

Article

Effect of Cross Nanowall Surface on the Onset Time of Explosive Boiling: A Molecular Dynamics Study

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Abstract: Explosive boiling is a fast-phase transition from an ultra-thin liquid film to vapor under an extremely high heat flux, which typically has been studied using the molecular dynamics simulation (MDS) method. The present MDS study investigated the explosive boiling of a liquid argon nanofilm over different solid copper surfaces with different nanowall patterns, including parallel and cross nanowalls. For each surface, atomic motion trajectories, the number of liquid and vapor argon atoms, heat flux, and, mainly, the onset time of explosive boiling were investigated. The simulation results indicated that explosive boiling occurs earlier on parallel and cross nanowall surfaces than on an ideally smooth surface, regardless of the topology and configuration of the nanowalls. Moreover, the results revealed that by using the cross nanowall surfaces, the onset time of explosive boiling decreased by 0.7–4% compared to the parallel nanowall surfaces. In addition, it was found that the onset time of explosive boiling strongly depends on the potential energy barrier and the movement space between nanowalls for both parallel and cross nanowall surfaces. Furthermore, the simulation findings showed that even though increasing the height of cross nanowalls increases the heat flux and temperature of the fluid argon domain, it does not necessarily result in a shorter onset time for explosive boiling. These findings demonstrate the capability of cross nanowall surfaces for explosive boiling, thereby being utilized in future surface design for thermal management applications.

Keywords: explosive boiling; molecular dynamics simulation; liquid nanofilm; nanostructured surface; onset time



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1. Introduction

Studying the phase change of extremely thin liquid films over a surface is crucial for both scientific understanding and practical uses. Phase transitions could happen in normal boiling or explosive boiling [1]. Explosive boiling requires heating the liquid to a significantly high temperature beyond its saturation temperature by laser heating or sudden immersion in a hot medium. Hence, a sharp pressure increase accompanies the phase transition, leading to the liquid being ejected from the surface in a very short time. Therefore, explosive boiling is highly violent and rapid, resembling an explosion [2,3].

Due to the miniaturization of microelectronic devices, heat dissipation has become a serious problem, which limits the development of some technologies, such as laser surgery and ink-jet technology [4,5]. In this scenario, explosive boiling could represent a powerful method to advance the heat transfer efficiency of hot surfaces. Consequently, improving our understanding of this phenomenon is a compelling and vital topic to increase the efficiency of new technologies' thermal energy conversion.

Experiments at a large scale have shown that surface roughness, including the topology (shape) and configuration (size) of nanostructures, significantly impacts explosive boiling heat transfer. Even though almost all solid surfaces exhibit some molecular-level roughness, it is possible to design unique nanopatterns on a flat surface with the evolution of nano-manipulating technology [6]. Subsequently, great possibilities to pursue more

efficient nanostructured surfaces for explosive boiling heat transfer have recently drawn significant attention.

Although researchers have been studying how ultra-thin liquid films explosively boil in recent years [7,8], fully understanding the physical processes has been difficult because explosive boiling occurs on a very tiny scale, happens very quickly, and involves extremely high heat and temperatures [3]. However, due to advancements in computer technology, it is now possible to study transport processes on the nanoscale through numerical simulations. In order to conduct molecular dynamics simulation (MDS) research, precise force field parameters, sufficient computational resources, and suitable modeling assumptions are essential. Regarding the simulation time and computational expense, the scale and complexity of systems present obstacles. Despite these limitations, the MDS method, which can describe any physical process at the atomic level and on a picosecond (ps) time scale, has shown promise as a powerful method for exploring explosive boiling on surfaces and has been successfully and widely used in recent years.

For the first time, Morshed et al. [1] investigated the influence of nanostructured solid surfaces on the explosive boiling performance of ultra-thin liquid films. They discovered that the presence of the separated cylindrical nanopillars with a height either equal to or more than the liquid film's thickness could result in a considerable increase in the liquid separation temperature. After their study, many MDS studies have been conducted to investigate the effect of different nanostructured surfaces on explosive boiling, as summarized and tabulated in Table 1.

Table 1. A review of the literature concerning MDS investigations of explosive and normal boiling on nanostructured surfaces.

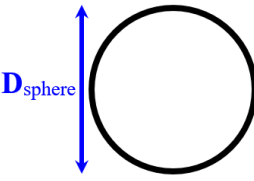
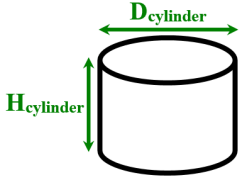
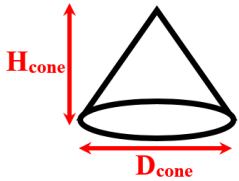
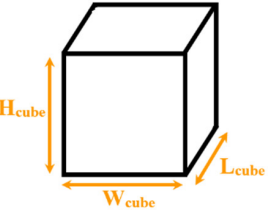
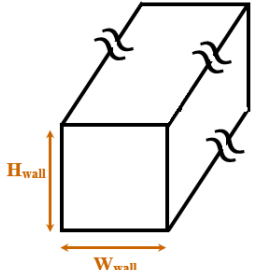
 Spherical nanopillar  Cylindrical nanopillar  Conical nanopillar  Cubical nanopillar  Cubical nanowall					
Study	Boiling Mode	Fluid/Solid Mediums	Nanostructure		Solid Surface Temperature (K)
			Topology (Shape)	Configuration (Size) *	
Morshed et al. [1]	Normal/ Explosive	Argon/ Platinum	Separated cylindrical nanopillars	$D_{cylinder} = 1.013$ $H_{cylinder} = 1.754\text{--}4.782$	130 and 300
Seyf and Zhang [6]	Normal/ Explosive	Argon/ Copper	Separated spherical nanopillars	$D_{sphere} = 1\text{--}3$	170 and 290
Seyf and Zhang [9]	Explosive	Argon/ Aluminum and Silver	Separated conical nanopillars	$D_{cone} = 1$ $H_{cone} = 2\text{--}5$	270

Table 1. Cont.

Study	Boiling Mode	Fluid/Solid Mediums	Nanostructure		Solid Surface Temperature (K)
			Topology (Shape)	Configuration (Size) *	
Wang et al. [10]	Normal/ Explosive	Argon/ Aluminum	Separated cubical nanopillars	$W_{\text{cube}} = 1.8$ $L_{\text{cube}} = 1.8$ $H_{\text{cube}} = 1.8225\text{--}4.455$	150 and 310
Fu et al. [11]	Explosive	Water/ Copper	Separated cubical nanopillars	$W_{\text{cube}} = 1.444\text{--}2.166$ $L_{\text{cube}} = 1.444\text{--}2.166$ $H_{\text{cube}} = 1.444\text{--}2.166$	1000
Zhang et al. [12]	Explosive	Argon/ Copper	Parallel cubical nanowalls	$W_{\text{wall}} = 1.808$ $H_{\text{wall}} = 1.266\text{--}3.434$	350
Liu et al. [13]	Explosive	Argon/ Copper	Random roughness surface	–	300
Zhang et al. [14]	Explosive	Water/ Copper	Separated cubical nanopillars	$W_{\text{cube}} = 1.444$ $L_{\text{cube}} = 1.444$ $H_{\text{cube}} = 1.444$	800
Liao and Duan [15]	Explosive	Argon/ Gold	Parallel cubical nanowalls	$W_{\text{wall}} = 0.612$ $H_{\text{wall}} = 0.816\text{--}2.040$	120–240
Liu et al. [16]	Explosive	Argon/ Copper	Random roughness surface	–	300
Qasemian et al. [17]	Explosive	Argon/ Aluminum and Copper	Separated conical nanopillars	$D_{\text{cone}} = 2.8$ $H_{\text{cone}} = 2$	350
Zhou et al. [18]	Explosive	Water/ Copper	Separated spherical and cylindrical nanopillars	$D_{\text{sphere}} = 1\text{--}1.44$ $D_{\text{cylinder}} = 6$ $H_{\text{cylinder}} = 1.8$	1000

* All dimensions are reported in nm (nanometer).

Zhou et al. [18] studied the effects of the size and number of separated spherical and cylindrical nanopillars on explosive boiling. Their findings demonstrated that the heat transfer performance improves with an increase in the number and size of nanostructures. Moreover, they confirmed that the cylindrical nanopillars could enhance the explosive boiling performance more than the spherical nanopillars. Similarly, the impact of the size of separated spherical nanopillars was investigated by Seyf and Zhang [6], who indicated that the explosive boiling performance improved when the nanostructure size increased. After that, in their subsequent study [9], they discovered that increasing the size of the separated conical nanopillars had a similar effect on the explosive boiling performance. Other studies about the effect of nanopillars on explosive boiling conducted by Zhang et al. [14], Wang et al. [10], and Fu et al. [11] showed that the addition of separated cubical nanopillars could significantly enhance the heat transfer efficiency, evaporation rate, separation temperature, and departure velocity. Qasemian et al. [17] researched the impact of aluminum and copper-separated conical nanopillars on explosive boiling. The research group found that utilizing separated conical nanopillars resulted in increased heat transfer and, consequently, accelerated evaporation of liquid layers. Moreover, they showed that the copper nanostructure was more effective in enhancing explosive boiling compared to the aluminum nanostructure. Zhang et al. [12] and Liao and Duan [15] researched the rapid boiling of extremely thin liquid layers on parallel cubical nanowalls. Their study revealed that this kind of nanostructure can significantly enhance heat transfer processes and much more violent explosive boiling than ideally smooth surfaces.

