and students assume a more active role and a greater shared commitment, evaluation of the coursework illustrated that students have indeed integrated the knowledge they already gained during the course in developing the project, showing improved understanding of the material-structure-property relationships. Feedback highlighted the value of bridging theory and practice, as well as the importance of communication in scientific and business contexts.

These results suggest that integrating project-based learning into early engineering education enhances technical and professional competencies, preparing students for research and industry challenges.

The Art of Overcoming: Challenge-Driven Learning

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G_2, Seminario 7 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

An experimental concept for accelerated learning was subjected to a trial, adopting an interdisciplinary approach that integrates insights and methodologies from multiple domains to optimise the learning process. The block seminar, “High-Performance Materials for Fusion Technology,” designed for engineering students, integrates insights from both engineering and physics through the combined expertise of a materials science researcher and a plasma physicist. Throughout the seminar, participants explore the challenges and innovations within fusion technology while gaining hands-on experience in problem solving, critical analysis, and effective communication. By employing an inverted classroom model, the program fuses intensive lectures with interactive workshops and project-based learning, fostering creative thinking and collaboration across disciplinary boundaries.

The curriculum emphasizes the synthesis of diverse perspectives to address the complex challenges inherent in fusion technology. Students explore the interplay between material performance and plasma interactions, engaging in case studies and hands-on exercises that illustrate real-world issues and innovative diagnostic techniques. A novel method is employed to activate creative thinking: students are first challenged to propose innovative solutions for new materials before being introduced to state-of-the-art approaches. This strategy has resulted in an enormous increase in the speed at which learning material is absorbed, stimulating deeper engagement and understanding.

The seminar not only enhances technical knowledge but also develops essential professional skills, including teamwork, critical thinking, and effective communication. A key component of the course is the final project—a 20-minute PowerPoint presentation conducted in a professional setting that simulates collaborative work in committees and tech research communities. This format aims to further develop advanced presentation and discussion skills.

By bridging the gap between academic theory and industry needs, this seminar equips graduates with the versatile expertise necessary to drive technological innovation and meet the evolving demands of higher education and industry.

Innovative Teaching in Materials Science: Methods, Challenges, and Opportunities

Prof. Paloma Fernández Sánchez¹

¹University Complutense, Madrid, Spain

G_2, Seminario 7 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Materials Science cannot be considered in isolation from its social context. Everything we use in daily life is made of “something,” and that “something” is, fundamentally, a material. As society evolves rapidly, so does the field of Materials Science, which plays a crucial role in technological advancements across multiple industries. Teaching and learning must adapt to these transformations, integrating the challenges and demands posed by an increasingly technology-driven world. However, traditional teaching methods often struggle to keep pace with the interdisciplinary and applied nature of the discipline.

This talk explores innovative approaches to modernizing Materials Science education, emphasizing active learning methodologies, digital tools, and industry collaboration. Problem-Based Learning (PBL) and flipped classroom strategies foster critical thinking and problem-solving skills by shifting the focus from passive knowledge reception to hands-on exploration of real-world material challenges. Additionally, virtual labs and simulation software enhance students’ understanding of complex material behaviors, bridging the gap between theoretical concepts and practical applications. The integration of Artificial Intelligence and Big Data further transforms learning, enabling predictive modeling and computational material design—key competencies for the future of the field.

By aligning education with societal and industry needs, this approach better prepares students for their professional careers, ensuring they develop both technical expertise and essential problem-solving skills. Collaborations between academia and industry provide students with project-based experiences that enhance their adaptability and innovative mindset. Ultimately, modernizing the teaching of Materials Science ensures that graduates are not only proficient in fundamental principles but also equipped to thrive in an ever-changing technological landscape.

Integrating Sustainable Material Selection in Engineering Education Through a Gamified Learning Approach

Dr. Waleed Ahmed¹, Dr. Essam Zaneldin¹, Dr. Lindita Bande¹, Dr. Omar Al Khatib¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Promoting sustainability in education requires integrating environmental considerations into engineering curricula from the early stages of design thinking. This paper explores the incorporation of sustainability principles within an Engineering Ethics Course Project, emphasizing the importance of material properties and recyclability in early stage design decision-making. The initiative engaged students in selecting appropriate sustainable materials by utilizing the Granta Material Intelligence Card Game, an interactive tool designed to enhance awareness of material families and their environmental impacts. Through this gamified approach, students better understood how material selection influences product lifecycle, recyclability, and overall sustainability. The implementation of this methodology fostered critical thinking, ethical responsibility, and engagement, preparing future engineers to make informed, sustainable choices in real world applications. This study highlights the effectiveness of integrating material intelligence into ethics education, demonstrating how hands-on activities can drive sustainability awareness and responsible engineering practices.

Developing Interdisciplinary Professional Engineering Skills at University

Dr. Faith Nightingale¹

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G_2, Seminario 7 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Engineers are required to have a number of hard and soft skills in order to be considered competent in their profession (Engineering Council, 2020). It is however widely reported that engineers lack soft skills which costs businesses money (The Institute of Engineering and Technology 2021; Winterbotham, et al. 2018). Therefore, it is a university's responsibility to ensure students develop the skills needed during their studies (Department of Education, 2017). However, there is a lack of consistency when teaching and developing soft skills which are usually taught sporadically and generically.

This talk will show how professional engineering skills are taught at Queen Mary Engineering School (QMES), Xi'an, China using a project-based, interdisciplinary approach. The talk will demonstrate activities that take place in all years in the Professional Engineering Skills modules to develop the skills that student engineers require such as through the Materials Library project, escape room challenges and the Engineering Logbook. By developing these activities that support students throughout their time at university, students develop professional skills that will support future academic or career applications. From research conducted, students recognise their development of these skills and acknowledge the importance of them.

By completing these activities, not only do students develop graduate attributes which aligns with the aims of QMUL and TEF (Department of Education, 2017), but they also learn through engineering themed projects which enables them to see the interdisciplinary relationship between engineering and soft skills. Developing activities that contain real-world engineering problems helps students see the relatability of professional skills in the workplace. Additionally, soft skills align with AHEP objectives for accreditation of a programme which has been achieved in QMES through these professional skills modules.

The aim of this talk is to show that supporting students to develop soft skills at university is not only worthwhile for the students but also supports inclusivity. These activities can be developed and embedded into any programme using a project-based pedagogic approach. It is beneficial for a university to also develop interdisciplinary education and skills modules to aid in accreditation and diversifying the curriculum.

Science for all ages: engaging the elderly in lifelong learning

Miss Marianela Gómez-Toledo¹, Dr. Khalid Boulahya¹, Dr. Abderrahim Bouaid¹, Mr. Damir T. Biskup¹, Miss Eva López-Rabanal¹, Miss Sara María Gutiérrez-Flórez¹, Dr. Elena Arroyo-de dompablo¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Universities generate knowledge that fosters progress and innovation. Consequently, it is essential to share this knowledge with society to encourage education and development. While scientific dissemination is often linked to younger generations, learning is a lifelong activity and, therefore, citizens of all ages should be included. Engaging elderly people in scientific activities not only helps integrate them into society but also promotes scientific culture. Presenting our findings to senior citizens has benefits beyond the mere transfer of knowledge. It contributes to their cognitive stimulation, encouraging critical thinking and problem-solving skills. Moreover, it can relieve feelings of isolation and loneliness, providing social interaction and a sense of purpose.

We have developed a science dissemination activity entitled “The energy of the future: A current problem”. The activity is part of the program “Ciencia en Residencia” (<https://www.ucm.es/otri/ciencia-en-residencia>), developed by the Office for the Transfer of Research Results of Universidad Complutense de Madrid. The program aims to bridge the gap between academia and society, illustrating the relevance of science to everyday life. The activity includes a talk that addressed the significant societal challenges related to energy, incorporating various interrelated aspects such as energy independence, environmental sustainability, and economics. As a particular example, in a 5-minute video (https://www.youtube.com/watch?v=h_ezQtmtJrg) we illustrate the materials design process for green hydrogen production. The participants were encouraged to engage actively through games, written exercises, and debates. In this communication, we present the results, observations and conclusions of carrying out the scientific dissemination activity with senior citizens in out in two retirement homes in Madrid (Spain).

The authors acknowledge MCIN/AEI/10.13039/501100011033 - “ERDF A way of making Europe” for the project ECSAWE-PID2022-139501OB-C22. This research is also part of the Teaching Innovation Project Nº 36 of the 2024/2025 call from Universidad Complutense de Madrid, and of the “Ciencia en Residencia” initiative of Oficina de Transferencia de Resultados de Investigación (OTRI) from Universidad Complutense de Madrid. The authors are grateful to “MANAVA” senior day center and the retirement home “Residencia Isabel la Católica” for hosting the activity.

Sherlock Holmes in the Laboratory: Material Properties to Solve a Mystery

Mrs. Sandra Tarancón Román¹, Dr. Jaime Orellana¹, Dr. Elena Tejado¹, Mrs. Aida Martínez Barja¹, Dr. José Ygnacio Pastor¹

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G_2, Seminario 7 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

In recent years, the gamification of laboratory practice has developed into a more dynamic approach using available technology. This method aims to make the educational process more appealing, motivating, and interactive by incorporating elements that break away from traditional teaching styles. Crucially, though, it never loses sight of the main objective: to apply the knowledge acquired in the classroom in a practical way.

One such application of gamification can be seen in a challenge presented to the students. The task is to uncover the identity of the most infamous assassin in Materials Land, a fictional world where every citizen is distinguished by a specific material. The students are given a clue, a piece of material discovered at the crime scene, known to belong to the murderer. From this clue, the students are required to extract as much information as possible about the material to identify it, which, in turn, leads them to unmask the villain.

The students, acting as Scotland Yard detectives, are tasked with solving the case. However, they are told that the key to uncovering the villain's identity lies in a tensile test, a laboratory procedure used to assess the strength of materials. To assist them in their investigation, they are granted access to the expertise of the world-renowned detective of Materials Land, Sherlock Holmes—Mike Ashby—who is equipped with an extensive database known as Granta-EduPack. This database allows the students to match the "criminal profile" of the material based on its specific properties, aiding them in identifying it.

Through analysing the test results, the students are able to identify the villain—the material—by comparing the data they collect to known profiles stored in the Granta-EduPack database. The success of the method lies in the fact that students apply their theoretical knowledge of materials science in a very practical context. Most students, by carefully examining their tensile test results and using the database to collate material characteristics, are able to successfully identify the material in question.

This approach encourages active student participation, making learning more interactive and enjoyable. As they engage with the challenge, students become more familiar with the use of laboratory equipment and develop a deeper understanding of how to analyse and interpret results. This method not only consolidates fundamental concepts of material properties but also does so in a way that is both fun and effective.

Transforming students into scholars: the approach of the Queen Mary Centre for Undergraduate Research

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G_2, Seminario 7 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Abstract

The present contribution traces the journey of the Queen Mary Centre for Undergraduate Research (QMCUR) and discusses the operational model and pedagogical strategies that are being used with the intention of transforming students into scholars. QMCUR was built by integrating well-established models of undergraduate research [1, 2] and addressing common challenges in promoting such initiatives [3, 4], by introducing innovative elements and tailored procedures to facilitate its foundation at Queen Mary.

The centre's pedagogical framework combines co-creation and inquiry-driven approaches, through which students are integrated into research groups and expected to independently conduct hands-on research, contributing to knowledge creation and dissemination under structured mentorship programs with their respective hosts. The pedagogical strategies employed are grounded in the principles of progressive education, democracy in learning, and methods that promote heutagogy, self-efficacy, and student emancipation. The success of this educational framework is evidenced by the numerous awards, prizes, research opportunities, and paid internships and placements secured by students as a direct result of their involvement at QMCUR.

The achievements of QMCUR students demonstrate how early involvement in co-creation activities and engagement in meaningful research strengthens academic skills, builds confidence, accelerates professional development, and significantly broadens future opportunities.

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- [4] A. Brew, L. Mantai, Academics' perceptions of the challenges and barriers to implementing research-based experiences for undergraduates, *Teaching in Higher Education*, 22(5), 551-568, (2017).

Welcome to Materland

Dr. Gloria P. Rodríguez Donoso^{1,5}, Dr Juan José Damborenea^{2,5}, Dr Ana Romero^{3,5}, Dr Rodrigo Moreno^{4,5}, Ms Dora Sierra¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

"Welcome to Materland" is an outreach project in Materials Science, Technology, and Engineering coordinated by the Spanish Materials Society (SOCIEMAT) and the University of Castilla-La Mancha (UCLM). It brings together more than 90 participants from 37 institutions (universities, research centers, and technology centers) across Spain.

The project's main objectives are:

- (i) to enhance public knowledge and understanding of Materials Science, Technology, and Engineering by showcasing its relevance to technological development;
- (ii) to introduce the fascinating world of materials to primary, secondary, and vocational education students, fostering scientific vocations in STEM fields; and
- (iii) to establish and consolidate a national network for the dissemination of Materials Science and Engineering, facilitating collaboration between researchers and educators while promoting research initiation activities for adolescents and young people.

To achieve these goals, a wide range of activities is carried out, structured into three main areas:

- a) Creation of outreach materials and dissemination activities – This includes seminars, talks, competitions, and exhibitions (e.g., Women in Materials; Materland: The Materials Around Us), as well as the podcast Conversations in Materland, which features engaging discussions between researchers on socially relevant, current, and general-interest topics related to materials.
- b) Introduction to research activities – This involves scientific workshops and projects in schools aimed at bringing scientific experimentation and research closer to young students, as well as training courses for non-university educators.
- c) National Materials Outreach Conference "Materdivulga" – A biennial congress dedicated to science communication in the field of materials.

Launched in 2021, the project has been funded by the Spanish Foundation for Science and Technology (FECYT) through various grant programs supporting scientific, technological, and innovation culture:

- Bienvenidos a Materland: Acercándonos al maravilloso mundo de los materiales (Welcome to Materland: Approaching the Wonderful World of Materials), FCT-20-15783 (2021–2022)
- Materland: La aventura continúa (Materland: The Adventure Continues), FCT-22-18133 (2023–2024)
- Descubriendo Materland (Discovering Materland), FCT-23-19226 (2024–2025)

Pioneering Women in Materials Science

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This work is part of the outreach activities carried out within the framework of two science communication projects funded by the Spanish Foundation for Science and Technology (FECYT) [1, 2]. Its main objective is to recover and highlight the contributions of women who have excelled in the field of Materials Science, Technology, and Engineering throughout history.

In general, the public is familiar with very few female scientists and even fewer engineers or technologists. This is due to several reasons, but primarily because, throughout history, women have been denied both knowledge (access to culture and education) and recognition. Despite these barriers, many historical and contemporary female role models exist, and it is crucial to make their contributions visible—especially to younger generations. Additional goals of this initiative include breaking down gender stereotypes that hinder women's access to STEM fields, particularly in leadership and decision-making positions, and bringing female role models in Materials Science and Engineering to rural areas where access to scientific knowledge is more limited.

Among the women whose lives and work are highlighted in this project are Constance Tipper (UK, 1894), Mária Telkes (Hungary, 1900), Stephanie Kwolek (USA, 1923), Mildred Dresselhaus (USA, 1930), María Vallet Regí (Spain, 1946), Alicia Durán (Argentina, 1950), and Rosa Menéndez (Spain, 1956), among others.

The activities designed to introduce these pioneers to girls, young students, and the broader society include an exhibition featuring informational panels and objects related to their work, talks, workshops, competitions, and more. Additionally, an interactive game, "Discover Women in Materials Science, Technology, and Engineering," has been developed. This game includes videos where Spanish PhD students and researchers present these pioneering women to inspire future generations.

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[2] Discovering Materland, Spanish Foundation for Science and Technology (FECYT), FCT-23-19226 (2024–2025)

OpenSemanticLab: Accelerating Materials Innovation through Semantic Integration and AI Workflows

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G_3, Seminario 7 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Materials research is inherently complex, involving intricate relationships between material properties, compositions, and processing methods. To expedite the journey from laboratory breakthroughs to market-ready solutions, there is a pressing need for integrated platforms that harness the power of materials informatics. We introduce OpenSemanticLab, an open-source platform designed to accelerate materials research by integrating semantic web technologies, linked-data schemas, and artificial intelligence (AI) workflows.

OpenSemanticLab serves as a comprehensive knowledge platform where shared resources are efficiently managed. Object-oriented linked-data schemas (OO-LD) are embedded to harmonize data across various domains, including Lab-Inventory Management Systems (LIMS) and Electronic Lab-Notebooks (ELN). This integration ensures that both unstructured and structured data are accessible and interoperable, fostering better collaboration among researchers and streamlining R&D processes. A standout feature of OpenSemanticLab is its incorporation of Large Language Models (LLMs) and deterministic agents orchestrated by AI workflows. By delegating time-consuming tasks—such as data entry, form completion, and data analysis—to AI agents, researchers can significantly reduce the time and effort required for routine activities. The platform employs retrieval-augmented-generation (RAG) using phrased Resource Description Framework (RDF) graphs and document embeddings to enhance data retrieval and analysis capabilities. In addition, a chat-based automatic tool selector allows users to find the forms they are looking for, access key information and speed up data analysis without the need for advanced programming skills. Through this AI-assisted approach, OpenSemanticLab allows scientists to produce and structure large amounts of validated and AI-accessible data.

In this regard the interoperable description of material properties is a key element in both material research and material related value chains, particular in the form of product passports. For example, various initiatives like BatteryPass and Catena-X have drafted machine readable schemas for battery characteristics. Despite modelling the same asset based on the same regulation different initiatives came to diverging results.

In addition we face various ontologies just for physical quantities and units while those for material properties and characteristics are still emerging (e.g. EMMO, PMDco, IOTMaterials). We therefor picked up the path and extend those initial collections to a growing catalog of interoperable data characteristics in order to ensure both FAIR research and compliance with industry requirements.

In this presentation, we will introduce the high-level architecture of OpenSemanticLab and illustrate how semantic technologies and AI workflows are seamlessly integrated to create a platform for linked-data. We will delve into case studies that demonstrate the platform's impact on research efficiency and collaboration.

Accelerating Materials Innovation: The Role of Materials Platforms and Databases in EU-Funded Projects

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Material informatics is transforming the innovation landscape by integrating data science, machine learning, and multiscale modeling to accelerate materials discovery and deployment. This study explores how these advanced methodologies enhance technology transfer, with a particular focus on the development and impact of materials platforms and databases across EU-funded projects. These initiatives have successfully enabled seamless data integration, interoperability, and predictive modeling, fostering collaboration between academia, industry, and policymakers. By examining key case studies, we open the discussion on how these platforms are streamlining the transition from fundamental research to commercial applications, driving efficiency, and reducing time-to-market for novel materials.

Integrating Materials AI: A New Scientific Process for the Lab-of-the-Future

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G_3, Seminario 7 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

AI and digitalization are about to fundamentally disrupt chemistry and materials science, with the opportunity to accelerate innovation by up to 10 times. However, technology alone will not be enough. To realize AI's full impact, we need to integrate AI into everyday lab processes.

As a spin-off from the Karlsruhe Institute of Technology (KIT), we are advancing the adoption of AI in chemical research through our R&D management and AI platform. This platform empowers chemists to use AI without specialized data science or coding expertise—similar to Apps on an iPhone.

In this presentation, we demonstrate our adaptive optimization for the fabrication of Metal-Organic Frameworks (MOFs), a versatile materials class relevant for many applications, such as gas separation or storage, sensors, photodetectors, and catalysts. Using AI-powered closed-loop optimization, we precisely control film properties such as orientation and surface roughness, surpassing traditional methods like OFAT and expert-driven trial-and-error.

Key technologies that we bring from development to commercially ready, plug-and-play software tools include:

1. Automated data extraction and machine learning for optimal synthesis predictions.
2. Adaptive experimental planning for autonomous optimization.
3. Large language models to streamline data management and accelerate knowledge extraction.

Our platform, EDISON-4.0™, bridges the gap between AI innovation and practical lab application, fostering the widespread adoption of AI in materials research. With self-learning AI and adaptive optimization, labs can accelerate material development and boost productivity by up to 10 times.

Transforming R&D Efficiency: The Role of Dataspace Management in Material Development

Dr. Lukas Morand, Mr. Yoav Nahshon, Mr. Matthias Büschelberger, Mr. Kiran Kumaraswamy, Dr. Dirk Helm

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G_3, Seminario 7 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

In the manufacturing industry, development cycles within R&D departments play a crucial role in the incremental improvement of products. However, these cycles are often lengthy and resource-intensive, hindering innovation and responsiveness to market demands. This contribution introduces the Dataspace Management System (DSMS), a comprehensive technology stack designed to power dataspaces and digital ecosystems, which addresses these challenges by improving the way materials and process data are handled. By connecting and harmonizing disparate data sources, DSMS facilitates a semantic-based overview of materials and process data as well as data-processing workflows, significantly enhancing development efficiency. Additionally, it allows for the seamless integration and management of custom applications for data analysis and post-processing. Through its user-friendly interface, DSMS simplifies the use of semantic technologies, making it accessible to various stakeholders along the development cycle (technicians, engineers, data scientists, R&D managers, ...), thereby facilitating collaboration among them. We demonstrate the applicability of the DSMS in case studies of materials engineering and manufacturing. Our findings illustrate how DSMS not only accelerates product development cycles but also enables a more agile and data-driven approach to materials innovation.

AI Explainability by Transparency for Surrogate Computation, Inference and Data Exploration in Material Informatics

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G_3, Seminario 7 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The use of data-based methods for predicting effective material properties and material design has been intensified recently with the availability of efficient approaches like Deep Learning. Even more the application of Large Language Models in many areas is transforming the way engineering tasks are performed. The development of this ap-proaches is very dynamic, and it is advancing as we speak, nevertheless for effective use in material science and in general in engineering, there are a few challenges that must be addressed and overcome.

In this work we present a research framework that address those challenges. Starting with the development of a transparent method for surrogate modelling that, in contrast with deep learning, is not as data intensive. The methodology is transparent in the sense that computed features for learning are based on mathematical principles. This is coupled with the use of Large Language Models for the efficient surrogate evaluation, data exploration and documentation that is merely used as a convenient interface to specific predefined data analysis functionality, aiming at avoiding hallucinations, that interacts with the user.

The framework uses a graph database to have full flexibility for learning and adapting. It can also be used to represent, if available, specific ontologies. A python-based backend is implemented as well as a convenient React and python-based frontend. Applications of the framework are demonstrated for the computation of surrogate models in predictive effective material properties from given two-point microstructure statistics as well as for computing a surrogate for forming simulations by given input process parameters. For interfacing with the data analysis results, an open-source Large Language Model is implemented and demonstrated .

Sustainable battery recycling using electrodialysis with X-ray fluorescence process control

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Recycling of lithium-ion batteries (LIBs) is important to secure the supply-chain of critical metals and to limit the demand for virgin raw materials. An important type of LIB contains lithium (Li), nickel (Ni), manganese (Mn) and cobalt (Co) as active material, referred to as NMC-type LIBs. Metals in spent NMC batteries are recycled by hydrometallurgical methods like leaching, solvent extraction and crystallization. Electrodialysis is being researched as a novel refining method in the recycling processes, requiring less chemicals and producing fewer by-products compared with conventional methods. A chelating agent such as ethylenediaminetetraacetic acid (EDTA) is added to the metal leachate, binding to nickel ions (Ni²⁺) and forming a negatively charged chelate. This compound is then separated from the other positively charged metal ions by an electric field across a series of ion exchange membranes. Cobalt ions (Co²⁺) and manganese ions (Mn²⁺) are later separated in a similar way, forming the second and third most stable chelates with EDTA. A precise assay of the metal content is paramount for accurately dosing the chelating agent, as superstoichiometric additions give higher metal recovery at lower selectivity while substoichiometric additions give lower recovery but improve selectivity. Inductively coupled plasma optical emission spectroscopy (ICP-OES) is the standard laboratory technique for assaying leachates, having a low detection limit (ppb-ppm range) but requiring time-consuming sample dilution before analysis. In this study, X-ray fluorescence (XRF) was used to monitor metal content in electrodialysis feed and product streams. XRF is a quick assaying method with low operating cost obviating sample dissolution prior to analysis, making it suitable for on-line tracking of elements during operation despite its inability to measure Li and other light elements in solution. A synthetic sulfate leachate of NMC 111 black mass (0.01 M of Ni²⁺, Mn²⁺ and Co²⁺, respectively) was mixed with 10% molar excess of EDTA for Ni separation. Electrodialysis was performed at pH 2, achieving Ni separation factors of 20.2, 18.4 and 6.61 toward Li, Mn and Co respectively. Samples were retrieved during separation, later assayed using a Thermo Fisher iCAP 7000 ICP-OES and an Xore Boxray XRF analyzer. A linear correlation between assays from the two methods was observed, with a least-squares regression showing coefficients of determination (R²) equaling 0.980, 0.999 and 0.999 for Ni, Mn and Co respectively. XRF is a promising technique for monitoring metal content in leachates and for production control, enabling upscaling of the electrodialysis process.

Electrochemical study for the separation and recovery of gold and copper from waste printed circuit boards leach solutions

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Hydrometallurgical processes have been extensively studied for the recovery of base and precious metals from electric waste. Waste Printed Circuit Boards (WPCBs) present a promising source of critical materials such as Cu and Au, but their complex composition makes the recovery of these metals from leachates challenging. This study aims to recover Cu and Au from leach liquors of real WPCBs extractions. Two different liquors are obtained from a sequential leaching process: The first mixture (M1) contains a high concentration of Cu (40 g/L) and other base metals (<7g/L). The second mixture (M2) contains Au (10 ppm) and Cu in a greater proportion (Cu:Au ratio of 1000:1) along with chlorides (1.5 M). Both the Cu and the chlorides hinder the selective extraction of the precious metal.

This study focuses on determining the optimal conditions for recovering selectively both metals by investigating the electrochemical behavior of mixtures M1 and M2 for Cu and Au recovery, respectively. Cyclic voltammetry (CV) and chronoamperometry (CA) techniques were employed to assess the recovery of these metals under varying conditions using a potentiostat-galvanostat (Metrohm, PGSTAT 302N). The experimental setup included a two-compartment cell with an Ag/AgCl reference electrode, a 1 cm² Ti substrate as the working electrode in the cathodic compartment, and a Pt wire as counter electrode in the anodic compartments.

The study for the Cu recovery in M1 was done in sulphate and chloride media, using different concentrations of CuCl₂, CuSO₄ and H₂SO₄. From the CV study, the operation potential for selective electrowinning was selected. A potentiostatic CA at the selected potential was performed with real M1 to recover Cu in a separate cell using a Ti plate (cathode) and a Pb plate (anode). The faradaic yield for Cu recovery and the deposit purity have been determined, proving a selective recovery of Cu.

The study of M2 was done in a separate cell, conducting CV and CA in different samples based on M2 composition, using HAuCl₄, CuCl₂, CuSO₄ and H₂SO₄. The study involved the CV of different gold, copper and chloride ratios, to determine the optimum conditions for the selective Au deposition. The maximum Cu:Au ratio, the chloride content and working potential were obtained. A potentiostatic chronoamperometry was held on real M2 to assess the selective gold deposition in such complex electrolyte.

Electrolytic leaching of critical materials from Waste Printed Circuit Boards: a sustainable method

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Waste Printed circuit boards (WPCBs) are becoming a global concern as they are an increasing source of toxic waste as well as a source of valuable materials. Pyrometallurgy is the most commonly used recycling method, but it consumes large amounts of energy and it has a low selectivity. Besides, the heterogeneity of their composition hampers an effective recovery, requiring a combination of technologies to recover its valuable materials. This work presents an environmentally friendly alternative. The process consists in a sequential leaching of base and precious metals using electrolysis in mild acid conditions at room temperature. The main advantages of the proposed method are low current density, inexpensive reagents, and short operation times.

