



# Study on the effect of foreign particle on bubble nucleation by using molecular dynamics simulation

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## ABSTRACT

To promote the engineering application of additive in enhancing nucleate boiling, the effect of foreign particles on bubble nucleation is investigated by the molecular dynamics simulation method. Some foreign atoms are added into the pure argon system with a proportion of 5%. The liquid is heated by a hydrophilic smooth platinum substrate to achieve bubble nucleation. The results show that foreign atoms have significant impacts on bubble nucleation. Compared with the pure liquid system, the bubble nucleation efficiencies in the aspects of the incipient nucleation time and temperature are promoted by the foreign atom with a smaller energy parameter than argon atom but decreased with the increasing energy parameter. Then, the intrinsic regime of the difference between pure liquid and mixed liquid in bubble nucleation is fully illustrated based on the competition between atomic potential energy and atomic kinetic energy, which are the restriction and impetus for bubble nucleation, respectively. Furthermore, based on the influencing regime of foreign atoms in bubble nucleation, a further application of foreign atoms in controlling the nucleation position is developed.

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## 1. Introduction

The nucleate boiling has the advantages of low superheat and high heat transfer efficiency in the applications of electronic cooling, power generation, refrigeration, and cryogenics [1,2]. Therefore, it has attracted considerable attention in the past decades, especially with the rapid development of Micro-Electro-Mechanical System (MEMS) and Nano-Electro-Mechanical System (NEMS) [3]. The nucleate boiling studies on the enhancement of heat transfer efficiency has been carried out by many scholars through the macroscopic experiment method [4–9]. The experiment results indicated that nanoparticles play an important role in promoting nucleate boiling [8]. The nucleate boiling generally includes three stages: bubble nucleation, bubble growth and coalescence, and bubble departure. The bubble nucleation is the initial stage of nucleate boiling, and clarifying the effect of foreign particles on the bubble nucleation is vital for its development and application in the engineering.

Molecular dynamics simulation method (MD) is a powerful tool for describing the micro behavior [9], and which has been widely used to study the bubble nucleation in recent years. Tsuda et al. [10] investigated the growth mechanism of cavitation bubble nuclei in a two-component fluid where the noncondensable gas was dissolved at a

certain molar fraction. A frequent coalescence process of bubble nucleus was observed in the two-component liquid, which was different from that in the one-component liquid with a competing growth process of the bubble nucleus. Suh et al. [11] studied the effect of foreign particles on bubble nucleation. The simulation systems with the foreign particles showed an overall increase in bubble formation, but the impact of foreign particle shape was inconclusive. Baidakov et al. [12] conducted a comparison between MD simulation results and classical nucleation theory to reveal a qualitative difference of bubble nucleation in a pure liquid and a solution (methane and nitrogen).

On the other hand, the studies of bubble nucleation in a one-component system are universal. Zhou et al. [13] investigated the nucleate boiling of pure liquid argon on patterned surfaces with different wettabilities. The wall temperature affected the bubble nucleation position, and the reasons for that were analyzed by the change trends of heat flux and the state points of argon during bubble nucleation processes. Zhang et al. [14] studied the effect of substrate wettability on the nucleation and growth of nanobubbles in a nanochannel with a groove. The heterogeneous nucleation happened on the hydrophobic groove, and the bubble nucleation position was changed to where inside the liquid film with the increase of hydrophilicity. Similarly, Bryukhanov et al. [15] investigated the formation of vapor bubbles in a hydrophobic smooth nanochannel. It was found that the probability of spontaneous bubble nucleation and its nucleation place depended on the liquid-solid interaction. Mukherjee et al. [16] investigated

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nucleate boiling on a grooved substrate. The average energy of the molecules on the groove was increased by applying a heat flux through the substrate, leading to the formation of a bubble nucleus. Moreover, the effects of groove geometry parameters on bubble nucleation were fully discussed. Chen et al. [17] studied the bubble nucleation on the grooved substrate with different wettability. An initial bubble nucleus existed in the strongly hydrophobic groove and slowly grew up with the heating. However, the strongly hydrophilic groove was covered with a layer of liquid atoms after bubble nucleation.

The above studies provide significant insights into bubble nucleation on the micro-scale. Both the substrate characteristics and foreign atoms have significant effects on bubble nucleation. However, the influencing mechanism of foreign particles has not been revealed yet, which hinders the further development of the foreign particles in the engineering application of enhancing nucleate boiling. Therefore, in this paper, the MD method is conducted to figure out the differences between pure liquid and mixed liquid in bubble nucleation, and the intrinsic regime of differences is further explored based on the competition of atomic potential energy and atomic kinetic energy. Moreover, based on the intrinsic regime, the further application of foreign atoms in controlling the nucleation position is developed.

## 2. Simulation system and method

As shown in Fig. 1, the simulation box is a cubic box with a size of 30.2 nm ( $x$ )  $\times$  5.0 nm ( $y$ )  $\times$  150.1 nm ( $z$ ). Five layers of dark blue platinum atoms (Pt) are placed at the bottom with the arrangement of face-centered cubic structures (FCC (111)). The three layers of platinum atoms at the bottom are set as the heat source, whose temperature is controlled by a Langevin thermostat. 97,000 liquid argon atoms (Ar) with the color of reddish-brown are placed on the substrate surface with an initial density of 1.367 g/cm<sup>3</sup>. 4850 foreign atoms (Br) with the color of green is added to the liquid and vapor regions, accounting for 5% of argon atoms. A periodic boundary is applied to the  $x$ -direction and  $y$ -direction, and the atom will come back to the simulation box from one side when it leaves on the opposite side. On the other hand, a reflecting wall is applied to the  $z$ -direction because of the existence of a metal substrate at the bottom. During the simulation, if an atom moves outside the reflecting wall in a time step by a distance delta, then it is put back inside the simulation box by the same delta, and the sign of the corresponding component of its velocity is flipped. Therefore, the atoms reflect from the top boundary without any losses of energy and momentum.

The interaction potential between two different atoms is described by the Lennard-Jones (L-J) potential.

$$\phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r} \right)^{12} - \left( \frac{\sigma}{r} \right)^6 \right] \quad (1)$$

$$\epsilon_{a-b} = \sqrt{\epsilon_a \epsilon_b} \quad (2)$$

$$\sigma_{a-b} = \frac{\sigma_a + \sigma_b}{2} \quad (3)$$

where  $\epsilon$  and  $\sigma$  express the energy parameter and length parameter, respectively. The subscripts  $a$  and  $b$  represent different types of atom.  $\epsilon_{a-b}$  and  $\sigma_{a-b}$  are calculated by Eqs. (2) and (3) based on the Lorentz-Berthelot combining rule [18]. The values of these parameters are listed in Table 1. It is worth stressing that the foreign atom Br is not a certain kind of atom, and four types of Br with different energy parameters are chosen to discuss its effect on bubble nucleation thoroughly. Based on the energy parameter of Ar, that of Br is adjusted by a scaling parameter  $\beta$  with the values of 0.5, 0.75, 1.25, and 1.5, respectively. On the other hand, the length parameter of Br is the same as that of Ar.