From the above studies, it is clear that nanostructured surfaces could drastically enhance the explosive boiling performance [19]. However, they have focused only on either separated nanopillars or parallel nanowalls without considering the influence of

connected ones. Using connected nanostructures, which could change the interaction of the nanofilm with the solid surface, could change the heat flux. Moreover, the fabrication of ideal parallel nanowalls is challenging because of some uncontrollable manufacturing processes; therefore, surfaces with cross nanowalls are inevitable. As far as the authors know, nobody has looked into how cross nanowall surfaces affect explosive boiling yet. This study focuses on the effect of both cross and parallel nanowalls, using the MDS method for the first time. In the simulations, we also check how changing the distance between nanowalls and the height of the cross nanowalls affects the onset time of explosive boiling.

In this paper, the simulation method is first described. After that, the validation of the molecular model is presented. Then, the influence of the surface topology and spacing on explosive boiling is examined for the parallel and cross nanowall surfaces. Then, further evaluation of the effect of the height of the cross nanowalls is discussed. Finally, this paper is completed with conclusions.

2. Simulation Method and Details

2.1. Simulation Details

Several cases with distinct surface topologies and configurations were studied to examine the cross nanowalls' impact on explosive boiling. The simulation procedure consisted of three steps: Step I: model development; Step II: computational runs; and Step III: post-processing analysis. The steps described here were mostly the same in all simulations, except for two cases. Information about the simulating exceptions (Cases I and II) is provided in Sections 3.1.1 and 3.1.2.

Although the simulation method can work with any combination of materials, argon (Ar) and copper (Cu) were chosen because their potential functions are easy to access and use [20]. The simplification involved ignoring gravity in all simulations (because surface interaction is much more significant for a liquid nanofilm than gravity [21]) and applying an additional spring force to each copper atom (see "Section 2.2.1. Force field and parameters" for more details).

The velocity Verlet integration was used to solve Newton's equation of motion. Several papers on the MDS method present the algorithm for solving atom motions (for example, see Refs. [22,23]). All simulations in this study were conducted utilizing the MDS code LAMMPS (patch_22Dec2022) [24], and further assessments were conducted by the OVITO software (Version 3.8.3) [25].

2.2. Model Development

2.2.1. Force Field and Parameters

The most crucial step in the MDS method is selecting a suitable intermolecular potential that characterizes the interaction between atoms and the movement of each atom. Since the present study focuses on the boiling of a liquid Ar nanofilm on a solid Cu surface, the interactions between them were modeled only by Van der Waals interactions, which have been widely used in several studies dealing with the MDS of Ar explosive boiling on metal surfaces (for example, see Refs. [1,6,10,12,26]) and have been demonstrated to be reliable. Consequently, the most frequent and well-known formulation of the Lennard-Jones 12-6 (L-J 12-6) function potential (U_{ij}) was applied to characterize the Cu-Cu, Ar-Ar, and Ar-Cu atomic interactions as follows [27]:

$$U_{ij} = 4\epsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] \quad (1)$$

The distance between atoms i and j is presented as r_{ij} . ϵ_{ij} represents how deep the energy well is, measured in electron volts (eV), while σ_{ij} is the distance where the interaction potential is zero, measured in angstroms (Å). Table 2 shows the energy and distance parameters for the Ar-Ar and Cu-Cu interactions [13]. However, $\epsilon_{\text{Ar-Cu}}$ and $\sigma_{\text{Ar-Cu}}$ were

determined in the way described below. The Lorentz combination rule (an arithmetic mean) was used to estimate the length parameter between the Ar and Cu atoms [28]:

$$\sigma_{\text{Ar-Cu}} = \frac{\sigma_{\text{Ar-Ar}} + \sigma_{\text{Cu-Cu}}}{2} \quad (2)$$

Table 2. Parameters of the force field.

Atom Pairs	σ (Å)	ϵ (eV)
Cu-Cu	1.9297	0.2047
Ar-Ar	3.4050	0.0104
Ar-Cu	2.6674	0.0065

For the energy parameter between the Ar and Cu atoms ($\epsilon_{\text{Ar-Cu}}$), a revised form of the Berthelot rule, which is a geometric mean, suggested by Din and Michaelides [29], was adopted as follows:

$$\epsilon_{\text{Ar-Cu}} = \alpha \sqrt{\epsilon_{\text{Ar-Ar}} \epsilon_{\text{Cu-Cu}}} \quad (3)$$

where “ α ” is the potential energy factor that could be applied to modify the wettability of the solid surface. In the present work, according to the results in Ref. [16], only the moderate hydrophilic ($\alpha = 0.14$) was considered. It is essential to point out that the word hydrophilicity refers to the wettability phenomena that occur when the liquid is water. If the liquid is other than water, this property should be referred to as lipophilicity. Nonetheless, “hydro” is frequently employed as a generic term regardless of the liquid [30].

Calculating the potential energy is the most time-consuming part of any MDS. When the distance between two atoms exceeds the cut-off radius, there is no interaction between the atoms; consequently, atoms with distances larger than the cut-off radius are eliminated from the energy computation. The cut-off radius was chosen to be 9 Å to ensure accurate calculations and speed up simulations (see Section SA of the Supplementary Material).

To keep the Cu atoms in their initial place during the simulations, we used a spring force for each atom. This allowed the Cu atoms to wiggle around their starting positions in the lattice. At each step, a force of $-Kr$ (eV/Å) was exerted, where K represents the spring constant (K (eV/Å²)) and r denotes the displacement of the atom from its initial position to its current position. To obtain a precise copper surface, you need to use the right spring force. The stiffness of the spring is connected to the Young’s modulus, so it can be approximated as defined in [31]:

$$K = Ed \quad (4)$$

E stands for the Young’s modulus, which is 128.2 GPa [32], and d is the lattice constant of copper (3.6147 Å). The data presented above, along with the correlation, yield a spring constant value of $K = 2.8926$ eV/Å².

2.2.2. Simulation Boxes

In this study, a rectangular simulation setup was used for all the simulation cases shown in Figure 1. It consisted of three main parts: a solid copper surface (with various shapes and layouts), a liquid argon domain, and a vapor argon domain. Since the number of copper layers varied on different surfaces, the simulation boxes’ heights were different in each case.

The solid copper surfaces were placed at the bottom of the simulation boxes. The solid copper surfaces were 54.2205×54.2205 Å² in size. The dimension values were chosen to be large enough (more than twice the 9 Å cut-off radius) to adhere to the minimum image convention. To learn more about how different shapes and arrangements affect explosive boiling, we made and simulated various parallel and cross nanowalls that all have the same width (3.6147 Å). The nanowalls were created on the smooth upper layer (surface F) to form various nanostructured surfaces. The sizes of all the copper surfaces used are listed in Table 3. Pictures of them can be found in Section SB of the Supplementary Material

(Figure S2). The surfaces named F, P, and C are perfectly smooth, parallel nanowall surfaces, and cross nanowall surfaces, respectively. The surface ratio at the Ar-Cu interface was calculated by dividing the wetted surface area by the nominal surface area [33].

Table 3. Simulation cases and corresponding topologies and configuration parameters.

The top and side schematic views of different copper surface topologies.			
Simulation Case ¹	Spacing (Å)	Height (Å)	Surface Ratio ²
1. Simulation Cases A: different topologies with different spacing:			
F	–	–	1
P-S1	50.6058		1.3333
P-S2	23.4956		1.6667
P-S3	14.4588		2.0000
P-S4	9.0368		2.3333
P-S5	7.2294		2.6667
P-S6	5.4220		3.0000
C-S1	50.6058	9.0368	1.6444
C-S2	23.4956		2.2445
C-S3	14.4588		2.8000
C-S4	9.0368		3.3111
C-S5	7.2294		3.7778
F	–		1
P-S1	50.6058		1.3333
2. Simulation Cases B: cross nanowall surfaces with different heights:			
C-H1		3.6147	1.4978
C-H2	23.4956	9.0368	2.2445
C-H3		12.6515	2.7422

¹ For convenience of reference, the simulation cases were labeled using two parts: the first part of the case name indicates the topology of the copper surface (F: smooth surface, P: parallel nanochannel surface, and C: cross nanochannel surface), and the second part of the case name shows the variable parameter for different configurations (S: spacing and H: height). ² Surface ratio = (the wetted surface area)/(the nominal surface area).

