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Bubble nucleation on various surfaces with inhomogeneous interface wettability based on molecular dynamics simulation

Yujie Chen[a], Yu Zou[b], Yi Wang[a], Dongxu Han[b], Bo Yu[b,*]

[a] National Engineering Laboratory for Pipeline Safety/MOE Key Laboratory of Petroleum Engineering/Beijing Key Laboratory of Urban Oil and Gas Distribution Technology, China University of Petroleum, Beijing 102249, China

[b] School of Mechanical Engineering, Beijing Key Laboratory of Pipeline Critical Technology and Equipment for Deepwater Oil & Gas Development, Beijing Institute of Petrochemical Technology, Beijing, 102617, China

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ABSTRACT

In this paper, non-equilibrium molecular dynamics simulation is performed to study the bubble nucleation behaviors on smooth and nanostructured surfaces with inhomogeneous interface wettability. The bubble nucleus turns up after the substrate temperature is set up to be 250 K. The atomic trajectory, argon density profiles and bubble nucleus volume are computed to compare the processes of bubble nucleation on different surfaces. First of all, comparisons are made between weak-hydrophilic smooth surfaces with different area of strong-hydrophilic region in the center. Results show that larger area of strong-hydrophilic region is beneficial for the formation and growth of bubble nucleus. Then, the strong-hydrophilic smooth region is replaced by introducing strong-hydrophilic nanostructure. Results show that the nanostructure surface is favorable for bubble nucleation and can improve the efficiency of nucleate boiling. Finally, the common strong-hydrophilic nanostructures of cylinder, cuboid and cone are constructed to explore their effects on bubble nucleation. Both the strong-hydrophilic area and the height of these nanostructures are the same. It is found that the nanostructure morphology has little influence on the efficiency of bubble nucleation.

1. Introduction

Nucleate boiling is one of the most challenging subjects in thermal fluid engineering, which has been widely used for cooling electronic devices, thermal management of aerospace and micro energy systems. Therefore, the physics essence of nucleate boiling is one of the research hotspots in recent decades [1]. However, the traditional methods [2–4] can't thoroughly study the mechanism of bubble nucleation due to its complexity and diversity [5,6]. The further study is required to satisfy an increasing emphasis on miniaturization of engineering systems with/without extremely fast processes and study the micro- and nano-scale nucleate boiling phenomena [7].

Molecular dynamics simulation (MD) is a method integrating physics, mathematics and chemistry, which has been widely applied to study the phenomena of nucleate boiling at microscopic scale [8]. Maruyama and Kimura [9] explored the mechanism of bubble nucleation by molecular dynamics simulation. It was found that bubble nucleus appeared when the system was stretched, and the more hydrophilic surface was suitable for bubble nucleation. Nagayama et al. [10] studied the influences of interface wettability on bubble nucleation in metal channels. Homogeneous nucleation occurred on the hydrophilic surface, while heterogeneous nucleation turned up on the hydrophobic surface. Besides, there was no bubble nucleation phenomenon happened on the non-wetting surface. She et al. [11] also analyzed the bubble nucleation behavior in metal channels, but there was a cavity in the bottom surface. The cavity provided larger effective volume to reduce the relative density of argon, which was conducive to the formation of bubble nucleus. Moreover, the bubble nucleation was premised on hydrophilic surface. Yamamoto and Matsumoto [12] studied the effects of different initial states of solid surface on bubble nucleation in the simulation system with a free-surface. The results showed that the bubble successfully nucleated on the surfaces with inhomogeneous heating temperature or interface wettability.

What the above research results have in common is that hydrophilic surface plays a vital role in bubble nucleation. The atomic interaction between solid and liquid atoms is stronger in more hydrophilic surface [13]. Therefore, the liquid on more hydrophilic region obtains more energy than other regions on the surface with inhomogeneous interface wettability, which is the key to bubble nucleation [12]. Moreover, the heat transfer between solid and liquid can be further strengthened with

* Corresponding author.
E-mail address: yubobox@vip.163.com (B. Yu).

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the increase of strong-hydrophilic area on the weak-hydrophilic surface, which may have a significant effect on bubble nucleation. However, the area of strong-hydrophilic region cannot be substantially increased, otherwise it will reduce the number of bubble nuclei on a surface with the limited area because the bubble nucleation is based on inhomogeneous interface wettability [12]. This problem can be solved by replacing smooth surface with the nanostructure surface. The strong-hydrophilic nanostructure supports larger heat transfer area with small ground occupation, and it may improve the efficiency of bubble nucleation while the number of bubble nuclei is kept unchanged.

Based on the above description and discussion, for a strong-hydrophilic region that is either smooth or nanostructured, positioned in the center of the weak-hydrophilic surface, its area size or nanostructure configurations may have significant effects on nucleate boiling. However, the related studies are lacking. Therefore, the bubble nucleation behaviors on smooth and nanostructured surfaces with inhomogeneous interface wettability are studied in this paper to fill the research gaps. The effects of strong-hydrophilic area, strong-hydrophilic nanostructures and its structural forms on bubble nucleation are investigated.

2. Simulation system and method

In this paper, the bubble nucleation behaviors on various platinum surfaces are simulated by molecular dynamics simulation method in the microcanonical ensemble (NVE). As shown in Fig. 1, the simulation system is a 14.9 nm (x) × 7.7 nm (y) × 35 nm (z) cuboid box, which consists of three parts: gaseous argon, liquid argon and platinum substrate. The gaseous argon sparsely distributes in the upper region. The liquid argon is tightly packed in the central region with the density of 1.367 g/cm^3, which contains 20,000 argon atoms. The solid metal platinum arrays in regular arrangement at the bottom. The boundary conditions in x and y directions are periodic. The reflecting wall is applied to the upper boundary in z direction. Argon atoms are reflected from the upper boundary without any loss of energy and momentum.