The present study is conducted by a Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [20], which is a popular open-

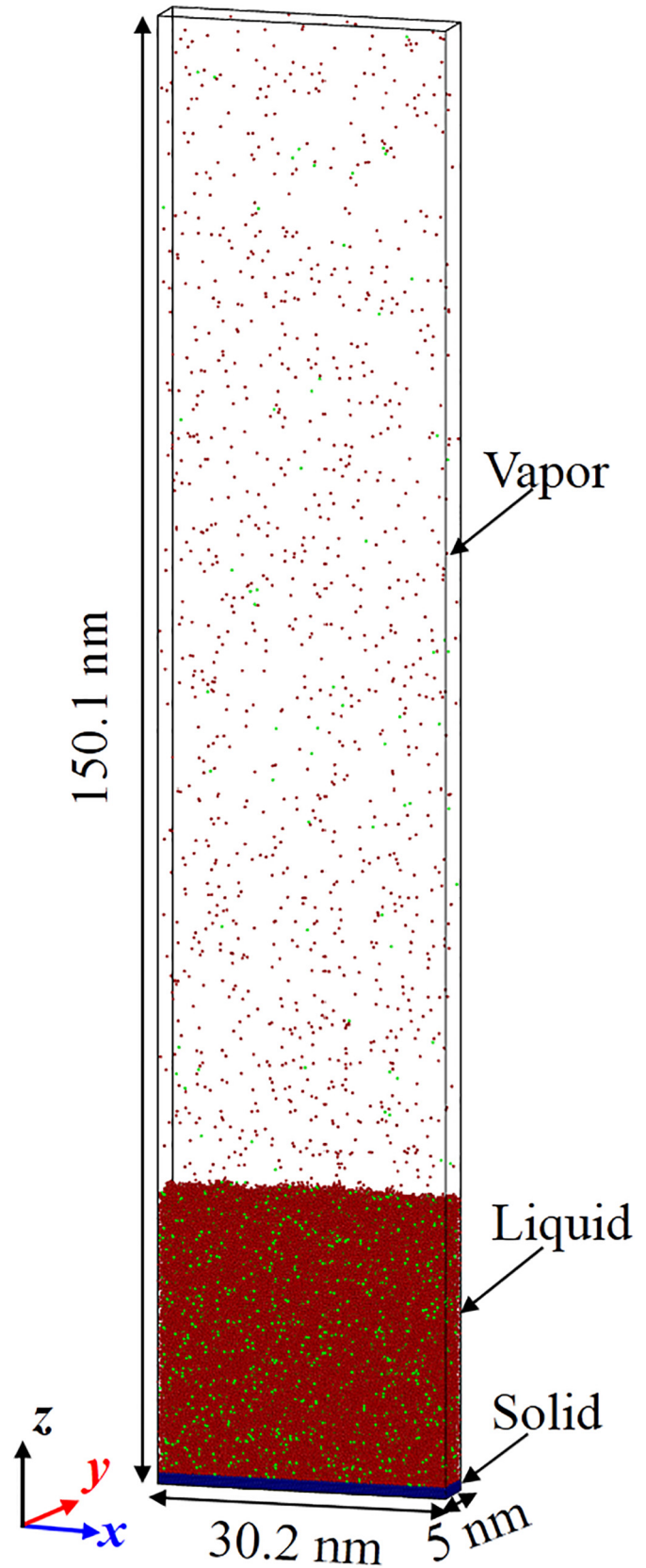


Fig. 1. Initial configuration of the simulation system.

source software for molecular dynamics simulation developed by the Sandia National Laboratory. During the simulation process, the cut-off radius  $r_c = 3.5\sigma_{Ar}$  and time step  $\Delta t = 5 fs$  are set to improve simulation efficiency, and the position and velocity of each atom are updated by a

**Table 1**  
Lennard-Jones parameters for Ar–Ar, Pt–Pt, and Br–Br [19].

Interaction type	$\epsilon/eV$	$\sigma/nm$
Ar–Ar	0.0104	0.3405
Pt–Pt	0.5219	0.2475
Br <sub>1</sub> –Br <sub>1</sub>	0.0052	0.3405
Br <sub>2</sub> –Br <sub>2</sub>	0.0078	0.3405
Br <sub>3</sub> –Br <sub>3</sub>	0.013	0.3405
Br <sub>4</sub> –Br <sub>4</sub>	0.0156	0.3405

Velocity-Verlet algorithm [21]. The simulations in this paper include two main stages: preparation and nonequilibrium. In the preparation stage, a 2.5 ns simulation in the canonical ensemble NVT is conducted to achieve an equilibrium state at 90 K. In the nonequilibrium simulation stage, the temperature of heat-source is raised to 145 K by the Langevin thermostat, and an additional 10 ns nonequilibrium simulation in the microcanonical ensemble NVE is conducted to study the liquid film phase transition. In both stages, the simulation data are output every 100 time-steps, and the atom trajectories are visualized by the open visualization tool OVITO [22].

### 3. Results and discussion

Based on the above simulation system and method, the comparisons between pure liquid and mixed liquid in bubble nucleation are conducted in this section, and a further application of foreign atom is developed. The detailed illustration is shown in the following parts.

#### 3.1. The comparison between pure liquid and mixed liquid in bubble nucleation

Different foreign atoms may have different effects on the bubble nucleation. Therefore, Four types of foreign atom Br with different energy parameters are selected as the representatives to conducted the comparisons between pure liquid and mixed liquid in bubble nucleation. As shown in Table 1, the energy parameter values of the foreign atoms are 0.5, 0.75, 1.25, and 1.5 times as much as that of argon atom, respectively, corresponding to the foreign atoms Br<sub>1</sub>, Br<sub>2</sub>, Br<sub>3</sub>, and Br<sub>4</sub>. On the other hand, the length parameter of foreign atoms is the same as that of the argon atom.

The representative snapshots of the bubble nucleation process in the systems with and without foreign atoms are illustrated in Fig. 2. For the pure liquid and mixed liquid, the bubble nuclei generate successfully in the vicinity of the substrate and grow up with the increasing time, but the nucleation position is unpredictable. After bubble nucleation, a layer of the liquid atom is restricted to the substrate surface with a thickness of about 15 Å, the reason for that will be explained in the next subsection. Compared with the pure argon liquid, the mixed liquid shows a significant impact on the incipient nucleation time. As shown in Fig. 3, no foreign atoms exist in the simulation system when the energy parameter is equal to 0.0104 eV. The incipient nucleation time of liquid is shortened by the foreign atoms (Br<sub>1</sub>, Br<sub>2</sub>) with a smaller energy parameter than the argon atom. On the contrary, the foreign atoms (Br<sub>3</sub>, Br<sub>4</sub>) with a larger energy parameter than the argon atom delays the formation of a bubble nucleus on the substrate. It is noteworthy that the nucleation time of liquid increases with the increase of the energy parameter of foreign atom except the mixed liquid with Br<sub>4</sub>, the reason for that will be illustrated in the next subsection as well. A conclusion can be drawn from the atomic trajectory that the foreign atom with weak atomic interaction in favor of shortening the incipient nucleation time.

Fig. 4 illustrates the temperature contours of the liquid region with and without foreign atom at the incipient nucleation time. The liquid absorbs thermal energy from the substrate, and its temperature is raised from the bottom to the top. It is noteworthy that some singular points with a high temperature in the top region because of the statistical

error caused by less vapor atom in there. At the incipient time of bubble nucleation, the mixed liquid with Br<sub>1</sub> or Br<sub>2</sub> obtains less thermal energy than pure liquid, but the mixed liquid with Br<sub>3</sub> or Br<sub>4</sub> turns the tables to absorb more thermal energy. Therefore, the foreign atom plays an essential role in incipient nucleation temperature.

Furthermore, the bubble nucleation region is locked to calculate the incipient nucleation temperature, which is a statistical mean value within 1000 time steps as shown in Fig. 5. For the different liquids, the incipient nucleation temperatures are in the range of 125 K–138 K and increase with the increase of energy parameters. The incipient nucleation temperatures are about 134.5 K and 125.3 K in the pure liquid and mixed liquid with foreign atom Br<sub>1</sub>, respectively, and the difference is up to 9.2 K. The incipient nucleation temperature of liquid argon is decreased remarkably by the foreign atom with small energy parameter. However, the effect of the foreign atom with a large energy parameter on the incipient nucleation temperature of liquid argon is the opposite.