In Figure S2 and the images in Table 3, it is evident that in all the simulation cases, the solid copper surface was divided into three different parts from bottom to top. The bottom part (the fixed region) was fixed at the bottom of the simulation box to avoid the thermal deformation of the simulation boxes. The four Cu layers after that, called the “phantom region”, had their temperature controlled with a thermostat to act like a heat source. The other layers conducted the heat from the phantom region to the liquid domain. Light green and dark green colors are used to show the nanowall and smooth surface differently, so it is easier to see their shapes and how they are arranged. In this study, the thinnest copper surface, labeled as surface F with nine monolayers, measured 14.4588 Å, which is still larger than the cut-off radius of 9 Å. Therefore, the effect of the copper thickness can be disregarded.

On the solid copper surfaces, liquid argon was placed with a thickness of 40.0147 Å. At 87.18 K, liquid argon was measured to have a density of 1.3962 g/cm³ [34]. Also, the liquid argon layer was thick enough to ensure that explosive boiling occurred.

To imitate a real phase change setup, we added 152 argon vapor atoms above the liquid argon area. At 87.18 K, the density of these atoms was measured to be 0.0057 g/cm³. At first, they took up a space that was 601.7080 Å. Because of this, it was ensured that the

space above the liquid in the Z-direction was much greater than the argon liquid layer's thickness. This means that the top limit did not really change how the boiling happened. Also, periodic boundary conditions were applied in the X- and Y-directions, while the non-periodic fixed boundary condition was applied in the Z-direction. This setup follows the instructions for the experiment [35].

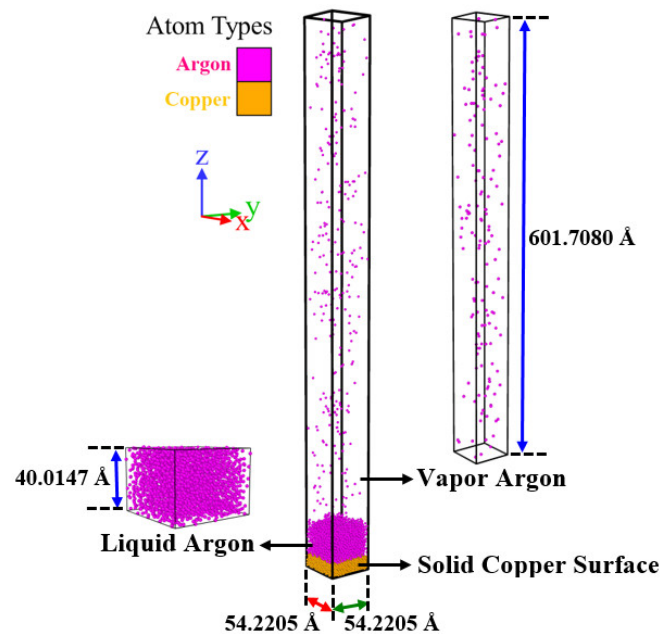


Figure 1. A typical representation of the initial setup of simulation systems.

2.3. Computational Runs

The simulations consisted of four major steps:

Step I (energy minimization): at the start of each simulation, we made sure the system's energy was as low as possible. We used the conjugate gradient (CG) to minimize the energy. We stopped when the energy tolerance was less than 0.00001 eV, and the force tolerance was less than 0.00001 eV/Å.

Step II (equilibrium preparation): during this stage, the simulation systems were adjusted to a constant temperature of 87.18 K [34]. This temperature was kept stable for 2000 ps using the Langevin thermostat. To avoid entering the liquid Ar atoms in the lattice structure of the solid copper surfaces, the liquid Ar atoms were initially located above the solid copper surfaces (during the simulation box construction), and, in this step, they fell onto the surfaces uniformly (see Section SD of the Supplementary Material (Figure S4) for simulation Case P-S2). Every simulated system achieved its equilibrium state in this step. Figure S5 (see Section SD of the Supplementary Material) shows a typical fluctuation of the temperature and total energy plot for simulation Case F. The temperature and total energy fluctuations were determined to be small, satisfying the equilibrium condition.

Step III (equilibrium relaxation): In this stage, the simulation continued for another 2000 ps. By applying the NVE ensemble, the argon fluid kept its atom count, volume, and energy constant, while the temperature of the copper surfaces stayed at 87.18 K using the NVT ensemble. We watched the temperatures of the argon and copper atoms and checked how many argon atoms were in liquid and vapor states to ensure everything settled into a stable condition. More details can be found in Section SE (Figures S6 and S7) of the Supplementary Material for simulation Case F.

In Step IV, the phantom monolayer atoms were heated to 250 K using Nose–Hoover thermostats to simulate explosive boiling. Concurrently, the remaining atoms interacted within the NVE ensemble, and simulations were carried out for 2000 ps. The duration of the run was selected to induce the sudden boiling of the liquid. Extending the duration could

result in the gradual vaporization of liquid argon, as depicted in Section SF (Figure S8) of the Supplementary Material for simulation Case F.

2.4. Post-Processing Analysis

The trajectories of the atoms in the simulation systems were recorded throughout the simulations, and the desired properties were calculated. The data and snapshot files were exported for post-processing and visualization every 1 ps.

Explosive boiling onset was determined as the time when a full vapor film measuring 20 Å in thickness formed on the solid surface. More details can be found in Section SG of the Supplementary Material.

The simulation systems for density investigations were separated into equal bins with a thickness of 2 Å along the Z-direction of the phase transition.

Based on the “Oxford” method [36] and the definition introduced by Wolde and Frenkel [37], which is remarkably successful in cluster definitions of argon in the MDS method [38], if the distance between two Ar atoms was less than $1.5\sigma_{\text{Ar-Ar}}$ ($=5.1075$ Å), they were considered to be part of the liquid phase. Otherwise, the atoms were considered in the vapor phase. This definition was applied to draw a distinction between the liquid and vapor Ar atoms.

The heat flux was calculated by [39]:

$$q = \frac{1}{A} \frac{\partial E_f}{\partial t} \quad (5)$$

A shows the interface area (54.2205×54.2205 Å²), while E_f represents the total energy of all the argon atoms (measured in eV). Figure 2 displays the heat flow in simulation Case F, measured in units of eV/(Å²ps) and GW/m². As you can see, the heat measurements fluctuate a lot. To fix this, the results were smoothed out using the FFT filter with a coefficient of 0.4 (see References [4,39] for more details). The blue curves in Figure 2 present the smoothed-out results.

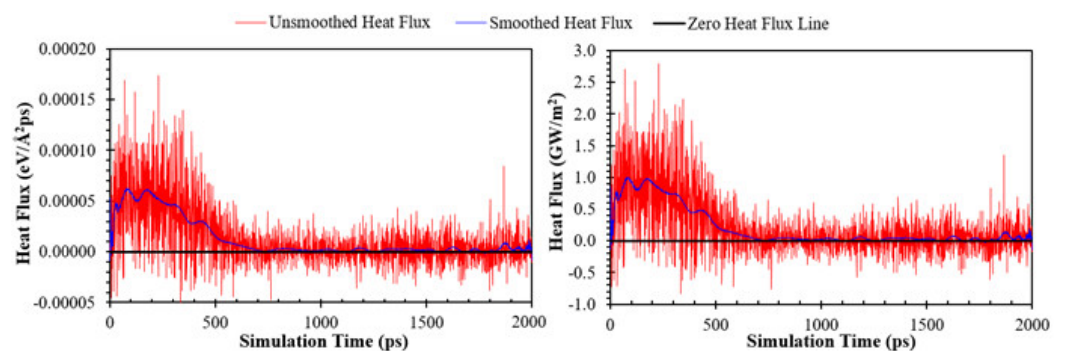


Figure 2. Simulation Case F: two different presentations of heat flux, unsmoothed and smoothed.

3. Result and Discussion

3.1. Model Validation

In this study, we simulated two different boxes to examine the validation of the force field and its parameters. One model simulated a liquid argon system (simulation Case I), and the other a system with liquid and vapor argon coexistence (simulation Case II). Density is a crucial factor for validating the MDS method. To assess its accuracy, this study calculated it and compared the results with data from the widely recognized NIST fluid properties database.

3.1.1. Simulation Case I: The Liquid Argon System

In this section, to ensure the reliability of the force field to reproduce the structural properties of the liquid argon, a liquid argon box with a dimension equal to $40.0002 \times 40.0002 \times 40.0002$ Å³ (consisting of 1360 Ar atoms) was subjected to a 2500 ps simulation

under an NPT (isothermal–isobaric) ensemble at 1 bar and 85 K. Notably, the NPT ensemble was used because the simulation box should be allowed to vary in size in order to obtain a well-density equilibrated system. Since the temperature and the total energy are key factors determining the equilibrium state, Figure S11 (see Section SH of the Supplementary Material) shows the fluctuation of the temperature and total energy for simulation Case I during the NPT simulation, which are found to be slight, which meets the equilibrium criteria, and illustrates that the simulation box has achieved its equilibrated state. Moreover, Figure 3 shows the change in the density and cell length.