First, WPCBs from a local company were selected and dismantled, crushed and separated using magnetic and pneumatic processes. The non-magnetic fraction (<2mm) was used in the leaching tests. The in-house leaching system includes a two-compartment cell, a glass column where the leaching takes place, two tanks and a pump. NaCl and H₂SO₄ were used as electrolytes in both compartments. The chloride concentration of both electrolytes was 1.5 M and the initial acid concentration was 0.05 M. The cell was operated in galvanostatic mode using a current density of 400 A·m⁻².

The process was divided in 3 sequential steps. The first step aims to leach the base metals with no extraction of precious metals, the second step focus on the extraction of precious metals and the third step was included to check the end of the leaching process. A concentration process was performed by reusing the electrolytes and introducing different batches of WPCBs, to increase the metal concentration in each solution and improve their potential recovery from these solutions. After the process, the remaining WPCBs were analyzed to verify the metal content of each batch. The concentration of Cu, Au, Ag and Pd was monitored during the leaching tests, with an accumulated extraction yield of 98%, 95%, 90% and 68%, respectively.

Thermal drying for safe, high-quality and high-yield recycling of battery cells with liquid electrolyte

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Sustainable lithium-ion and sodium-ion battery markets require efficient and effective recycling technologies for end-of-life batteries. Batteries represent a complex type of waste, composed of various materials that must be carefully separated and processed. In novel recycling processes, the individual materials are first liberated by shredding or disassembling the cells, resulting in the release of various gases and vapors. These volatiles include the constituents of the liquid electrolyte that fills the porous network of electrodes and separator, as well as gases produced by decomposition and side reactions during battery operation, some of which are toxic. Since these substances pose a serious risk to process safety and the environment, and also negatively affect the quality and recovery yield of critical and precious materials, a thermal drying step is implemented to remove them from the material flow to the required low residual levels.

The objective of this work is to identify and quantify volatiles from battery cells and to determine their release kinetics in the recycling process, depending on the material- and process-related properties such as the disassembly depth, macrostructure of the material (e.g. particle size and geometry) and the drying boundary conditions. For the experimental studies, the mass change (over time) of a battery cell during drying under controlled process conditions is recorded. The composition of the exhaust gas from the drying process is analyzed using FT-IR spectrometry.

Results on the release kinetics of volatiles, especially of electrolyte and electrolyte degradation products, under different process conditions are presented. In particular, the influence of the drying temperature on the formation of unwanted reaction products will be demonstrated. Additionally, the study assesses the effects of cell formation, cycling, and aging on the gas and vapor release and evaluates potential benefits of solvent extraction prior to thermal drying. The experimental results support the optimization of the drying process parameters and assist in the design of the recycling process, focusing on the targeted and strategic placement of thermal treatment within the process chain. This study will lead to more ecologic and economic industrial-scale recycling processes for ion-based batteries with liquid electrolyte which ultimately help to increase material circularity and provide high-quality secondary resources.

This work contributes to the research performed at Material Research Center for Energy Systems (MZE). The authors would like to acknowledge financial support of the Federal ministry of Education and Research (BMBF) via the SynBatt project “DiRecReg” (03XP0553C).

Ink formulation from spent NiMH batteries

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H1_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The list of critical raw materials for the European Union is continuously expanding, with an increasing number directly affecting the ceramic industry. Notable among these critical raw materials are Co, Ni, Li, B, Sr, Ce, and Pr, which are widely used in the ceramic sector.

These materials are considered critical due to their economic importance and the risk of supply disruption. All of them are mined in countries outside Europe, and the refining processes are mainly carried out in China, which is the major supplier of many of these raw materials.

Therefore, securing alternative sources of raw materials is essential, which necessitates the exploration of end-of-life products containing critical raw materials and the development of recovery processes that are both environmentally friendly and economically viable.

A NiMH battery cell is made of a cathode, whose active material, in the charged state, is nickel oxyhydroxide (NiOOH), and an anode, mainly composed of hydrogen in the form of a metal hydride. The metal alloy is responsible for hydrogen storage and those normally used are the rare-earth (Misch metal) alloys based on lanthanum nickel (LaNi₅), known as the AB₅ class of alloys, in which La is sometimes partially substituted by Co, Ce, Nd, or Pr.

In this study, a separation process for the components of a NiMH battery was developed, using mechanical processes and considering the magnetic properties of the different materials. As a result, the active materials from both the cathode and anode were separated, and their potential use as secondary raw materials for the formulation of functional inkjet inks—capable of generating heat transfer systems—was explored. The results are at the laboratory scale, and further work is underway to advance to the pilot plant level before industrial-scale implementation.

Synthesis of LNMC cathode from recovered precursors from secondary source materials

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In recent years, the global lithium-ion battery market has grown by around 13% and is estimated to reach \$87.5 billion by 2027 due to the demand for portable electronic devices and electric vehicles, which is enhanced by the goals set by the European Union to achieve carbon neutrality by 2050.

LNMC cathodes, which are crucial for their high energy density, thermal stability, and long cycle life, depend on scarce raw materials like lithium, nickel, manganese, and cobalt.

For this reason, the recovery and recycling of critical metals from secondary sources, such as spent lithium-ion batteries, could be a promising solution, as it would reduce environmental impact and the dependence on primary sources.

This work focuses on the synthesis of LNMC cathodes using recovered precursors from secondary sources, lithium-ion batteries specifically.

Each precursor is obtained through specific recovery processes based on pyrometallurgical and hydrometallurgical methods. The recovery begins with a solid material known as black mass, which is obtained through crushing processes of spent lithium-ion batteries. This material is subjected to a carbothermic reduction followed by hydrolysis, allowing the selective extraction of lithium as a carbonate. Meanwhile, the insoluble solid residue is subjected to a hydrometallurgical route involving leaching. The resulting leachate is treated with oxalic acid, a precipitating agent, to recover a Ni-Mn-Co mixed oxalate. These steps ensure efficient separation and recovery of high-purity precursors for cathode synthesis.

The LNMC cathode synthesis procedure is based on a first step of solid reactive milling where the precursors are mixed for two hours in a planetary mill in stoichiometric quantities for a specific LNMC cathode. The mixture is then subjected to a heat treatment in order to decompose the precursors and make them more susceptible to the reaction. Finally, the temperature is raised to sinter the mixture. The sintering step was carried out in an oxygen atmosphere to maintain oxidative conditions.

The obtained black powder, which is characterized by analytical techniques such as XRD, SEM and ICP-OES, is identified as NMC cathode with a specific stoichiometry.

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Selective recovery of rare earth elements from electric vehicle motor NdFeB type magnets

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H1_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Electric mobility is a fundamental solution to reduce the environmental impact of mobility, as it contributes to reduce greenhouse gas emissions and improve air quality in cities. However, this transition to electric vehicles is intimately linked to the increase of critical raw material use. An example is the exploitation of rare earths, essential elements in the manufacture of motors and batteries that allow these cars to operate efficiently. Every electric car contains around 2 kg of NdFeB type magnets, about 30% of which is neodymium, a valuable and scarce resource that must be recovered and reused. This growing demand has increased the need to ensure a responsible and sustainable supply of these elements, which are not only crucial to the performance of electric motors, but also presents geopolitical and environmental challenges.

This work develops a rare earth recovery process, that starts from sintered NdFeB magnets obtained after the dismantling of electric car motors. The precursor material is a provided powder obtained through a hydrogen decrepitation process (HPMS: Hydrogen Processing of Magnetic Scrap). Subsequently, this powder was treated by chlorination roasting process, followed by liquid-liquid extraction stages using selective extraction agents in order to eliminate the iron and obtain a solution rich in rare earths. A successive stage of selective separation by liquid-liquid extraction technique allows the obtention of separate rare earth compounds that undergo a calcination process to obtain the REE oxides, which have further potential applications.

The final products have been characterized by techniques such as Inductively Coupled Plasma – Optical Emission Spectroscopy (ICP-OES), X-Ray Diffraction (XRD), Infrared Spectroscopy, and Scanning Electron Microscopy (SEM). The analyzed materials are identified as Neodymium and Holmium oxalates and oxides.

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Recycling and Calcination Behavior of Leaching Sludge from Secondary Batteries

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As the electric vehicle and electronics industries continue to grow rapidly worldwide, the demand for secondary batteries has also increased significantly. This surge has led to a rising concern regarding the efficient recycling of waste secondary batteries, which is emerging as a critical environmental and economic issue. Among various waste by-products, Fe-Al leach residual sludge is typically managed through landfilling or chemical treatment. However, these conventional disposal methods pose serious long-term environmental risks, such as soil and water contamination, while also incurring high treatment costs. Therefore, developing alternative approaches to effectively recycle and upcycle this sludge is essential.

Leach sludge primarily consists of approximately 95% aluminum hydroxide ($\text{Al}_2(\text{OH})_3$) and contains small amounts of valuable metals, including Ni, Co, and Fe. Additionally, aluminum oxide (Al_2O_3) is widely used across industries such as electronics, petroleum, chemicals, refractories, and ceramics, with demand continuing to rise. However, securing a stable supply of raw materials has become an increasing concern due to potential export restrictions imposed by bauxite-producing countries. This highlights the urgent need to explore alternative sources for aluminum oxide production and sustainable material recovery solutions.

To address these issues, this study aims to analyze the calcination behavior of Fe-Al leaching residual sludge from the secondary battery impurity removal process and investigate its potential for upcycling into high-value-added materials. By converting this waste into a valuable resource, we reduce the environmental impact associated with secondary battery waste disposal and promote a circular economy, and we expect that our findings will contribute to advancing green recycling technologies, increasing resource efficiency, and promoting sustainability in the battery industry.

Enhancing Purity of Cu-Based Alloys Recovered from WEEE through Oxidative Refining

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With the increasing use of electronic devices worldwide, the efficient recycling of waste electrical and electronic equipment (WEEE) has become essential in addressing the growing challenge of electronic waste and its environmental consequences. In 2019 alone, 53.6 million metric tons of e-waste were generated, highlighting the urgent demand for more effective recycling methods. However, only 17% of this waste is currently recycled, leading to the continuous loss of valuable materials such as copper, gold, and silver. One of the primary obstacles in WEEE recycling is the difficulty of efficiently separating and purifying these valuable metals, a crucial step in minimizing environmental impact and conserving resources.

This study explores the oxidative refining process as a technique for purifying metals recovered from waste printed circuit boards (PCBs), a major component of WEEE. The research focuses on the FeO-CaO-SiO₂ slag system and its effectiveness in removing impurities while enhancing the purity of recovered copper alloys. The FeO-CaO-SiO₂ slag system was chosen due to its low melting point and viscosity, properties that are vital for efficient slag formation and effective metal-slag phase separation during the refining process. The findings indicate that optimizing the FeO, CaO, and SiO₂ composition within the slag can significantly improve impurity removal and enhance the purity of the recovered metals.

Black mass recovery from lithium-ion battery recycling: interplay of efficiency and chemical composition

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The unprecedented demand for lithium-ion batteries, which inevitably reach the end of their lifecycle, is driving the growth of the battery recycling industry. Recycling these batteries is crucial not only for environmental sustainability but also for their significant economic potential: lithium-ion batteries contain critical raw materials, such as lithium, cobalt, nickel, and manganese, in concentrations often higher than those found in natural resources.

Recycling typically begins with shredding, followed by sieving to recover the “black mass,” a fine powder rich in valuable metals, depending on the specific battery chemistry. One of the main challenges in reintroducing black mass into the battery production cycle is achieving high purity with minimal contaminants, which is essential for its further refinement into high-purity individual components via hydrometallurgical processes. As in many industrial separation processes, there is often a trade-off between recovery efficiency and product quality. Thus, careful optimization is necessary to balance material recovery with purity, ensuring both economic viability and environmental sustainability.

This study systematically examined sieved fractions of black mass, focusing on optimizing sieve mesh sizes to enhance the recovery of active material. The results demonstrate that selecting appropriate sieve mesh sizes significantly improves active material recovery while reducing contaminant levels. A detailed chemical analysis of the refined black mass confirms its improved purity, reinforcing the effectiveness of this optimization approach.

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Optimization of parameters to obtain metallic cobalt from lithium-ion batteries with microwaves irradiation process

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With the increasing volumes of spent lithium-ion batteries from electric vehicles and the concurrent increase in raw materials cost for cathode production, finding effective methods for recycling battery materials has become critically important. This study investigates a pyrometallurgical approach using microwave irradiation to achieve carbothermal reduction of LiCoO_2 . Infrared thermal camera was employed for temperature measurements, allowing to optimize the process parameters to obtain metallic cobalt. Specifically, the research included microwave experiments on mixed black mass samples of anode and cathode materials in different proportions, treated at varying power levels and exposure times under standard atmospheric pressure. The effect of the process parameters and therefore of the temperature on microstructure was studied with SEM-EDS and XRD analysis. The feasibility of wet magnetic separation method between cobalt and lithium compounds formed during the reaction was also evaluated. The results obtained from the final separation process indicated that individual compounds can be obtained at the end of the cycle; moreover, the optimization of time, temperature and microwave power during the tests allowed to obtain metallic cobalt.

Reduced graphene oxide supported on polyurethane foams for metal recovery from e-waste

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H1_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The growth of global population and digitalization is rising the global demand of materials. In the last decade, critical raw materials (CRMs) have received much attention, due to their importance in strategic sectors such as the transition to climate change, aerospace, and safety. Waste from electric and electronic equipment (WEEE) represents an enormous resource due to their wide metal composition. However, nowadays, the majority of waste materials is wrongly discarded or misplaced, producing a huge loss of valuable metals.

WEEE can be treated in different ways to recover the contained critical raw materials, spanning from pyrometallurgical treatments to hydrometallurgical ones. The adsorption step, used into hydrometallurgical plants after various leaching steps, is a versatile technique because of its high recovery efficiency, short extraction time, high enrichment factor, simplicity, and low cost. The adsorption process makes also use of a wide variety of sorbents with different characteristics, such as silica- and carbon-based, green, and polymeric materials.

Graphene based materials have shown a great potential in this field of application, also owing to their high specific surface area. In this work, we exploit the adsorption behaviour of a 3D object composed by reduced graphene oxide (rGO) supported on commercial polyurethane (PU) flexible foams of 20 PPI. PU foams have been dip coated with a rGO aqueous dispersion, obtained after a mild reduction of commercial GO with L-ascorbic acid, performed under magnetic stirring at room temperature and pressure. The excess of dispersion on the foam has been removed by the use of compressed air; then, the coating has been consolidated in the oven at a temperature of 40 °C for 1 hour. The foams have been used to remove and recover different metals that can be found in e-waste.

Lanthanum, copper, and silver were selected as representative of e-waste critical (and strategic) raw materials. Adsorption was carried out on simulated mono- and multi- ionic solutions at different initial concentrations, from 1 mg/L to 1 g/L. The volume of the contacted solution was 100 mL. The experiments were performed under magnetic stirring at room temperature and pressure. The solution was analysed via ICP-OES before and after the adsorption experiment, to determine its composition. Preliminary results revealed a higher affinity of the rGO-coated foams for silver ions, being able to reach a capture efficiency of 59 wt.%. Moreover, SEM analysis performed at high magnifications revealed the presence of silver clusters on the surface of rGO.

BATCycle: green chemistry for recycling Li-ion NMC-111 Cathode material.

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Lithium-ion batteries (LIBs) are one of the most common batteries used in Electric Vehicles (EVs) due to high energy and power density and longer-life span. Alongside EVs increased production, the demand for LIBs has risen as well. For metal recovery from LIBs, end-of-life is the most used feedstock in the recycling industry, nonetheless rejected scrap from production of cathodes is also a high source of material. Production waste rates of LIBs are reported to be approximately 5% to 30%, which may vary with manufacturers.

Among LIB chemistries, Nickel Manganese Cobalt (NMC) cathodes are preferred for applications that require continuous cycling. Considering their high concentrations of critical materials, such as Cobalt and Lithium, NMC recycling is crucial. [3] Electrochemical recycling of LIBs, due to its selective metal recovery, is a growing interest in recycling companies. However, because of NMC complex chemical composition the recovery rate of high purity metals from electrochemical processes is limited. [4]

This study proposes a green chemistry approach for recycling of NMC-111 production waste. A pretreatment has already been designed. A treatment to selectively recover all critical materials that compose the active material are then tested and studied. Using only methanesulfonic acid as electrolyte, and NaOH for precipitation, to recover metal oxide compounds from the active material in multiple stages of the process at room temperature. The study also presents the use of a drum electrode setup as the working electrode, which increases the dissolution kinetics of the material in the electrochemical cell.

Eco-friendly electrospun lignin membranes for sustainable precious metal recovery from e-waste

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H1_2, Seminario 1 + 2 Room (Level +1), settembre 17, 2025, 14:30 - 16:30

Advances in technology have led to a significant increase in the consumption of electrical and electronic equipment, resulting in the generation of large quantities of waste electrical and electronic equipment (WEEE). This waste contains hazardous substances such as lead, mercury and flame retardants, which release harmful dioxins during incineration, posing serious environmental and health problems [1]. WEEE is a rich source of base metals (Cu, Fe, Ni and Zn) and precious metals (Ag, Au, Pt and Pd). For example, one tonne of electronic waste can yield up to 0.2 tonnes of copper, while discarded mobile phones are particularly rich in gold. Consequently, WEEE serves as an important reservoir of precious metals, making their sustainable recovery critical to meeting global metal demand and advancing the circular economy [1].

This study explores an environmentally sustainable strategy for the recovery of precious metals from WEEE, focusing on the valorisation of biowaste using biomolecules such as humic acids (HA) and lignin (L) as functional components of biocompatible polymeric matrices (e.g. polyvinylpyrrolidone, PVP). These biomolecules were incorporated into electrospun fibers. The resulting materials were subjected to an extensive physicochemical characterization and tested as biosorbents for the selective extraction of precious metals (e.g. Au, Pd) under optimal pH conditions with varying concentrations of metal ions in solutions mimicking real leachates. SEM microscopy confirmed the formation of uniform, defect-free fibers, while swelling tests demonstrated the exceptional water absorption capacity of the mats without structural degradation.

Preliminary adsorption experiments showed very good adsorption performance for Au³⁺ ions at pH 3, with negligible interaction with Cu²⁺ ions. The selectivity of the sorbents was evaluated in multi-metal solutions, confirming that effective adsorption requires simultaneous adsorption and reduction processes, which can be due to the high concentration of carboxylic and phenolic groups in the chemical structure of biowaste [2].

Biowaste-based sorbents represent a promising, environmentally friendly solution for the recovery of metals from WEEE, in line with the principles of the circular economy. It also offers an environmentally sustainable and cost-effective alternative to conventional electrochemical reduction techniques.

This work was supported by MITE (ora MASE - Ministero dell'Ambiente e della Sicurezza Energetica) Progetto di ricerca PESoMeNo – "Processi rigenerativi ecoSostenibili per il recupero e la valorizzazione di Metalli Nobili da RAEE".

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Enhanced Metal Recovery from spent Lithium-Ion Batteries Using ChCl:PTSA Deep Eutectic Solvents: A Study on Conventional and Microwave-Assisted Leaching Process

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H1_2, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

With the increasing demand for lithium-ion batteries, the quantity of end-of-life batteries is also rising. Due to the valuable metals they contain and the environmental hazards they pose, the recovery of lithium-ion batteries at the end of their lifespan has become essential. Moreover, maintaining high metal extraction efficiency while minimizing environmental impact is critically important in recovery processes. At this point, deep eutectic solvents (DES) emerge as a promising alternative due to their several advantages, including their organic composition, reusability, biodegradability, the ability to achieve high metal extraction efficiency through synergistic effects, and minimal water consumption.

In this study, the recovery of metals contained in the cathode active powder of end-of-life NMC type batteries was investigated using solvometallurgical method. Choline chloride (ChCl) and p-toluenesulfonic acid (PTSA) were synthesised in 1:1 molar ratio and used as DES. In conventional leaching experiments, temperature, time, reductant addition, solid/liquid ratio were optimised for maximum metal recovery. Similarly, the effect of operating conditions on leaching efficiency was investigated for microwave assisted leaching process. As a result of conventional leaching experiments, Li, Mn, Co and Ni metals were completely leached into ChCl:PTSA solution at 100°C, 2 hours and 1/50 solid/liquid ratio conditions. When 5 wt% fructose was added to DES, approximately 100% yield was obtained under the same conditions at 60°C. Additionally, a series of experiments were conducted to determine the effect of microwave assistance on the leaching efficiency, and the results were compared with those obtained using the conventional leaching method. According to the results, at a solid/liquid ratio of 1/20 and 100°C for just 10 minutes, all metals were dissolved nearly 100% efficiency.

Sustainable Recovery of Rare Earth Elements from Nd-Fe-B Swarf via Hydrogen Plasma Reduction

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H1_2, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Rare earth permanent magnets (REPMs) are critical components in electric vehicles, wind turbines, and consumer electronics due to their excellent magnetic properties. REPMs on the basis of Nd-Fe-B typically contain 29–31 wt.% rare earth elements (REEs), primarily neodymium (Nd), praseodymium (Pr), dysprosium (Dy), and terbium (Tb). Approximately 80% of global Nd consumption is dedicated to REPM production, and Nd-Fe-B demand is expected to exceed 260,000 tons per year by 2035, driven largely by electrification and the transition to renewable energy sources.

However, REE mining and refining present serious environmental and geopolitical challenges. Extraction generates toxic waste, including acid-leaching agents, heavy metals, and radioactive byproducts like thorium and uranium, which contaminate the environment and pose health risks to urban areas. Geopolitically, supply chains are vulnerable to disruptions and import dependency due to the concentrated production and processing in specific regions. As a result, recycling of REPMs is becoming increasingly important as an economically and environmentally sustainable alternative to primary production.

This study focuses on the recovery of REEs from Nd-Fe-B grinding swarf, a significant yet underutilized waste generated during REPM production. It is estimated that 6–73 wt.% of the REPM material is lost as swarf, making it a major untapped source for critical materials. Nd-Fe-B magnet swarf can contain up to 37 wt.% REEs, such as Nd and Dy. Current hydrometallurgical and pyrometallurgical methods for recycling swarf face substantial limitations. Hydrometallurgical processes, although effective in extracting REEs, require large volumes of leaching media and can produce hazardous waste, making their sustainability questionable. In contrast, pyrometallurgical approaches demand high energy input, precise temperature control, and often result in slag formation, which limits the overall efficiency. These limitations underscore the necessity for a more effective and sustainable recycling strategy.

In this study we demonstrate a novel approach using hydrogen plasma reduction (HPR) as an energy-efficient and environmentally sustainable method to recover and separate the various REEs from the swarf without generating hazardous by-products with high recovery rates. We investigate key process parameters of the HPR method to evaluate its feasibility for REE recovery. Advanced characterization techniques are employed to provide insight into phase transformations, reduction kinetics, microstructure and the purity of the recovered phases. We will discuss whether HPR can serve as a viable recycling and extraction pathway for REPM swarf, offering a sustainable and environmentally responsible solution to reduce reliance on primary REE production in the future.

Electrochemical leaching of CIGS PV panels for recovery of CRMs

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H1_2, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Copper-Indium-Gallium-di-Selenide or CIGS panels are one of the promising alternatives in the market for thin-film solar technologies. CIGS panels are lightweight, durable and use less semiconductor materials as compared to Si-based PV modules [1, 2]. According to EU CRM materials report 2023, indium gallium and copper which are raw materials for CIGS panels are rated as critical materials subject

to their high supply risk and moderate economic importance [3]. The development of robust recycling methodologies for copper indium gallium selenide (CIGS) photovoltaic panels and associated production

waste presents a viable pathway towards securing the supply of critical raw materials (CRMs). While a range of recycling processes have been explored, many current approaches demonstrate limitations. Specifically, challenges remain in achieving both efficient material separation and high material purity within a single process. Furthermore, certain methodologies necessitate operation under highly toxic conditions, resulting in the generation of secondary waste streams which require further management. Within this research electrochemical leaching for separation and recovery of materials from CIGS solar panels is studied. The scope of study is to determine efficiency of semiconductor coating separation from glass in H₃C-SO₂-OH (Methanesulphonic Acid). Using ICP-OES/MS and XPS techniques the dissolution and de-coating efficiencies are calculated. The investigation includes the observing effective

separation of the glass and coating material at different acid concentrations in novel drum electrode[4].

Within the study, sustainability analysis of the processes from ecological, safety and social aspects are briefly discussed.

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Hydrogen Processing of Recycled NdFeB Powders via HPMS and Production of New Magnets

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H1_2, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Neodymium Iron Boron ($\text{Nd}_2\text{Fe}_{14}\text{B}$) magnets are essential components in modern technology, including electronics, renewable energy systems, electric vehicles, and household appliances. The increasing demand for rare earths, coupled with supply chain vulnerabilities and environmental concerns, underlines the urgency of developing efficient and sustainable recycling strategies to reduce dependence on primary raw materials and support a circular economy. This recycling approach supports the objectives of the Critical Raw Materials (CRM) Act, aiming to recycle at least 25% of the EU's annual raw material consumption by 2030 while promoting circular economy practices and strengthening supply chain sustainability. This approach utilizes a closed-loop recycling process for NdFeB magnets, employing Hydrogen-Processing of Magnet Scrap (HPMS), a technique patented by researchers at the University of Birmingham. Through this method, dense NdFeB magnets from end-of-life devices are efficiently converted into hydrogenated powder, which is then refined via jet-milling to reduce particle size. Subsequently, the recycled powder is degassed to eliminate hydrogen, restoring its original composition, microstructure, and magnetic properties, ultimately enabling the production of new magnets. This work explores optimal annealing conditions for dehydrogenation in vacuum varying temperatures up to 900°C, heating rates and dwell times for the final production of bonded magnets by injection moulding and also optimal parameters for the fabrication of sintered magnets by spark plasma sintering. The degassed final powder suitable for bonded magnet production exhibits competitive properties compared to virgin material, achieving a coercive field of 434 kA/m. SPS sintered magnets present a remanence magnetization of 1.26 T and a coercive field of approximately 1200 kA/m, comparable to magnets found in the market (N40).

Thermodynamic Approach for Metal Recovery from Black Powder of Used Secondary Batteries through Pyrometallurgical Process

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The increasing use of secondary batteries has resulted in a significant accumulation of waste batteries, raising environmental concerns and the need for efficient recycling methods. Black powder, a by-product of waste battery recycling, contains valuable metals such as cobalt, nickel, and lithium. Recovering these metals through a pyrometallurgical process offers a promising solution for sustainable resource management.

In this study, a thermodynamic approach was applied to optimize metal recovery from black powder using a pyrometallurgical process. To enhance the phase separation between reduced metals and slag, the viscosity variation of slag was analyzed by modifying its composition. Additionally, equilibrium phase changes at different temperatures were investigated to determine optimal operating conditions. These thermodynamic calculations were conducted using the FactSage software. The results provide insight into improving the efficiency of metal recovery by controlling slag properties and reaction conditions.

Electrochemical recovery of metals and silicon from c-Si photovoltaic module

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H1_2, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The popularity of photovoltaic energy has soared in recent decades due to its affordability, ease of installation, and minimal environmental footprint [1]. As the number of photovoltaic panels installed continues to rise, so will the amount of waste generated, considering that these panels have a lifespan of approximately 25 years [2]. c-Si PV panels contains glass (75 wt%), Al (10 wt%), polymers (8 wt%), Cu (0.8 wt%), and other metals (such as Pb, Sn, Zn and Ag) (>1 wt%), and also Si (5 wt%)[3], which is a critical material for the European union [4].