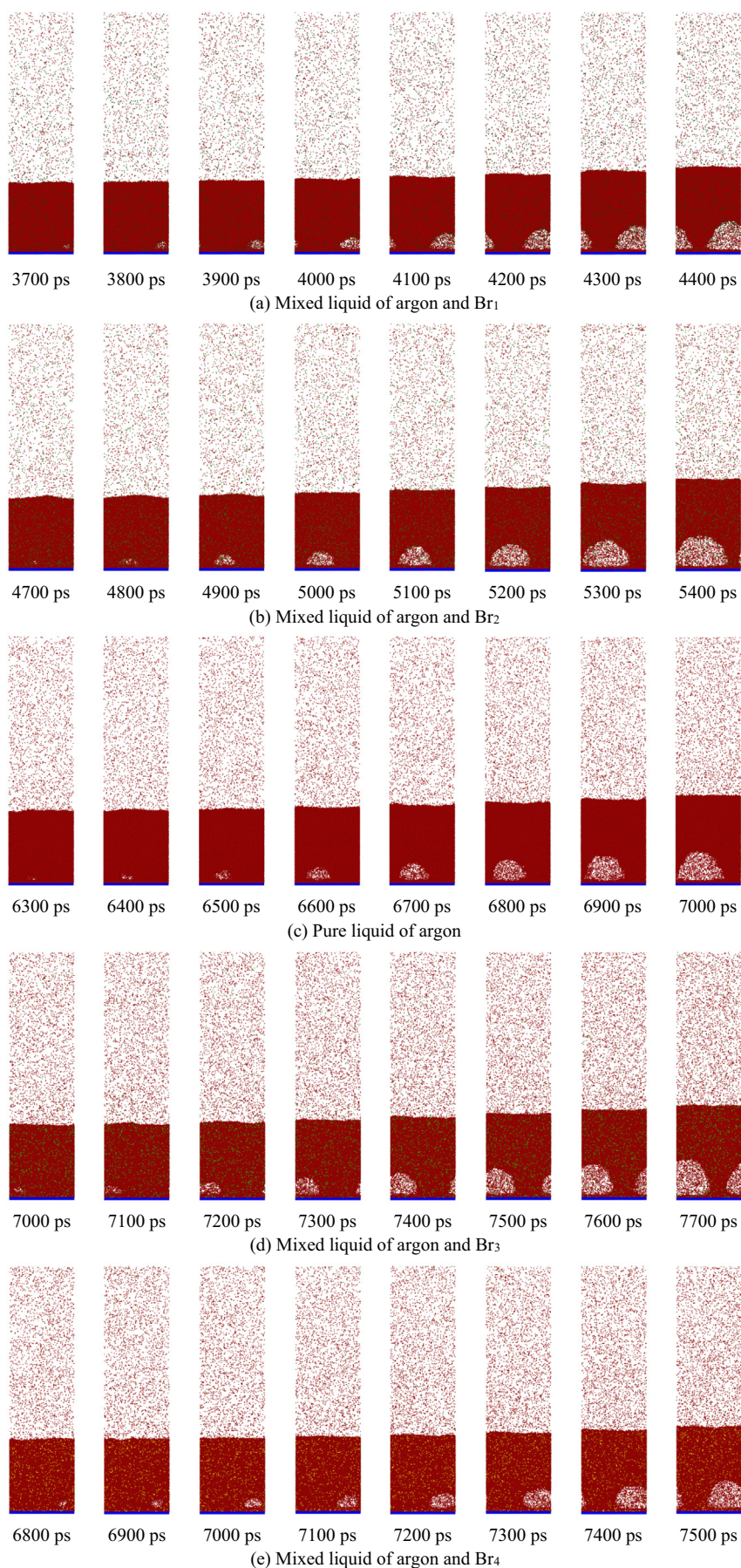
In summary, the comparisons are made between the liquids with and without foreign atom in bubble nucleation. The foreign atom with a small energy parameter has a positive impact on reducing both the incipient nucleation time and nucleation temperature. However, the effects are opposite for the foreign atom with a large energy parameter.

#### 3.2. The regime of the difference between pure liquid and mixed liquid in bubble nucleation

The differences of liquids with and without foreign atom in bubble nucleation efficiency have been illustrated in the 3.1 section. Further, in this subsection, the intrinsic regime of the difference is explained. For the simple L-J liquid argon, the evaporation is related to the escape of molecules from a potential well in the field established by the liquid-vapor interface [23]. In the present study, the argon atoms only have two types of energy: potential energy and kinetic energy. The atomic kinetic energy is the impetus for escaping and directly related to macro temperature, the change of which is the trigger for the macro phase transition. The bubble nucleation inside liquid can be viewed as a similar process to the evaporation at the liquid-vapor interface. If some liquid atoms obtain enough kinetic energy to break their potential restriction, they will be converted into the bubble nucleus. Therefore, the competition between these two types of energy is an available tool to explain the difference of bubble nucleation efficiency between pure liquid and mixed liquid.

Firstly, the comparison of potential restriction exerted on the liquid atom is made between the pure liquid and mixed liquid. Some of the thermal energy from the heating substrate is converted into the potential energy of the liquid during the nonequilibrium simulation stage, which affects the comparison result of potential restriction because of the difference among different liquids in the energy exchange. Therefore, the potential energy distribution in the liquid region with and without foreign atom is calculated at the initial time of the nonequilibrium simulation stage, as shown in Fig. 6. The potential energy in both liquid and metal regions is less than zero, indicating the potential energy is a barrier for the bubble nucleation. The potential restrictions (absolute value of potential energy) on the liquids with and without foreign atom are different, which is stronger on the pure argon liquid than the mixed liquid with Br<sub>1</sub> or Br<sub>2</sub>. Moreover, the potential restriction on the mixed liquid with Br<sub>3</sub> or Br<sub>4</sub> is further enhanced. Namely, the foreign atom with a smaller energy parameter than the argon atom prefers to decrease the potential barrier of bubble nucleation. Fig. 7 shows the diffusion coefficients of the argon atom and foreign atom in mixed liquids. The diffusion coefficient is Å<sup>2</sup>/ps for the argon atom in the pure liquid, and which is decreased by 3.5% and 6.4% by foreign atoms Br<sub>3</sub> and Br<sub>4</sub> in the mixed liquids, respectively. On the contrary, the diffusivity of the argon atom in the mixed liquids is improved by 2.1% and 7.8% by foreign atoms Br<sub>2</sub> and Br<sub>1</sub>. The change of the diffusion coefficient of argon atoms further illustrates that the foreign atom with a smaller energy parameter in favor of decreasing the potential restriction on liquid atoms.





**Fig. 2.** Representative snapshots of the bubble nucleation process in the systems with and without foreign atoms.

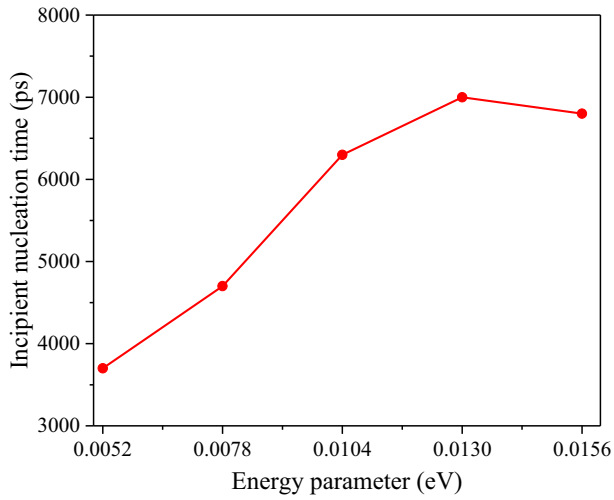


Fig. 3. Change trend of incipient nucleation time with the increasing atomic energy parameter.