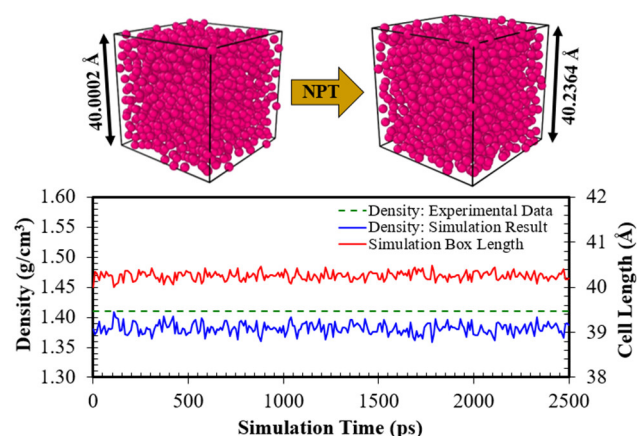


Figure 3. Simulation Case I's cell length and density during the NPT simulation.

With the density bouncing constantly around the value of 1.3829 g/cm^3 , which agrees well with the experimental data (1.4096 g/cm^3 [34]), the plot demonstrates that the system is stable. Moreover, the radial distribution function (RDF) predicted by the molecular simulation is compared with the experimental data, as shown in Figure 4. The experimental data were obtained from J. L. Yamell et al. [40], measured at 85 K.

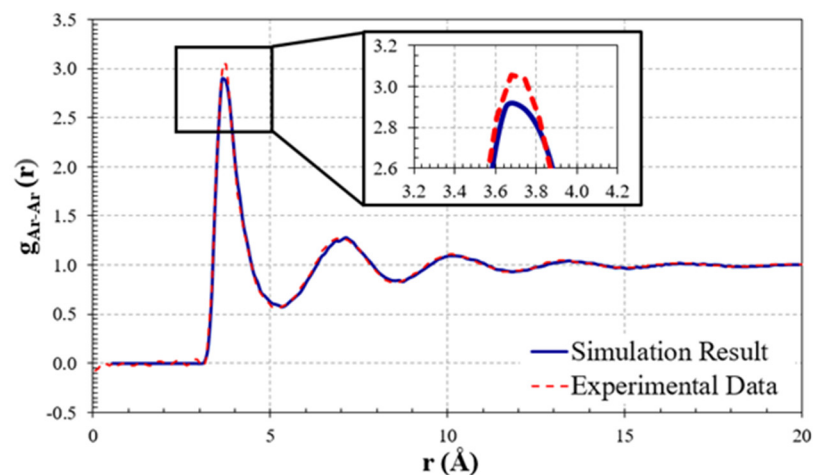


Figure 4. Comparison between experimental and simulated RDFs of liquid argon. The experimental data are from Ref. [40].

As can be seen, the MDS result matches the experimental measurement excellently, and the two curves are practically indistinguishable, especially for the second and third peaks. However, the MDS slightly underestimated the value of the first peak. This is somewhat expected since the experimental RDF has been measured with an atomic density of $0.02125 \text{ atom/\AA}^3$ [40], but the average atomic density for the simulation was $0.02085 \text{ atom/\AA}^3$. This is reasonable because the particles neighboring each other are closer when the density increases. This leads to a higher value for the first peak in the experimen-

tal data. This is also compatible with the assertion that the force field underestimated the liquid density (see Figure 3). Generally, there is reasonably good agreement between the MDS results and the experimental data.

3.1.2. Simulation Case II: The Liquid–Vapor Argon Coexistence System

A setup, known as simulation Case II, was developed to test the accuracy of the model in handling the balance between liquid and vapor argon. This is depicted in Figure 5. The liquid film was $39.9995 \times 39.9995 \times 39.9995 \text{ \AA}^3$ in size, made up of 1347 Ar atoms. On each side, there was a vapor space measuring $39.9995 \times 39.9995 \times 400.0579 \text{ \AA}^3$, housing 55 Ar atoms. During a 2500 ps period of settling at 87.18 K (the temperature at which argon boils at 1 bar [34]) in an NVT ensemble, it is noticed that there are only small changes in the total energy and temperature, which shows that things are stable (Figure S12).

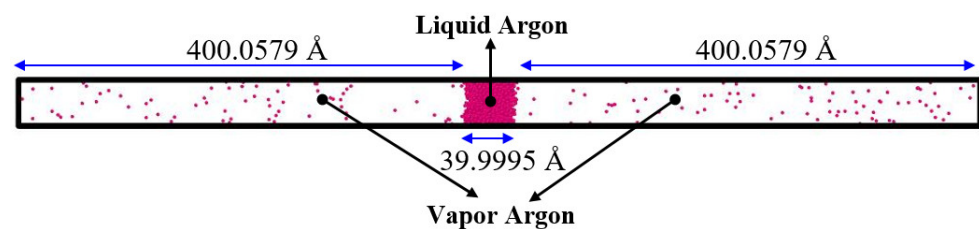


Figure 5. Case II simulation's initial setup.

Figure 6 shows that the liquid and vapor densities match well in both the simulation and real-world tests. To find the average density along the Z-axis, we divided the system into 210 sections.

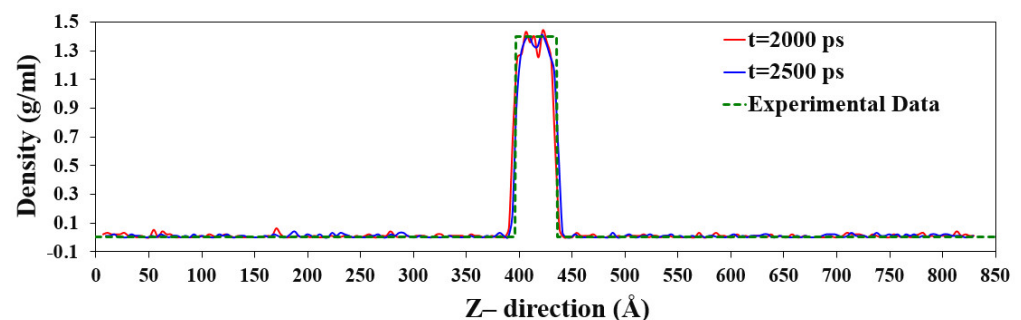


Figure 6. An examination of the experimental data and the density profile along the Z-axis (at 2000 and 2500 ps) for Case II of the simulation. Refer to [34] for the experimental data.

Moreover, snapshots from the simulations after 2000, 2250, and 2500 ps are presented in Figure 7. As can be seen, the boundary between the liquid and vapor phases is almost constant. Even though escaping and reentering atoms into the liquid phase could change the surface density, it is not very significant.

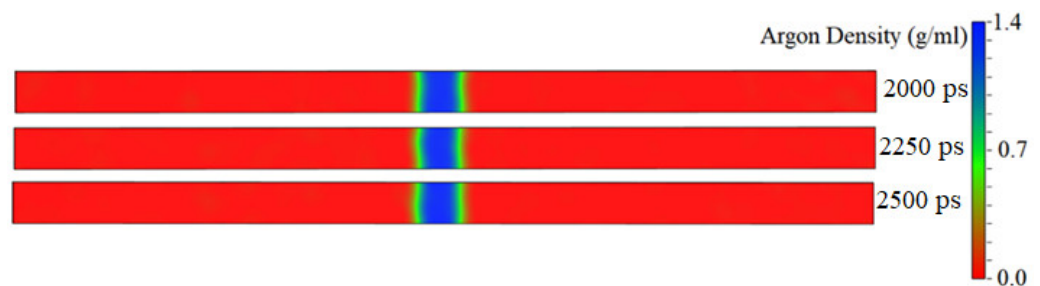


Figure 7. Snapshots of density profiles of simulation Case II at 2000, 2250, and 2500 ps.

Furthermore, as shown in the Supplementary Material (Video S1), during the simulation, liquid Ar atoms are evaporating from the liquid surface. However, they are reentering the liquid just as fast as they are escaping from it, which provides a molecular viewpoint on the two-phase equilibrium.

3.2. Simulation Cases A: Effects of Surface Topology and Spacing

Figure 8 shows when liquid argon boils explosively on different solid copper surfaces. These surfaces have different shapes. The full snapshots are illustrated in Figure S13 (see Section SI of the Supplementary Material) for a better inspection. The three main findings can be summarized as follows:

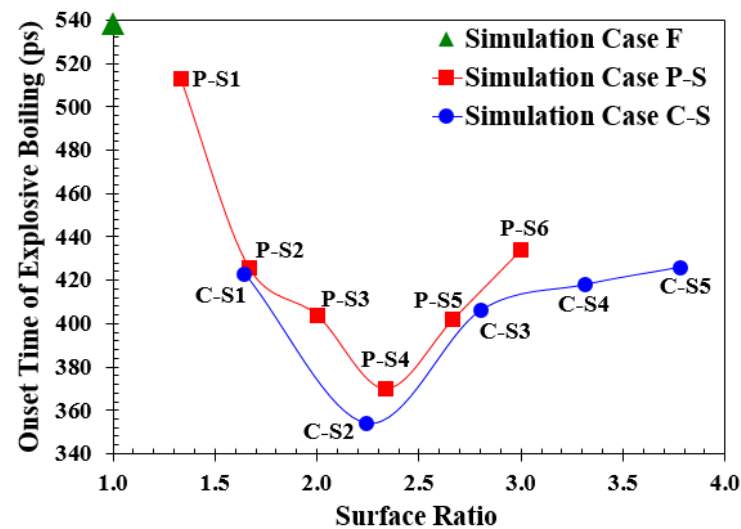


Figure 8. Changes in the onset time of explosive boiling versus increasing the surface ratio (the wetted surface area/the nominal surface area) for various topologies.