Si wafers were recovered from the end-of life Photovoltaic module by delamination of glass and back sheet in a solvent bath followed by the thermal decomposition of EVA by means of pyrolysis. Subsequently, it was treated electrochemically to separate metals such as Al, Cu, Sn, Pb and Ag in 1mol/L H₃C-SO₂-OH with 1mol/L HCl (1:1 v/v). The electrochemical treatment was conducted using an indigenously built drum electrode with platinised titanium inlet mesh. Si, Cu and Sn were recovered in 99%, 98% and 82% purity respectively. The three-step c-Si PV panel recycling process ensures recovery of the PV glass, the back sheet, Si, Cu, Sn and EVA as pyrolytic oil. According to a close-loop recycling approach, the recovered silicon and metals are used in an additive manufacturing process to prepare flexible PV-module.

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Optimization of thermal pretreatment parameters to enhance black mass recovery in lithium-ion battery recycling

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The progressive electrification of transportation is driving a significant increase in the production of lithium-ion batteries in recent years. These batteries contain elements classified as critical, such as lithium, cobalt, nickel, and graphite. Despite ongoing research to minimize their presence in new batteries, these elements remain essential in modern battery technology.

To mitigate the environmental impact of the extraction of these elements from minerals, it is crucial to increase the recycling rate of batteries that reach the end of their life cycle. To promote this recycling, the European Union has established a series of targets in the new Battery Regulation that came into force in 2023, setting recovery targets of 95% for cobalt and nickel by 2030.

Once the possibility of extending their life in stationary storage devices is discarded, post-consumer batteries can be subjected to a dismantling process followed by shredding and a series of separation processes that result in the production of a black mass. This black mass then undergoes a refining stage where the metals are recovered and can be used as precursors in the manufacture of electrodes for new battery cells.

Reducing impurities in the black mass is key to achieving better performance in the refining process, and the application of a thermal process to the shredded material has been shown to be effective on that purpose, thereby increasing the quality of the black mass. This work presents the results of a study conducted to investigate the influence of different parameters of this thermal process on both the recovery yield of the black mass and its quality.

Sustainable ceramics: Circular economy implementation and prospects

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H2_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The ceramics industry is at a turning point shifting from a traditional linear economic model towards a sustainable circular economic approach. The ceramics manufacturing process has been energy-intensive. Ceramics recycling is hindered due to technical, regulatory, and financial barriers. This practice has contributed to 19 million tons of carbon dioxide (CO₂) yearly emissions within the European Union with the ceramic brick industry contributing 2.7% of global CO₂ emissions. Though studies have investigated energy efficiency and emission reduction in the ceramics industry, there is little focus on integrating circular economy principles through its value chain. This work aims to identify prominent advancements in three major areas: raw material optimization, product durability and resource recovery. This work employs a qualitative approach by synthesizing insights from peer-reviewed studies and real-world examples from 2000 to 2025 to identify emerging trends, obstacles, and opportunities in implementing sustainable practices. It emphasizes novel materials, manufacturing processes, digital technology, and energy-efficient solutions regarding industry developments, opportunities, and challenges. A contribution of this paper lies in its relevance to Sustainable Development Goals 11 (Sustainable cities and communities), 12 (Responsible production and consumption), and 13 (Combat climate change and its impacts), specifically by reducing carbon emissions and conserving natural resources. Results show an increase in the diffusion of practices like material recovery and energy-efficient technologies; while factors like barriers to high implementation costs and complex regulatory systems are presented. A supportive policy framework should be emphasized to maintain technological innovation and cross-industry collaboration as a recommendation to overcome these barriers and drive a circular economy principle within the ceramics industry.

Rigid polyurethane foams with a reduced petrochemical content

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The prevailing emphasis on sustainability and the reuse of waste is precipitating a novel research direction. Rigid polyurethane foams (RPUFs) have recently seen a surge in utilization, primarily for the purpose of thermal insulation in buildings, but also in a variety of other applications. The popularity of PUR can be attributed primarily to its ability to adapt properties to meet specific application requirements [1, 2].

A potential opportunity to reduce the amount of petrochemicals in RPUF production is the use of bio-polyols derived from renewable feedstocks. The most commonly used feedstocks are natural oils and their derivatives (soybean oil, castor oil, palm oil, rapeseed oil and sunflower oil) [3, 4]. The issue with the raw materials cited is that they are food products. The utilization of these materials in the building industry has been demonstrated to engender an augmentation in demand, a phenomenon with the potential to culminate in elevated food prices or the exacerbation of the global hunger issue. Consequently, it is imperative to explore the potential of utilizing waste raw materials in the production of bio-polyols.

The research focuses on the characterization of fats recovered from municipal wastewater as a raw material for the production of bio-polyols. The subsequent phase involves the utilization of a ring-opening epoxidation process to synthesize bio-polyols from the fat fraction that has been recovered. The final stage of the research will entail the design of a rigid polyurethane foam system and the evaluation of the basic application properties. The RPUFs contain 5% and 10% bio-polyol from sewage sludge fats in exchange for polyol produced from petrochemicals. The effect of bio-polyol addition on foam morphology, apparent density, hardness and brittleness was characterized.

Acknowledgements

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Assessment of earthen soil binder for 3DP

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H2_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The use of earthen soil-based materials for 3D printing (3DP) has emerged as a promising avenue in the pursuit of sustainable construction practices. This study presents a comprehensive review of existing literature on the application of earthen soil in 3DP, focusing on its challenges, potential, and opportunities within the framework of a circular economy. Earthen soil, being abundant and locally available in most regions, offers immense potential as a low-cost, eco-friendly material for additive manufacturing in construction. The review examines different aspects of earthen soil for 3DP, including material formulation, rheological properties, structural performance, and the influence of natural additives such as fibers and nanoclay. Key challenges such as shrinkage, cracking, and limited strength are discussed, alongside innovations in material modification and process optimization to overcome these limitations. Additionally, the study highlights the potential for integrating earthen soil-based materials into sustainable construction practices, reducing resource extraction and minimizing waste generation. This work aims to provide insights into the opportunities for leveraging earthen soil in advancing 3D printing technologies for construction, emphasizing its role in creating low-carbon, resource-efficient, and locally adaptive solutions.

Investigation of the impact of reducing the albedo of the coloured wall tiles of an Italian building heritage of the Second Twentieth Century for sustainable restoration purposes

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Restoring Italy's mid-20th century architectural heritage involves addressing the increasing demand for summer cooling, which has outpaced winter heating needs since the early 2000s. A promising solution is the renovation with solar reflective (SR) materials that can lower air temperatures and reduce reliance on air conditioning. However, it is essential that the renovation process respects the architectural and stylistic characteristics that define these structures by preserving their appearance and chemical-physical properties.

Inkjet-printed colored ceramic wall tiles are excellent materials for this purpose, as they can achieve solar reflectance (SR) properties by using appropriate engobe formulations and special infrared (IR)-reflective inks, often referred to as cool materials. Furthermore, tile production allows for the incorporation of secondary raw materials (SRMs) thereby reducing the environmental impact of the tiles and contributing to sustainable urban regeneration.

This study aimed to develop cool colored wall tiles that could potentially be applied to renovate an Italian building representative of the mid-20th century, specifically Bologna's former Library Pelagalli. Particularly, we investigated several engobe formulations with the highest possible SR value while ensuring that it contains at least 30 wt. % of SRMs. A selected formulation was then used to prepare inkjet-colored cool wall tiles featuring industrial IR-reflective inks. The thermal, physical and optical properties of such tiles were then used to perform a microclimate and fluid dynamics analysis during a day characterized by a heat wave (hypothetical ex-post). The same analysis was also performed with the properties of the conventional tiles currently placed in the building (ex-ante).

The preparation of the SR engobe was studied by examining several SRMs. We investigated the thermal (emissivity, specific heat, thermal conductivity), aesthetic (colour, gloss), physical (density), and optical properties (absorption, solar reflectance) of the tiles after firing at 1205 °C in a 50-minute cold-to-cold industrial firing cycle. It was discovered that an engobe formulation containing 33 wt.% of SRM allows the production of coloured cool tiles, which have solar reflectance (SR) values that are 7% to 90% higher than those of the original coloured tiles currently from the Bologna's building.

The change in albedo can affect the thermal conditions of the representative building. To analyse this effect, the properties of the developed cool-coloured tiles were input into ENVI-met software for a microclimate and fluid dynamics analysis. The results indicate that using these tiles can contribute to the sustainable urban regeneration of buildings from the second half of the twentieth century.

Building with Rammed Earth: Characterization and Optimization of Earth Mixes from a Monticello d'Alba Case Study

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H2_1, Seminario 1 + 2 Room (Level +1), settembre 17, 2025, 17:00 - 19:00

This study explores the potential of rammed earth (RE) as a sustainable construction material by evaluating the mechanical and compositional properties of an earth-based mixture designed for structural applications.

The investigation focuses on "Casa del Thè," a pavilion built using a tailored RE mixture (Tmix), combining quarry waste-soil (Tb) and vineyard soil (Tv). Comprehensive geotechnical (Atterberg Limits, Specific Gravity, Granulometry) and chemical and materials characterizations (ATR-FTIR, TGA, XRD, XRF) characterized the constituents. Optimal water content for compaction was determined using Standard Proctor tests, for both Tb and Tmix, followed by UCS tests to compare their mechanical behaviors. To evaluate the compressive strength (UCS) of the mixture, cylindrical samples were made at the construction site. The mixture was then recreated in the laboratory using the same ratios to ensure better control over the preparation methodology.

A granulometric optimization was achieved computationally by blending Tb with other soils to approximate an ideal grain size distribution for RE, resulting in an optimized mixture with an average UCS of 0.99 MPa.

Results indicated that while the initial Tmix yielded a UCS of 1.67 MPa, the optimized mixture demonstrated a slight UCS reduction, highlighting a trade-off between granulometric refinement and compressive strength.

Comparative analysis of on-site and lab-prepared samples revealed that Tb and Tmix achieved UCS values of 1.44 MPa and 1.24 MPa, respectively, underscoring the influence of preparation methods on material performance. Overall, the findings suggest that with targeted adjustments in soil composition and compaction, rammed earth can be effectively adapted for broader, sustainable structural applications.

Development of Hemp insulation Biopanel with Tannin-Based Adhesives: A Sustainable Solution for Green Construction

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H2_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The European SNUG project has among its objectives developing innovative solutions for manufacturing sustainable materials, with a particular focus on the construction and habitat industries. A key breakthrough of the project is the creation of hemp-based biopanel with tannin-based adhesives, designed to replace traditional materials derived from non-renewable and highly polluting sources. The tannin-based adhesive is developed by CHIMAR, production protocols and material characterization are handled by AIDIMME and KEAS scale up to a industrial level the bio-panels.

Tannins, natural phenolic compounds found in various plant species, have been explored as a potential alternative to the ingredients of synthetic adhesive formulations, that are traditionally used in construction materials. The tannin-based resins developed by CHIMAR are formaldehyde-free and exhibit excellent bonding capabilities with various biomasses, including hemp, making them ideal for particleboard production. These resins provide a biodegradable, non-toxic solution that aligns with the principles of sustainability.

Hemp, a renewable natural resource with exceptional mechanical properties, serves as an ideal material for manufacturing insulating panels. The use of hemp shives as a substitute for wood in bio-panels enhances both the mechanical properties and sustainability of the resulting boards.

The bio-based tannin adhesives not only enhance the mechanical performance of hemp panels but also ensure a high level of sustainability, offering a greener adhesive solution for a wide range of industrial applications.

AIDIMME has researched tannin-based adhesives and hemp shives formulations, determining the best resin-to-fiber ratios for panel production. Their findings suggest 10–12% resin concentration for optimal performance.

AIDIMME have also assessed fire reaction, mechanical, durability and sustainability properties. Additionally, a Life Cycle Analysis is underway to compare the environmental impact of these bio-panels to conventional synthetic materials.

KEAS leverages the lower bulk density of hemp shives, a byproduct of the textile industry, to create boards with better insulation. This approach supports industrial symbiosis and involves KEAS adjusting the industrial production lines to incorporate hemp as a wood substitute.

Preliminary findings show that hemp bio-panels with tannin-based adhesives not only provide a sustainable alternative but also match or surpass conventional materials like wood panels and petrochemical composites. These advantages make hemp bio-panels a viable choice for eco-friendly buildings, supporting circular economy principles. This research highlights the potential of hemp and tannins in creating innovative, sustainable construction materials, advancing Europe's push for greener building practices.

Keywords: Biopanel, Hemp, Tannins, Natural adhesives, Sustainability, SNUG Project, Green construction.

Recent advances in microencapsulated phase change materials for energy-efficient buildings

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H2_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

Phase Change Materials (PCMs) has been recognized for their ability to release as well as store the substantial heat in response to variation in ambient temperature which provides an innovative solution for enhancing thermal regulation in building design. Although the recent literature is more focused on the incorporation of the microencapsulated phase change materials (MPCMs) into various building materials. This review will thoroughly categorize the recent advances in the MPCMs based on their material composition and phase change characteristics, offering a brief overview of their diverse applications in building thermal regulation. Initially, different types of MPCMs will be discussed which is followed by synthesis techniques and their simulation using multiple softwares like EnergyPlus, TRNSYS, and ANSYS Fluent etc. The pros and cons of different PCMs will also be overviewed and compared to each other. Moreover, it compiles the study on the MPCMs into building materials like roofs, walls, paints, floors, cement, bricks, and windows. This review will also address the gaps in between the existing research work. In summary, this work highlights the recent advancements and offers valuable insights into MPCM applications across various building components, providing as a key resource for scientists, engineers, and professionals in academia and industries.

Use of cement paste containing foundry wastes as anodes for electrochemical chloride extraction in concrete

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

One of the difficulties involved in the use of reinforced concrete is the corrosion of the embedded bars. The low density of iron oxides compared to the metal state causes internal stresses to be generated in the concrete structure, leading to cracks and potentially causing structural failures, of which many cases have been documented. Ideally, the strong alkalinity of the cement would allow the formation of a passive layer in the rebars, which could avoid the corrosion problem; however, the fact is that this situation is unlikely due to the presence, for example, of chlorides (very common in marine environments). This acidifies the conditions in which the reinforcement is found, accelerating the process of localized corrosion. In order to avoid the degradation of the metal reinforcements, there are two strategies: hindering the advance of chlorides or removing them from the concrete element. This study focuses on the second point, using electrochemistry to extract chlorides from reinforced concrete elements that have been manufactured with added NaCl. To reduce the concentration of the aggressive ions, a conductive element, an anode, is placed on the surface of the structure to be treated and an electrical potential is subsequently applied. In this way, the chloride ions are forced towards the surface, away from the metal reinforcement, thus reducing the risk of localized corrosion. In this study, the anodes were made from cement paste to which 6 mm long carbon fibres are added. The anodes also contain between 15-30% of the cement mass of residues obtained from the cast iron foundry industry.

Overview of agricultural waste-based SCMs from Kenya for climate care and a circular economy

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

More climate sparing cement production has been target of industry and researchers since the building industry is coping with a growing demand (1) (2) (3). This is produced by the climate- and energy-intensive burning of clinker at roughly 1450 °C, whereas the majority of emissions are released due to the decomposition of limestone (CaCO_3) to reactive CaO (4) (5) (6). In order to abate this, furnaces' bottom ash is utilized as supplementary cementitious materials (SCM) if the composition is adapted as the UGR showed in Granada (7). However, the reaction of which depend on the right mineral oxide content (CaO , SiO_2 , Al_2O_3) and proportioning.

Any such ash producing process has a positive carbon footprint, meaning that significant CO_2 equivalents are emitted into the atmosphere. This general research question aims at finding suitable ash from biomass waste, which could theoretically generate the necessity of testing hundreds of biomasses. In a later step, however, operating an artificial intelligence system will sort the data and prioritize those that are worth deepening.

Kenya has significant amounts of biomass waste, whereby healthy growing biomass will be excluded from ash production. The Bundesanstalt für Materialforschung und -prüfung (BAM), the Meru University of Science and Technology (MUST) and SRH Universities are researching the potential for climate relief through circularity and provide the data relevant for this publication. Funded by the Volkswagen foundation that consortium is studying the Kenyan case as a pilot relevant for many parts of the African continent. About forty percent of that East African country's population elaborates 21% of the national economy (11) and hereby deals with significant waste materials from biomass such as shells, peels and pruning. Not only Biomass waste like maize, cassava, bamboo or sugarcane bagasse is interesting, but also invasive plants such as mesquite.

As a first step, this research will set up a model, a database to record which biomass waste is produced where and what the water content amounts to. In the 2nd step samples are taken systematically and ashed above 650 °C for varied times, so determining the ash content from the biomass waste. The 3rd step is measuring mineral content with a focus on CaO , SiO_2 , Al_2O_3 through X-ray fluorescence (XRF) analysis. These three steps presented here will be followed by determining the pozzolanic properties along with compressive strength, spread flow and other relevant indicators.

Recycling of Rigid Polyurethane Foam with Solid Filler: Flammability and Thermal Conductivity Analysis of Newly Synthesized Materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

Rigid polyurethane foam (RPUF) is a widely used thermal insulation material, but its production depends on fossil raw materials, which is not sustainable. The transition to a circular economy is a growing trend in materials science. Studies in the literature consider the use of waste materials as fillers to reduce dependence on fossil resources in insulation products [1, 2]. The recycling of modified polyurethane materials with additives remains incompletely investigated.

The complex problem of the availability of raw materials for RPUF synthesis and their recycling is the subject of this study. Composites made with recycled raw materials obtained from waste polyurethane foam modified with fly ash (FA) are presented. Although numerous studies have examined the properties of FA-modified RPUF, its recycling remains unexplored [3, 4]. Ground foam was used as a filler to produce a new composite, and recovered polyol served as a base component.

To evaluate the effect of recycled raw materials on the properties of RPUF, samples with 10–30% recycled polyol and 5–10 wt.% granulate were produced. The microstructure was analyzed using a scanning electron microscope (SEM), thermal conductivity was measured by the hot disk method, and flammability was tested using a cone calorimeter.

Microstructural analysis showed that increasing the recycled polyol content resulted in a slight increase in cell diameter and changes in cell wall thickness. The addition of granules reduces cell diameter by increasing the reaction mixture's viscosity, which hinders the nucleation process. Thermal conductivity measurements showed a slight increase with the addition of recycled material, confirming that insulating properties were maintained. In conclusion, incorporating recycled raw materials into RPUF reduces landfill waste and fossil raw material use, without significantly compromising material properties.

Acknowledgments

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Utilization of Wind Turbine Waste in Cementitious Materials: Circularity and Sustainability

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The increasing decommissioning of wind turbines has created a challenge in waste management. This study proposes an innovative cementitious composition that partially replaces Portland cement with wind turbine waste (RAG), oxy-combustion ashes (OXI), and polymeric waste (PS), contributing to the circular economy in construction. The mechanical properties and feasibility of these materials for structural and non-structural applications were evaluated.

The waste materials were characterized using XRD. Mixes were prepared with 10% and 20% cement weight replacement using RAG, OXI, and PS. Compression and flexural strength tests were conducted at 7 and 28 days according to UNE-EN 196-1. Additionally, carbon footprint and water consumption were analyzed.

The results indicate that mixes with up to 15% OXI and RAG substitution exhibit mechanical strengths equivalent to or superior to conventional cement. Water absorption was reduced by up to 36% in mixes with porcelain adhesive cement. The "MIX" composition (6.67% OXI + 6.67% RAG + 6.67% PS) provides an optimal balance between strength and circularity, significantly reducing the carbon footprint.

It is concluded that incorporating these waste materials into cementitious compositions is both technically and environmentally viable, effectively reducing industrial waste and aligning with the principles of the circular economy.

Sustainable Geopolymer Catalytic Supports from Construction and Demolition Waste and Metakaolin Activated with Alternative Siliceous Waste-Derived Activators

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H2_1, Seminario 1 + 2 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

This research proposes the synthesis of innovative geopolymer-based catalytic supports derived from a precursor blend of construction and demolition waste (CDW) and metakaolin (MK) activated with alternative solid activators synthesized from siliceous waste. The objective of this research is to obtain advanced catalytic supports for environmental remediation application, such as CO₂ capture and pollutant degradation, which also contribute to the circular economy by reusing waste materials.

In this study the precursor consists of a mix of CDW and MK in equal proportions, combining the abundant availability of CDW with the high reactivity of MK. The activation process employs a novel solid activator produced by mixing a silica-rich waste, such as waste glass or spent diatomaceous earth, with sodium hydroxide in a defined proportion. This mixture is subjected to thermal treatment at 300 °C to synthesize sodium silicate, which functions as the activator in the geopolymerization process. Following activation, the resulting alkali-activated materials are dried, ground, and subsequently treated with a slightly acid solution of ammonium chloride. A final calcination step at 550 °C is performed to develop the microstructure necessary for catalytic functionality, with an emphasis on creating a high BET surface area and a pore size distribution predominantly within the 2–50 nm range. Preliminary assessments show that the alternative activator and an optimal liquid to solid ratio promote the formation of a geopolymer matrix with a tailored porous architecture, essential for catalytic efficiency. The materials synthesized using this method exhibit a good catalytic performance. Furthermore, the low-temperature processing route for the alternative activator results in potential energy savings and a reduced environmental impact, aligning with sustainable production and circular economy principles.

The results of this research pose CDW and MK as valid precursors in the manufacture of geopolymer-based catalytic supports and contribute to the development of sustainable construction materials and innovative remediation technologies, offering a practical route for mitigating environmental pollution.

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Thermochemical Synthesis of a Sodium Silicate Activator from Refractory Casting Bag Residues for Sustainable Geopolymer Production

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

The development of sustainable alternatives to conventional alkali activators in geopolymer production is strategic given that their use represents the main environmental impact associated with geopolymer manufacture. This study presents a novel approach for synthesizing a sodium silicate activator from a scarcely utilized residue derived from the degradation of refractory casting bags employed in the ferroalloy industry. It is generated as a by-product in electric arc furnace operations during the production of ferroalloys such as silicomanganese, and remains largely unexploited, thus representing both an environmental challenge and an opportunity for valorization within a circular economy framework.

The primary objective of this research is to utilize this refractory casting bag residue (RCBR) in the thermochemical synthesis of sodium silicate by mixing it with sodium hydroxide (NaOH) and subjecting the mixture to a thermal treatment at 300 °C. The activator is designed to achieve a molar ratio of 1:1 (SiO₂:Na₂O), and subsequent processing via planetary mill, obtaining a fine, homogeneous powder. This solid activator is then employed in the production of one-part geopolymers, aiming to replace commercial activators. Comprehensive characterization of the synthesized activator was conducted using Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD). The technological properties of the resulting geopolymers were also evaluated through common standardized tests.

Preliminary findings indicate that the sodium silicate activator produced from RCBR exhibits a reduced content of inert phases (in comparison with alternative activators from other residual sources) and facilitates the manufacture of geopolymers with mechanical strengths comparable to those achieved using commercial activators. These results suggest that RCBR can serve as a viable raw material for the production of sustainable activators, thereby reducing environmental impacts and promoting waste valorization. This study not only offers a promising alternative to commercial activators but also contributes to sustainable waste management practices in high-temperature industrial processes aligning with current policies in circular economy.

Acknowledgements: This work has been funded by the project Catalytic supports obtained by the geopolymerisation of CDW for the transformation of CO₂ into products with energy applications (CATGEOCO₂), (M.1.B.B TA_000602) of the Operational Plan for Research and Knowledge Transfer of the University of Jaen 2023 financed by the Operational Programme Feder Andalucía 2021-2027.

Chemical and Thermal Analysis of PLA Degradation and Stability Across Recycling Cycles for 3D Printing

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),

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PLA (polylactic acid) is a biodegradable and compostable polymer derived from renewable resources such as corn starch or sugarcane. Its use is particularly relevant in 3D printing due to its versatility and biocompatibility. Currently, pressure on its production is increasing due to the implementation of regulations and restrictions on single-use fossil-based plastics in various countries. However, our project advocates for promoting the reuse of PLA, given its wide potential, in order to avoid the mistakes made with single-use plastics, such as the "use and dispose" mentality. At present, extrusion is the main method employed for its recovery, though the number of reuse cycles remains highly limited.

This study evaluated the chemical changes in recycled PLA products using ATR-IR spectroscopy, as well as the thermal changes through thermogravimetric analysis. Our findings suggest that, beyond structural modifications of the polymer, controlling the loss, stability, and recovery of additives in the recycled material is crucial for improving product quality and optimizing its performance in future applications. Adequate management of these additives will significantly extend the reuse cycles of the material.

Advancing the Future of High-Performance Materials: Bio-Based Epoxy Resins for Sustainable Innovations

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H3_2, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Extensively employed in aerospace, automotive, construction, and renewable energy, traditional epoxy resins are burdened by a reliance on bisphenol A (BPA)—a hazardous petrochemical—along with non-recyclability and minimal bio-based content. Recent innovations have sought to resolve these issues by developing cutting-edge materials combining environmental sustainability with exceptional thermomechanical properties.

Our recent work focused on the development of >140 formulations of bio-based epoxy resins (1–4) with a bio-renewable content from 86% to 99% while exceeding the performance benchmarks of conventional materials. The resins boast impressive thermomechanical characteristics: storage moduli ~2.1 and 3.7 GPa, Young's moduli from 0.6 to 1.5 GPa, and glass transition ranging from 110 to 220 °C. Additionally, they exhibit thermal stability > 300 °C and minimal water absorption (0–0.5%). Free from BPA, compliant with green chemistry principles and REACH regulations, these resins align with stringent safety and sustainability standards. When reinforced with carbon or vegetable fibers, these bio-based resins enable the creation of composite materials with remarkable properties (5,6). The composites show storage moduli ~ 43 GPa and compressive strengths ~ 400 MPa. Their interlaminar shear strength, ~ 63 MPa, shows strong fiber-matrix adhesion, confirmed by SEM. These materials support the principles of circular economy through their Recyclable, Repairable, and Reshapable properties. Sectors as aerospace, renewable energy, and automotive manufacturing stand to benefit from these innovations, which reduce reliance on fossil fuels, cut greenhouse gas emissions, and offer sustainable end-of-life solutions.

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Ionic liquids for biopolymer dissolution and regenerated fiber spinning

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H3_2, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Biopolymers derived from renewable resources are gaining attention for their sustainability and potential to replace synthetic materials in various applications. However, the natural forms in which these biopolymers exist—often in highly organized, crystalline, or fibrous structures—present significant challenges in processing. For example, cellulose in plant cell wall forms a highly packed, crystalline structure, making it challenging to be dissolved or extracted using conventional solvents.

In recent years, ionic liquids (ILs), particularly super base-based ILs, have emerged as promising solvents for the dissolution and processing of biopolymers. The ILs can disrupt the hydrogen bonding in biopolymers and facilitate the dissolution. In this work, we present our recent developments in using super base-based ionic liquids for the dissolution of cellulose and proteins extracted from biomass and waste streams, with a particular focus on fiber spinning and the production of sustainable textiles.

The biopolymer dopes, prepared by dissolving cellulose and proteins in these ionic liquids, provide a pathway for high-performance fiber production with customizable properties. One application is the incorporation of functional particles during the dope preparation step to produce fibers with tailored functionalities, such as UV sensing, which can be integrated into smart textiles.