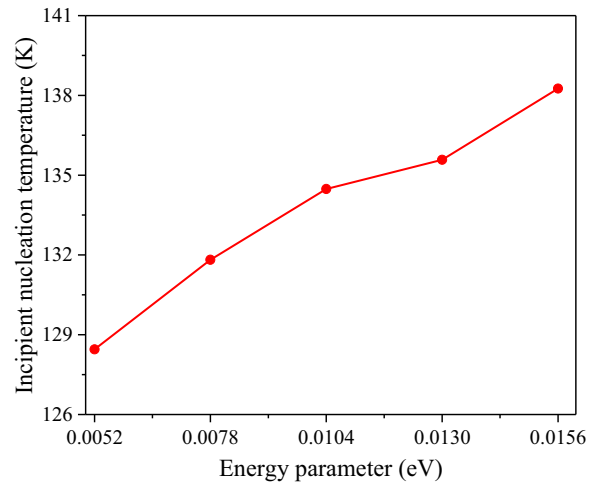


Fig. 5. Change trend of incipient nucleation temperature with the increase of potential energy.

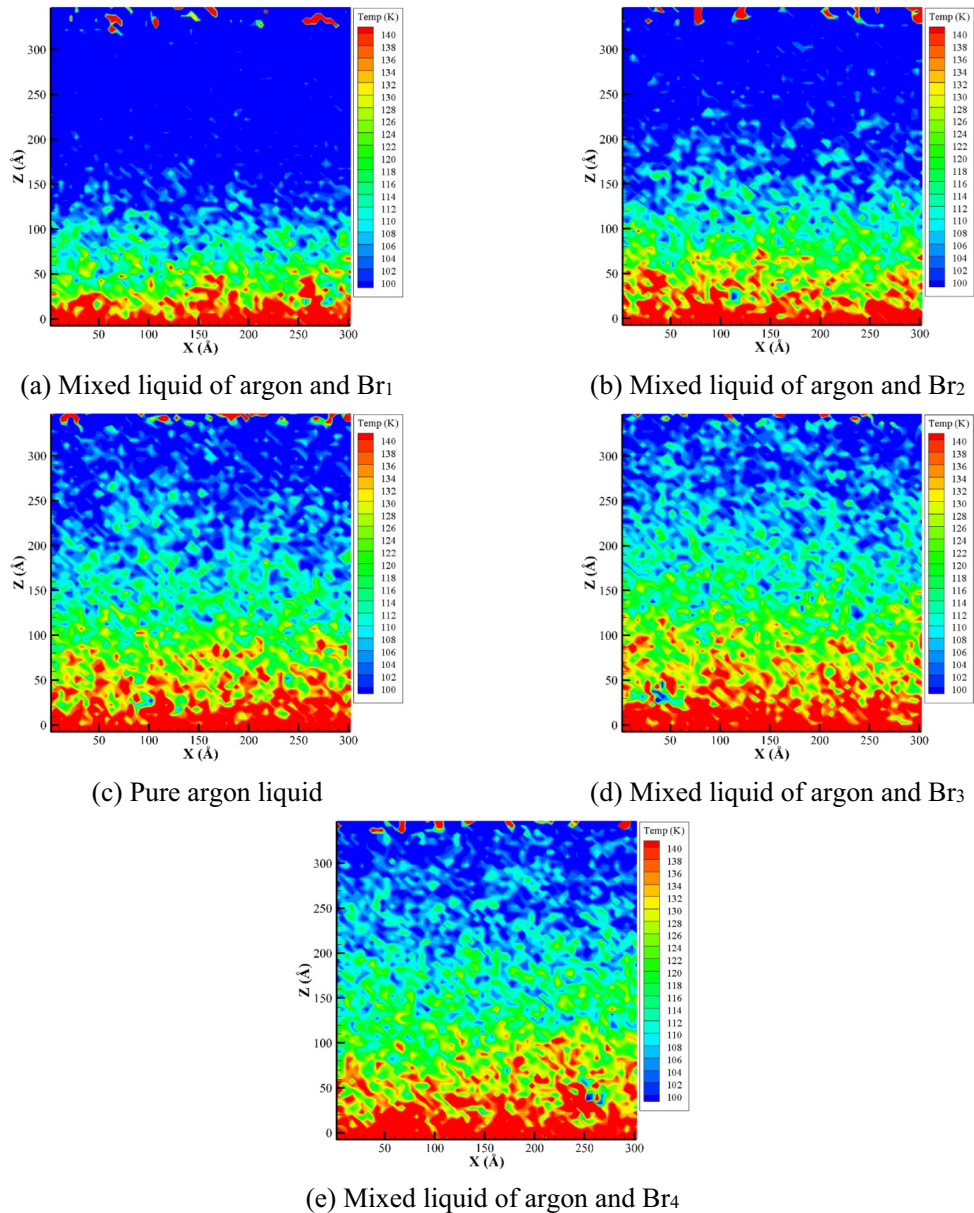


Fig. 4. Temperature contours of the liquid region with and without foreign atoms at the incipient nucleation time.



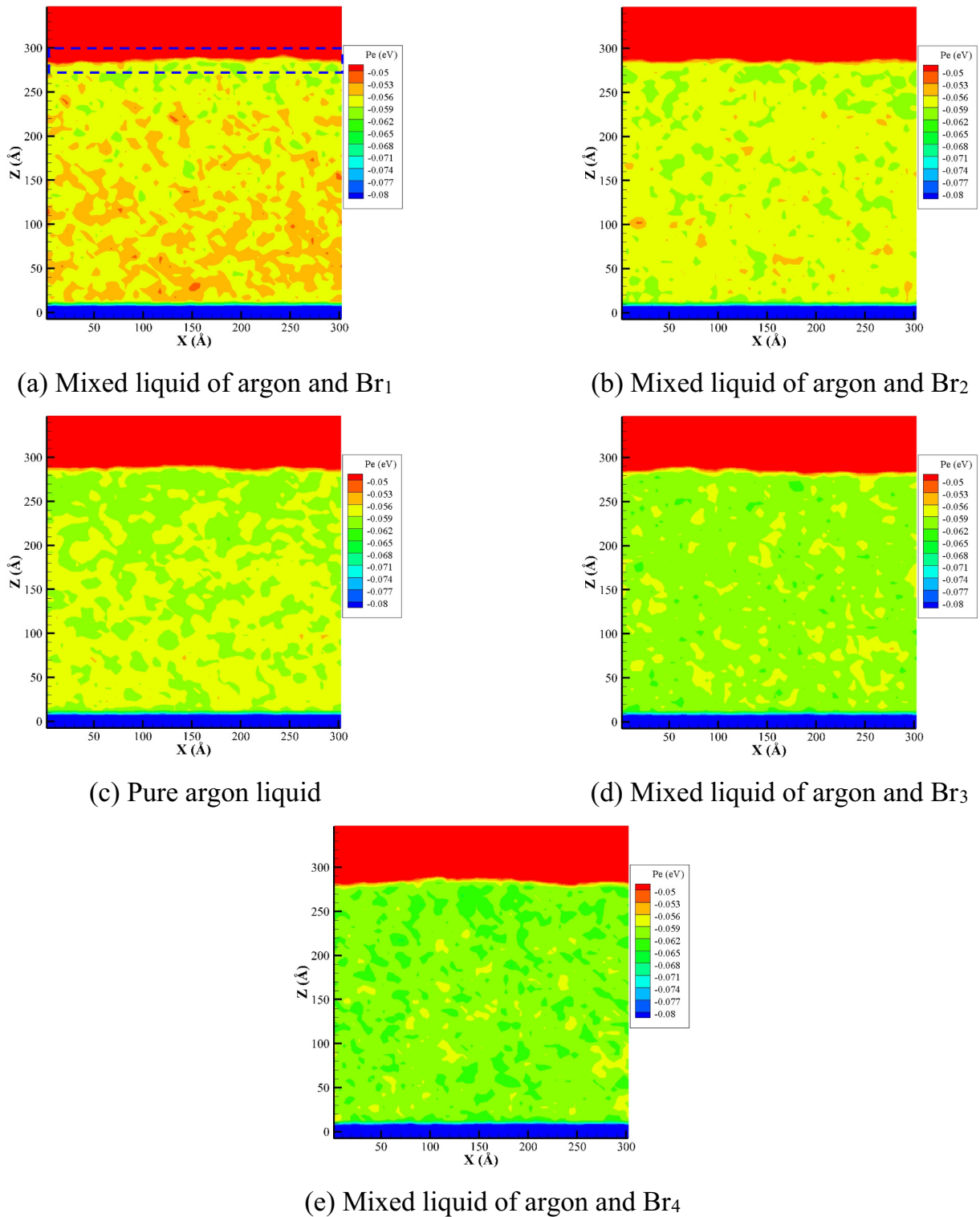


Fig. 6. Potential energy contours of the liquid region with and without foreign atom at the initial time step of the nonequilibrium simulation stage.