Finding #1: the onset time of explosive boiling over the ideally smooth surface (simulation Case F) is 538 ps, longer than the nanostructured surfaces (354–513 ps).

Finding #2: For the parallel nanowall surfaces with different spacing, the onset time of explosive boiling reduces from 513 ps (for simulation Case P-S1) to 370 ps (for simulation Case P-S4) and then increases to 434 ps (for simulation Case P-S6). The same trend can be seen for the cross nanowall surfaces (simulation Cases C-S).

Finding #3: the cross nanowall surfaces show a shorter onset time than the parallel nanowall surfaces.

Finding #1 suggests that nanowalls could make explosive boiling happen sooner. Nanowalls make the liquid argon nanofilms touch more of the solid copper surface. Hence, when more liquid argon gathers at the interface, it helps heat move faster from the solid to the liquid argon. This makes explosive boiling start more quickly. Towards the end of this section, a detailed examination will be conducted to explore how nanostructured surfaces impact the beginning of explosive boiling. This will involve discussing the measurements of heat flow, the temperature of argon atoms, and the quantities of liquid and vapor argon atoms.

Herein, it is presumptive that the effects of the potential energy barrier and the movement space for liquid Ar atoms are what led to Findings #2 and #3. In the following, to investigate the effect of these factors on the onset time of explosive boiling, the parallel nanowall surfaces are chosen (due to more explicit view pictures and easy observation), and the mechanism of explosive boiling from the molecular point of view is discussed. The discussion could be extended to cross nanowall surfaces.

Figures 9 and S14 display how heat flows through argon fluid in narrow channels with different distances between them. When the solid became hotter from the thermostat, the heat flow reached its highest point. Then, it went down to a fairly low level. During

this period, the shift from the solid–liquid boundary to the solid–vapor boundary takes place, resulting in a notable increase in interfacial thermal resistance, known as the Kapitza thermal resistance, and consequently reducing the heat flux. After the liquid cluster and its tail move away from the surface, the heat flows almost stop completely.

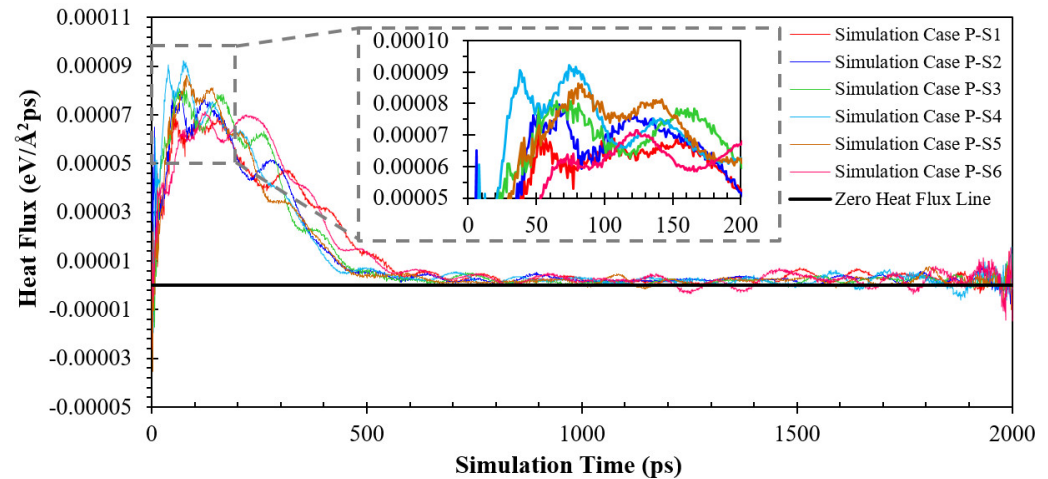


Figure 9. Variation in heat flux ($\text{eV}/\text{\AA}^2\text{ps}$) of fluid argon domain on solid copper surfaces for various parallel nanowall surfaces.

Considering the highest heat flow as the key indicator [41], Figure 9 also demonstrates that as the nanochannel spacing decreases, the heat flow initially increases from $3.406 \times 10^{-5} \text{ eV}/\text{\AA}^2\text{ps}$ (for simulation Case P-S1) to $9.167 \times 10^{-5} \text{ eV}/\text{\AA}^2\text{ps}$ (for simulation Case P-S4), then decreases to $7.080 \times 10^{-5} \text{ eV}/\text{\AA}^2\text{ps}$ (for simulation Case P-S6). This happens because of how the potential energy between liquid argon and copper atoms affects the way heat moves. Therefore, Figure 10 shows how the potential energy per Ar atom varies across different parallel nanowall surfaces. Figure 10 shows that most of the potential energy is near the surface, particularly around the nanowalls. Therefore, using nanowalls makes the liquid Ar interact more strongly with the surface, which makes it heat up faster and boil explosively sooner. It is interesting that when we reduced the gap between the nanowalls more, the heat flow decreased in simulation Cases P-S5 and P-S6.

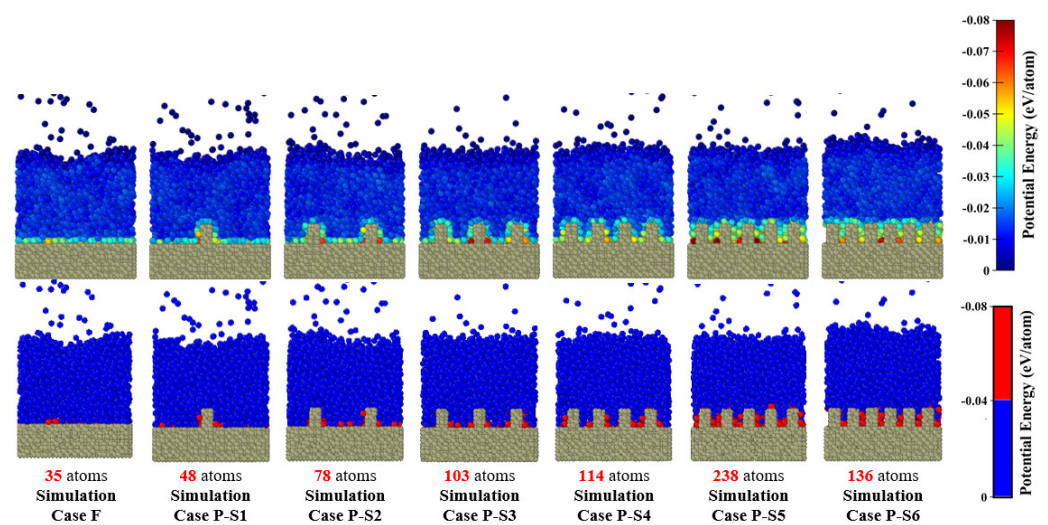


Figure 10. Comparison of potential energy per Ar atoms distributions and number of Ar atoms with high potential energy (-0.04 – $0.08 \text{ eV}/\text{atom}$) for the ideally smooth surface and various parallel nanowall surfaces.

Thus, the exact moment when explosive boiling starts is not only influenced by the interaction potential energy's value; there are other factors involved too. So, to understand it better, we need to look at how the Ar atoms move along their paths.

Figure 11 shows the paths of 31 randomly picked liquid argon atoms between the nanowalls in simulation cases P-S4, P-S5, and P-S6. Examining Figure 11 reveals that the Ar atoms move more effectively in the larger space (simulation Case P-S4) compared to the smaller spaces (simulation Cases P-S5 and P-S6). Thus, besides the energy from interactions, the size of the space where liquid atoms move around also plays a big role in causing explosive boiling. When the interactions between the solid and liquid are strong and the available space for movement is limited, the liquid Ar atoms become restricted in their motion. When the movement of liquid atoms is restricted, they collide less frequently, resulting in a lower heat transfer rate (as seen in Figure 9). Furthermore, overcoming the high potential energy barrier takes more time, which explains the relatively delayed onset of explosive boiling.