Additionally, we explore the production of hybrid fibers by blending cellulose with keratin, extracted from waste wool textiles. Keratin, by itself, lacks sufficient mechanical strength to form fibers. However, by dissolving keratin alongside cellulose, we achieve a spinnable hybrid dope. The resulting hybrid fibers exhibit high mechanical strength derived from cellulose and improved hydrophobicity from the keratin, highlighting the potential of biopolymer-based textiles in high-performance applications. This approach also contributes to reducing the reliance on synthetic polymers and promoting a circular economy by utilizing waste-derived resources.

Despite the advantages of super base-based ionic liquids, challenges remain in their application, including their susceptibility to hydrothermal hydrolysis during recycling and sensitivity to moisture during dissolution process. To address these issues, we have explored various cations and anions to improve the stability and recyclability of the ionic liquids.

This work presents a promising approach to overcoming the challenges in biopolymer processing and highlights the potential of ionic liquids in the development of sustainable, functional textile fibers, contributing to a circular economy.

Positron Annihilation Spectroscopy: Unlocking Atomic Insights for Next-Gen Energy Materials

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
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We introduce the Positron Research Infrastructure (pELBE) at the ELBE linear accelerator, hosted at HZDR, as part of the ReMade@ARI (REcyclable MAterials DEvelopment at Analytical Research Infrastructures) project under the Horizon Europe program. [1]

Positrons, as the anti-particles of electrons, provide a highly sensitive, non-destructive probe for detecting defects at low concentrations in a wide range of materials, including metals, semiconductors, polymers, and porous materials.

pELBE offers a wide range of advanced positron annihilation spectroscopy techniques for the precise characterization of point and extended defects, their agglomerations, and nano-, micro- and mesoporous systems, both with interconnected and isolated pore structures.

This method is used to understand key properties of advanced materials at the atomic level, such as: identifying defect structures in carbon-capture materials like MOFs to enhance their efficiency, optimizing free volume in bio-based polymer membranes, investigation of fatigue in polymeric materials, or determining pore size distribution in nanofiltration membranes designed for sustainable resource recovery and circular economy applications.

The established role of positron annihilation spectroscopy in materials research makes it a powerful tool for material innovation.

[1] - <https://remade-project.eu/>

High-cell-density strategies to maximise bacterial production of biopolymers from real by-products

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H3_1, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Polyhydroxyalkanoates (PHAs) are biological polyesters synthesised by bacteria and viewed as a replacement for petrochemical plastic in many different applications. However, they suffer from suboptimal thermal and mechanical properties. An improvement in their material properties (for example: flexibility, crystallinity and toughness) is obtained when the microbial biosynthesis of PHA can produce a variety of carbon lengths in the PHA sidechains. This can be tailored depending on both the fed carbon source and the choice of microorganism. An economically viable and circular approach where the chemical structure of these biopolymers is tailored by using a variety of chemically related precursors to PHA and where these precursors are coming from real world by-products can expand the potential applications of these polymers and improve their material properties. A mathematical modelling approach targeting high-cell density (HCD) cultivation is paramount if one wants to increase yields and volumetric productivities of the bioprocess. Using real world by-products (dairy side-stream feedstocks, grass treatment by-products and waste-originated fatty acids) we cultivated a range of bacterial PHA producers using a bioreactor-based approach aiming at a HCD cultivation. Pulse-feed cultivations of *Burkholderia sacchari* IPT101 using a dairy-side stream as the sole carbon source produced a bacterial biomass of 120 g/L (as cell dry weight, CDW) with 25% of polyhydroxybutyrate (PHB). Individual fed-batch cultivations of *Pseudomonas putida* CA3, *Pseudomonas chlororaphis* IMD555 and *Burkholderia sacchari* IPT101 using a by-product of grass treatment as the main carbon source and fatty acids by-products as PHA inducers produced microbial biomass up to 90, 37 and 44.5 g/L of CDW, respectively containing 33%, 65% and 10% of PHA, respectively (Cerrone et al. 2014, Cerrone et al 2015). Fed-batch cultivation of *Pseudomonas umsongensis* GO16 using a mixture of fatty acids (by-products from a specialty chemical-producing company) as a unique carbon source produced a blend of short chain length (scl) and medium chain length (mcl)-PHA up to 25 g/L of CDW with 55% of PHA (Cerrone et al. 2023). This last bacterial strain is the only known strain capable of producing blends of scl-PHA and mcl-PHA, manufacturing therefore natural biocomposites.

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Development of mycelium-based composite materials through valorization of agro-industrial wastes

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H3_1, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

Global environmental awareness and strict legislation are currently driving research towards the implementation of sustainable and environmentally friendly processes, aiming also to minimize dependence on non-renewable resources in line with the principles of the circular economy. Mycelium-based materials have emerged as natural and sustainable alternatives to conventional synthetic plastics. Valorization of agro-industrial residues as alternative nutrient sources for mycelia/fungi growth meets multiple sustainability objectives, minimizing both the environmental pollution from waste disposal and the final production cost of materials.

Walnut shells, a zero-value agro-industrial lignocellulosic by-product generated in thousands of tons from walnut processing industries worldwide, could be a sustainable feedstock to produce mycelium-based composites. The present study focuses on the valorization of walnut shells through the cultivation of different basidiomycete fungi (mushroom-producing fungi) for the development of 3D mycelium-based materials. Our results provide insights into the morphological, physicochemical and mechanical properties of 3D mycelium-based composite materials relevant to various engineering applications. These materials exhibit good mechanical strength, hydrophobic properties and thermal stability, offering a promising, sustainable light-weight alternative to conventional plastics, with low energy consumption. Additionally, the mycelium-based composites showed enhanced oil removal from different emulsions with a wide range of oil content. Our findings will help in the development of eco-friendly and durable mycelium-based composites alternatives to conventional synthetic plastics and composites that are non-biodegradable, high in emissions and costly.

Keywords: mycelium, lignocellulosic residues, biocomposites, green materials, mechanical properties

Vegetable oils as source of building blocks for high added value materials

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H3_1, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The valorization of biomass into high added value applications require the development of enabling technologies that can transform these biomass into materials with desirable performances. Here, I will show how byproducts of vegetable oil can be transformed into interesting building blocks for the synthesis of new materials. Coatings for sustainable leather, plasticizers for bioplastics and foams are only few examples of materials that can be made out of these building blocks.

The valorization method is based on trans esterification of the triglycerides and epoxidation of the insaturations in the fatty acid, to create a library of building blocks with different functionalities.

The applications that I will present, show how biobased materials, when engineered together, can be a credible alternative for high performance materials. Foams can be created using only oils and vegetable biomass. Oil-based coating can provide excellent water resistance to leather and cotton, without changing the breathability, flexibility and the microstructure of the substrate. Biobased plasticizers can facilitate the processing of bioplastics. These high performing materials synthesized from waste and byproducts are an example of circular economy in material enabled by green chemistry.

Biobased Antioxidants: A sustainable solution to thermomechanical degradation of recycled polypropylene

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H3_2, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

The increase in environmental concern and the regulatory restrictions on synthetic additives in plastics have steered the need for sustainable alternatives. Many conventional antioxidants effectively protect plastics from thermo-oxidative degradation but raise concerns due to their potential toxicity, migration into food contact materials, and poor biodegradability. To address these challenges, this study explores the possibility of using benign bio-based materials as antioxidants in recycled polypropylene. Natural compounds such as clove oil, quercetin, tocopherol, and their combination (quercetin and tocopherol) were evaluated to determine their potential ability to replace the synthetic antioxidants. Their interaction with secondary antioxidants is also studied. The objective is to assess their ability to enhance thermal stability, ultraviolet degradation, oxidative resistance, and mechanical properties of recycled PP under oxidative and weathering conditions.

The results demonstrate that all tested antioxidants improved the thermal and oxidative stability of recycled PP compared to the unstabilized recycled PP. Thermogravimetric analysis (TGA) revealed enhanced thermal resistance, with oxygen induction time (OIT) and oxidative onset temperature (OOT) data confirming significant antioxidant activity, particularly for the quercetin and tocopherol combination, which exhibited a synergistic effect. The OIT values increased to 80 minutes under an oxygen atmosphere at 200°C. OOT values for quercetin and quercetin-tocopherol combination showed higher values, 258°C and 268°C, respectively. UV aging tests highlighted the ability of the antioxidants to mitigate degradation induced by UV light and moisture, with quercetin and its combination with tocopherol providing the most pronounced long-term stabilization. Mechanical testing of aged and unaged samples indicated that biobased combinations effectively maintained tensile and impact properties. Clove oil, although showing moderate stabilization effects, presents a promising bio-based option due to its ease of incorporation into the polymer matrix.

Among all formulations, the quercetin-tocopherol combination displayed superior overall performance, achieving an optimal balance between thermal stability, oxidative resistance, and retention of mechanical properties after aging. The findings contribute to advancing environmentally friendly solutions in polymer stabilization, reducing reliance on conventional synthetic additives.

A semi-industrial prototype bearing ceramic materials for Carbon Capture and Storage

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POSTER SESSION 2. September 17 (13:00-14:30 & 16:30-17:00) and 18 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 17, 2025, 13:10 - 14:30

In order to meet the European Union's CO₂ targets, CO₂ capture and storage (CCS) as well as CO₂ capture and utilization (CCU) techniques are being implemented for the industry. Moreover, to overcome the new challenges in the industry decarbonization, the study of mineralization and thermal catalytic hydrogenation processes are required unless these technologies are mature today. These mature technologies need the development of pilot plants for the specific industrial processes.

Herein, we will describe the results obtained within the construction of a prototype for CO₂ capture from industrial streams. This prototype is based on different sorbent materials including a modified ceramic material revalorized from industrial wastes. These novel materials are characterized, formulated and tested in the semi-industrial pilot plant, to study their capacity of carbon capture and storage. Moreover, the reactivation or regeneration of the spent materials are studied and evaluated.

COPPER AND ZINC REMOVAL BY BIOCHAR-BASED MATERIALS

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H3_1, Seminario 4 + 5 Room (Level +1), settembre 17, 2025, 10:30 - 13:10

The use of zinc oxide (ZnO) and copper (Cu) salts in livestock farming, particularly in monogastric animals, has contributed over the past thirty years to environmental issues such as eutrophication. Despite zinc and copper are essential elements in the animal's diet, these feed additives are mainly excreted in the animal's feces, resulting in their accumulation in the ecosystem. Various approaches can be employed to prevent high accumulation levels of Zn and Cu, among which adsorption is one of the simplest and most environment-friendly methods for pollutant capture. In this scenario, biochar is the residual carbonaceous by-product generated by the thermochemical conversion - gasification and pyrolysis processes - that is emerging as a circular and sustainable sorbent material, due to its physico-chemical properties. Biochar is known to contribute to the mitigation of climate change, specifically in the CO₂ capture as recalcitrant carbon stable for hundreds of years.

In this study, biochar obtained by chestnut waste has been studied as potential sorbent for copper and zinc in simulated conditions. Six different biochars, generated by both pyrolysis and gasification at BEElab (Università di Modena e Reggio Emilia, Italy), were tested for metals capture at different initial metals concentrations (3.3 mM – 100 mM). A maximum metal's capture of 99% and 53% was found for copper and zinc, respectively.

The biochar obtained by gasification process emerged as the most effective sorbent for the metals' removal, probably due to its textural, morphological and physico-chemical characteristics; namely, in terms of surface area and porosity.

Moreover, biochar was immobilized in 3-D structured materials in cooperation with Opigeo S.r.l (Grisignano di Zocco, Vicenza) to move towards industrial application, and to overcome the limits connected with the use of biochar in powder form. Preliminary batch tests with simulated copper solution showed a metal capture efficiency in the range of 14-44% when an initial copper solution 100 mM was applied.

Synthesis of lignin-based resin using epoxidized cross-linkers from bio-sources.

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H3_2, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

Epoxy resins are an important class of thermosetting polymers, representing 70% of the total polymeric resin market. One of the main fossil-based aromatic monomers used for their synthesis is bis(4-hydroxyphenylene)-2, 2-propane, also known as bisphenol A (BPA). Still, this compound is toxic to human health and the environment.

For replacing BPA, a promising natural solution is lignin due to its aromatic structure, making it an attractive natural replacement for aromatic monomers. Lignin is the most abundant aromatic biopolymer present in nature and is a highly available byproduct from pulp and paper industries.

Extracted lignin has a variety of chemical structures that depend on the extraction method and the plant source, strongly impacting the mechanical properties, solubility, thermal stability, and reactivity. There are some methods, such as lignin fractionation or chemical modifications (i.e., epoxidation), which help to increase lignin reactivity and obtain a less dispersed structure with more homogeneous and reproducible properties but reduce the potential of lignin in sustainable bio-based materials because of the use organic solvents and the increase of the processing steps. Furthermore, fractionated lignin is not commercially available on an industrial scale. More sustainable approaches are based on reactive melt processing of technical lignin without any purification steps before or after the chemical modification. Moreover, most lignin-based resins use non-renewable cross-linkers, increasing the negative impacts on the environment.

In the literature, some studies used bio-based cross-linkers in lignin-based resins, but the lignin must be modified to increase the epoxy content.

This work proposes a new strategy to produce fully bio-based epoxy resins that improve the sustainability of the final product by valorizing unmodified technical lignin and exploiting its natural advantages in combination with non-toxic bio-based epoxidized cross-linkers.

Direct chemical conversion of *Pleurotus ostreatus* whole mycelium into biodegradable films

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H3_1, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The indiscriminate use of petroleum-based plastics for single-use food packaging has caused serious environmental issues due to their non-biodegradable nature. Consequently, there has been growing interest in developing new bio-based and biodegradable materials, especially for the specific application. Fungal biomass represents an abundant and inexpensive source of biopolymers with excellent potential for sustainable materials. However, tailoring fungal biomass into materials with specific properties requires precise control over the manufacturing process. This research project adopted a green chemistry approach to develop new sustainable biobased materials, adhering to the principles of zero waste and circular economy. Raw mycelium biomass (*Pleurotus ostreatus*) was directly converted into eco-friendly materials using low-energy, non-toxic, and cost-effective, water-based alkaline treatments. To adapt these materials for food packaging, processing conditions, such as solution incubation time, and glycerol plasticizer content were systematically varied. The morphological and physicochemical properties of the resulting materials were investigated, as well as their mechanical properties and water vapor permeability. Crucially, the research also assessed the migration of material components into food simulants and the biodegradability of the developed films, essential for safe and environmentally sustainable food packaging. This work provides a comprehensive analysis of the relationship between the alkaline treatment duration and plasticizer content on the mechanical performance of mycelium-derived films. The resulting films exhibited promising mechanical properties, surpassing those of previously developed mycelium-derived films, making them suitable for food packaging applications. These findings offer a valuable new approach to developing mycelium-based materials through green chemical methods and represent a significant step towards a sustainable future in food packaging.

Influence of processing methods on the crack resistance for a polypropylene/recyclate blend and the virgin material

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H3_2, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 14:30 - 16:30

In recent years, there has been a growing trend toward processing more recyclates and producing blends of virgin materials with recyclates for new products. Recyclates' properties depend on the feedstock, the treatment, and subsequent processing. Each additional processing step not only raises costs but also increases the thermal and/or mechanical stress on the materials. In industrial practices, pure materials are usually blended with recyclates in a single extrusion process to avoid the need for additional compounding. However, improving the mixing quality, which is particularly important when working with recycled materials, is usually achieved by pre-compounding the material before extrusion. As a result, understanding the effects of both processing methods is highly relevant.

This study investigates how different processing methods, such as direct extrusion and compounding, affect the short-term properties and crack resistance of virgin polypropylene (PP), recycled PP, and a blend consisting of 90% virgin PP and 10% recycled material. To assess the impact of various processing histories, all three materials were either extruded once, extruded twice, or compounded, resulting in nine different thermal and mechanical histories.

For the subsequent determination of the mechanical parameters (tensile test, Charpy impact test) and crack resistance using CRB tests, compression-molded sheets were produced. In addition, the MFR values were also measured to receive an overview of the rheological properties of the materials. This allows the influence of the higher thermal and shear stress caused by the twin screw and the second extrusion process to be measured. It was found that the manufacturing methods had no significant influence on Young's modulus, yield stress, or impact strength of the blends. In contrast, the notched impact strength and crack resistance were notably affected, which could have a significant impact on product performance.

Ecotechnology applied to the manufacturing of ecological material by biomineralization processes with the *Sporosarcina pasteurii* bacteria

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H3_3, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 17:00 - 19:00

The integration of microorganisms into the manufacturing of biomaterials represents an innovative advance in sustainable construction. This study explores the potential of regenerative biotechnology applied to architecture, with a particular focus on the use of the *Sporosarcina pasteurii* bacteria to solidify granulated materials and produce resistant structures through 3D printing. This technique not only reduces environmental impact by minimizing energy consumption, but also aligns with the principles of the circular economy by transforming organic waste into valuable resources.

The cement industry is responsible for approximately 8% of global carbon dioxide (CO₂) emissions, being one of the main sources of greenhouse gases. This problem has driven the development of innovative and sustainable solutions in the construction field. In this context, the use of the *Sporosarcina pasteurii* bacteria represents a promising alternative. This bacteria has the ability to induce biomineralization by precipitating calcium carbonate, a process that allows granular materials to be solidified in a sustainable way, without the need for traditional chemical binders and with a considerable decrease in energy use.

This project combines biotechnology and 3D printing to manufacture biocemented tiles. The methodology is structured in several phases: (1) cultivation and optimization of the growth of *Sporosarcina pasteurii* under controlled conditions; (2) design and manufacture of plastic matrices by 3D printing, using CAD software to obtain precise structures; (3) preparation and inoculation of the matrices with bacteria to promote the biomineralization process; and (4) characterization of the tiles obtained using physical-chemical analysis techniques and mechanical tests to evaluate resistance and durability.

From an economic perspective, the production of these biomaterials presents reduced costs compared to conventional materials, particularly on a large scale. Their application in extreme environments, such as the desert or even Mars, could facilitate autonomous construction through 3D printing with in situ materials.

From M.A.R.T.E. (Microbiology and Regenerative and Techno-Ecological Architecture) research group we lead this emerging field, exploring new possibilities for the integration of biotechnology and sustainable architecture. The implementation of these advances in the construction industry could mark the beginning of a new era in materials manufacturing, promoting innovative and environmentally responsible solutions.

Preliminary results show that this technology not only reduces the environmental impact of construction materials, but also allows the incorporation of pigmenting bacteria to provide aesthetic value. This innovation has the potential to transform the industry, reducing the use of non-renewable resources and promoting more sustainable construction practices.

The scaling and use of solid sorbents for decarbonisation of industrial CO₂ emitters

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H3_1, Seminario 4 + 5 Room (Level +1), septiembre 17, 2025, 10:30 - 13:10

The road to decarbonisation is perhaps facing a turbulent future, particularly in the short term. Despite the absence of a unified approach to reducing carbon, Europe continues to be a leader in this transition, and has moved from 80% reduction targets in greenhouse gas emissions by 2050 to a Net Zero target. Many other countries have similar targets.

Metal organic frameworks (MOFs) represent a next generation route to sequestering CO₂ from flue gas, with the greatest chance of reducing the energy penalty to the operator. Currently, amine-based technologies are being deployed, though the environmental concerns and high regeneration energy usage show the overall inefficiency of these materials.

There are many researchers around the world making MOFs in batch and flow. At present, scale of production tends to be quite low i.e. grams to 10's or 100's of grams, which has not helped in the 'take up' of the new and exciting material. Through the use of novel continuous mixing reactors, we have been able to take grams per hour to kg's per hour to tons per hour production rates. The paper will explain this road to scale up from our initial paper on continuous flow synthesis in 2012¹. Each MOF requires a different approach to synthesis, but many can be manufactured hydrothermally.

Promethean Particles has a 1000tn/year production plant in Nottingham and is planning significantly larger production in the next few years.

Beyond the manufacture of MOFs, there is still work to be done around MOF performance, particularly at higher TRL levels. Those seeking to use MOFs for CO₂ sequestering generally investigate selectivity, uptake kinetics and capacity i.e. the ability of the MOF in question to selectively remove CO₂, the rate of gas uptake into the MOF structure and the overall CO₂ wt% uptake, respectively. These are all important characteristics but the practical application of MOFs in industrial systems will require much more work. This paper will also detail some of these areas e.g. Life-Cycle Assessment (LCA) is a tool allowing for a complete cradle-to-cradle overview of a product's life-cycle, using real-world data to inform computer models of the processes involved in manufacturing, using, disposing and recycling materials. We carried out LCA on a particular MOF, to identify the areas of high environmental impact, and to evaluate changes that could reduce these. This paper will present LCA data as well as an appraisal of potential for recycling approaches.

Modelling microstructure evolution during reduction of iron oxide pellets

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H4_1 - Hydrogen metallurgy I, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The urgent need to reduce greenhouse gas emissions in steel metallurgy, driven by the challenges of climate change, is catalyzing a paradigm shift and transforming long-established industrial processes. A transition towards a clean hydrogen-based direct reduction of iron, for example, requires a deep understanding of the interdependencies among all process parameters. Such insights can be achieved through robust, physically sound process modeling with high extrapolative power.

We present a one-dimensional micro-reaction model with explicit time stepping capable of predicting and optimizing the reduction process of industrial iron ore pellets exposed to various reducing gas streams. In addition to reduction kinetics and mass transport, our simulation incorporates thermodynamics and microstructure evolution, thereby providing a comprehensive understanding of the thermochemical and thermophysical phenomena involved. Compared to other micro-reaction models, our thermodynamics-based approach reduces the number of fitting parameters while still accounting for all relevant gas-solid, gas-gas, and partitioning reactions.

This method enables the reliable integration and optimization of key input parameters, such as kinetic parameters, iron oxide pellet properties, as well as pure and mixed reduction gas streams. Ultimately, it supports the integration of hydrogen into industrial processes, contributing to a reduced carbon footprint in steel metallurgy.

Theoretical predictions and high-resolution experimental observations of lenticular hematite formations in partially oxidised magnetite powder

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H4_2 - Hydrogen metallurgy II, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

The reduction of iron oxides into pure iron is the most energy intensive and polluting process in steelmaking. Pre-oxidation of magnetite to hematite is an effective approach to increase its reducibility in ironmaking due to the associated microstructure refinements and defect formation during oxidation, thus creating an opportunity for optimisation of the process. In this study, we investigate the crystallographic orientation relationship between hematite and magnetite and their interfacial structures down to the atomic scale in order to elucidate the growth mechanism of hematite in magnetite during oxidation. We first build a theoretical model for the advancement of the hematite/magnetite interface by identifying disconnections (i. e., steps with dislocation character) suitable for the accomplishment of the phase transformation, according to the topological model of interfacial defects, and calculated their Burgers vectors and step heights. The role of the disconnections in partially compensating for the lattice misfit on the interface plane is also noted. We then investigate a magnetite powder oxidised in air at 700 °C for 30 min via electron microscopy. We observe lenticular hematite formations and confirm that their relationship with the magnetite matrix follows the Shoji-Nishiyama orientation relationship ($(111)_{\text{mag}} \parallel (0001)_{\text{hem}}$, $[1-10]_{\text{mag}} \parallel [10-10]_{\text{hem}}$) using electron backscatter diffraction (EBSD). We analyse one of these hematite plates with a high-resolution transmission electron microscope (TEM), characterising the hematite/magnetite interface as a faceted interface containing steps through high-angle annular dark-field (HAADF) imaging. Coherent terraces of interface parallel to $(0001)_{\text{hem}}$ and $(111)_{\text{mag}}$ are seen to be separated by the steps. The dislocation content of the steps is found through Burgers circuit mapping to correspond to that of the transformation disconnections predicted by the theoretical model. We thus validate the proposed growth mechanism of hematite plates in magnetite mediated by interfacial disconnections.

Thermodynamic-guided sustainable alloy design via hydrogen-based direct reduction of metal oxide mixtures

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H4_2 - Hydrogen metallurgy II, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

More than 2 billion tons of metals and alloys are produced annually to facilitate economic growth and meet the demands of rapid civilization. However, conventional alloy production routes, which use carbon-based reductants, emit CO₂ as a by-product and contribute approximately 40% of all industrial greenhouse gas emissions. The co-reduction of metal oxide mixtures using hydrogen as a reductant offers a one-step approach toward sustainable alloy production. In this study, we propose a thermodynamic model to predict the effect of temperature and composition on the reducibility of NiO+Cr₂O₃ and Fe₂O₃+Cr₂O₃ mixtures using CALPHAD approach. Based on the thermodynamic prediction, hydrogen-based direct reduction was performed to produce Fe-10Cr alloy by reducing the corresponding oxide mixtures at 900 and 1100 °C, as well as Fe-50Cr alloy at 1100 °C. The reduction kinetics of the binary oxide mixtures were quantitatively analyzed by thermogravimetry analysis, while the microstructure of the reduced samples was characterized by X-ray diffraction and scanning electron microscopy. The experimental results were consistent with the thermodynamic predictions. Furthermore, the findings demonstrated that mixing different oxides enables the reduction of highly stable oxides (here, Cr₂O₃, which in the pure oxide form cannot be reduced by pure hydrogen at 1100 °C), offering a potential pathway for sustainable alloy production.

Scope 3 emissions in secondary steelmaking: relevance and impact on CFP

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H4_3 - Sustainable steel production and processing, Seminario 4 + 5 Room (Level +1), settembre 15, 2025, 17:00 - 19:00

As international regulations and stakeholder expectations tighten, transparency and accuracy have become increasingly important for GHG assessment and reporting. Nevertheless, steelmaking companies struggle to incorporate Scope 3 emissions, caused by the industry value chain, in their reports due to the complexity of the supply chain and the lack of incentives or regulatory requirements pushing for more transparent reporting.

In particular, stainless-steel production is heavily impacted by Scope 3 emissions due to its high content of alloying elements (e.g. Cr, Ni and Mo), which leads to intense ferroalloy and raw materials consumption.

In this work a product carbon footprint (CFP) study for stainless-steel production via Electric Arc Furnace (EAF) was performed, incorporating both direct and indirect emissions along the value chain, adopting a cradle-to-gate boundary. Primary data for raw materials and energy consumption were gathered at facility level, while secondary data from ecoinvent 3.10 were used to characterize upstream processes such as raw materials extraction.

The steelworks under investigation featured three main areas—steel shop, forging line and rolling line. The steel shop direct CO₂ emissions were calculated via mass balance, considering carbon content in cast steel, raw materials, electrodes, EAF dust and EAF slag. Electric energy and methane consumption were directly measured for EAF and LF while other contributions were allocated based on the manufactured steel mass. Forging line and rolling line were subdivided into divisions, zones, and working centres. Emissions were allocated linking data on electricity and methane consumption to specific products through a combination of mass, processing time, and temperature-based allocation factors. Additional indirect emissions from transport, waste disposal and other auxiliary operations were evenly distributed across the product portfolio.

The results show that emissions distribution is heavily influenced by the product steel grade (i.e. chemical composition) as this parameter is the main driver for raw materials consumption (i.e. ferroalloys). In fact, Scope 3 emissions are always higher than 60% of total emissions for every analysed steel category (i.e. austenitic, ferritic, martensitic and duplex steel); in particular Ni, Cr and Mo are the most impactful elements. Finally, Scope 1 and Scope 2 emissions are driven by CH₄ and electricity consumption, which are both dependent on the steel grade (e.g. thermal treatments) and on the product format (i.e. product diameter and section). For example, an austenitic bar with diameter ranging from 110 to 160 mm features a CFP difference equal to 11.5% mainly due to the different diameter.