The reason for the difference in potential energy distribution can be illustrated by the potential energy between the argon atom and foreign atom. As shown in Fig. 8, the interatomic potential energy decreases with the increase of potential parameters (the absolute value of potential energy is the potential restriction). Therefore, the foreign atoms Br<sub>1</sub> and Br<sub>2</sub> distributing uniformly in the liquid region lead to the decrease of the potential barrier for bubble nucleation, but which is strengthened instead by the foreign atoms Br<sub>3</sub> and Br<sub>4</sub> with a large interaction with argon atom. The larger the atomic potential restriction is, the more

atomic kinetic energy is needed to achieve nucleating. The potential restriction on the atoms at the liquid-vapor interface is very weak, and these atoms tend to become a part of vapor, as shown in Fig. 6(a).

Then, the comparison of atomic kinetic energy obtained from the heating substrate is made between the pure liquid and mixed liquid. At the initial time of the nonequilibrium stage (2500 ps), the atomic kinetic energy of liquid atoms is uniform because of the whole system achieving an equilibrium stage at 90 K. Therefore, the comparison between liquids with and without foreign atom in

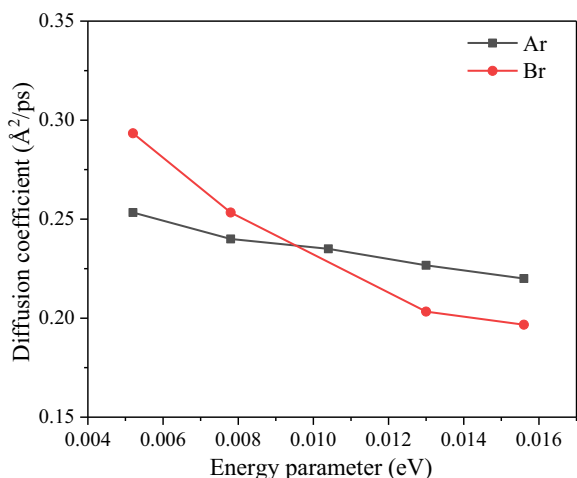


Fig. 7. Diffusion coefficients of argon atom and foreign atom in mixed liquids.

the kinetic energy distributions is conducted at 3000 ps, as shown in Fig. 9. It is hard to distinguish the differences between the liquids with and without foreign atoms in the kinetic energy distributions because the argon atoms dominate the heat transfer. Besides, the temperature trends of pure liquid and mixed liquids before 3000 ps are obtained to make a further comparison of heat transfer, as shown in Fig. 10. The temperature trends show that the foreign atom with a stronger energy parameter in favor of improving heat transfer efficiency. Namely, the mixed liquid with Br<sub>3</sub> or Br<sub>4</sub> tend to obtain more thermal energy than pure liquid to increase their kinetic energy within the same time, but the effect of Br<sub>1</sub> and Br<sub>2</sub> is on the contrary. On the other hand, The magnitude of liquid kinetic energy at 3000 ps is about a quarter of liquid potential energy at the initial time of the nonequilibrium stage. Therefore, the liquid atoms need to absorb more thermal energy to improve their kinetic energy and decrease their potential restriction.

The foreign atom shows a similar effect on the change of both the atomic potential energy and atomic kinetic energy. It is hard to explain the difference between pure liquid and mixed liquid in bubble nucleation through the individual comparison of atomic kinetic energy or atomic potential energy. Therefore, the further comparison between the pure liquid and mixed liquid in the

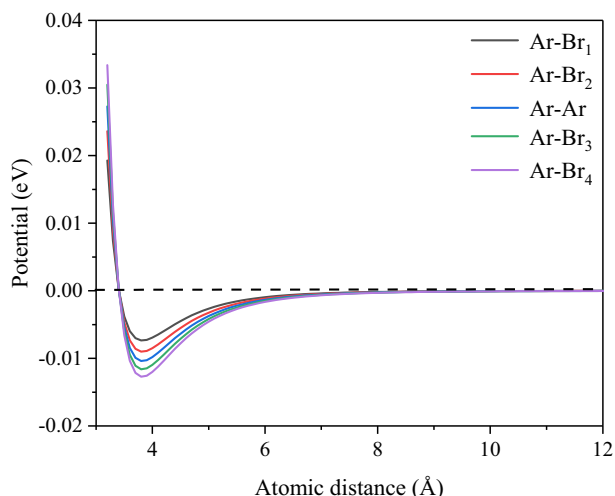


Fig. 8. Trends of potential between different atoms with the change of atomic distance.

competition of atomic potential energy and atomic kinetic energy is needed. Fig. 11 illustrates the contours of total energy (the sum of atomic kinetic energy and atomic potential energy) in different liquids at 3700 ps, which is the incipient nucleation time of mixed liquid with Br<sub>1</sub>. The liquid atoms in the vicinity of substrate absorb thermal energy from the heating substrate to increase their kinetic energy and decrease their potential restriction. At 3700 ps, in the mixed liquid with Br<sub>1</sub>, the kinetic energy of some liquid atoms clinging the substrate wins the competition with their potential energy, leading the formation of bubble nucleus, as shown in Fig. 11 (a). It is attractive that the position of where atomic kinetic energy larger than atomic potential energy coincides with the bubble nucleation position inside the mixed liquid with Br<sub>1</sub>, as shown in Fig. 2(a). At the same time, the total energy distributions in the other liquids are less than zero, limiting the happening of bubble nucleation before 3700 ps, as shown in Figs. 11(b), (c), (d), and (e). For the mixed liquid with Br<sub>1</sub>, the heat exchange efficiency is lowest among the pure liquid and mixed liquids, as shown in Fig. 10, thus the temperature of the bubble nucleation region is lowest at the incipient nucleation time of 3700 ps. Based on the above analysis and comparison, the advantage of mixed liquid with Br<sub>1</sub> in both incipient nucleation time and nucleation temperature is verified. On the other hand, for the vapor region in all cases, the total energy is equal or larger than zero, indicating the availability of the ideal for illustrating the difference regime between the pure liquid and mixed liquid based on the competition of atomic potential energy and atomic kinetic energy. On the contrary, the potential restriction on the atoms clinging to the substrate surface is so large that they are hard to get rid of the substrate limitation and cover the substrate surface all the time.

Fig. 12 shows the competition results of atomic kinetic energy and atomic potential energy in pure liquid and another three kinds of mixed liquid. Similarly, the position of where atomic kinetic energy larger than atomic potential energy coincides with the bubble nucleation position at the incipient nucleation time. On the other hand, the happening of some liquid atoms breaking their potential restriction inside the liquid is much earlier in the mixed liquid with Br<sub>2</sub>, followed by the pure liquid, the mixed liquid with Br<sub>4</sub>, and the mixed liquid with Br<sub>3</sub>. This trend successfully explains the difference of incipient nucleation time between different liquids.