The bubble nucleus successfully turns up on the smooth surface whose left-half region is hydrophilic and right-half region is neutral in the reference [12]. Therefore, the surface wettability consists of strong hydrophilicity and weak hydrophilicity in this paper. As shown in Fig. 2, the simulation systems include two weak-hydrophilic smooth surfaces that both contain a strong-hydrophilic region in the center but with different area, and three weak-hydrophilic nanostructured surfaces that each surface is constructed with a strong-hydrophilic nanostructure but with different morphology, namely cuboid, cylindrical and conic. It is noteworthy that the central blue region represents for strong-hydrophilic and the rest red-orange region is weak-hydrophilic in all surfaces. The concrete geometric parameters of heating surfaces are listed in Table 1, and smooth surface B has larger strong-hydrophilic area than smooth surface A. The smooth surface consists of seven layers of platinum atoms with the arrangement of face-centered cubic (FCC (1 1 1)) [14]. The two layers at bottom are considered to be “phantom atoms” which acted as the heat source [15]. The temperature of “phantom atoms” is controlled by Langevin thermostat. The top five layers are set as thermal conductivity layer. A spring force is applied to each platinum atom to ensure the atoms vibrate around their equilibrium positions during the simulation process. The magnitude of spring constant is 2.925 eV/Å.

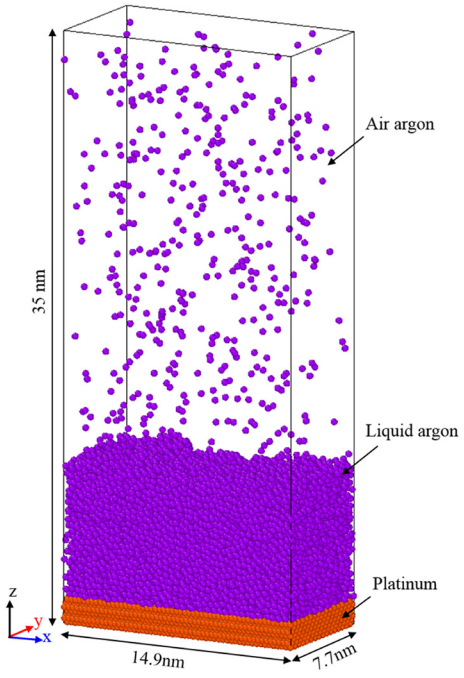

Fig. 1. The simulation system.

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [16] is performed to carry out all simulations, which mainly include two stages: equilibrium stage and data acquisition stage. In equilibrium stage, the Langevin thermostat is applied to control the temperature of “phantom atoms” at 90 K, and 4 ns simulation is conducted to make sure the simulation system reaches equilibrium state. In data acquisition stage, the temperature of heat source is set up to be 250 K for carrying out another 1.5 ns non-equilibrium simulation. The simulation data is output every 200-time steps, and atoms trajectories are visualized by OVITO [17].

The interaction between the platinum atoms can be accurately computed by EAM potential, which requires a significant amount of computing resource. While in present study, the simulations only focus on the heat transfer between metal and liquid atoms rather than inside the metal atoms. Therefore, Lennard-Jones (12–6) potential is more suitable for simulations in this paper, and the interactions of Ar-Ar and Pt-Pt are described as Eq. (1) [18].

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

where ε is the energy parameter, σ is the length parameter. The detailed values are listed in Table 2.

For the interaction between argon and platinum atoms, another modified form of Lennard-Jones potential is adopted [20]. It is a combination of the potential models used by Din [21] and Barrat [22].

$$\phi_{Pt-Ar}(r) = 4\varepsilon_{Pt-Ar}\left[\left(\frac{\sigma_{Pt-Ar}}{r}\right)^{12} - \beta\left(\frac{\sigma_{Pt-Ar}}{r}\right)^{6}\right] \tag{2}$$

$$\sigma_{Pt-Ar} = \frac{\sigma_{Pt} + \sigma_{Ar}}{2} \tag{3}$$

$$\varepsilon_{Pt-Ar} = \alpha\sqrt{\varepsilon_{Pt}\varepsilon_{Ar}} \tag{4}$$

where σ_{Pt-Ar} and ε_{Pt-Ar} are energy parameter and length parameter between platinum and argon atoms, which are based on the Lorentz–Berthelot combining rule [23]. β and α are related to the surface wettability, the specific values are listed in Table 3.

All simulations are carried out with a time step of 5 fs, the cutoff distance r_c is set as $3.5\sigma_{Ar}$. The position and velocity of atom at each step are calculated by using Velocity-Verlet algorithm [24].

$$\vec{r}\,(t+\Delta t) = \vec{r}\,(t) + \vec{v}\,(t)\Delta t + \frac{1}{2}\vec{a}\,(t)\Delta t^2 \tag{5}$$

$$\vec{v}\,(t+\Delta t) = \vec{v}\,(t) + \frac{1}{2}[\vec{a}\,(t) + \vec{a}\,(t+\Delta t)]\Delta t \tag{6}$$

where $\vec{r}$ is the position vector, $\vec{v}$ is the velocity vector, $\vec{a}$ is the acceleration vector,Δt is the time step for integration.

The absorbed heat flux of argon is computed to investigate the