Direct reduction of iron oxides by hydrogen: Elucidating microstructure effects in single crystal and polycrystalline hematite

Dr. Barak Ratzker¹, Dr. Martina Ruffino¹, Mr. Shiv Shankar¹, Prof. Dierk Raabe¹, Dr. Yan Ma^{1,2}

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H4_1 - Hydrogen metallurgy I, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The aim of reducing CO₂ emissions in the metal industry necessitates developing more sustainable metallurgical processing pathways. One of the most promising approaches is the solid-state hydrogen-based direct reduction (HyDR) of metal oxides. Extensive work has been conducted to study the influence of reducing conditions (e.g., time, temperature, gas composition, etc.) and material properties (e.g., metal oxide composition, gangue elements, powder particle size, etc.) on the HyDR process. Gaining a fundamental understanding of microstructural factors affecting the reduction behavior assists in further optimizing the process and the reactor design. In the present study, we investigated the reduction kinetics of single crystal and dense polycrystalline hematite (without initial percolating pores) exposed to pure H₂ at 700 °C using thermogravimetric analysis. Furthermore, the microstructure of partially reduced specimens was thoroughly characterized by scanning electron microscopy and electron backscatter diffraction to elucidate the microstructure evolution during the reduction process. The critical steps of porosity development alongside the formation of reduced oxides and metallic iron were thoroughly examined. Studying single crystal samples enabled us to assess the microstructure development for different crystallographic plane facets and analyze the orientation relationships between the different oxide phases. In addition, the polycrystalline hematite samples with various grain sizes revealed the effect of grain boundaries on the reduction behavior. The microstructural insights shed light on the importance of the microstructure aspects for HyDR of metal oxides.

Solid-state recycling of aluminium AA6060: effect of thermomechanical coupling on oxidation during extrusion

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H4_4 - Aluminum Recycling, Seminario 8 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The electrolysis of alumina to obtain aluminium from ore requires a lot of electricity. Recycling avoids electrolysis by reusing waste in its metallic form. Wrought aluminium, approximately 40% of recycled aluminium in 2007, undergoes a remelting process and is then shaped through plastic deformation. Hot extrusion is a commonly used process to produce wrought aluminium profiles.

In the solid-state recycling process, to reduce energy consumption, waste is shaped without a remelting step. The studied process is divided into three stages: industrial AA6060 chips are compacted to form a chip billet, the billet is heated to the forming temperature, and it is hot extruded. However, during the process carried out at 450 and 550 °C, magnesium oxides grow on the chips surface and form a network in the extrudates [1]. This network, at prior chip boundaries, leads to mechanical losses in directions normal to the extrusion direction [2]. An acceleration of the kinetics is measured during extrusion, making this stage the main source of oxides. The purpose of this study is to understand the effect of the thermomechanical coupling on oxidation during extrusion.

First, to reproduce the extrusion ex-situ, massive samples and aluminium chips compressed at 450 and 550 °C with a Gleeble3500 are analysed. Then, a study is conducted on samples taken during the extrusion process and on the extrudates. Two heat treatment conditions are compared: 450 °C and 550 °C for 45 minutes, together with two extrusion temperatures: 380 and 450 °C. To quantify and/or describe the nature of the oxide, a multi-technique and multi-scale approach is used. The oxygen concentration is measured by inert gas fusion (IGF) at each stage, the nature of the surface oxides is determined by X-ray photoelectron spectroscopy (XPS), and the dimensions and nature of the oxide network in aluminium are measured using transmission electron microscopy (TEM) coupled with energy dispersive X-ray spectroscopy (EDS). The microstructural evolution due to hot deformation is followed by electron backscatter diffraction (EBSD). These chemical analysis results and oxide quantification, coupled with microstructural evolution, allow to describe the acceleration of oxidation kinetics during extrusion and determining its causes in order to suggest ways of optimizing the process.

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Computational prediction of the effect of process parameters and pellet properties on the hydrogen direct reduction of iron oxide pellets

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H4_2 - Hydrogen metallurgy II, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

The urgent need to reduce greenhouse gas emissions in steel metallurgy, driven by the challenges of climate change, is catalyzing a paradigm shift and transforming long-established industrial processes. A transition towards a clean hydrogen-based direct reduction of iron, for example, requires a deep understanding of the interdependencies among all process parameters. Such insights can be achieved through robust, physically sound process modeling with high extrapolative power.

We demonstrate that our one-dimensional thermodynamics-based micro-reaction model can simulate the direct reduction of porous industrial iron ore pellets exposed to pure or mixed reducing gas atmosphere. With our novel approach we can predict how porosity and convergence degree are affected by process parameters - like temperature or the reduction gas composition - and materials properties - like the pellet porosity, composition and diameter. Model predictions are validated through comparison with experimental data from pellet reduction processes and microstructure analysis of reduced iron oxide pellets.

Our simulations offer detailed insights into the system's dynamic behavior, including chemical, thermophysical, and transport phenomena within the pellets. Ultimately, our predictions support the integration of hydrogen into industrial processes, contributing to a reduced carbon footprint in steel metallurgy.

Heating and melting behavior of hot briquetted iron (HBI) under isothermal conditions for sustainable electric steelmaking

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H4_3 - Sustainable steel production and processing, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

In the carbon-neutral era, the scarcity of high-quality scrap for electric arc furnace (EAF) steelmaking has led to an increased focus on direct reduced iron (DRI) and hot briquetted iron (HBI) as sustainable alternatives. While EAF processes traditionally rely on scrap, a transition to DRI/HBI-based operations introduces challenges due to difference in heating and melting behaviors of DRI/HBI. The current study investigates the melting behavior of industrial HBI under isothermal heating conditions to optimize its use in sustainable steel production.

Three types of industrial HBI – standard (ST), high-SiO₂ (HS), and high-carbon (HC) – were characterized at 1250oC, 1300oC, and 1350oC using a vertical furnace to investigate the effects of gangue oxide and carbon content in HBI on heating and melting behavior. The cross-sections of the HBI samples were examined using SEM-EDS.

The experimental results showed that gangue composition and intrinsic carbon content significantly influence melting behavior. ST-HBI forms CaO-SiO₂-based slag at 1300oC, whereas HS-HBI forms FeO-SiO₂-based slag at 1250oC. The presence of SiO₂ influences slag separation during heating and melting. However, MgO gangue oxide remained in all samples, indicating that MgO does not significantly influence melting behavior. In HC-HBI, the presence of Fe₃C accelerates melting, leading to the complete separation of liquid metal and slag at 1350oC. These findings highlight the need to optimize HBI composition for efficient melting and slag separation, thereby reducing energy consumption and improving melting efficiency in EAF process.

Sustainable manufacturing of FeCrCoMnNi high-entropy alloy (HEA) using ferroalloys feedstock via slagging methods

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H4_5 - Advanced Materials & Life Cycle Strategies, Seminario 8 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Ferroalloys play an indispensable role in the materials world, especially in the steelmaking process. In the current study, commercial ferroalloys, such as high-carbon ferromanganese (HCFeMn), low-carbon ferrochromium (LCFeCr) and ferronickel (FeNi), are utilized in the manufacturing of the ultra-clean FeCrCoMnNi-based high-entropy alloy (HEA) in view of the cost-effectiveness and the sustainability of manufacturing process. However, elemental impurities such as carbon, oxygen, sulfur and other trace elements in ferroalloys can affect the mechanical and corrosion properties of HEA.

The present study explores the deoxidation and desulfurization behaviors of FeCrCoMnNi HEA with varying carbon content (0.3, 0.7, and 1.8 at%) using a CaO-Al₂O₃-MgO slag in an induction melting furnace at 1773 K. The results indicate that different carbon levels significantly affect the grain size, nano twinning, and carbide size, as observed through EBSD and SEM analyses. These microstructural changes influence mechanical properties, including yield strength, ultimate tensile strength, and elongation, as revealed by tensile testing.

Additionally, the corrosion properties of the three types of C-alloyed HEA were examined in 0.1 mol H₂SO₄, with corrosion film composition characterized using XPS method. The study discusses the effects of carbon content on microstructure development, strengthening mechanisms, and corrosion resistance.

Life cycle assessment for a holistic approach to sustainable steel design

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H4_5 - Advanced Materials & Life Cycle Strategies, Seminario 8 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Steel production is undergoing a significant transition toward a circular, recycling-based process, leading to changes in chemical composition. This shift is driven by the presence of contaminated scrap fractions, introducing impurities such as copper, and an increasing emphasis on the environmental impact of raw materials. To enhance circularity, the recyclability and reusability of steel depends on the controlled mixing of different iron sources and scrap, as well as the selection of alloying elements.

In addition to physical material optimization, integrating materials into the digital representation of production processes is crucial. The Digital Material Shadow provides a standardized approach to material digitalization, enabling more accurate and efficient process modeling.[1]

When developing alloy concepts, the focus must extend beyond cost and material properties to include environmental impact. A holistic optimization approach is essential, as the environmental footprint arises not only from raw materials but also from production processes.[2] Alloy composition can influence production parameters and even modify entire process steps. For instance, air-hardening steels form a martensitic structure through air cooling alone, eliminating the need for downstream heat treatment. This process modification significantly reduces energy consumption and emissions.[3]

To assess the environmental impact of steel grades, Life Cycle Assessment (LCA) is applied in accordance with DIN EN ISO 14040/14044 standards. The analysis follows a “cradle-to-gate” approach, evaluating aspects such as CO₂ footprint, toxicity, energy, and water consumption. [4]

Building on this foundation, a holistic analysis concept incorporating the Digital Material Shadow was developed and implemented. Individual steels were assessed up to the industrial semi-finished product stage through an ecological evaluation of melting processes. By integrating environmental impact, costs, and material properties, a comprehensive assessment was conducted, enabling a data-driven and sustainable decision-making process for alloy design.

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One step alloy-making from oxides: From thermodynamic design maps to atomic-scale chemistry

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H4_2 - Hydrogen metallurgy II, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Metallurgical production traditionally involves three steps: extracting metals from ores, mixing them into alloys by liquid processing and thermomechanical processing to achieve the desired microstructures. This sequential approach, practiced since the Bronze Age, reaches its limit today because of the urgent demand for a sustainable economy: almost 10% of all greenhouse gas emissions are because of the use of fossil reductants and high-temperature metallurgical processing. In this talk, we will discuss a H₂ redox-inspired alloy synthesis strategy, turning oxides into sustainable bulk alloys in one single solid-state process step. We ask three fundamental questions: (1) What are the thermodynamic processing guidelines? (2) What are the rate-limiting kinetic processes at play? (3) What are the chemical characteristics of the redox-alloying fronts? By taking Fe-Ni invar alloy as a demonstrator case, we will address these questions in quantitative depth via theoretical calculations, in situ synchrotron X-ray experiments, and the cutting-edge correlative 4D scanning transmission electron microscopy (STEM)-atom probe tomography (APT) analyses. We will also discuss a hypothesis concerning tailored metal-oxide interface for improving oxide reducibility. Finally, we will outline an “one step metallurgy” concept conceived to further dissolve some of the classical borders between extractive and physical metallurgy.

Science of Dirty Alloys: improving the recyclability of Al alloys

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H4_4 - Aluminum Recycling, Seminario 8 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Theoretically, aluminum alloys, like most metallic alloys, are infinitely recyclable. In the case of aluminum alloys, the energy involved in the recycling process represents only 5% of the energy required for primary production. However, recycling presents some difficulties, as alloying elements from certain series are poisons to be avoided for others. Therefore, their mixing in the recycling process must be strictly limited, as such contamination leads to a reduction in the properties of so-called secondary aluminum, particularly ductility, which in turn reduces the potential applications for the use of this recycled aluminum. This decrease is usually attributed to the presence of Fe-rich brittle intermetallic compounds (IMC). The objective of this work is to improve the recycling sector's ability to produce alloys of interest for a wide range of applications, in particular by closing the loop on wrought grades such as 5xxx and 6xxx alloys without any downgrade to casting alloys. To do so, the methodology relies on a combination of experimental approaches and thermodynamic calculations to better understand the impact of impurities on the microstructure and improve the predictive capacity of numerical simulation tools in compositional spaces they were not optimized for, to assess the impact of composition shift on the formation of detrimental IMC. To reproduce the consequences of recycling on the composition of secondary aluminum, industrial alloys have been enriched to reach up to 0.5w% Fe, 0.9w% Si, 1.0w% Mn and 4.7w% Mg.

The nature, size, shape and distribution of IMC have been successfully investigated by advanced techniques such as EDS, EBSD and XRD. Both massive samples and isolated IMC have been studied, thanks to a new take on a matrix selective dissolution technique (so called "Sibut" technique). This technique allowed a precise quantification of the different IMC in the enriched alloys through XRD and Rietveld refinement. The influence of several processing parameters on IMC such as cooling rate or homogenizing heat treatment have been studied. Experimental results have been also compared with numerical phase transformation models and thermodynamical calculations in order to challenge and optimize current databases.

UTILIZATION OF MICROWAVE ENERGY IN ZINC WASTE PROCESSING

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The aim of the EU in the area of securing critical and strategic metals is to achieve raw material and energy security. By using domestic raw material resources and recycling waste, the need for their supply from other countries will be reduced. The application of microwave energy in waste treatment represents an innovative way of recovery metals. Flue dust containing Zn, Fe and other metals are a dangerous by-product, arising not only during the production of steel in an electric arc furnace, but also during the subsequent galvanization of steel products. The aim of pyrometallurgical and hydrometallurgical methods of flue dust processing is the recovery of valuable elements in accordance with the most advantageous economic and environmental procedures. However, metal recovery is often limited by the existence of a stable spinel structure of ZnFe_2O_4 phase present in the dust particles. The advantage of microwave radiation is the acceleration of ongoing processes and the heating selectivity on base of dielectric and magnetic properties of irradiated materials.

Microwave absorption materials containing metals, especially Fe, effectively absorb electromagnetic waves, on the other hand, transmission materials allow electromagnetic waves to pass through. The advantage of microwave pretreatment of zinc dust is the transformation of refractory minerals present (e.g. ZnFe_2O_4) into easily leachable zinc oxides. Experiments of microwave-assisted extraction of flue dust from an electric arc furnace in microwave field confirmed zinc recovery above 97%.

A higher yield of zinc compared to conventional leaching was achieved by the interaction between the electromagnetic field and the heated material. Microwave heating offers a promising alternative for zinc recovery from flue dust, combining energy efficiency, environment and high speed of processing. Laboratory tests, thermodynamics and kinetics of the microwave assisted extraction process will help to optimize the parameters of microwave heating. The microwave power regulation, increase in temperature and dielectric properties knowledge of treated materials will lead to the possibility of reducing the amount of leaching agents and to the efficiency of the methodology processing.

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Methodology to design a new high performance HPDC aluminium alloy with a high recycled content

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H4_4 - Aluminum Recycling, Seminario 8 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The European Green Deal generates to the automotive industry a need to evolve towards a greener and more sustainable system for achieving a net-zero emission of Greenhouse Gases (GHG) in Europe by 2050, and to secure itself a stable future. In order to achieve this objective, the materials have been improved and new developments performed over the last years. In order to reach this target, the vehicles have to be as light as possible and, of course, there is the necessity to move towards a global electrification of the road transport. Both solutions involve the use of innovative and light materials for improving energy efficiency and aluminium alloys are the core of this material evolution. Structural parts require high mechanical properties, as 10% elongation at fracture and, at least 100 MPa yield strength, as they have a crash-relevant function. For this kind of applications, the automotive sector has always used primary alloys, while secondary alloys only for non-structural parts as engine blocks or housings. The reason behind this is the detrimental effect that iron and other impurities, commonly present in the aluminium scrap, have in the alloy castability and mechanical properties.

In this study, the effect that different elements have in the most common alloy used for HPDC structural applications, AlSi10MnMg alloy have been investigated. Relevant alloy properties, such as alloy flowability, and mechanical properties after T5 and annealing heat treatments were analyzed. The effect of different levels of the main alloying elements (Si, Mg and Sr), as well as the main impurities commonly present in the scrap (Fe and Cu), were investigated. The results show that, while the Mg level has a strong influence in the hardening achieved after a T5 heat treatment, it does affect very little the yield strength and maximum strength achieved after an annealing. Alternately, the Cu level does not significantly affect the alloy strength after a T5 heat treatment, but highly affect the alloy strength after the annealing.

Circular economy of aluminium alloy to extrusion process: From dismantled batteries to batteries.

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H4_4 - Aluminum Recycling, Seminario 8 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

The automotive industry has played a decisive role in the economy and it has been the responsible of important advances in new materials, processes and designs. In the last years the huge increment in the use of electrical vehicles has lead to the increase on the amount of aluminium employed in each vehicle. At the same time, the bauxite, principal source of primary aluminium is considered a Critical Raw Material since 2020, open the opportunity to increase and approach one of the most relevant properties of the aluminium alloys, their recyclability.

Aluminium alloys can be recycled infinitely without losing their properties, with a clear tendency to increase the use of secondary alloys. Unfortunately, the scrap is usually mixed and contaminated, restricting the use of secondary alloys until the present days to low performance applications. The most common and undesirable impurity in recycled Al-Si alloys is Iron. Due to the low solubility of Fe in Al, secondary phases are usually formed in Al Alloys, decreasing the mechanical properties and increasing their porosity. The light alloys research group of Eurecat is focused on the research and development of high-performance aluminium alloys with high scrap ratio, evaluating the effect of the principal impurities and alloying elements on alloy properties and their effect in an extrusion process, in this case. Eurecat leads the research in this area, thanks to the participation in different European projects. In particular, FREE4LIB project has allowed the demonstration the possibility of closing the cycle of extrusion aluminium alloys used in the battery of electrical vehicles.

The dismantled batteries were supply by ACCUREC. The sorting of the scrap was made depending on the Si content. The scrap with more than 1% of Si, was used to produce casting alloys and the scrap with less than 1%, to produce extrusion alloys. The extrudability of the secondary alloys obtained 100% from dismantled batteries were studied with an special extrusion device developed by EURECAT. The microstructure and mechanical properties of the extruded profiles obtained were also analysed. The extrusion alloy obtained directly from the battery scrap, has a chemical composition similar to 6082 but with a higher Cu content, however, the results suggest than a Cu level near to 0,2% do not have a detrimental effect in the mechanical properties or alloy extrudability, allowing the use of aluminium alloys with higher Cu contents to produce extruded profiles for high performance applications.

Evaluating sustainable steam shaft production strategies through Life Cycle Assessment

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H4_1 - Hydrogen metallurgy I, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Historically, product development has been a source of waste in the forging industry. This is often due to failed attempts to manufacture new steel parts, either due to quality defects or critical failures along the manufacturing process. While there are always risks in producing new steel grades and parts, these can be greatly minimized by integrating computerized tools into the design phase. This enables engineers to select optimal parameters and eliminate problematic ones. Although simulation-based tools such as FE thermal modelling are currently well-established in forging companies, artificial intelligence has emerged as a natural progression to optimize product design. Reinosa Forgings & Castings (RFC) is currently exploring the potential of these analytical techniques in combination with traditional FE modelling to predict the creep properties of a novel steam shaft before it is put into service. In this way, the trial and error approach can be avoided by selecting the most appropriate manufacturing parameters route to achieve the desired properties in the final product. To understand the environmental impact of these innovations, an analysis of a non-optimized process is proposed as the basis of the study. The study includes a life cycle assessment (LCA) to assess the environmental footprint of manufacturing steam shafts from recycled steel, highlighting how existing residue streams at RFC are revalorized, contributing to the circular economy. The analysis initially follows a 'cradle-to-gate' approach, prioritizing processes such as EAF melting, refining, and casting, proposing scenarios to measure the impact of by-product revalorization. Primary data was collected directly from industrial operations, supplemented with secondary data from Ecoinvent v3.10, and modelled using Umberto 11.14.1. The assessment of environmental impacts was based on the production of one tonne of ingot as the functional unit. Initial results indicate that RFC's processes where residue streams are revalorized present a reduction on environmental impact of as much as 15% in comparison with processes performed elsewhere where these streams are disposed as waste. Finally, by utilizing the synergies of AI-tools and LCA, the present study aims to be able to extend the lifespan of critical industrial components where the core product is utilized, i.e. energy generation turbines, on a broader 'cradle-to-grave' approach.

Interplay of scrap introduced tramp elements and non-metallic inclusions in steels on wetting conditions and deformation behavior of inclusions

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H4_3 - Sustainable steel production and processing, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Increasing steel scrap recycling rates is essential to achieve the ambitious climate targets set by the European Union. Low-quality scrap containing elevated levels of tramp elements such as copper, nickel, molybdenum, and tin, introduces these elements into the steel cycle. However, their complete separation in the melt by metallurgical processes is impossible. Due to various effects on steel properties, such as delayed phase transformation or hot-shortness, the tramp element content is restricted to low levels for many steel grades. Recent research therefore focuses on the development of more tramp element tolerant compositions. Furthermore, increased tramp element contents also lead to issue during processing of liquid steels, e.g., most dissolved elements lower the surface tension favoring the formation of non-metallic inclusions (NMIs).

During continuous casting, attachment of NMIs onto the submerged entry nozzle and resulting clogging may even lead to interruption of casting and, thus, increasing production costs. This behavior is favored by an agglomeration tendency of NMIs and a high wetting angle between steel and oxides. This is why one focus of this study is the wetting behavior of steel on various materials with chemical compositions matching those of refractories and NMIs. It is shown that most tramp elements decrease the wetting angle.

Since tramp elements affect phase transformations and can accumulate at NMIs, the influence on the surrounding steel matrix of NMIs is the second important point of this work. Thereby, the deformation behavior of NMIs in steels with and without tramp elements is evaluated using quenching and deformation dilatometry in combination with Scanning Electron Microscopy (SEM) to obtain the aspect ratio before and after deformation. While the influence of tramp elements on the deformation of hard NMIs was negligible, softer NMIs' deformation behavior was altered by the presence of certain tramp elements.

Solid-state recycling of AA6006 via chips compaction and hot rolling

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H4_4 - Aluminum Recycling, Seminario 8 Room (Level +1), septiembre 16, 2025, 14:30 - 16:30

Solid-state recycling techniques for aluminum have been studied for years as a potential alternative to conventional recycling methods that rely on remelting, due to their lower energy consumption and reduced environmental impact. This study explores the solid-state recycling of AA6006 chips through compaction and consequent hot rolling, with the aim of producing a continuous bulk material. The focus has been set on the effects on material properties of different process parameters, including compaction pressure, rolling temperature and rolling reduction ratio. The final mechanical properties were defined through tensile and hardness tests. Microstructural evolution was monitored throughout different process steps involving optical microscopy, Scanning Electron Microscopy (SEM) and Electron Backscattered Diffraction (EBSD). Correlations have been found between microstructural features and mechanical properties. Preliminary results indicate that this approach has potential for producing high-density materials with promising mechanical properties, providing a viable alternative for more sustainable aluminum recycling in a circular economy perspective aimed at minimizing wastes.

Solvometallurgical process for copper and cobalt extraction from DRC oxide ores using Di-(2-ethyl hexyl)phosphoric acid

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H4_5 - Advanced Materials & Life Cycle Strategies, Seminario 8 Room (Level +1), septembre 16, 2025, 17:00 - 19:00

Conventional metallurgical process of metals like copper and cobalt from their primary resources are often energy and emissions intensive. Herein we report an alternative solvometallurgical process to extract copper and cobalt from Kamwale ore site in Democratic Republic of Congo. Copper and cobalt bearing minerals were found as malachite and heterogenite, respectively. In this study, di-(2-ethyl hexyl)phosphoric acid (D2EHPA) diluted in kerosene was used for selective Cu and Co dissolution. To reduce Co(III) to Co(II), sodium metabisulfite or copper were studied separately. The influence of leaching parameters like the extractant and reducing agent amounts, solid-to-organic ratio, leaching temperature and time were investigated. Under optimal conditions, >98% of Cu and >87% of Co can be leached with no Fe extraction. While Co dissolution is chemically controlled, Cu dissolution is also impacted by diffusion control. The speciation of dissolved Cu and Co in D2EHPA by UV-Vis spectroscopy showed the formation of Cu(II) and Co(II)-D2EHPA complexes. Following the leaching, the loaded organic phase was stripped using diluted sulfuric acid solution. Several stripping parameters were optimized including pH, organic-to-aqueous ratio and contact time. This way, >93% Cu and >99% Co can be stripped from the organic phase which effectively regenerates consumed D2EHPA for reuse as confirmed by FTIR analysis.

UTILIZATION OF MICROWAVE ENERGY IN OBTAINING METALS FROM SULPHIDIC ORES

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The processing of the necessary metals as well as the sustainability of their production is currently closely related to the modernization of the technological procedures of their obtaining. Progressive technologies, which are increasingly being used in various industrial areas, include the application of high-frequency electromagnetic radiation. The advantage of the application of microwave energy in the processes of heating materials is the replacement of the conventional heat source. Copper, as one of the main industrial metals, is obtained from naturally occurring ore deposits as a primary raw material, or as a secondary raw material in the form of electronic wastes and wastes generated during production.

In nature, copper occurs in the form of sulphides (chalcopyrite, bornite, tetrahedrite, tennantite), oxides (cuprite), hydroxycarbonates (malachite, azurite, tyrolite), or silicates (chrysocolla).

However, the quality of the primary bearings decreases and the cost of mining and rock transport requires a large amount of energy. The obtaining metals from refractory ores is also difficult process requiring energy-intensive treated processes and leaching in environmentally undesirable leaching agents. When complex sulphide ores are heated in a microwave field, useful components containing metals such as Cu, Fe, Zn, Sb, Ag, Au are heated. There is no heating for tailings components with Si and Ba content.

For this reason, it is advantageous and economically prospective to treat primary ores with a lower metal content. The use of microwave energy thus represents an innovative method of thermal pretreatment of sulphidic ores before the subsequent processes of hydrometallurgical obtaining of strategic metals. The heating complex ores in a microwave field will cause disturbance of minerals structure and break down mineral grains. The result will be an intensification of crushing and grinding processes, reduced requirements for the amount and type of leaching agents, and better leachability of metals.

Acknowledgments:

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Unravelling the copper precipitation mechanism at the grain boundaries and intergranular cementite in copper alloyed ferritic steels: steps towards enhanced understanding and use of copper in steel scrap.

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H4_5 - Advanced Materials & Life Cycle Strategies, Seminario 8 Room (Level +1), septiembre 16, 2025,
17:00 - 19:00

The need to accommodate copper in steels is becoming increasingly important due to the rising accumulation of copper in steel scrap, driven by the transition from fuel combustion vehicles to electric vehicles. This shift is a necessary step toward circularity and reducing carbon dioxide emissions from the steel industry.

Copper precipitation is one of the most promising strengthening mechanisms in steels, offering enhanced fatigue resistance, ductility, and strength. These benefits contribute to improved lifespan and weight reduction in ferritic steels. While copper precipitation within the matrix is well understood and extensively studied, its behavior at grain boundaries and intergranular carbides has not been studied, investigated, or considered in the design of copper-alloyed steels. This is despite its critical influence on grain boundary strength, material properties, crack initiation and propagation resistance, and, ultimately, structural integrity and fatigue life.

This study presents novel findings on the accelerated precipitation mechanism of copper at intergranular cementite. Using a combination of transmission electron microscopy (TEM), atom probe tomography (APT), and in-situ small-angle X-ray scattering (SAXS), along with MatCalc© simulations, we systematically investigate medium- and ultra-low-carbon copper-alloyed ferritic steels. The study examines the effect of carbon content and reveals an accelerated Cu-precipitation mechanism at grain boundaries during austenite decomposition and isothermal aging.

Unravelling this unique mechanism—its relation to austenite decomposition, cementite formation, and varying carbon content—provides valuable insights for optimizing copper-containing ferritic steels and potentially leveraging intergranular Cu precipitation for grain boundary engineering to enhance mechanical properties. By refining heat treatment processes, chemical composition design, and product development, these findings contribute to extending product lifespan and increasing the viability of higher copper concentrations in steel recycling, making sustainable steel production more feasible.