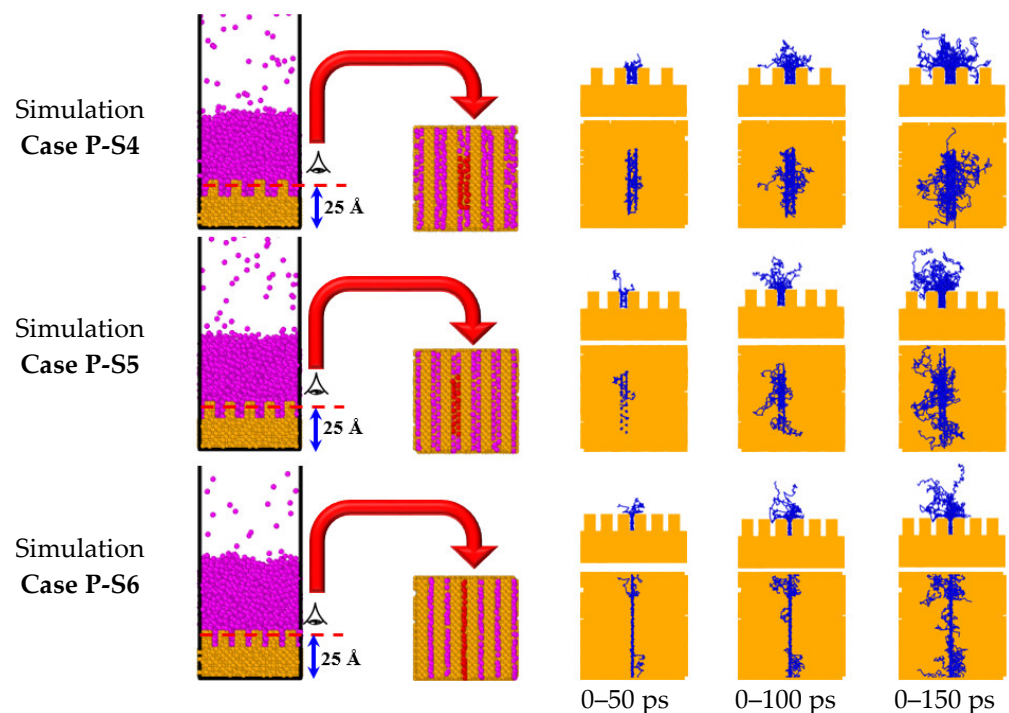


Figure 11. Projections of trajectory lines of Ar atom motion between the nanowalls for various parallel nanowall surfaces.

When considering explosive boiling, adjusting the spacing between channels can significantly impact performance. Decreasing the channel spacing improves explosive boiling by increasing the interaction potential energy. However, there is a critical point: if the channel spacing becomes too small, increasing the surface ratio will actually reduce the heat transfer. This applies to both parallel and cross nanowall surfaces. So, while reducing the spacing initially helps, exceeding the critical threshold negatively affects the onset of explosive boiling.

This discussion can also elucidate the shorter onset time for cross nanowall surfaces (Finding #3). Cross nanowall surfaces, despite having nearly identical surface ratios to parallel ones, offer an increased mobility space for Ar atoms. For instance, although simulation Cases P-S4 and C-S2 exhibit almost equal surface ratios (2.3333 and 2.2445, respectively), the spacing length for simulation Case C-S2 is 23.4956 Å, nearly double that of simulation Case P-S4 (9.0368 Å). Consequently, liquid Ar atoms are likely to escape more rapidly from cross nanowall surfaces compared to parallel ones, thereby potentially accelerating explosive boiling and reducing its onset time.

To better compare the heat transfer characteristics for different surface topologies, the ideally smooth surface (simulation Case F) and two nanostructured surfaces with almost equal surface ratios (simulation Cases P-S4 and C-S2) are selected and discussed in the following.

The heat fluxes for simulation Cases F, P-S4, and C-S2 in $\text{eV}/(\text{\AA}^2\text{ps})$ and GW/m^2 are presented in Figure 12 and Figure S15, respectively. It is seen that due to the presence of nanowalls, the solid–liquid interface area and interaction between the solid copper and liquid film increase, leading to a substantial difference between the heat fluxes of the perfectly smooth surface (simulation Case F) and nanostructured surfaces (simulation Cases P-S4 and C-S2). In addition, the heat flux on surfaces with cross nanowalls is greater than that on surfaces with parallel nanowalls.

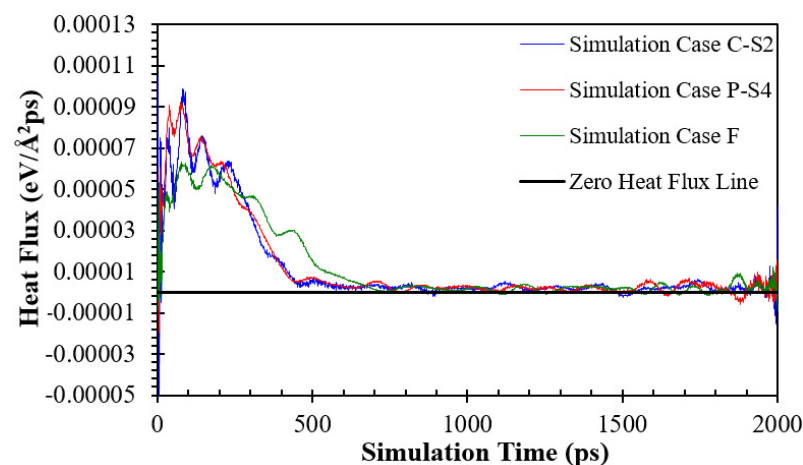


Figure 12. Variation in heat flux ($\text{eV}/(\text{\AA}^2\text{ps})$) of fluid argon domain on solid copper surfaces for simulation Cases F, P-S4, and C-S2.

The simulation results of the temperature history of Ar atoms are shown in Figure 13. The Ar temperature represents the temperature of all argon atoms, including the liquid and vapor atoms. The plot is limited to 600 ps to have a clear view of the onset time of explosive boiling. For the simulation cases with parallel and cross nanowalls (simulation Cases P-S4 and C-S2, respectively), Ar atoms become more heated than the ideally smooth surface (simulation Case F), as described in the last section. Moreover, with the presence of nanostructures, the distance from the solid surface to the top liquid argon layer decreases. As a result, the temperature of the liquid Ar atom on the nanostructured surface is higher than on the ideally smooth surface. Even though for simulation Cases P-S4 and C-S2, the average conduction path of the liquid films is practically identical, simulation Case C-S2 shows a slightly higher argon temperature because of its slightly higher heat flux (see Figure 12).

Figure 14 illustrates the amount of liquid and vapor atoms present in the system during the non-equilibrium explosive boiling. The fluctuation in vapor atom quantity indicates the rate of evaporation in the system. The quantity of liquid Argon atoms falls in all the simulated scenarios following the onset time. The liquid argon atom count reduces sooner in simulation Cases C-S2 and P-S4 compared to simulation Case F, indicating a greater evaporation rate on nanostructured surfaces. Nanostructured surfaces with larger heating areas and higher heat flux lead to rapid liquid evaporation during boiling, resulting in a swift alteration in the liquid-to-vapor ratio in the system.

Furthermore, the results indicate that even though the evaporation ratios of surfaces with nanostructures are nearly comparable, simulation Case C-S2 is slightly greater than that of simulation Case P-S4 due to the larger space for moving Ar atoms and, consequently, a higher heat flux, as described before. It is interesting for all the simulation cases that the liquid cluster before the detachment absorbs high values of heat flux from the heated

substrate. Therefore, the liquid argon clusters still maintain a high evaporation rate even after detachment.

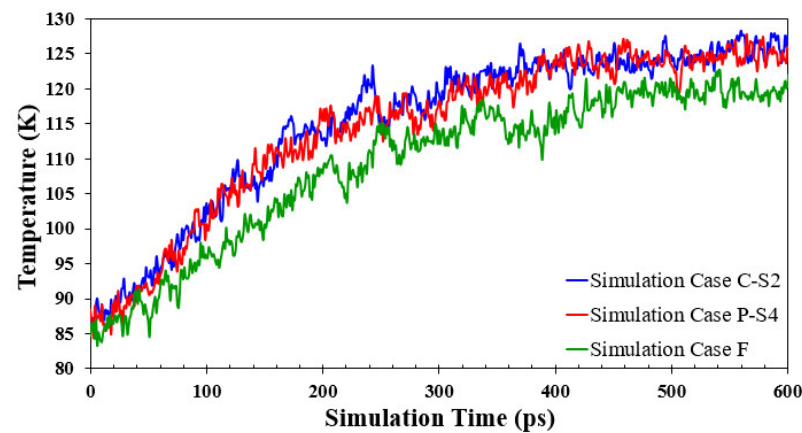


Figure 13. Temperature history of fluid argon domain for simulation Cases F, P-S4, and C-S2.

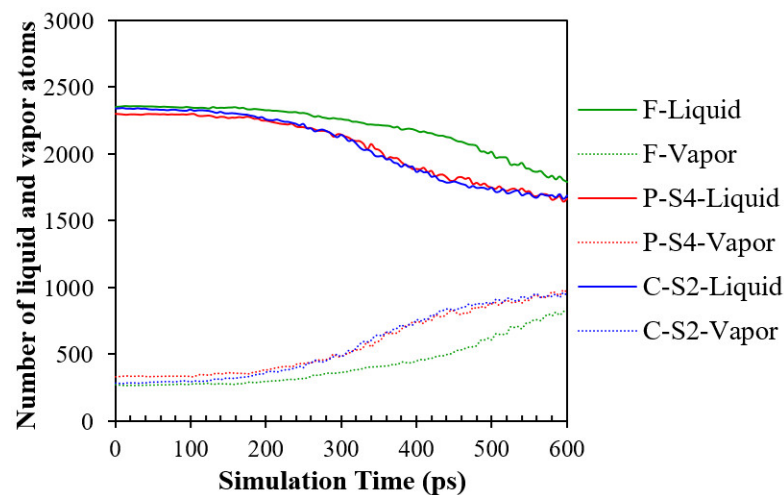


Figure 14. The number of liquid and vapor Ar atoms as a function of time for simulation Cases F, P-S4, and C-S2.