In summary, the reason for the difference between pure liquid and mixed liquid in bubble nucleation efficiency is efficiently illustrated based on the competition of atomic potential energy and atomic kinetic energy. The exchange efficiency of atomic kinetic energy is dominated by the argon atoms, which take up 95% of mixed liquid. The potential restriction on the liquid atoms strengthens with the increase of energy parameters. The position with a weak potential barrier for bubble nucleation is around a foreign atom in the mixed liquid with Br<sub>1</sub> and Br<sub>2</sub>. As a result, the bubble nucleation efficiency of liquid argon is promoted by foreign atoms Br<sub>1</sub> and Br<sub>2</sub>. On the contrary, the position with a weak potential barrier for bubble nucleation is around an argon atom in the mixed liquid with Br<sub>3</sub> or Br<sub>4</sub>. Even so, the argon atom needs more kinetic energy to achieve bubble nucleation under the effect of surrounding foreign atom Br<sub>3</sub> or Br<sub>4</sub>. Therefore, the bubble nucleation efficiency of liquid argon is weakened by foreign atoms Br<sub>3</sub> and Br<sub>4</sub>. On the other hand, the exchange efficiency of atomic kinetic energy in mixed liquid with Br<sub>4</sub> is slightly higher than that in mixed liquid with Br<sub>3</sub>. Moreover, in the simulation process, the kinetic energy tends to distribute uniformly in the liquid region, but not for the potential energy. Therefore, the atomic kinetic energy breaking atomic potential restriction in one region with less foreign atom around in the mixed liquid with Br<sub>4</sub> is more quickly than that of the mixed liquid with Br<sub>3</sub>, and the incipient nucleation time of the mixed liquid with Br<sub>4</sub> is earlier than that of the mixed liquid with Br<sub>3</sub>.

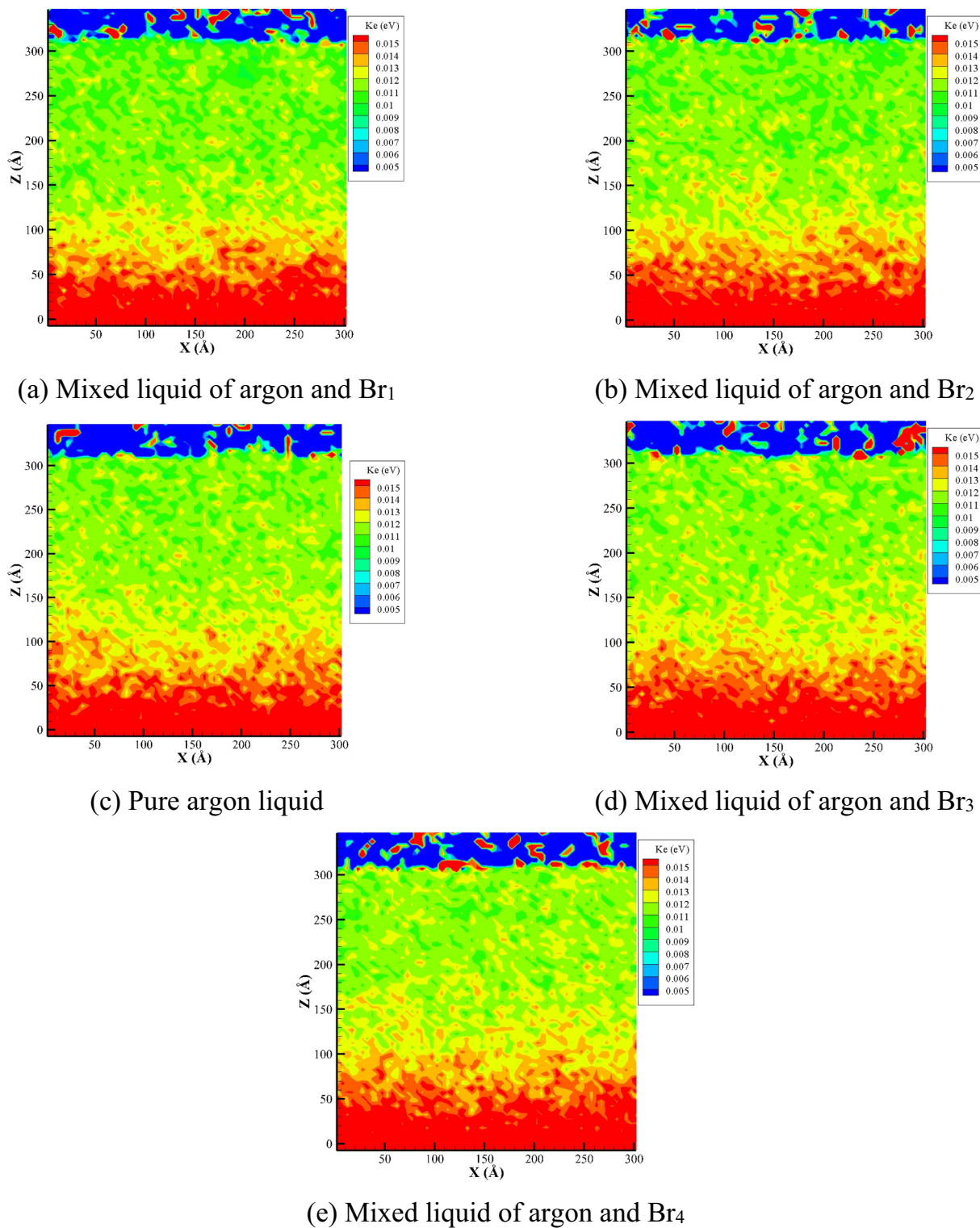


Fig. 9. Kinetic energy contours of the liquid region with and without foreign atom at 3000 ps.

### 3.3. The application of foreign atom on controlling the bubble nucleation position

From the above studies, we can find that the bubble nucleation position is unpredictable. If the foreign atoms with a small energy parameter are only added to some local region of liquid argon system, the bubble nucleus will generate firstly in there based on the analysis in Subsection 3.2. Therefore, 350 foreign atoms Br<sub>1</sub> are placed on the

center of the substrate to study its effect on bubble nucleation position and efficiency further.

Fig. 13 illustrates the representative snapshots of the bubble nucleation process in the liquid argon with foreign atoms on the substrate center. The bubble nucleus turns up on the center of the substrate, which is the same as the pre-setting position. However, the bubble nucleation position is not on the substrate surface, which is still covered by a layer of liquid atoms because of the large potential restriction from the



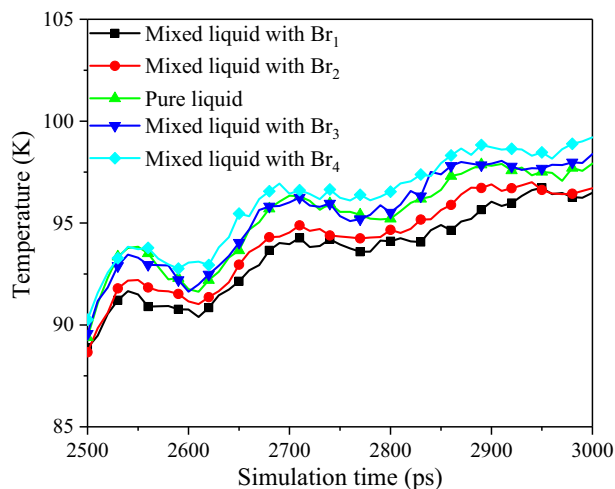


Fig. 10. Temperature trends of pure liquid and mixed liquids.

substrate. On the other hand, the incipient nucleation time and temperature respectively are 3200 ps and 124.0 K, which are smaller than that of uniform mixed liquid with foreign atom Br<sub>1</sub>. The results indicate that the bubble nucleation position can be controlled by added the foreign atom in a local pre-setting position. Moreover, the bubble nucleation efficiency is further improved by less foreign atoms.