Hydrogen-based direct reduction and decomposition of mill scale at 400°C-700°C

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H4_1 - Hydrogen metallurgy I, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

The transition towards a more sustainable society requires the urgent decarbonization of the steel industry. Indeed, this sector is responsible for around 5% of the CO₂ emissions in the European Union and 7% worldwide [1]. In 2016, 70% of the world steel production was done via Blast Furnace or Basic Oxygen Furnace [2], using carbon as a reducing agent. Hydrogen-based direct reduction (HyDR) is a promising alternative to produce metallic iron with a lower CO₂ impact [3].

However, the behavior of the various iron sources during direct reduction is not yet fully understood. In this work, we studied the HyDR kinetics of mill scale, an industrial iron-rich oxide waste produced during the thermo-mechanical processing of steel. Mill scale mainly consists of wüstite (about 80%) with small amounts of impurities (Mn-0.4, Al-0.05, Si-0.04, Cr-0.02, Cu-0.02, Ni-0.02 in wt%). The studied iron oxides fines have a particle size range between 45-106 µm.

Isothermal reduction kinetics were analyzed using a thermogravimetric analyzer. The influence of both deep pre-oxidation (using dry air at 700°C, 800°C or 900°C) and reduction temperatures (400°C, 450°C, 500°C and 700°C) on crushed mill scale powder was studied in pure hydrogen. The evolution of the impurities within the powder during its reduction was measured by ICP, SEM-EDS and STEM-EDS analyses.

Pre-oxidation consistently resulted in faster reduction rates, with the highest kinetics obtained with a pre-oxidation temperature of 800°C followed by a reduction at 500°C. Interrupted tests were carried out at 500°C, with and without pre-oxidation, to assess the reaction mechanisms of the intermediate steps during direct reduction. The eutectoid wüstite decomposition at 500°C was also quantified. This is done with microstructural analyses (SEM, EDX, EBSD, XRD) coupled with kinetic fittings. For each reaction mechanism, the rate constant and activation energy was calculated and compared with the HyDR behavior of other Fe sources.

[1] IEA (2020), Iron and Steel Technology Roadmap, IEA, Paris <https://www.iea.org/reports/iron-and-steel-technology-roadmap>.

[2] Ariyama, T., Sato, M., Nouchi, T., & Koichi, T. (2016). *Isij International*, 56, 1681-1696.

[3] Wang, P., Ryberg, M., Yang, Y., Feng, K., Kara, S., Hauschild, M., Chen, W-Q. (2021). *Nature Communications* 12, 2066.

Sustainable production of iron and steel via electric steelmaking routes for mitigation of CO₂ emissions

Prof. Joohyun Park¹

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H4_3 - Sustainable steel production and processing, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

It is known that 7-8% emissions of CO₂ arise from the steel industry sector. Hence, many steel companies are trying to develop the electric arc furnace (EAF) and/or electric smelting furnace (ESF) processes instead of blast furnace (BF) – basic oxygen furnace (BOF) integrated routes by employing high amounts of direct-reduced iron (DRI) and/or hot-briquetted iron (HBI) to reduce CO₂ emissions. The DRI/HBI as substitutes for virgin scrap in EAF has been used because DRI/HBI does not have tramp elements. Unfortunately, however, commercially available DRI contains relatively high levels of phosphorus and gangue oxides, which adversely affects not only the steel properties but also the operation efficiency. Alternatively, integrated steel mills have focused on the ESF process by keeping conventional BOF to produce high-end quality products. The H₂-reduced DRI are potentially charged in ESF in conjunction with fluxes and carbon sources, producing hot metal. In the present lecture, the challenging points should be carefully considered to achieve the improved and stable EAF or ESF technology on the way to green steel will be reviewed, and the recent experimental and modeling research will be discussed. The slag chemistry is one of key parameters affecting the operation efficiency in electric steelmaking processes in view of FeO reduction behavior.

Thermochemical aspects of the substitution of natural gas by hydrogen in blister copper deoxidation during fire refining

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H4_2 - Hydrogen metallurgy II, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

High-purity copper, valued for its excellent conductivity, is essential for the energy and digital transitions. During blister copper deoxidation, the oxygen concentration in the melt is reduced to below 0.15 wt.% by bubbling, typically, natural gas (methane). This deoxidation process generates water vapor and carbon dioxide (CO₂) and has an average efficiency of 30 %. Replacing natural gas with hydrogen presents a promising strategy to lower CO₂ emissions and to increase the reduction efficiency in copper production. In addition to process parameter optimization, the design of more efficient refining strategies requires a deep understanding of the thermodynamics of Cu-O-S systems, including the presence of multiple minor impurities (As, Ni, Pb, Ag, Sb, etc...).

This study comparatively evaluates key thermodynamic aspects of the deoxidation process of Cu-S-O melts by methane and pure hydrogen by using the FactSage 8.3 software. The deoxidation dependence on temperature, oxygen, and sulfur contents, as well as minor impurity levels, are analyzed. In addition, given that industrial furnaces operate with a methane burner, the analysis incorporates a thermodynamic comparison of the methane-oxygen and hydrogen-oxygen flame products and their interactions with the liquid copper surface.

The results indicate that, regarding gas bubbling into liquid copper, since methane requires to run first through an endothermic decomposition before reacting with dissolved oxygen, hydrogen exhibits a better deoxidation performance over a broader range of gas temperatures compared to methane. Additionally, the nature and content of impurities are identified as key parameters governing the efficiency of copper deoxidation through the oxygen activity in liquid copper and the final solid microstructure. In respect of burner operation, the oxygen-to-fuel ratio is identified as the primary factor influencing both the atmosphere temperature and the fraction of reductant species. A comparative analysis reveals a higher fraction of reductant species in oxygen-methane adiabatic flames with respect to oxygen-hydrogen flames, and a more reductant behavior on liquid surface.

The results of this study enhance our understanding of molten metals refining based on 100 % hydrogen bubbling and combustion, which will aid the development of more sustainable and efficient metallurgical processes.

TiC-Containing Ferritic Steels: A Path Toward Lightweight, High-Performance, and Sustainable Vehicles

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H4_5 - Advanced Materials & Life Cycle Strategies, Seminario 8 Room (Level +1), septiembre 16, 2025,
17:00 - 19:00

Future vehicle designs prioritize weight reduction to lower carbon dioxide emissions while maintaining maximum safety, including high shock absorption capacity. While high- and medium-manganese steels offer excellent strength-ductility combinations, they present industrial challenges and do not fully align with sustainability standards due to their high environmental impact. This makes the optimization of ferritic steels a crucial and more sustainable alternative.

Titanium carbides (TiC) as precipitating phases provide a promising approach to enhancing ferritic steel through precipitation strengthening while simultaneously controlling recrystallization degree. However, despite their potential for achieving the desired mechanical properties, the complex interaction between precipitation and recrystallization—depending on temperature, annealing time, and Ti content—poses significant challenges in optimizing steel design.

This study aims to unravel the complex relationship between Ti content, recrystallization mechanisms, and precipitation formation. A combination of advanced characterization techniques—including scanning transmission electron microscopy (S-TEM), atom probe tomography (APT), electron backscatter diffraction (EBSD), and in-situ small-angle X-ray scattering (SAXS)—is employed to investigate the interplay between processing parameters, precipitation behavior, recrystallization degree, and their collective impact on mechanical properties.

The insights from this study enable a more effective utilization of TiC to optimize precipitation strengthening while achieving the ideal recrystallization degree and optimal mechanical properties. This understanding contributes to the development and optimization of TiC-containing ferritic steel grades as environmentally friendly alternatives, meeting the evolving demands of the automotive industry and aligning with standards for sustainable steel production and use.

Iron recovery from EAF slags through hydrogen-based reduction

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H4_2 - Hydrogen metallurgy II, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

The steel production in the electric arc furnace (EAF) is continually growing as more steel is recycled. The iron content in EAF slags is significantly higher than conventional BF slags, which makes them attractive as potential Fe sources. It is estimated in 25 million tons the total iron content of the EAF slag produced in 2023 . Therefore, the development of sustainable iron recovery methods from EAF slags will enhance the circularity of the steel industry. Our thermochemical calculations for the hydrogen-based reduction of molten slags show that recovering high-purity Fe is thermodynamically feasible and could offer advantages over carbon-based processes.

This study proposes the experimental framework for the design of hydrogen-based iron recovery processes from industrial EAF black slags. Firstly, the chemistry and mineralogy of different industrial EAF slags were characterized. Elemental analysis was conducted using X-ray fluorescence (XRF), crystalline and amorphous phases were determined through Rietveld refinement of X-ray diffraction (XRD) patterns, and the morpho-compositional study of the slags was performed by scanning electron microscopy (SEM) and energy dispersive X-ray (EDX) spectroscopy microanalysis. The iron is mainly distributed in the amorphous phase and the RO phase (Fe,Mn,Mg)O.

In order to design adequate reduction heat treatments, thermodynamic equilibrium calculations by FactSage 8.3 were combined with phenomenological models to predict the foaming index of the slags under a variety of hydrogen injection flow rates and temperatures. It has been verified that, for fixed H₂ injection conditions, the chemical composition of slags influences the optimum temperature range to get the proper fraction of solid phases coexisting with the liquid slag and, thereby, the slag foam height. Finally, experimental validation was carried out using an innovative laboratory-scale melting furnace, equipped with a mini-lance to bubble hydrogen-based gas mixtures into the molten slag and a micro-gas chromatograph for the off-gas semi-continuous analyses. To evaluate the iron recovery efficiency after reduction, slag samples were subjected to both slow and quenching cooling routines and their chemistry and mineralogy were characterized.

The results of this study enabled the identification of experimental optimal working ranges, as well as the first experimental validation of our theoretical hypothesis. This knowledge will allow us to develop hydrogen-based metallurgical processes for slags, either to use them as alternative iron sources or to reduce the CO₂ emissions in EAF steel production.

Hydrogen use in valorization of bauxite residue to extract iron and alumina

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H4_1 - Hydrogen metallurgy I, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Bauxite residue (de-watered red mud) has been a long-lasting environmental problem in the alumina production from bauxite ores via the commercial Bayer process. The current world stockpiled bauxite residue is estimated over 4 billion tones, with annual addition of over 175 million tons. It has high alkalinity and hence is harmful if it leaks to the nature, and several red mud catastrophes happened shows its risks. As bauxite residue is a hazardous waste, it must be safely stored, valorized via sustainable approaches, or its generation prevented. The continues growth of aluminum and alumina industry is accompanied with more bauxite residue production in future, and hence it is crucially important to solve this waste problem. Bauxite residue contains high amounts of metal oxides such iron oxides, alumina, silica, titanium oxides, and it contains rare earth elements such as Sc, Ga, etc. Regarding the chemical characteristics of the bauxite residue, it is a potential secondary source for the extraction of some metals such as Fe, Al, RREs. Obviously, the establishment of new methods to valorize bauxite residue must be with no or insignificant hazardous waste generation. In an approach in Harare EU project, sustainable methods for bauxite residue valorization using hydrogen gas as a reductant to reduce iron oxides is demonstrated in lab and pilot scales. In an approach, which is called Ca-route, bauxite residue is mixed with lime fine, pelletized via different techniques, and then reduced by hydrogen gas at elevated temperatures. The reduced material is then post-treated, and iron is separated from the coexisting non-metallic components. The pre-reduced pellets obtained by hydrogen reduction contain iron particles distributed in the non-metallic oxide matrix, which is mostly calcium-aluminate. Alumina is leached from the oxide matrix of the reduced pellets via alkaline leaching by sodium carbonate solutions. Applying advanced materials characterization techniques, the formation of suitable phases with proper physical characteristics were studied and the process conditions were optimized. The mechanisms of reduction reactions and the role of pellets components in formation of metallic iron and leachable calcium-aluminate phases were proposed. It was found that upscaling of hydrogen reduction from lab scale stationary bed reactor to a pilot rotary furnace yields better reduced product in term of iron particles sizes. Materials analysis and thermodynamics calculations, the mechanisms involved in iron particles formation and growth were proposed.

Sustainable metal production via hydrogen- and ammonia-based direct reduction of metal oxides

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H4_1 - Hydrogen metallurgy I, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Fossil-free metal production is critical for reducing the substantial CO₂ emissions from the metal industry, which accounts for approximately 10% of global emissions and is a major contributor to climate change. Hydrogen-based direct reduction of metal oxides, including the use of hydrogen carriers such as ammonia, represents one of the most promising strategies for mitigating these emissions. In this study, we investigate the reduction behavior of metal oxides (e.g., iron oxide and mixtures of iron and nickel oxides) using hydrogen and ammonia, with a particular focus on the spatial and temporal evolution of the microstructure during the multistep solid-gas reaction. Advanced characterization techniques were employed to analyze phase transformations, porosity, and local chemistry throughout the reduction process. The fundamental reaction mechanisms are discussed, providing new insights into the sustainable production of metals and alloys via hydrogen- and ammonia-based direct reduction, ultimately enabling a pathway to metal production with minimal CO₂ footprint.

Effect of Surface and Thermal Reconditioning on the Re-Use Potential of Quenched and Tempered Martensitic Steel in a Circular Steel Economy

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H4_3 - Sustainable steel production and processing, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Sustainable engineering practices necessitate extending the lifespan of steel components, particularly in a circular steel economy, where re-use strategies can significantly reduce material consumption and carbon footprint. This study investigates the effect of surface (mechanical + electropolishing) and thermal reconditioning on the fatigue life extension of quenched and tempered martensitic steel subjected to cyclic loading.

To assess re-use potential, specimens are pre-loaded up to 75% of their fatigue life under controlled fatigue conditions. The damage state of these specimens is characterized using non-destructive testing (NDT), scanning electron microscopy (SEM), and plasma focused ion beam (PFIB) lamella extraction to analyze subsurface crack propagation and damage depth.

Following initial damage assessment, surface reconditioning (mechanical + electropolishing) and thermal reconditioning are performed to evaluate their impact on microstructural recovery, residual stress redistribution, and fatigue resistance. Additionally, the study examines the influence of frequency, geometry, and specimen size on fatigue performance to establish the most effective reconditioning strategies for steel component re-use.

The findings contribute to the development of a residual life assessment model for steel structures, providing insights into the reusability of pre-damaged components and advancing sustainable material utilization in engineering applications.

Effect of Tramp Elements on Hot Shortness in Steel Products

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H4_3 - Sustainable steel production and processing, Seminario 4 + 5 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

The introduction of the Carbon Border Adjustment Mechanism (CBAM) has significantly enhanced steel production via the Electric Arc Furnace (EAF) process, thereby improving the recycling rate of steel scrap. Steel scrap frequently contains tramp elements, such as copper (Cu) and tin (Sn), which conventional refining processes cannot eliminate, and which accumulate during the steel recycling process. Specifically, Cu exhibits greater oxidation resistance than iron (Fe), remaining unoxidized during heat treatment and hot-rolling processes, leading to its accumulation at the steel surface. When the concentration of Cu surpasses the solubility limit of the base steel matrix, it precipitates at the interface between the steel surface and the oxide scale, resulting in the formation of a Cu-rich liquid phase. During high-temperature processing, such as hot rolling, this copper-rich liquid phase penetrates along the grain boundaries of the steel, causing hot shortness, which significantly impairs the hot workability of the steel.

The phenomenon of Cu-induced hot shortness is influenced by several factors, including the chemical composition of the steel. Nickel (Ni), as a residual element, raises the melting point of the Cu-rich phase and enhances the solubility of Cu in the austenite steel matrix, facilitating the back-diffusion of Cu into the matrix. This phenomenon has been extensively studied to mitigate the Cu-rich liquid phase at the steel/scale interface. The critical Cu equivalent is regarded as a key parameter, quantifying the relative contributions of various elements to crack formation and indicating that surface cracks caused by the Cu-rich phase may arise when the value exceeds a defined critical upper limit. However, a definitive standard remains elusive due to the varying effects of each constituent element.

This study analyzed the chemical composition of steel produced in domestic EAF steelworks in Korea to assess the current levels of tramp elements. High-temperature oxidation experiments demonstrated the formation of the copper-rich liquid phase and its chemical composition, which aligns reasonably with thermodynamic calculation results. Further thermodynamic calculations were conducted to investigate the influence of tramp elements on the formation of the Cu-rich liquid phase during the high-temperature oxidation process. A novel Cu equivalent formula is proposed to evaluate hot shortness in steel products derived from the EAF process in Korea.

This study establishes that the experimental results can be theoretically reproduced through thermodynamic calculations, indicating that these calculations serve as a suitable tool for predicting the formation of the Cu-rich liquid phase and the consequent hot shortness.

Graduate School Circular E-Cars: Development and establishment of a circular economy for e-cars in the Rhenish Mining Area

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The Graduate School Circular E-Cars aims to develop and establish a circular economy for e-cars in the Rhenish Mining Area. For this purpose, the entire value chain is addressed, from material preparation and design to questions of reuse.

Circular E-Cars is organized across four locations: RWTH Aachen University, the University of Siegen, FH Münster, and the Wuppertal Institute. Within this framework, the Steel Institute (IEHK) of RWTH Aachen University focuses on resource recovery, metal refining, and the innovative design of materials and products.

Key aspects include non-destructive assessment of damage status in structural and functional components, as well as the design of new high-strength, recyclable alloys. Additionally, the melting of recycled materials with comparable quality standards and comprehensive material testing are core tasks of the IEHK within this Graduate School.

Circular materials characterisation with synchrotron X-rays: an update on the European project ReMade@ARI

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H6_1, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

ReMade@ARI is a European project that provides free and assisted access to fifty analytical research infrastructures across Europe. The project is supported by Europe, UK and Switzerland at a level of 15 million EUR and runs until August 2026.

The aim of the project is to boost circular materials research through access to synchrotrons, neutron sources, lasers, electron microscopes, ion and positron beams, and high magnetic field facilities. ReMade@ARI offers services that goes beyond the usual level of support at ARIs. This includes consultation on project ideas, free access to the research facilities, experiment assistance and travel support. This opportunity is open to researchers from both academia and industry and is particularly beneficial to first time users or experienced users wishing to learn a new complementary technique.

Three years into the ReMade@ARI project, we can now report on its success stories of circular materials characterisation. ReMade@ARI attracted 192 research proposals for standard access (transnational access, TNA) in the first four access rounds, of which 124 were accepted. In addition, there were 25 requests from industry of which 19 have already been accepted, and it is noteworthy that more than half were from small and medium enterprises (SMEs). These achievements underscore the project's success and its potential to support diverse research needs.

Users still have the opportunity to apply for access through ReMade@ARI. The deadline for the final call for standard access is 08 October 2025, while tailored SME access is available through rolling applications until 15 April 2026. SME access can be confidential, without obligation to publish results, and includes specific assistance for data analysis.

Our presentation will demonstrate how researchers and industry partners can access these opportunities and make the most of the support provided by ReMade@ARI. To inspire prospective applicants, we will also showcase highlights from the project's achievements, including examples of cutting-edge research carried out at the synchrotron facilities ESRF and ALBA. Whether you are new to these facilities or looking to expand your research toolkit, this session will offer practical advice and showcase the potential of ReMade@ARI.

Website: remade-project.eu

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A Digital Platform for Circular Management of Critical Raw Material: Emission Estimation Module

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The management of critical raw materials (CRM) is an important endeavour for the re-industrialization of Western economies in a context of geo-political tensions. European economies need to increase domestic supply to secure the global competitiveness of industries, especially in the EU's strategic sectors (i.e. renewable energies, e-mobility, cloud and cutting-edge technologies). Extraction and processing of material resources (fossil fuels, minerals, non-metallic minerals and biomass) account for over 55 % of greenhouse gas emissions (GHG) and 40 % of particulate matter health related impacts globally. The expansion of the EU mining industry faces several challenges and increased CRM production will lead to the increase of air emissions.

The European Union has co-financed numerous projects related to the mining industries such as the Smart EcoMine Hub. Competition for access to raw materials has led to the need for more efficient management of the raw material supply chain. Therefore, this paper presents recent achievements in raw material management, such as Digital Twins, and proposes a novel collaborative digital platform designed as a part of the ROTATE project. The new platform aims to: i) foster collaboration among mining stakeholders to reduce the environmental footprint associated with the mining and quarrying (M&Q) sector required to obtain these materials; ii) define workflow management for mining-related calculations, such as process and environmental assessment for energy and resources efficiency model and the modules on decision making, energy efficiency, biodiversity, risk assessment and emission estimation; iii) allow the integration of several IT tools provided by different stakeholders.

The aim of this work is to present the emission estimation module's outcomes linked to the assessment of atmospheric emissions, including dust, CO₂, and NO_x, which form the basis of roadmaps for the reduction of atmospheric emissions in quarries. Some calculations of this module use near-real time meteorological data provided by WEkEO which is an EU cloud-based platform accessing updated and timely Copernicus data directly from the original sources.

The emission estimation is presented for the Canteras Industriales pilot quarry in Granada, Spain.

Everglass: The new role of glass in a sustainable society. Technology for the integral recycling of glass

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Glass recycling uses mature technology limited by high energy consumption to melt tons of glass and the inflexibility of a heavy-duty system. Current technology only allows the recycling of certain glasses and a very small amount of waste generated. A new technology is required to allow the integral recycling of all types of glass, drastically reducing the carbon footprint. EverGLASS proposes to develop a radically new technology called "glass laser transformation" for on-site glass recycling and the generation of customized or technical products. The vision is ambitious, as it aims to bring to the consumer market a novel technology to enable virtually infinite reuse of glass. It proposes an alternative approach to the traditional centralized recycling process (particularly where this model is not possible, generating thousands of tons of glass waste annually taken to landfills). The new technology goes beyond the current limitations of the systems (high energy use, expensive and rigid process, strong logistical requirement), adopting a highly environmentally friendly model that will allow flexibility in the use of the material and in the process. Therefore, EverGLASS has the potential to revolutionize recycling as a concept. It also addresses one of the main problems with recycling, user participation, in an innovative way by allowing the personalization of recycled items of different use. This project brings together experts from advanced laser technologies (UVIGO, Spain), glass and ceramics science (ICV-CSIC, Spain), glass processing and engineering (TnUAD, Slovakia), risk and impact assessment (ACTALIA, France), Social Sciences (ESCI, Germany) and numerical simulation (ITWM, Germany).

Key words: glass, recycling, circular economy, close loop recycling, open loop recycling, laser processing

Acknowledgements

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SUSTAINABLE USE OF ELECTRIC ARC AND LADLE FURNACE SLAGS AS CONVENTIONAL FILLER REPLACEMENT FOR NITRILE BUTADIENE RUBBER

Ph.D. Anna Gobetti¹, Prof. Giovanna Cornacchia¹, Prof. Marcello Gelfi¹, Ing. Giorgio Ramorino¹

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H6_6, Seminario 1 + 2 Room (Level +1), settembre 16, 2025, 17:00 - 19:00

The increasing demand for sustainable materials and the urgent need to reduce industrial waste have driven the exploration of innovative reuse applications for steel slag. This study investigates the potential of electric arc furnace (EAF) slag and ladle furnace (LF) slag as alternative fillers in nitrile-butadiene rubber (NBR) composites, replacing conventional fillers such as calcium carbonate.

The primary objective of this study is to evaluate the mechanical properties, processability, and environmental impact of NBR composites incorporating EAF and LF slag in comparison to those containing conventional calcium carbonate at equal filler volume fraction of 10%. This research aims to promote industrial symbiosis by converting steel industry waste into valuable raw materials for the rubber sector.

The study includes a detailed characterization of EAF and LF slag, focusing on their chemical composition, particle size distribution, and morphology. NBR composites were prepared with varying volume fractions of slag and calcium carbonate. Mechanical properties, including hardness, tensile strength, compression strength, and permanent set, were assessed. Additionally, a life cycle assessment (LCA) was conducted to compare the environmental impacts of using EAF slag versus calcium carbonate.

The results demonstrate that both EAF and LF slag exhibit morphological and chemical characteristics comparable to calcium carbonate. Rheometric analysis indicates that slag-filled NBR compounds have similar processability to those filled with calcium carbonate. Mechanical testing reveals that slag-filled NBR composites achieve comparable hardness, compression strength, and elastic modulus to calcium carbonate-filled composites. Notably, slag-filled NBR shows a higher tensile strain at break. The LCA highlights significant environmental benefits, showing reductions of at least 89% in all assessed impact categories when using slag as a filler.

This study provides compelling evidence for the feasibility and environmental advantages of using EAF and LF slag as sustainable fillers in NBR composites. The findings support industrial symbiosis, reducing waste disposal costs and promoting a circular economy. This research sets a foundation for further exploration and implementation of steel slag in rubber applications, contributing to sustainable materials management and environmental impact reduction.

Porous glass-derived products using vitrified ashes from municipal solid waste incinerators

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H6_5, Seminario 1 + 2 Room (Level +1), settembre 16, 2025, 10:30 - 13:30

Implementing circular economy approaches in materials processing and technologies is an important goal from environmental and socio-economical viewpoints because of the decrease in global resources and the constant increase of solid wastes. In this context, we used vitrified bottom ashes from municipal solid waste incinerators as a starting material to produce glass-ceramic foams for possible use in the thermal insulation of buildings. Sinter-crystallization of the material will be studied by thermal analyses (hot stage microscopy and differential scanning calorimetry). The morphological characteristics and chemical composition of the ashes, vitrified material and final porous products will be assessed by scanning electron microscopy and energy dispersive spectroscopy, respectively. The porous architecture will be investigated by combining micro-computed tomography analysis and permeability assessment. Specifically, permeability will be determined by using an acoustic method that involves measuring the pressure drop generated by an alternating airflow through the sample, using an oscillating piston (which creates the flow) and a low-frequency microphone detecting the drop. The advantage of this method is its relative ease of execution, speed and accuracy, especially for highly porous samples without causing any damage to them. The mechanical behaviour of the foams will be investigated by compressive tests and the release of heavy metal ions will be evaluated by leaching tests according to the current standards in order to confirm the suitability and safety of the product.

Enhancing the Wear Properties of CoCrMo Alloy for Orthopedic Application by High-Power Impulse Magnetron Sputtering Nitriding Treatment: Life Cycle Assessment and Critical Raw Material Analysis

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H6_6, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Technological developments in orthopaedic prostheses are mainly focused on improving the biocompatibility and tribocorrosion behavior of used materials in biological environment. CoCrMo alloys are widely applied in medical implants due to efficient biocompatibility and high mechanical characteristics. Previous studies demonstrated the possibility of further increasing their wear and corrosion resistance to overcome concerns about ions and wear debris release in service. Literature works reported different techniques mainly based on thermal treatment or coating approach with the aim to improve the functional characteristics of CoCrMo alloys. Recently, the use of high-power impulse magnetron sputtering (HiPIMS) nitriding treatments has proven effective in enhancing the surface properties of selected alloys. HiPIMS nitriding is advantageous in terms of reducing raw material use and processing time (Ehiasarian & Hovsepian, 2024; Zin et al., 2025). Due to the novelty of tribological improving approach together with the encouraging results, a Life Cycle Assessment (LCA) of the HiPIMS nitriding process at the lab-scale for CoCrMo alloys is presented. The environmental hot-spots have been analysed for two different nitriding treatments, using Mo and Ta targets. The results showed that the electrical consumption was the main impacting driver. The environmental assessment was useful to evaluate possible technological arrangements to decrease the total environmental impact of the treatment. A complementary study was performed on the criticality analysis of the raw materials used as targets during nitriding. The Critical Raw Material (CRM) assessment was performed using the European Commission methods, based on Supply risk and Economic importance indicators (Blengini et al., 2017). LCA at the laboratory scale coupled with CRM evaluation is crucial for identifying the environmental hot-spots at the early stage of development of novel technologies to provide insights for their sustainable development at industrial scale. For this reason, starting from these preliminary environmental results, LCA analysis could be an important approach in the next step of development of nitriding treatment by means of HiPIMS technique in ICMATE laboratories.