The study of the density profiles is important because it indicates the density and velocity of the liquid argon cluster. Figure 15 shows the Z-direction density distribution in the fluid domain for simulation Cases F, P-S4, and C-S2 at various times.

Three distinct zones can be seen in the density profiles. With a relatively high density, the liquid phase forms the first region, the liquid–vapor interface forms the second, and the vapor phase forms the third. Because there are a few atoms in the vapor region, the local density in this area exhibits some scattering. The peak values of the density profile at the onset time of explosive boiling for simulation Cases F, P-S4, and C-S2 are 2.6605, 2.6113, and 2.5397 mol/L, respectively. This means that using the cross nanowall surface leads to a floating liquid argon cluster with a lower density compared to the ideally smooth and parallel nanowall surfaces. It relies mainly on the fact that the cross nanowall surface could increase the Ar temperature and evaporation rate higher than the others (Figure 13). Moreover, because of a low-density floating liquid argon cluster for simulation Case C-S2, its upward velocity is higher.

For a better visual demonstration of explosive boiling on different surface topologies, Videos S2, S3, and S4 are provided for simulation Cases F, P-S4, and C-S2, respectively.

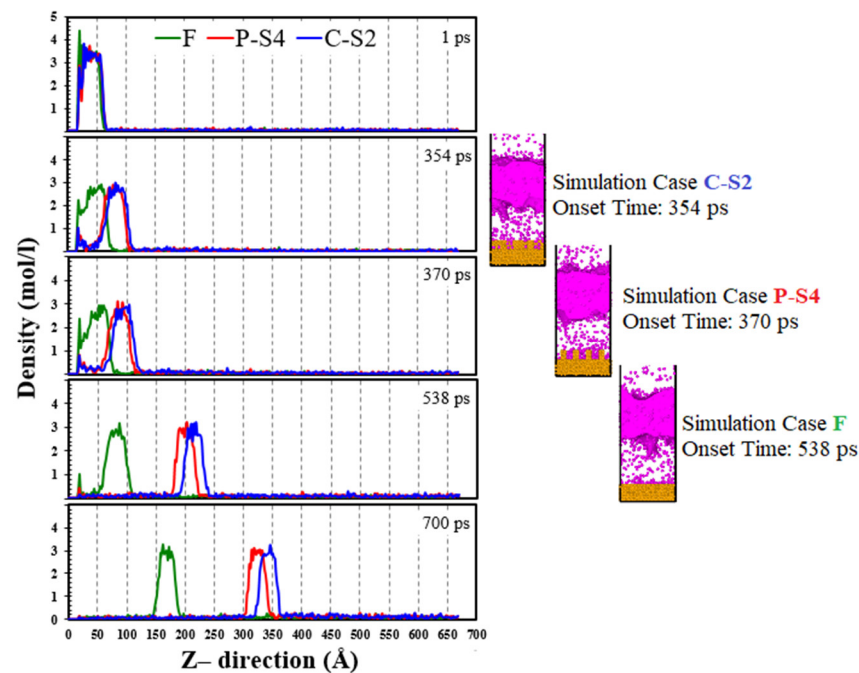


Figure 15. Density profile of the fluid argon domain in the Z-direction for simulation Cases F, P-S4, and C-S2 at various times.

3.3. Simulation Cases B: Effects of Nanowall Height

In this section, aiming to understand the influence of the height of nanowalls on the onset time, the nanowall height for the cross nanowall surfaces was changed, whereas the spacing was kept fixed. Three different heights (3.6147 Å (simulation Case C-H1), 9.0368 Å (simulation Case C-H2), and 12.6515 Å (simulation Case C-H3)) were investigated.

The onset time of explosive boiling on cross nanowall surfaces with varying heights is depicted in Figure 16. The full snapshots are illustrated in Figure S16 (see Section SJ of the Supplementary Material) for a better inspection.

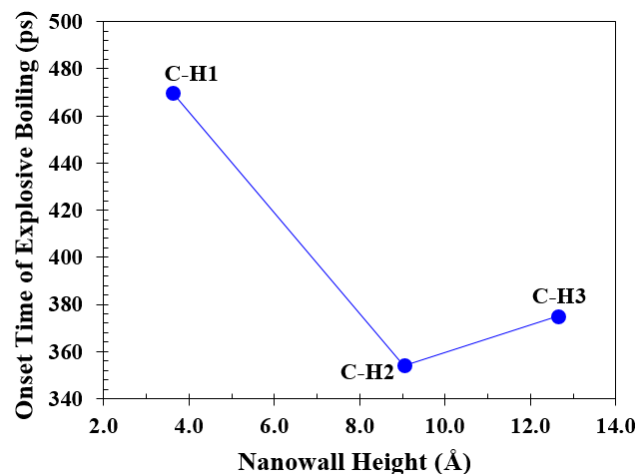


Figure 16. Variations in the onset time of explosive boiling as the height of the nanowall is increased for the cross nanowall topology.

As shown in Figure 16, a reduction from 470 ps (for simulation Case C-H1) to 354 ps (for simulation Case C-H2) and then an increase to 375 ps (for simulation Case C-H3) occurs in the onset time.

The heat fluxes for simulation Cases C-H1, C-H2, and C-H3 in $\text{eV}/(\text{\AA}^2\text{ps})$ and GW/m^2 are presented in Figure 17 and Figure S17, respectively. It can be seen that the maximum

heat flux increases as the nanowall height increases because the solid–liquid interface area increases. Therefore, increasing the nanowall height means the fluid argon domain could obtain more energy, resulting in a higher argon temperature, as shown in Figure 18. However, interestingly, more increases in the nanowall height resulted in postponing the onset of explosive boiling.

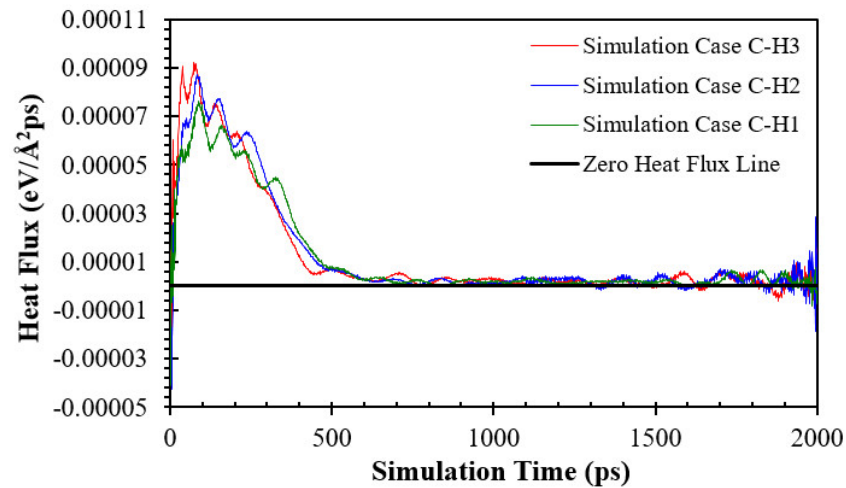


Figure 17. Variation in heat flux ($\text{eV}/(\text{\AA}^2\text{ps})$) of fluid argon domain on solid copper surfaces for simulation Cases C-H1, C-H2, and C-H3.

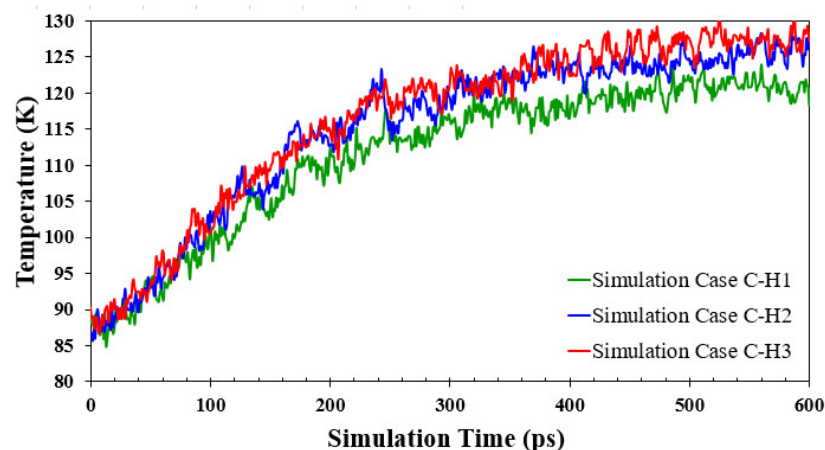


Figure 18. Temperature history of fluid argon domain for simulation Cases C-H1, C-H2, and C-H3.