4. Conclusions

In this paper, the comparisons between pure liquid and mixed liquid are conducted to illustrate the effect of foreign atom on bubble nucleation by using the molecular dynamics simulation, and the intrinsic regime of difference is fully illustrated based on the competition of atomic potential energy and atomic kinetic energy. Furthermore, the foreign atoms are adapted to control the bubble nucleation position and improve bubble nucleation efficiency. The conclusions are summarized as follows:

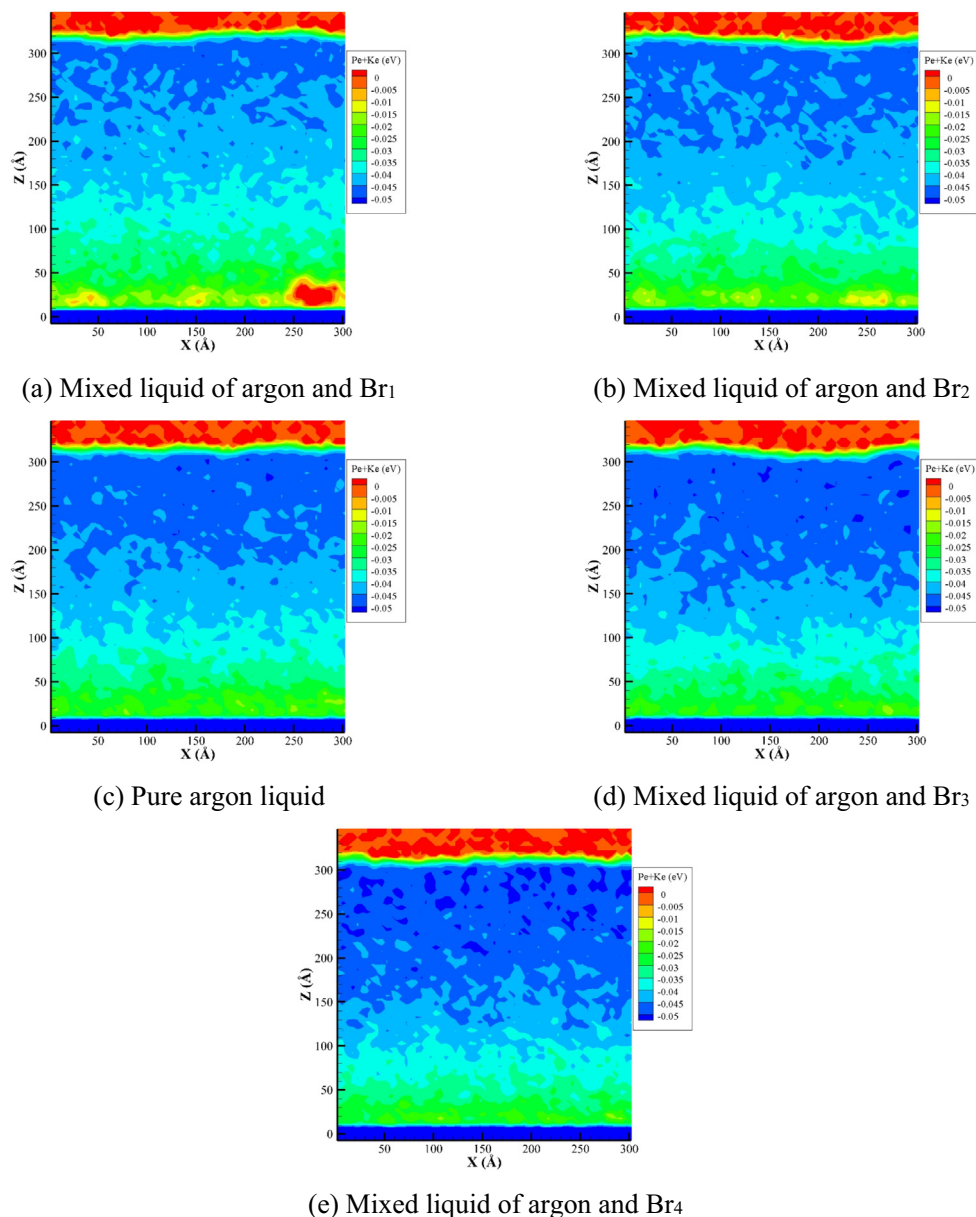
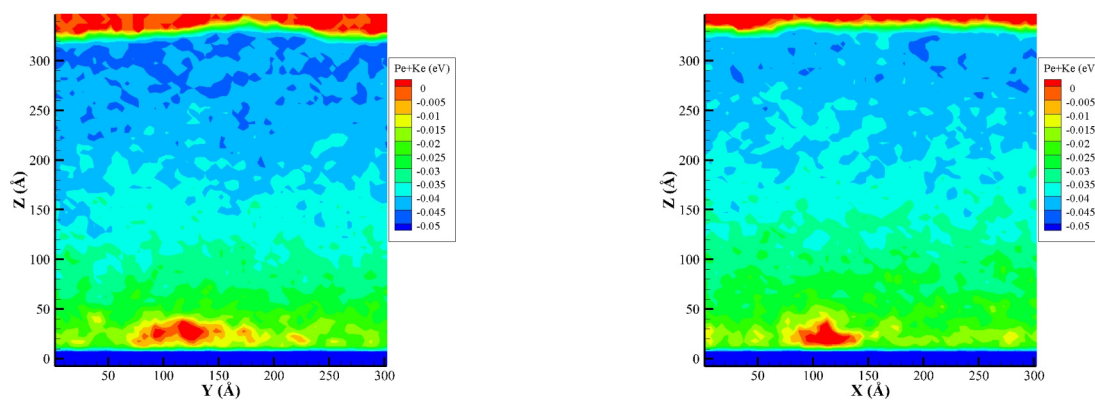
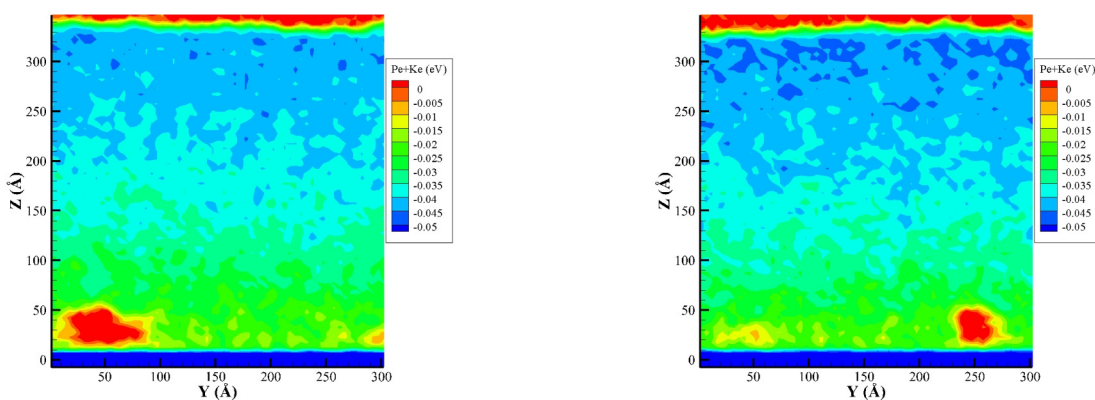


Fig. 11. Contours of the total energy at 3700 ps.

(a) Mixed liquid of argon and Br<sub>2</sub> (4700 ps)

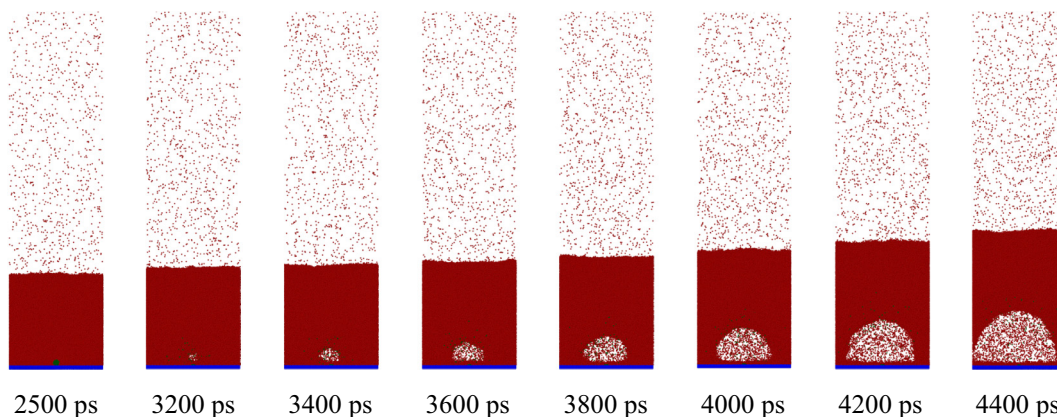
(b) Pure argon liquid (6300 ps)

(c) Mixed liquid of argon and Br<sub>3</sub> (7000 ps)(d) Mixed liquid of argon and Br<sub>4</sub> (6800 ps)**Fig. 12.** Contours of the total energy at the incipient nucleation time.