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Cost-Effective Approach to Maraging Steel Development Using Mixes of Commodity Alloys

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H6_5, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 10:30 - 13:30

Currently, to achieve high-performance steels like the maraging family with improved strength-to-ductility ratios, alloying elements are required, which are considered critical due to their scarcity, cost, or carbon footprint. Elements like Ni or Co are among these and are crucial to achieving the desired microstructures in advanced maraging steels. Hence, instead of using these elements separately in the production of maraging compositions, an alternative would be the employment of other alloys already containing these elements. As these “commodity” alloys are also manufactured on a large scale, their cost is diminished, and they enable circularity by being recycled. Therefore, the development of high-performance maraging steels using commodity alloys containing essential alloying elements was investigated in this work. Arc melting and additive manufacturing (AM) processes, specifically laser powder bed fusion (LPBF), were employed to produce compositions as close as possible to existing maraging steel grades, including 18Ni-300, MAR-50 Co-free, and MAR-60 steels. Both arc melting and LPBF were used to create the alloys under different conditions, enabling a comparative analysis of the resulting properties and the evaluation of the two production techniques. Furthermore, the study focused on analyzing the structural and microstructural features of the produced alloys, as well as evaluating their mechanical properties. Microstructural characterization consisted mainly of SEM, EDS, XRD, EBSD, and TEM explorations. Besides, hardness measurements were employed together with Profilometry-based Indentation Plastometry (PIP) to assess their mechanical performance. As these steels’ properties heavily depend on their thermal history to ensure their peak performance by precipitation strengthening, heat treatments were applied to optimize the microstructure and enhance the steels’ properties. This approach offers a sustainable and cost-effective method for developing high-performance steels using available scrap from commodity alloys, reducing reliance on rare and expensive critical alloying elements in pure form.

Keywords: Maraging steels, Commodity alloys, Arc melting, Additive manufacturing (AM), Laser powder bed fusion (LPBF).

Thermomechanical analysis of biochar-containing polymer-based composites by Dynamic Mechanical Analysis

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Carbon-based reinforced polymers have attracted significant attention among the different composite materials, due to their versatile nature and fascinating physiochemical properties. The incorporation of carbon fillers within a polymer matrix can lead to major improvements concerning the mechanical, electrical, thermal and tribological properties of the composite material, making them materials of choice for a variety of advanced applications [1]. However, the non-environmentally friendly and expensive nature of typical carbon-based additives including carbon nanotubes, carbon nanofibers and graphene, has raised concerns about their potential integration in a variety of larger scale applications. The necessity of finding eco-friendlier solutions has led to major developments in carbon-based polymer additives derived from natural resources. Such carbon-based fillers usually combine environmental friendliness, recyclability, cost-effectiveness and lightweight structures with excellent thermomechanical and electrical properties. In addition, thermoplastics including polyesters, polyolefins such as polyethylene and polypropylene, polystyrene, nylon and Teflon are gaining increased attention nowadays due to their lower manufacturing costs, high-impact resistance and reprocessing ability and thus recyclability through simple remelting processes [2].

In the present study, biochar fillers deriving from agricultural wastes are utilized as reinforcement materials for selected thermoplastic matrices. More specifically, agricultural wastes are carbonized by employing a large-scale pyrolysis method, followed by their co-processing with thermoplastic materials by means of twin-roll milling, resulting to biochar-containing thermoplastics. The produced composites in which the biochar content was systematically varied, were investigated in respect to their morphological and thermomechanical characteristics by means of scanning electron microscopy (SEM) and dynamic mechanical analysis (DMA), respectively.

Acknowledgments

This work was funded by the European Union Recovery and Resilience Facility of the NextGenerationEU instrument, through the Research and Innovation Foundation (Project: CODEVELOP-AG-SH-HE/0823/0140).

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Investigation of the Tensile Strength of Biochar-containing Thermoplastics

Mrs. Viktoria Theodorou¹, Mr. Paraskevas Kyriacou¹, Dr. Ioannis Ioannou¹, Mr. Spyridon Rallis², Mrs. Nikoletta Karydi², Mr. Charalampos Botsas², Mr. Panagiotis Katsikakis², Mr. David Stephen Garnett³, Mr. Nicos Larkos^{4,5}, Dr. Andreas Grigoriou⁶, Mr. Charis Mikkides⁶, Prof. Theodorou Krasia-Christoforou¹

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Nowadays carbon-rich materials derived from biomass waste known as biochar have gathered increasing attention as sustainable alternatives to carbon-based fillers. Traditional carbon-based nanofillers that are typically employed as additives in polymers to enhance their thermomechanical performance, are neither environmentally friendly nor economically viable. Several scientific studies suggest that the incorporation of biochar into polymer matrices may lead to polymer composites exhibiting superior properties compared to their pristine polymer counterparts, offering comparable or even enhanced mechanical performance compared to those reinforced with expensive carbon nanofillers. This study is structured into two key phases: First, the production of eco-friendly biochar-based thermoplastic composite and second, their mechanical characterization by performing tensile tests under ambient conditions. Sample preparation involved a pyrolysis step that was employed to convert biomass feedstock into a carbonaceous material, followed by a twin-roll milling process to produce composite plates with specific thicknesses. Tensile tests were performed according to ASTM D638 to determine the elastic constant (Young Modulus) and tensile strength of the resulting “green” composites. Overall, this research highlights the potential of utilizing biomass waste to create environmentally friendly products, with biochar emerging as a highly promising, renewable filler in polymer composites. [1-3]

Acknowledgements:

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From cheese-making waste to compostable cheese packaging films: physicochemical and environmental assessment

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H6_2, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Approximately 180 - 190 million tonnes of whey are produced every year worldwide. In particular, around 80 - 90% of the milk required for cheese manufacture becomes whey. In this work, whey protein extracted from cheese-making by-products was analysed as a potential alternative for both food waste valorisation and food packaging waste reduction. With this aim, a complete study of whey protein-based films, from the extraction of the protein to the biodegradation of the film, considering the film manufacture, was carried out in this work. The whey used in this study to extract whey protein was collected from a local farm in the Basque Country. This biowaste was selected for its accessibility and availability. To ensure the maximum protein recovery from whey, ultrafiltration processes were performed. Two fractions were obtained from the ultrafiltration process: a filtrated cheese whey with a content reduced in protein and a purified fraction mainly composed of protein, achieving a final protein content of 91.6 % wt, with the presence of some carbohydrates, such as lactose, as shown by Fourier transform infrared (FTIR) spectroscopy, X-ray diffraction (XRD) and scanning electron microscopy (SEM) analyses. This whey protein, extracted from local cheese whey, was used to produce food packaging films by compression, resulting in transparent and easy-to-handle films. Since the amino acid analysis showed that glutamic and aspartic acids were the major amonoacids in whey protein, films were tested using ethanol as fatty food simulant. The solubility outcomes showed that films were suitable for fatty foods, such as cheese, following this way circular economy strategy. Furthermore, the films were found biodegradable under industrial composting conditions, highlighting the more sustainable character of these packaging films.

Valorization of grape marc extract to develop active gelatin films

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00),
Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The development of active films is essential for extending food shelf life, minimizing spoilage, and reducing food waste. In this context, a novel approach was explored to create gelatin-based active films using choline chloride and citric acid natural deep eutectic solvent (DES) to dissolve chitin (Chi), valorized from fruit fly pupae. Films were manufactured by compression molding, a processing method that can be easily scaled-up, and Chi/DES amounts were varied from 20 to 80 wt %. Resulting films were homogenous, showing no agglomeration and a compact structure, as observed by SEM analysis, providing good mechanical properties in terms of film resistance and flexibility due to the new interactions formed among the components of the film forming formulation, as provided by FTIR and DSC analyses. In particular, a notable decrease of α -helix/random coil and an increase of β -turn were observed in gelatin with the increase of Chi/DES, irrespective of the DES content. Moreover, the incorporation of high percentages of Chi/DES (> 40 wt %) caused a slight decrease of β -sheet. These variations of the secondary structure indicate the physical interactions between gelatin and Chi/DES, which modify the protein secondary structure and, consequently, the film properties. Since the films prepared with 40 wt % Chi/DES showed high UV protection and good mechanical performance for food packaging (tensile strength of 10 MPa and elongation at break of 31 %), these films were selected to prepare active films. In particular, to provide the films with antioxidant properties, red grape marc extract was incorporated into the film forming formulation. The incorporation of this extract not only maintained the mechanical properties of the films but also improved its barrier properties and created a network that promoted the sustained release of the extract. These bioactive-containing films demonstrated oxidation inhibition capacity and, thus, their potential to extend food shelf-life.

A Comparative Life Cycle Assessment of Catalytic Converters: Recycled vs. Conventionally Sourced Platinum Group Metals

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H6_2, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Automotive catalytic converters (catalysts), introduced in the 1970s, have undergone continuous evolution to meet increasingly stringent emission standards. Their primary function is to mitigate air pollution from incomplete fuel combustion by catalytically converting hazardous gases, such as carbon monoxide, hydrocarbons, and nitrogen oxides, into carbon dioxide and water vapor. These converters typically comprise a platinum group metal (PGM)-based monolith core housed within an outer steel shell. PGMs -including platinum, palladium, rhodium, ruthenium, iridium, and osmium- are highly valued for their unique properties. Their exceptional catalytic activity, chemical inertness, corrosion resistance, thermoelectric stability, and aesthetic appeal facilitate their widespread use across diverse industries. Applications range from catalytic converters and hydrogen fuel cells to biomedical implants, aerospace components, and jewellery. However, the limited natural abundance of PGMs (estimated at 66,000 tons globally) necessitates efficient recovery strategies for sustainable production. Currently, the predominant methods for recovering PGMs from end-of-life (EoL) products, such as spent catalysts, are hydrometallurgical and pyrometallurgical processes. Hydrometallurgical methods involve dissolving PGMs in acidic solutions, while pyrometallurgical techniques concentrate them through smelting or roasting. The EU funded PEACOC project presents an integrated approach to PGM recovery, incorporating innovative technologies such as microwave-assisted leaching (MWAL), gas-diffusion electro crystallization (GDEx), superconducting magnetic density separation (MDS), ultra-fast sensor-based sorting (UFS), and the NOVA process. This integrated system aims to provide an efficient and scalable solution for extracting PGMs from EoL resources, including automotive catalysts and electronic waste, with feasibility demonstrated at a pre-commercial pilot scale. A life cycle assessment (LCA) will evaluate the environmental impact of the entire PGM recovery process chain, from EoL product collection to final PGM valorisation. This study will specifically compare the environmental performance of catalytic converters manufactured using PGMs recovered via PEACOC's innovative solutions against those produced using conventional methods. Furthermore, it will identify opportunities to minimize the environmental footprint and ensure the new processes contribute to sustainable practices within the automotive sector.

Raman I(D)/I(G) Analysis of Carbon-Based Materials Derived from *Mauritia flexuosa* (Aguaje) Residues

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

There is great interest in obtaining increasingly efficient, economical, and biodegradable materials. Low-cost carbon-rich materials have become a green

alternative for producing graphene-like materials for energy storage devices, sensors, and composite materials applications. For this reason, a one-step process for reforming *Mauritia flexuosa* (aguaje) residues under oxidation conditions with ferrocene is proved.

Aguaje is a fruit whose pulp demand increases over time, generating residues as its seeds. Ferrocene is applied as an oxidizing catalyst via direct carbonization in a

muffled furnace at 450 °C under atmosphere conditions. Contact time (15 to 30 min), particle granulometry (around 180 to 250 µm), and ferrocene ratio (5 to 15 %) influence

the transformation of an amorphous carbon phase to a graphene-like structure of sp² hybridization. The ratio of intensity D (structural defects) and G (sp² carbon pairs in

chains and rings) bands on Raman spectra was used as a response. Raman, FTIR, and SEM techniques characterized the structure of the obtained materials. It is

observed that the D/G ratio increase required a longer time with higher size-particle.

Electrochemical properties are evaluated with cyclic voltammetry on a ferro/ferri system with all synthesized materials.

CE-RISE (Circular Economy Resource Information System): A Digital Infrastructure for sharing information and connecting stakeholders along the circular supply chain

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H6_5, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 10:30 - 13:30

The European Green Deal, through its Circular Economy Action Plan, introduced transformative measures to enable circular economy in the manufacturing sector. Policies like Ecodesign for Sustainable Products Regulation and Critical Raw Materials Act set clear targets for products and materials to optimize resource use and efficiency across the supply chain. To support this, a key objective of the CE-RISE project is to develop indicators based on product composition, material criticality, and safety concerns. This will allow first assessing and later communicating a product's potential for circular economy applications through a dedicated digital infrastructure, building on tools such as the Digital Product Passport (DPP). Therefore, CE-RISE will allow informed decision-making throughout a product's or material's life cycle.

The CE-RISE digital infrastructure uses data stored in DPPs, and user-supplied data, to perform key calculation routines for monitoring and assessing circularity, accessible through an online platform. The platform incorporates indicators to measure a product's potential for effective circular economy implementation and quantifies actual contributions through circularity ratios, such as the proportion of secondary raw materials used. These indicators, together with a socio-economic and environmental impact assessment, provide insights into both the feasibility of circular economy practices and their broader implications. By connecting these metrics, the framework ensures transparent evaluation of a product's circularity, assessing its alignment with circular economy principles and its impact on material efficiency and environmental/social sustainability.

The infrastructure adds value to actors along the whole value chain, such as original equipment manufacturers or post-use operators, as well as consumers. The combined set of indicators, circularity ratios, and socio-economic and environmental assessment, help guide and inform them in different ways. In the presentation we will show how manufacturers benefit using the platform to meet regulatory requirements, such as incorporating recycled or remanufactured materials, and efficiently reporting compliance in a quantified manner. Consumers benefit from precise and easily accessible indicator scores, enabling them to make well-informed purchasing decisions. Finally, post-use operators rely on the platform to access reliable data and tools to support material/ product recovery and reintegration into the supply chain.

We will present the CE-RISE conceptual framework with the developed indicators to assess the extent to which end-of-life products and materials can contribute to enhancing sustainable supply chain management. First insights from the use cases, representing the various perspectives of manufacturers, post-use operators and consumers, demonstrate the value of the CE-RISE digital infrastructure in aiding them materialize the circular transition.

From Waste to Value: Harnessing Green Technologies for Residue Valorization and Circular Textile Innovation

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H6_1, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

Forestry and agriculture industries generate tons of waste each year, driving a global quest for sustainable and circular waste management solutions. As circular economies gain traction, innovative strategies to maximize residue utility while minimizing ecological impact have gained importance. Upcycling byproducts through bioconversion and resource recovery offers potential for value creation and market expansion across various sectors. Several pollutant industries, like the textile, are putting great effort into the development of more sustainable processes and bio-based solutions empowering decarbonization and zero-waste.

In this sense, the be@t project - Bioeconomy at textiles - is transforming Portugal's textile and apparel sector with its approach: "From nature to people, in a circular and sustainable way". This initiative aims to overhaul the entire textile value chain by introducing innovative, sustainable solutions promoting circular bioeconomy.

One strategy involves valorizing forestry and agro-industrial residues by extracting bioactive compounds and pigments to mitigate the negative ecological impacts of synthetic dyes, while conferring health benefits to textiles. The project offers opportunities for value addition and market diversification. For that, greener extraction technologies (energy-efficient processes), have been employed, which offer advantages such as reduced solvent consumption, shorter extraction times, and higher yields.

This study explored biomass from eucalyptus and banana leaves to obtain bioactive compounds and pigments using ultrasound-assisted extraction combined with eco-friendly solvents. Extracts were characterized for bioactivity and incorporated into formulations for spray-coating (known for minimal material waste and reduced energy consumption) in different natural fibers like cotton and linen. Alongside this approach, micronized banana leaf residue, resulted from the extraction process, was also used as raw material for textile coating, envisioning a full circular process, conferring coloration and residual bioactivity. The spray-coated textiles were assessed for relevant properties for the sector (washing and light fastness) as well as the functional properties (antioxidant, antimicrobial and UV protection), demonstrating promising results as sustainable alternatives to conventional dyeing and functionalization products.

This work highlights the potential of forestry and agro-industrial residues as valuable resources within a circular bioeconomy framework. The results underscore the feasibility and the advantages of integrating greener technologies and bio-based solutions into industrial processes, such as textile manufacturing, to promote sustainability and reduce environmental impact, aligned with global decarbonization and zero-waste goals.

The authors acknowledge financial support from the integrated project be@t – Textile Bioeconomy (TC-C12-i01, Sustainable Bioeconomy No. 02/C12- i01.01/2022), promoted by the Recovery and Resilience Plan (RRP), Next Generation EU, for the period 2021-2026.

Solid-State Upcycling Of Aluminium Alloy Machining Residues

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H6_6, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The conventional subtractive manufacturing processes generate a considerable amount of machining residues in the form of machining chips which are generally regarded as low-value scrap.

This study investigates the feasibility of using a mechanical milling technique for converting scrap machining chips into aluminum alloy powder suitable for additive manufacturing (AM), particularly laser powder bed fusion (LPBF) and laser direct energy deposition (DED). Mechanical shearing combined with ball milling is employed to convert the scrap material into a powder form that can be utilized in AM. Considering the requirements of these processes, the particle size distribution, particle shape, flowability, and spreadability of the resulting powder are analyzed and compared to a similar-grade commercial alloy to assess its suitability for purpose. Additionally, the evolution of the microstructure from the starting material to the ball-milled product is observed and discussed. The results of this study provide insights into the potential of upcycling the scrap machining chips into useful feedstock for AM processes. The findings of this research contribute to the development of an energy-efficient and environmentally friendly method for producing aluminum alloy powders suitable for AM applications.

Recovery and efficiency improvement of a TiO₂-rich waste: the case of tionite

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

The depletion of natural resources and the progressive environmental deterioration have emphasized the need for more sustainable chemical processes. A common solution is sustainable remediation, which involves removing pollutants released in the environment. Photocatalysis, particularly using titanium dioxide (TiO₂), proved efficient in degrading a wide range of organic contaminants at ambient conditions. However, due to the high environmental impact of TiO₂ production and market volume, more sustainable practices in TiO₂ preparation are needed. Traditional TiO₂ production, namely mineral extraction and liquid-phase synthesis, require high energy and solvent consumption. TiO₂ extraction from wastes has been considered, but the solution still has a strong environmental impact. Therefore, the direct use of Ti-rich residues or their improvement through mild chemical procedures remain more sustainable options but poorly explored. This scenario prompted us to investigate and optimize a TiO₂-rich waste material, known as tionite, obtained by the recovery and neutralization of the insoluble components from the TiO₂ production by sulfate process. Considering the rising interest toward circular economy, the final goal is to close the loop of TiO₂ industrial production through the application of tionite as a sustainable photocatalyst.

Tionite obtained using Ca(OH)₂ as a neutralizing agent showed NPs with various shapes made of a combination of TiO₂, mainly in the rutile phase, aluminosilicates and a significant amount of CaSO₄·2H₂O. Since preliminary photocatalytic tests conducted on tionite showed no significant photodegradation yields, a treatment based on NaOH neutralization was carried out to simplify tionite composition and improve its photoactivity. The new tionite shows a more homogeneous morphology consisting of titania NPs and aluminosilicate sheets with different counterions. To further simplify tionite composition, mild treatments with HF or NaOH were carried out to remove SiO₂-based components, as confirmed by a multi-technique characterization.

The obtained tionite samples, having different physico-chemical characteristics, were tested for different photocatalytic applications. At first, samples were employed in both traditional photocatalysis and photo-Fenton processes, but no significant decay was observed. On the other hand, remarkable selectivities were obtained in the application of tionite samples for the partial oxidation of ferulic acid to vanillin, an industrially relevant compound. The application of tionites in peroxymonosulfate (PMS)-assisted catalysis demonstrated a remarkable efficiency in PMS activation and 4-chlorophenol (4-CP) degradation for all samples.

In conclusion, TiO₂-based materials not only can reduce environmental pollution by degrading organic molecules, but the development of sustainable strategies for their production and preparation is possible.

Green ironmaking at higher H₂ gas pressures: Reduction kinetics and microstructure evolution of hematite

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H6_4, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Steel production is a key factor in the global transition toward sustainability, however, it is the largest source of CO₂ emissions in the industrial sector, contributing 7–8% of global emissions. Hydrogen-based direct reduction (HyDR) has attracted immense attention as a promising solution for producing sustainable iron from iron ores without CO₂ emissions. This solid-gas reduction process with H₂ occurs in multiple sequential steps, converting hematite into magnetite, then wüstite, and finally metallic iron at temperatures above 570°C. While previous studies indicate that H₂ gas pressure influences the reduction kinetics and microstructural evolution of iron ore during HyDR, the fundamental reaction mechanisms governing each step remain poorly understood. Here, we perform in-situ synchrotron high-energy X-ray diffraction during HyDR to monitor real-time phase transformation kinetics of hematite at different H₂ gas pressures at 1, 10, 50, and 100 bar at 700 °C. The microstructure evolution of the reduced hematite specimens was characterized using scanning electron microscopy equipped with the electron backscatter diffraction (EBSD) technique. Furthermore, the influence of H₂ gas pressures on the three-dimensional pore structure of reduced iron was analyzed using X-ray nano-computed tomography. The results offer valuable insights into the pivotal role of H₂ gas pressures in HyDR, paving the way for improving the reduction efficiency of HyDR.

Bridging Material Science and Life Cycle Assessment: Integrating OpenSemanticLab with openLCA for Comprehensive Early-Stage Sustainability Optimization

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H6_5, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 10:30 - 13:30

Safety and sustainability by design (SSbD) are increasingly critical in material science, especially in the pursuit of a circular economy. However, these considerations are often absent in the early stages of material development, where key decisions determine the direction and impact of research. This gap arises from a disconnect between material scientists and sustainability experts, which is amplified by diverging data structures and a lack of a common language between both domains. To address this challenge, we present an innovative approach that integrates OpenSemanticLab with openLCA, effectively building a digital bridge between material science and Life Cycle Assessment (LCA).

Our methodology involves the creation of linked data schema for an electronic lab notebook (ELN) compatible with the openLCA data schema. By utilizing JSON-LD, shaped with JSON-SCHEMAS, we generate a user-friendly web interface through the OpenSemanticLab software stack. This interface empowers material scientists to input data on processes and materials directly from the lab using only a web browser, without requiring any knowledge of JSON-LD or openLCA. This accessibility ensures that sustainability considerations are seamlessly integrated into everyday laboratory practices.

Beyond capturing general material and process properties, our system also incorporates economic and technical performance indicators, as well as Quantitative Structure-Activity Relationship (QSAR) toxicity metrics. This comprehensive data collection enables global multi-target optimization, allowing researchers to simultaneously consider safety, sustainability, performance, and cost factors in material development. By integrating these diverse metrics early in the research process, we facilitate more informed decision-making aligned with SSbD principles.

Building a system that enables the creation of a knowledge graph of experimental setups that can be automatically converted into openLCA workflows and processes was made possible by integrating OSL with openLCA via a Python plugin application. This tool queries and selects process entities, automatically assigns them to the appropriate format and generates an openLCA ZIP archive for import. LCA experts can then perform semi-automated or fully automated predefined assessments, evaluate various scenarios and provide immediate, valuable feedback to material researchers. By incorporating economic and technical performance indicators alongside QSAR toxicity metrics, the platform enables a holistic assessment of materials fostering early-stage innovation that aligns with circular economy principles.

We demonstrate this approach with a case study on paper-based electronics showcasing the potential of coupling materials and sustainability research from the outset. The integration not only facilitates the incorporation of SSbD principles but also enhances collaboration between disciplines contributing to resource optimization and waste reduction.

Maximising value and positive impact in campus-based circular economies of coffee

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H6_6, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

Our project, Circular Action for People and Planet: Using Coffee and Creativity in Innovative Networks and Operations (CAPPUCCINO), explores the creation of circular economy models of coffee based on university campuses by upcycling spent coffee grounds (SCGs) from on-campus coffee shops as a multi-product feedstock. SCGs are an abundant waste material on university campuses and current practices around their disposal leave a lot to be desired: key issues we have identified include human behaviour (e.g. café staff and community attitudes to disposal units, leading to significant contamination), patchy collection schedules, non-local non-sustainable transportation, and conversion into a carbon-emitting fuel pellet final product.

Herein, we present our vision and current work towards tackling this problem, in collaboration with partners in the United States of America and Brazil, in order to sustainably extract maximum material and chemical value from SCGs whilst simultaneously using the initiative for enhanced community engagement.

The model—which, crucially, can be adapted and optimised to different campuses—is segmented into three parts: Collection, Processing, and Product Creation. In Collection, we present strategies for mitigating the possibility of SCG contamination and discuss the opportunity for student engagement with the project. In Processing, we present a multi-step extraction of chemicals and materials. In Product Creation, we discuss the multitude of final products that can then be used either by research groups based within the university or by consumers. This final part of the model also offers fertile ground for the development of educational initiatives within the university and public engagement and outreach initiatives with local communities, as well as enterprise opportunities for the creation of sustainable ventures and a bottom-up approach to decentralised circular economies.

CAPPUCCINO presents a new, decentralised approach of integrating research, innovation, education and engagement on university campuses. In so doing, we hope to instigate a positive shift regarding the role of universities in the creation of sustainable value, broadly writ, highlighting the critical role of materials circularity in this endeavour.

RECOVERY AND VALORIZATION OF SILICA FROM FLUORO-DERIVATIVES INDUSTRY WASTE FOR ADVANCED TECHNOLOGICAL APPLICATIONS

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H6_5, Seminario 1 + 2 Room (Level +1), settembre 16, 2025, 10:30 - 13:30

In recent years, the recovery of silica from waste or end-of-life products has become a challenging issue as an effective waste management strategy and a sustainable circular economy model. In this context, the aim of the present work is the valorisation and reuse of silica as by-product of the recovery process to obtain CaF_2 as secondary raw material from hexafluoro silicic acid H_2SiF_6 (FSA), which is a hazardous by-product of phosphate and fluoride industry.

The main objective is to set the large-scale recovery process, based on the NH_4OH reaction with FSA, to directly provide silica particles with specific structural and morphological characteristics, aimed at reusing silica for highest value applications such as reinforcing filler for elastomeric nanocomposites with high mechanical properties for tyre industry. The conditions of process and post-process treatments were modulated to obtain FSA-derived silica with high surface area and controlled size, shape, aggregation and textural features by varying process temperature (3-20°C), pH (7.8-10), silica powder washing solution (acid/basic) and drying method (oven/fluid bed/spray drying) conditions.

FSA-derived silica was morphologically and structurally characterized by SEM and TEM microscopy, XRD, TGA and nitrogen physisorption BET. Composition and purity were assessed by XRF, solid state NMR and XPS spectroscopy for the elemental surface analysis of silica particles.

FSA-derived silica was tested as reinforcing filler for elastomer nanocomposites upon incorporation in Isoprene (IR) and Styrene Butadiene (SBR) matrix. The reinforcement properties of the filler was analysed by studying the vulcanization curves (at 170°C for 15 min.) of the rubber nanocomposites, showing comparability with those of rubber nanocomposites prepared with commercial silica filler commonly used in the rubber industry. The mechanical behaviour at low deformation of nanocomposites prepared with FSA-derived silica, acquired by determining the strain dependence of the shear modulus G , confirms the good properties of the material prepared by reusing the silica from waste, comparable with that obtained using the commercial reference.