As discussed in the previous section, the potential energy and movement spacing are the key parameters that could determine the onset time of explosive boiling. In this section, the movement spacing was the same ($23.4956 \text{ \AA}$) for all the simulation cases. Considering only the impact of the interaction potential energy (illustrated in Figure 19), the lower interaction potential energy for simulation Case C-H1 is the main reason for its reduced heat transfer and prolonged onset time. Nevertheless, the effect of the interaction potential energies on simulation Cases C-H2 and C-H3 is unusual.

The interaction potential energies and heat flux increased as the nanowall height was increased (from 9.0368 for simulation Case C-H2 to 12.6515 for simulation Case C-H3). Nonetheless, it also delays the onset of explosive boiling. Bai et al. [42] showed that the heat flux was enhanced, and the explosive boiling onset time was lowered by raising the height of the parallel nanowalls. Thus, the trend of the present work disputes the results in Ref. [42]. However, it can be explained by the difference in wettability. Bai et al. [42] used water and copper as the liquid nanofilm and solid surface, respectively. The energy parameter for the water–copper interaction is much larger than that for argon–copper.

This significant energy parameter (0.0342 eV) causes the water molecules to stay between the nanowalls during explosive boiling, and the cluster liquid separation starts above the nanowalls. Nevertheless, in this study, explosive boiling starts between the nanowalls because of the lower energy parameter for the argon–copper interaction (0.0065 eV). In this situation, when the height of the nanowall is significant compared to the thickness of the liquid nanofilm, increasing the height of the nanowall may negatively impact the onset time. In other words, although more liquid atoms between higher nanowalls could absorb more heat and reach a higher temperature, they could not overcome the incredible interaction potential energy barrier and start explosive boiling. It is evident from Figure 19 that simulation Case C-H3 contains a considerably greater quantity of Ar atoms with high interaction potential energies (-0.04 – -0.08 eV/atom) near the nanowalls in comparison to simulation Case C-H2.

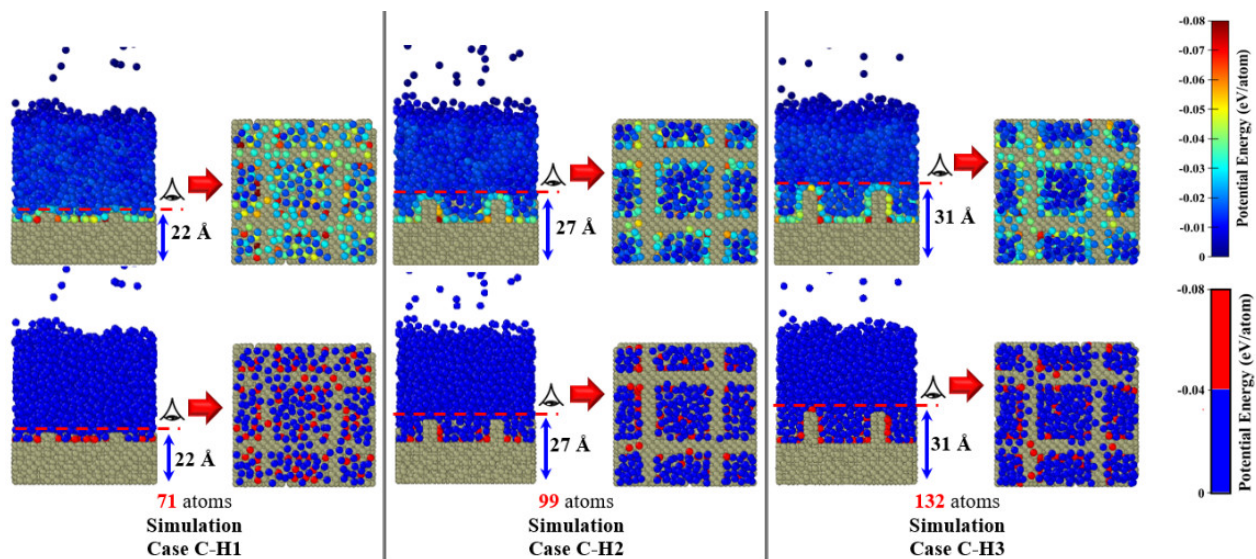


Figure 19. Comparison of the number of Ar atoms with high potential energy (-0.04 – -0.08 eV/atom) for simulation Cases C-H1, C-H2, and C-H3.

4. Conclusions

This study used molecular dynamics simulation to see how quickly liquid argon starts boiling explosively on three different types of solid copper surfaces: a perfectly smooth surface, a parallel nanowall surface, and a cross nanowall surface. The findings showed that the time it takes for explosive boiling to start (the onset time) mainly depends on three factors: how much surface area there is between the solid and liquid (the interface area), the required energy barrier to surpass, and how much space the liquid argon atoms have to move between nanowalls (the movement space). In summary, there were the following findings:

- (1) The nanowalls make the interface area greater, allowing more heat to move from the solid to the liquid. This means that on the parallel and cross nanowall surfaces, explosive boiling happens faster than on the smooth surface.
- (2) The cross nanowalls, which have the same interface area as parallel ones, showed an earlier onset time for explosive boiling. This is because they provide greater movement space, so liquid argon atoms can escape more quickly from cross nanowalls than from parallel ones.
- (3) Decreasing the spaces between nanochannels decreases the onset time because it increases the interface area. But if we make the spaces even smaller than a certain point, it could slow down the movement of liquid atoms and postpone the explosive boiling.

- (4) Increasing the height of the nanowalls can decrease the onset time because it increases the interface area. However, if the nanowalls become too high, they can create a strong barrier, which takes longer to overcome and consequently postpones the onset time.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/en17051107/s1>. Figure S1. L-J 12-6 potential curve for Ar and Cu. Figure S2. Oblique, top, and side views of different solid copper surface topologies and configurations. Figure S3. Representative snapshots of phase change of the liquid argon nanofilms with different thicknesses for simulation Case F. Figure S4. Representative snapshots of simulation Case P-S2 at the beginning and end of the equilibrium preparation. Figure S5. Fluctuation of temperature and total energy during the equilibrium preparation for simulation Case F. Figure S6. Fluctuation of the temperature of Ar and Cu atoms during the equilibrium relaxation for simulation Case F. Figure S7. The number of liquid and vapor atoms as a function of time during the equilibrium relaxation for simulation Case F. Figure S8. Representative snapshots of trajectories of atoms for simulation Case F during 16 ns of non-equilibrium simulation. Figure S9. The selected slab for simulation Case F. Figure S10. The experimental phase diagram of argon and the trend of explosive boiling for simulation Case F. Figure S11. Fluctuation of temperature and total energy of simulation Case I during the NPT simulation. Figure S12. Fluctuation of temperature and total energy of simulation Case II during the NVT simulation. Figure S13. Representative snapshots of trajectories of atoms for simulation Cases A. Figure S14. Variation in heat flux (GW/m^2) of fluid argon domain on solid copper surfaces for various parallel nanowall surfaces. Figure S15. Variation in heat flux (GW/m^2) of fluid argon domain on solid copper surfaces for simulation Cases F, P-S4, and C-S2. Figure S16. Representative snapshots of trajectories of atoms for simulation Cases B. Figure S17. Variation in heat flux (GW/m^2) of fluid argon domain on solid copper surfaces for simulation Cases C-H1, C-H2, and C-H3. Video S1: Simulation Case II during the NVT simulation. Video S2: Simulation Case F during the non-equilibrium explosive boiling simulation. Video S3: Simulation Case P-S4 during the non-equilibrium explosive boiling simulation. Video S4: Simulation Case C-S2 during the non-equilibrium explosive boiling simulation. References [43–45] are cited in the supplementary materials.

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Conflicts of Interest: The authors declare no conflicts of interest.

Nomenclature

A	Nominal surface area	($\text{\AA}^2$)
$\text{\AA}$	Angstrom	-
d	Lattice constant	($\text{\AA}$)
E	Young’s Modulus	(GPa)
E_f	Total energy of fluid atoms.	(eV)
FCC	Face-centered-cubic	-
GW	Gigawatt	-
K	Spring constant	($\text{eV}/\text{\AA}^2$)
L-J 12-6	Lennard-Jones 12-6	-
m	Meter	-
MDS	Molecular dynamics simulation	-
NVE	Microcanonical ensemble	-
NPT	Isothermal–isobaric ensemble	-
NVT	Canonical ensemble	-
OVITO	Open Visualization Tool	-

ps	Picosecond	-
q	Heat flux	(eV/Å ² ps)
r	Distance between the particles	(Å)
RDF	Radial distribution function	-
t	Time	(ps)
T	Temperature	(K)
U	Potential energy	(eV)
Greek Symbols		
α	Potential energy factor	-
ε	Energy parameter for L-J 12-6 potential	(eV)
σ	Length parameter for L-J 12-6 potential	(Å)
Subscripts		
Ar	Argon	
Cu	Copper	
i	Particle i	
j	Particle j	

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