- (1) The bubble nucleation phenomenon happens inside both pure liquid and mixed liquid with different foreign atoms on the smooth hydrophilic substrate with a temperature of 145 K, and the foreign atom plays a significant role in bubble nucleation efficiency. The foreign atom with a smaller energy parameter than the argon atom significantly improves the bubble nucleation efficiency in the aspects of incipient nucleation temperature and nucleation time. However, the foreign atom with a larger energy parameter than the argon atom has an opposite impact.
- (2) The intrinsic regime of the differences between pure liquid and mixed liquid is fully explained based on the competition of

atomic potential energy and atomic kinetic energy. Both the exchange efficiency of atomic kinetic energy and the potential restriction on the liquid atom are weakened by the foreign atoms with a small energy parameter than argon atom, but the reduction of the latter is more significant than the former. As a result, the bubble nucleation efficiency is improved. On the contrary, the foreign atoms with a large energy parameter cause a considerable potential restriction on liquid atoms, leading to a decrease of bubble nucleation efficiency.

- (3) The adding of foreign atoms is an available method to control the bubble nucleation position. The foreign atoms are added to a

**Fig. 13.** Representative snapshots of the bubble nucleation process in the systems with foreign atoms on the substrate center.

local region inside the liquid, where the potential barrier for bubble nucleation is reduced significantly, leading the formation of a bubble nucleus on the pre-setting position in a short time. Therefore, different types of foreign atoms can be adapted to control the intensity of nucleate boiling in different regions.

### CRedit authorship contribution statement

**Yu-Jie Chen:**Methodology, Software, Data curation, Writing - original draft.**Bo Yu:**Validation, Methodology, Supervision, Conceptualization.**Yu Zou:**Conceptualization, Visualization.**Bing-Nan Chen:** Investigation, Visualization.**Wen-Quan Tao:**Writing - review & editing.

### Declaration of competing interest

I am the corresponding author of this paper. I warrant that the manuscript has neither been nor simultaneously submitted to other journals and the work is not an infringement of any existing copyright and will indemnify the publisher against any breach of such warranty.

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### References

- [1] H.R. Seyf, Y. Zhang, Effect of nanotextured array of conical features on explosive boiling over a flat substrate: a nonequilibrium molecular dynamics study, *International Journal of Heat & Mass Transfer* 66 (11) (2013) 613–624.
- [2] V.P. Carey, Thermodynamic analysis of the intrinsic stability of superheated liquid in a micromechanical actuator with elastic walls, *Nanoscale and Microscale Thermophysical Engineering* 4 (2) (2000) 109–123.
- [3] W. Zhou, Y. Li, M. Li, J. Wei, W. Tao, Bubble nucleation over patterned surfaces with different wettabilities: molecular dynamics investigation, *Int. J. Heat Mass Transf.* 136 (2019) 1–9.
- [4] B. Bourdon, P.D. Marco, R. Rioboo, M. Marengo, J.D. Conincka, Enhancing the onset of pool boiling by wettability modification on nanometrically smooth surfaces, *International Communications in Heat & Mass Transfer* 45 (7) (2013) 11–15.
- [5] B. Bourdon, R. Rioboo, M. Marengo, E. Gosselin, J.D. Conincka, Influence of the wettability on the boiling onset, *Langmuir* 28 (2) (2012) 1618–1624.
- [6] S. Das, B. Saha, S. Bhaumik, Experimental study of nucleate pool boiling heat transfer of water by surface functionalization with SiO<sub>2</sub> nanostructure, *Exp. Thermal Fluid Sci.* 81 (2017) 454–465.
- [7] H. Jo, H.S. Ahn, S. Kang, M.H. Kim, A study of nucleate boiling heat transfer on hydrophilic, hydrophobic and heterogeneous wetting surfaces, *Int. J. Heat Mass Transf.* 54 (25–26) (2011) 5643–5652.
- [8] H. Kim, J. Kim, M.H. Kim, Effect of nanoparticles on CHF enhancement in pool boiling of nano-fluids, *Int. J. Heat Mass Transf.* 49 (25–26) (2006) 5070–5074.
- [9] X. Chen, L. Hou, W. Li, S. Li, Influence of electric field on the viscosity of waxy crude oil and micro property of paraffin: a molecular dynamics simulation study, *J. Mol. Liq.* 272 (2018) 973–981.
- [10] S.I. Tsuda, S. Takagi, Y. Matsumoto, A study on the growth of cavitation bubble nuclei using large-scale molecular dynamics simulations, *Fluid Dynamics Research* 40 (7–8) (2008) 606–615.
- [11] D. Suh, M. Nakamura, K. Yasuoka, Heterogeneous nucleation of bubbles by molecular dynamics, *J. Phys. Conf. Ser.* 656 (2015) 12037.
- [12] V.G. Baidakov, V.M. Bryukhanov, Molecular dynamics simulation of bubble nucleation in two-component Lennard-Jones solutions, *Chem. Phys. Lett.* 713 (2018) 85–90.
- [13] W. Zhou, Y. Li, M. Li, J. Wei, W. Tao, Bubble nucleation over patterned surfaces with different wettabilities: molecular dynamics investigation, *Int. J. Heat Mass Transf.* 136 (2019) 1–9.
- [14] L. Zhang, J. Xu, J. Lei, Molecular dynamics simulation of bubble nucleation in a nanochannel with a groove, *AIP Adv.* 9 (3) (2019).
- [15] V.M. Bryukhanov, V.G. Baidakov, S.P. Protsenko, Molecular dynamics simulation of nanobubbles on hydrophobic surface, *Interfacial Phenomena and Heat Transfer* 5 (2) (2017) 153–163.
- [16] S. Mukherjee, S. Datta, A.K. Das, Molecular dynamics study of boiling heat transfer over structured surfaces, *ASME. J. Heat Transfer.* 140 (5) (2018) 54503–054503–54505.
- [17] Y. Chen, J. Li, B. Yu, D. Sun, Y. Zou, D. Han, Nanoscale study of bubble nucleation on a groove substrate using molecular dynamics simulation, *Langmuir* 34 (47) (2018) 14234–14248.
- [18] J. Delhommelle, P. Millie, Inadequacy of the Lorentz–Berthelot combining rules for accurate predictions of equilibrium properties by molecular simulation, *Mol. Phys.* 99 (2001) 619–625.
- [19] Y. Chen, Y. Zou, B. Yu, D. Sun, X. Chen, Effects of surface wettability on rapid boiling and bubble nucleation: a molecular dynamics study, *Nanoscale and Microscale Thermophysical Engineering* 22 (2018) 198–212.
- [20] S. Plimpton, Fast parallel algorithms for short-range molecular dynamics, *J. Comput. Phys.* 117 (1993) 1–19.
- [21] M.P. Allen, D.J. Tildesley, J.R. Banavar, *Computer Simulation of Liquids*, Oxford University Press, New York, 1987.
- [22] A. Stukowski, Visualization and analysis of atomistic simulation data with ovito—the open visualization tool, *Modelling & Simulation in Materials Science & Engineering* 18 (2010) 2154–2162.
- [23] V.K. Shen, P.G. Debenedetti, A kinetic theory of homogeneous bubble nucleation, *J. Chem. Phys.* 118 (2003) 768–782.