The results indicate that FSA-derived silica has demonstrated interesting features alongside comparable performances to those of commercial silica as reinforcing filler for rubber composites with high mechanical properties, allowing to consider it as a valuable and convenient alternative from a waste recovery process to conventional silica filler in large scale tyre manufactures.

Mapping Circularity, Responsibility and Sustainability in Power Electronics Research: A Bibliometric Analysis

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H6_1, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 9:20 - 10:20

The sustainability of power electronics is an increasingly pressing issue, given the criticality of materials like cobalt, rare earth elements and gallium, all vital to global energy and digital transitions. These materials are often sourced from geopolitically unstable regions, raising concerns over resource depletion, exploitative labour practices and the concentration of supply chains in the Global North. These challenges represent one facet of the broader sustainability issues in electronics manufacturing. Circular economy strategies, including recycling, remanufacturing and material recovery, are explored as solutions. However, the integration of social responsibility, particularly issues related to responsible manufacturing, supply chain justice and social life cycle assessment, into power electronics research aimed at supporting the global energy transition remains underexplored[1].

In this bibliometric analysis, VOSviewer software tool is employed to assess the co-occurrence of circularity and social responsibility and terms related to power electronics research including integration and design, mapping the prevalence and thematic focus of these issues in academic discourse. Web of Science serves as the exclusive data source, with a structured search strategy identifying relevant publications from 2010 to the present. A targeted set of keywords relating to power electronics, circular economy, ethics, sustainability justice and the global energy transition are applied using Boolean operators to ensure comprehensive retrieval. The dataset is refined through inclusion and exclusion criteria, filtering out irrelevant studies and duplicates. Bibliometric techniques, including co-occurrence analysis to identify dominant research clusters, co-citation analysis to pinpoint influential works and citation network analysis to map scholarly influence, are used. Visualisation of trends in VOSviewer identifies key intersections between the technical and social dimensions of circularity in power electronics. Temporal keyword analysis tracks the evolution of ethical concerns, highlighting priorities such as responsible manufacturing and supply chain justice within the global energy transition.

Thematic analysis using NVivo explores how social considerations like social life cycle assessments and sustainable design are represented in power electronics research, offering a holistic view of how these issues are integrated into developments supporting the global energy transition. A manual/semi-automated approach is used to identify links to funding sources, policy documents and industry connections, providing an overview of the broader social and economic forces shaping the field. Potential biases in the Web of Science database, particularly the underrepresentation of research from the Global South, are acknowledged. The study also reflects on the systemic marginalisation of knowledge production from regions most affected by extractive practices.

[1] Sustainability 2024(16)2221. <https://doi.org/10.3390/su16052221>

Upcycling bio-based side streams for 3D printing of sustainable bioplastic filaments

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H6_6, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The valorisation of industrial side streams into high-performance biomaterials represents a key strategy for advancing circular economy principles in materials science. In this study, bio-based byproducts were investigated as sustainable feedstocks for the development of 3D-printable thermoplastic bioplastics, targeting applications in fused filament fabrication (FFF). Non-purified starch recovered from potato washing slurries was processed into a hydrophilic and flexible thermoplastic material, which could be extruded as a filament but exhibited excessive moisture sensitivity and lacked structural integrity for direct FFF processing. To enhance its printability, leather-rich byproducts derived from footwear industry, underutilized tomato wastes, and coffee byproducts (coffee silverskin and spent coffee grounds) were used, allowing to tune the physicochemical and mechanical performance, and FFF capacity of thermoplastic starch-based filaments. The results demonstrated the feasibility of upcycling bio-based side streams into engineered bioplastic filaments with potential for sustainable manufacturing. This approach contributed to waste valorisation in the agrifood and footwear industries, while offering a viable route for the eco-friendly production of customized 3D-printed biopolymeric structures, promoting innovation at the intersection of biopolymers, additive manufacturing, and green materials design. Acknowledgments: This work was developed within the scope of the project “FAIST – Fbrica gil, Inteligente, Sustentvel e Tecnolgica” (Project no. 66 with the application C644917018-00000031), financed by PRR – Plano de Recuperao e Resilincia under the Next Generation EU from the European Union, and CICECO - Aveiro Institute of Materials, UIDB/50011/2020 (DOI 10.54499/UIDB/50011/2020), UIDP/50011/2020 (DOI 10.54499/UIDP/50011/2020) & LA/P/0006/2020 (DOI 10.54499/LA/P/0006/2020), financed by national funds through the FCT/MCTES (PIDDAC). FCT is also thanked for the Individual Call to Scientific Employment Stimulus (IG, <https://doi.org/10.54499/CEECIND/00430/2017/CP1459/CT0032>). The Portuguese companies A Saloinha, Carit, FEB Cafs, and Hit Tomato are also acknowledged for supplied the bio-based side streams.

Driving the Circularity of Materials with Digital Solutions: A Case Study on Integration with the CE-RISE Information System

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H6_3, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

Transitioning to a circular economy (CE) requires a robust information framework to enable transparency of material sourcing, use, and recovery. Digitalization can play a key role in improving transparency, traceability, and efficiency across industries. The CE-RISE (Circular Economy Resource Information System) project, funded by the European Union (EU) under Horizon Europe, is developing an advanced system to facilitate data sharing across the value chain. In July 2024, the Ecodesign for Sustainable Products Regulation (ESPR) came into effect, requiring Digital Product Passports (DPPs) full implementation expected by 2030. DPPs provide essential data on product composition and its environmental impact, amongst others. CE-RISE aims to implement an intelligent data system that integrates DPPs, RE-indicators (such as recyclability and repairability), lifecycle assessments, and socio-economic indicators. By enabling better traceability, predictive maintenance, and informed decision-making, this digital infrastructure will help increase product circularity and reduce waste.

This presentation explores how CE-RISE leverages digital tools to drive circularity. CE-RISE will provide detailed end-of-life options and information, empowering consumers, manufacturers, and repairers to make informed decisions. We examine how materials data management software can enhance the information system by providing more comprehensive information about materials' properties and processes among others. As part of this project, we focus on integrating Ansys Granta MI Enterprise with CE-RISE systems to support decision-makers in developing circular strategies based on materials in products. We propose a framework within the CE-RISE project, that links with DPP systems and a product Bill of Materials (BoM) to generate reports on restricted substances in materials, assessed against legislation. Additionally, the framework delivers sustainability data, including climate impact (CO₂-eq) and material attributes such as recyclability and biodegradability. This enables a deeper understanding of products' sustainability credentials.

Hybrid nanomaterials from biowastes for sustainable agriculture

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H6_6, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 17:00 - 19:00

The use of nano-fertilizers can heavily support transition towards a more sustainable farming system, by exploring eco compatible materials able to enhance nutritional efficiency, biotic and abiotic stress tolerance, and/or crop quality.

At the same time, the huge amount of waste generated, 338 million tonnes per year worldwide, with biowaste (BW) being the widest component, has caused economic and technological challenges to reduce and mitigate its environmental impacts due to improper management [2]. Indeed, BWs are emerging as a cheap and abundant source of chemical and biological richness, in view of their multiple properties including metal ion chelating, as well as intrinsic red-ox behaviour involving antioxidant and antimicrobial activity. Among BWs, lignin and humic acids exhibit great efficacy in improving plant growth and nutrition [3]. Furthermore, molecular combination of BWs with an inorganic nanostructured phase can address the issues related to high heterogeneity, provide stability and boost intrinsic bioactive features [4]. In this context, hydroxyapatite (HA), is an ideal component for forming hybrids with lignin (L), expanding its applications. Moreover, encapsulation of hybrid nanostructures into electrospun fibers can provide with 2D and 3D constructs mimicking soil structure.

Herein, it is highlighted the bio-stimulant potential of hybrid nanomaterials derived from BW valorization according to a biomimetic approach. Notably, hybrid BW-apatite nanostructures have been designed and encapsulated into electrospun polylactic acid (PLA) fibers. On one hand, obtained nanostructured materials exhibit marked antioxidant activity as well as widespread potent biocide action towards phytopathogenic bacteria and fungi. On the other hand, they promote proliferation of microorganisms beneficial to the soil microbiome. Following a holistic approach to sustainability, this study provides with organo-mineral systems with multifunctional activity and boosted efficacy .

[1] Chemosphere 292 (2022) 133451

[2] Environmental Pollution 324 (2023) 121363

[3] Journal of Cleaner Production 366 (2022) 132832

[4] International Journal of Biological Macromolecules, 2024, 280, 135946

Reuse of Plastic Waste in the Agricultural Sector: Another Step Towards Sustainability

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Plastic consumption has experienced exponential growth, leading to the accumulation of waste in landfills around the world. For this reason, various countries and institutions promote the reduction of plastic use and the increase of its recycling to protect the environment. However, although this effort aims to reach all scenarios, some of them are ignored, such as the agricultural sector. The management of plastic waste from agricultural and livestock use is hindered by the lack of interest from companies and institutions, and as a result, a large portion of the waste generated ends up scattered across fields and forests. This research aims to find a new use for the plastic waste generated in the agricultural sector, a solution that is more attractive and encourages companies to recycle it. This study focuses solely on packing ropes or raffia ropes: polypropylene ropes used to compact different types of grasses for livestock consumption. A clear influence of degradation on the properties of this material was observed. To determine these properties, different test specimens were manufactured, and subjected to compression and bending tests, accompanied by optical analysis to understand the behavior of the material throughout the study.

Replacing boric acid in industrial nickel electroplating: toward REACH compliant electrolytes

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H6_2, Seminario 1 + 2 Room (Level +1), settembre 15, 2025, 10:50 - 13:10

Boric acid plays a crucial role in industrial nickel electroplating, acting as a buffering agent to stabilize pH and improve deposit quality. However, due to its classification as a substance of very high concern (SVHC) under the REACH regulation (EC No 1907/2006), industry faces increasing pressure to find suitable alternatives. Substituting boric acid is challenging, not only for its consolidated role in the plating industry but also for its intrinsic qualities: high bath stability, grain refinement, exceptional pH stabilization. Alternative buffering agents must therefore ensure equivalent pH control, without compromising bath stability, in front of comparable coating properties.

The substitution is crucial for well-established practices like bright nickel plating, but it also constitutes an important step toward the development of nickel-based composites. These are deposited by dispersing functional nanoparticles in an electrodeposited nickel matrix. Such particles can be either hard ceramic particles (B_4C , Al_2O_3 ...), suitable to improve the wear resistance of the layer, or solid lubricant particles (graphene, MoS_2 ...), which confer low friction coefficient and self-lubricating properties [1]. Hard composites, in particular, are promising for the replacement of hard chromium coatings. This action is vital for a wealth of industrial applications, as the hexavalent chromium species required for hard chromium plating are harmful for human health.

The ongoing research is focusing on boron-free buffers for the deposition of both pure nickel coatings and nano-composite layers, but industrial-scale implementation remains complex. The electroplating sector must balance regulatory requirements with technical feasibility to ensure sustainable and efficient nickel deposition. In this context, the MOZART European project aims at implementing electrolytes compliant to the REACH normative for the electrodeposition of nickel-based materials as alternatives to hard chromium.

The present work aims at discussing, in the framework of the MOZART project, the feasibility of boric acid replacement for the industrial electrodeposition of nickel. The laboratory practice is discussed in parallel with the industrial practice, considering the point of view of the partners of the project. The influence of some alternative buffers, mainly belonging to the class of carboxylic acids [2], on the properties of the coatings obtained is evaluated. Then, the impact of such alternative buffers on LCA is evaluated, with a particular focus on bath longevity and disposal procedures.

[1] R. Karmakar et al., *Met. Mater. Int.* 27, 2134–2145 (2021)

[2] H. Riechmann et al., *Trans. Inst. Met. Fin.* 95(2), 73-77 (2017)

Valorization of Construction and Demolition Waste in Ceramic Tile Industry: A Sustainable and Circular Economy Perspective

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H6_4, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Construction and demolition waste (CDW) accounts for one-third of the total solid waste generated annually. This waste typology has a low recycling rate due to several inherent characteristics, including its high heterogeneity and the absence of a unified management policy that enables these materials to be obtained in a form suitable for

upcycling applications. The ceramic tile industry plays a significant role in the European economy, particularly in countries like Spain and Italy. For example, in Spain, this industry accounted for 15,000 direct jobs and €4.864 billion in revenue in 2023. However, it is also a sector with high energy and natural resource demands, being responsible for 143.823 tons of CO₂ emissions not covered by free allowances in 2023 [1].

Therefore, the transition of this industry towards a circular economy model and decarbonisation is essential for achieving a greener future.

This work explores strategies aimed at increasing the sustainability of the ceramic tile industry, with a special focus on the recovery of CDW and low-impact practices.

Firstly, it explores a system for quantifying construction materials based on chemometrics applied to Raman and SWIR spectroscopies. This methodology quantifies the brick and concrete content in real CDW samples, providing a tool for applications where material composition is critical, such as in recycled ceramic tiles. [2] Secondly, the easibility of manufacturing ceramic tiles with 55 wt% of real CDW at a high level of industrial readiness (TRL 7) is demonstrated. After various experimental assessments, industrial

production of recycled ceramic tiles was achieved, containing 89% ceramic debris and 11% mixed CDW. These tiles exhibited flexural strength and water absorption values that classify them under BI and BIII typologies of ISO13006, respectively, confirming their industrial viability.

In addition, the development of a traceability tool based on a photoluminescent ink compatible with ceramic glaze is explored. For the first time, a photoluminescent pigment based on (Ca,Sr)(Na,K)AlSi₃O₈:Eu³⁺ was designed, characterised, and scaled industrially. Applied via inkjet printing, the pigment remains invisible under visible light but becomes visible under UV light, enabling smartphone-readable traceability. [3] Finally, cold sintering was explored as a sustainable manufacturing route. Compositions with up to 95% CDW showed flexural strength above required thresholds by the standard, which increased significantly after post-treatment at 1100 °C without compromising dimensional stability [4,5]. In this way, the study proposes a multi-strategy advancement in sustainability for the ceramic tile industry.

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Development of a thermoplastic starch-based compound for extrusion of biodegradable foams

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H6_2, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 10:50 - 13:10

Starch foams have gained attention due to growing concerns regarding their non-biodegradable counterparts. Since the early 90s, starch foams have been extensively used in niche applications, such as extruded foam peanuts, where they offer a positive balance between cost, cushioning performance, and ease of disposal through composting or water dissolution. However, poor processability, weak mechanical properties, and low water resistance have limited a wide utilization of starch foams as packaging solutions. To improve starch foams processability, researchers have explored their plasticization, chemical modification, and blending with other polymer or additives. These advances, coupled with stricter environmental regulations targeting expanded or extruded polystyrene (EPS and XPS), have contributed to a revived interest in starch-based foams. This study aims to develop a starch-based material suitable for extrusion foaming through the compounding of a modified thermoplastic starch (TPS) and an expandable grade of polylactic acid (PLA). The extrudability of the TPS/PLA blends with different TPS contents (0–100 wt.%) was evaluated by analyzing their thermal properties (DSC and TGA) and processing behavior (screw torque, melt viscosity, and melt flow index). Moreover, selected TPS/PLA blends foamability with a chemical blowing agent (CBA) was evaluated using a laboratory-scale twin-screw extruder. Apparent density, compression behavior, and foam morphology were monitored as a function of the TPS/PLA ratio of the blends. Furthermore, the effects of CBA concentration, screw speed, and die temperature on the starch foam structure and physicochemical properties were also analyzed. Interestingly, as TPS content increased, the melt transition temperature decreased, leading to higher flowability and lower screw torque under similar extrusion conditions. These results highlight the opportunity of leveraging the material composition and processing conditions to obtain starch foams with enhanced properties which can contribute to higher material circularity in the packaging industry.

Acknowledgments

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Circularity for Metal Additive Manufacturing: a review

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H6_5, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 10:30 - 13:30

Material production contributes to 25% of global CO₂ emissions, highlighting an urgent need to transition towards a more circular economy. Metal Additive Manufacturing (AM) offers the potential to revolutionise industrial production by enabling complex geometries and improving material efficiency. However, sustainability challenges persist, particularly concerning metal feedstock. The use of recycled feedstock in AM remains underexplored, necessitating further investigation. This research explores circularity in metal AM feedstock. This research will be undertaken through a systematic literature review and meta-analysis. The study will encompass Powder Bed Fusion (PBF) and Directed Energy Deposition (DED) processes, focusing on metals that have been previously investigated for recycling. First, feedstock minimum quality requirements will be examined. Then, various metal waste streams both inside and outside the AM chain (e.g. machining scrap, end-of-life components, and residual material from AM processes), will be identified. The selection and pre-processing stages (e.g., cleaning, shredding) required to prepare these materials for reuse will also be explored. Next, conversion methods (e.g. powder atomization, ball milling and wire drawing) will be researched to determine their suitability for transforming pre-processed metal waste into viable PBF and DED feedstock. The study will also investigate the impact of using recycled materials on feedstock quality, processability, and on the resulting microstructure and mechanical properties. A comparative analysis will be conducted between parts fabricated using recycled versus virgin feedstock, evaluating differences in the presence, quantity and morphology of various phases, precipitates and defects. These microstructural variations will be correlated with the mechanical performance of the parts. Integrating recycled materials into AM aligns with sustainability objectives of reducing raw material extraction, minimising waste generation, and lowering environmental impact. The findings will contribute to the broader effort of advancing circular economy principles in AM, paving the way for more resource-efficient and sustainable manufacturing practices.

Recycled Inconel 718 Powder for sustainable metal additive manufacturing

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H6_4, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 17:00 - 19:00

Inconel 718 is widely used in additive manufacturing (AM) due to its exceptional corrosion resistance and superior mechanical strength. However, the reuse of powder in AM processes raises significant challenges, as alterations in powder properties can potentially compromise the performance of fabricated components. This study explores the feasibility of reusing Inconel 718 powder by evaluating a mixture composed of 50% cyclone-collected used powder and virgin powder, with virgin powder serving as the baseline for comparison. Comprehensive characterization of the powders was conducted, focusing on particle size distribution, flowability, and chemical composition. To determine the impact of powder reuse on part quality, defect analysis was performed on laser powder bed fusion (L-PBF) specimens using light microscopy to assess porosity and defect distribution. Mechanical properties were further evaluated through tensile and fatigue testing. The results revealed that pore distribution trends were consistent between the virgin and blended powders, with pore sizes consistently below approximately 70 microns. Tensile testing demonstrated negligible differences in yield and ultimate tensile strength between the two powder types. Interestingly, fatigue testing indicated enhanced performance in components produced from the blended powder. These findings suggest that incorporating partially recycled Inconel 718 powder in AM processes is not only feasible but also advantageous, offering a sustainable and cost-effective solution without sacrificing mechanical performance. This study underscores the potential for optimizing powder reuse in AM, contributing to both economic and environmental benefits in advanced manufacturing.

Safe and Sustainable by Design Framework: An Exploratory Case Study in Additive Manufacturing with a Focus on Surface Functionalization of Parts with Complex Geometry

Mrs. Khadija Sarquah^{1,2}, Marta Revello^{1,2}, Maja Jelic¹, Prof. Dr Gesa Beck^{1,2}

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H6_5, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 10:30 - 13:30

The growing environmental challenges for materials exploration and production have necessitated a global adoption of sustainable practices to minimise resource depletion, waste and global warming. Additive manufacturing (AM) is a potential technology for increasing resource economy and environmental performance in manufacturing systems. Recent research, however, has demonstrated that the design and functionalisation of complex manufactured parts affects the sustainability of AM. The EU Safe and Sustainable by Design Framework as an iterative guideline aims to minimise environmental and social impacts throughout a product's life cycle while enhancing overall functionality and economic value. This study explores the application of SSbD to the design of complex shaped parts via additive manufacturing and surface functionality based on laser technologies. Four use cases were studied in different fields of application: biomedical (femoral component of a knee implant), aerospace (clamp band), and aviation (pivot bracket and lever). The study involved a life cycle mapping of the use case supply chain followed by a Material Energy Toxins (MET) analysis that expanded to include Criticality, Environment (land), and Social elements, referred to as C-MET-ES. Qualitative and quantitative data were analysed for C-MET-ES matrix, hotspot analysis using ranking, weighting, and expert group evaluation. A chemical hazards risk and gender dimensions assessment identified specific concerns related to post-processing. The results provide recommendations towards material changes and improvement of resource efficiency in target use cases via additive manufacturing, laser post-processing, and in-line monitoring. The outcome of this study contributes to a well-defined eco design checklist and optimisation potentials in the AM and laser processing of parts with complex geometry.

Technoeconomic and Performance Assessment of Refuse Derived Fuel (RDF) Production: A Response Surface Methodology (RSM) Approach

Khadija Sarquah^{1,2,3}, Prof. Dr. Satyanarayana Narra², Prof. Dr. Gesa Beck^{1,3}, Nana Sarfo Agyemang Derkyi⁴, Dr. Edward Awafo⁴, Prof. Dr. Michael Nelles², Prof. Dr. Michael Hartmann¹

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H6_5, Seminario 1 + 2 Room (Level +1), septiembre 16, 2025, 10:30 - 13:30

Utilising alternative fuel from waste as a substitute fuel contributes to energy diversity, economic value addition, and environmental benefits of sustainable waste management. For the coprocessing of alternative fuels such as refuse-derived fuel (RDF), it is essential to assess feasibility and investment viability. Response surface methodology (RSM) - Design of experiments (DoE) is a statistical approach that designs and analyses complex relationships between multiple variables, resulting in reliable and objective outcomes. This study aims to assess the economic viability of the refuse derived fuel production from municipal solid waste as a substitute fuel and process optimisation potentials in a case study. The economic analysis includes the net present value (NPV), profitability index (PI) and simple payback (SPB) for the feasibility check. Operating variables were optimised with the desirability approach of RSM to assess the optimum output using Minitab software. Input variables of production capacity, discount rate, life span and response or output variables of net present value, profitability index and simple payback were considered. The results estimate the predominant economic parameter on the response functions of the financial indicators. The sensitivity analysis predicts the effects of lifetime and interest ratios on the output variables. RSM-DoE application presented sensitivity analysis of the most significant parameters affecting the viability of the proposed energy recovery from MSW. Thus, process optimization with technoeconomic analysis is helpful in decisions for integrated waste management systems.

Advanced Thermal Insulation Composite Material for Sustainable Construction Using Palm Fiber and Basalt Waste

Dr. Waleed Ahmed¹, PhD Candidate Noura Al Mazrouei¹, Professor Ali Al Marzouqi¹

¹Uae University, Al Ain, United Arab Emirates

POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

This research explores the development of an innovative composite material using waste basalt rock, biodegradable polylactic acid (PLA), and palm waste. The study aims to address environmental challenges by repurposing waste into a high-performance material suitable for modern construction applications. A key research focus is the use of waste basalt rock, which is often discarded as domestic waste. Instead of accumulating in landfills, the fine basalt is processed into a concrete aggregate, improving the mechanical properties of basalt-based concrete while reducing environmental impact. This aligns with circular economy principles by converting waste into a valuable construction resource. The second component is biodegradable PLA, a thermoplastic polymer commonly used in eco-friendly packaging. PLA is a sustainable alternative to petroleum-based plastics, offering the advantage of biodegradability while retaining strength and flexibility. Its incorporation into the composite enhances durability while addressing plastic waste concerns. Additionally, the study includes palm waste, comprising leaves and wood, as a reinforcing component. This agricultural byproduct not only reduces organic waste but also contributes to the composite's mechanical performance and aesthetic properties. The resulting material demonstrates promising characteristics for civil engineering applications. It exhibits high compressive strength and excellent thermal insulation, making it suitable for energy-efficient and durable construction materials. Its adaptability allows for applications across various structural components, enhancing sustainability in the building sector. We highlight the significant advancement in waste management and material science. Upcycling basalt rock, biodegradable PLA, and palm waste presents a sustainable and high-performance composite with broad applications in construction and insulation. The findings contribute to the ongoing development of environmentally friendly materials, paving the way for more sustainable and resilient infrastructure solutions.

Magnets in Resilient Supply Chains

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H6_3, Seminario 1 + 2 Room (Level +1), septiembre 15, 2025, 14:30 - 16:30

The supply of magnets and critical materials, such as rare-earth elements (REEs), is of paramount importance for Europe, particularly in the context of the growing demand for electric vehicles and renewable energy technologies. Europe relies heavily on imports for these materials, making the region vulnerable to supply chain disruptions and geopolitical risks. Ensuring a stable and sustainable supply of REEs is crucial for the development of electric vehicle traction motors (EVTMs) and other green technologies, which are central to the European Union's transition towards a low-carbon economy.

Consequently, the need for innovative approaches to secure and optimize the use of these critical materials has never been more urgent. This MAGELLAN project aims to address these challenges by developing a sustainable and cost-effective REE permanent magnet value chain, enhancing Europe's autonomy and resilience in the face of material shortages.

The main objectives include advanced recycling and manufacturing technologies, incorporating efficient material reuse through Powder Injection Moulding. Additionally, the work focuses on optimizing EVTMs rotor design to improve motor assembly, performance, and facilitate End-of-Life dismantling. Another key goal is enhancing magnet recovery and recycling to minimize REE losses and promote standardized labelling for improved reuse.

The results of this project are expected to contribute to the reduction of pollutant emissions by incorporating a higher amount of recycled material in the production of new magnets, making the European magnet-related industry more resilient and competitive.

Measuring Circularity in Practice: Insights from Repairability Assessment

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POSTER SESSION 1. September 15 (13:15-14:30 & 16:30-17:00) and 16 (13:00-14:30 & 16:30-17:00), Posters area (Level +1), septiembre 15, 2025, 13:15 - 14:30

Material circularity is becoming increasingly important in today's economy and is a central focus of both industry and policy agendas. Achieving circularity requires robust, consistent metrics that can evaluate circular economy strategies across all levels of a product, beginning at the material level. From design for reuse to functional recycling, each strategy offers different opportunities for circularity. To understand their real impact, these strategies must be measured in a comparable and transparent way.

Within the CE-RISE project, we have developed a set of indicators to support such evaluations. This poster presents the methodology behind these indicators, using the repairability indicator as an example. By applying these indicators, we aim to provide a practical basis for assessing how much circularity products can unlock.

Among circular strategies, repair plays a central role due to its close relation with current and emerging regulations. Policies such as the Right to Repair and the Ecodesign Directive are shaping expectations for how products should be designed to enable easier repair. However, to evaluate how well these regulations are applied in practice, and to assess the efforts made by manufacturers, a common assessment is needed.

One relevant initiative in this area is the EN 45554 standard, which provides a methodological basis for assessing the repairability of energy-related products. Based on this standard, several repairability indexes have been developed, including the French Repairability Index and the iFixit Repairability Score. While these indexes offer useful perspectives, they differ in scope, scoring logic, and applicability across product categories.

Within the CE-RISE framework, these existing indexes have been compared and evaluated using real-world cases from industry partners. As a result, a new tool called the Repairability Indicator has been developed. This indicator uses a scoring system that considers both design-related parameters (e.g., modularity, accessibility of components) and support-related parameters (e.g., availability of documentation and spare parts over time).

Each parameter is scored individually, and the combined result reflects how repairable a product is in practice. The aim is to provide a flexible tool that can be adapted to different product groups while offering a fair, consistent basis for comparison.

In our poster presentation, we will introduce the EN 45554 standard, review key existing repairability indexes, and present the Repairability Indicator developed within CE-RISE. By combining and adapting current approaches, this tool helps move toward a more harmonized method for assessing repairability and supports clearer tracking of circular economy progress across sectors.

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