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Molecular dynamics simulation of bubble nucleation on nanostructure surface

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ABSTRACT

In this paper, the bubble nucleation of ultra-thin liquid argon film on a platinum surface is studied by molecular dynamics simulation. In the simulations, the liquid is heated by the middle part and cooled by the two sides of the platinum surface. Observation of bubble nucleation is performed after increasing the temperature of heating zone. The space and time evolution of argon density distribution and the size of bubble are monitored to investigate the nucleation processes above surfaces with and without nanostructures. The results illustrate that nanostructure surface increases the solid-liquid contacting area and the degree of surface temperature non-uniformity, which results in the enhancement of heating intensity and higher rate of nucleation. Comparisons are made among surfaces with different nanostructures, with which it is further found that the heat flux increases with the height of nanostructures. Higher nanostructure reduces nucleation duration.

1. Introduction

As an important form of pool boiling, nucleate boiling is featured of high efficiency of heat transfer. The industry has seen a broad application prospects of nucleate boiling in the forefront of aerospace, electronic integration, new energy and micro and nano scale engineering [1,2]. Bubble nucleus, playing a decisive role in nucleate boiling [3], is a research hotspot within mechanism-level in recent years. The traditional experimental methods [4,5] could only qualitatively describe the process of bubble nucleation at macroscopic scale, by which the nucleation mechanism is of great difficulty to be revealed thoroughly. Obviously, these studies cannot match the applications of nucleate boiling in the rapidly developed micro and nano scale engineering [6].

With the development of computer science over past several decades, the molecular dynamics simulation has become a powerful tool to study the mechanism of bubble nucleation at molecular scale [7]. Maruyama and Kinmura [8] adopted molecular dynamics simulation to study heterogeneous nucleation of bubble on solid surface. The nucleus arose by gradually separating the parallel metal surfaces. Chen et al. [9] studied both heterogeneous and homogeneous nucleation in the isothermal-isobaric (NPT) and isothermal-isostress ($NP_{zz}T$) ensembles. The simulation results illustrated the instability of homogeneous bubble nucleus in the NPT ensemble whereas the stability of heterogeneous bubble nucleus. The nucleation temperature was related to atom interactions between solid surface and heated object. Nagayama et al. [10] researched on nucleation phenomenon in a nanochannel and found that bubble nucleation was associated with the solid-liquid interface wettability. The homogeneous nucleation turned up above the hydrophilic surface, the heterogeneous nucleation appeared above the hydrophobic surface, and no bubble nucleus generated above the non-wetting surface. She et al. [11] adopted a platinum surface with a cavity to analyze the process of bubble formation. Results showed that the cavity could provide a larger effective volume for liquid argon, thus the relative density of the argon was lower, which was conducive to the formation of bubble nuclei. Yamamoto and Matsumoto [12] investigated the initial state of nucleate boiling on ideally smooth surface, within which situations bubble nucleus occurred on the surface with inhomogenous temperature or interface wettability. Inaoka et al. [13] introduced a uniform gravitational field to all particles as well as the inhomogenous surface temperature. It was presented that the pool boiling curve and the general behavior were consistent with those observed in experiments.

The molecular dynamics simulation of bubble nucleation has achieved a series of achievements. However, most of the researches focused on the smooth surface without considering

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Nomenclature

Ar	argon
e	potential and kinetic (eV)
H	height of the nanostructure (nm)
m	molecular mass (g/mol)
N	number of molecules
P	pressure (bar)
Pt	platinum
r_c	cut off distance (Å)
S	stress tensor
T	temperature (K)
v	3 × 3 matrix-vector
x	coordinate in *x*-direction
y	coordinate in *y*-direction
z	coordinate in *z*-direction

Greek symbols

σ	length parameter of LJ potential (Å)
ε	energy parameter of LJ potential (eV)
ρ	density (g/cm^3)
φ	potential energy (J)
Δt	time step (ps)

Subscripts

Ar	argon
c	cut-off
Pt	platinum

the influence of surface nanostructure on bubble nucleation. In fact, the surface is a smooth wall on macro-scale, while with uneven nanostructures on nanoscale. The presence of nanostructure alters the contact area between solid and liquid, which may make differences in the absorption of heat flux by the argon [14]. Therefore, the differences may affect the nucleation process, which make the study of bubble nucleation on surface with nanostructure necessary. In this paper, the bubble nucleation of argon above platinum surface is studied by molecular dynamics simulations, and the differences between smooth and nanostructure surfaces are compared. On this basis, the influences of nanostructures with different heights on the growth process of bubble nucleus are investigated to study the advantages of boiling heat transfer. Besides, an optimal nanostructure height is obtained by further studying on the efficiency of bubble nucleation above surfaces with higher nanostructures.

2. Simulation method

In this paper, the processes of bubble nucleation are simulated by molecular dynamics simulation method in the microcanonical ensemble (NVE). The simulation system is an 11 nm (x) × 11 nm (y) × 29 nm (z) cuboid box, consisting of three parts: gaseous argon, liquid argon and metal platinum surface. As shown in Fig. 1, the purple area packed with sparse particles is the gas region; the purple area packed with dense particles is liquid phase, which contains 26,000–28,000 argon atoms with the whole density of 1.367 g/cm^3; the blue area is solid platinum surface (fcc(1 1 1)) [15] composed of seven layers of platinum atoms with the thickness of 1.6 nm. The position of solid-liquid interface is 0 Å in z direction. Fig. 2 shows the constructions of smooth and nanostructure surfaces. The heating region with red[1] color in the middle of the surface, and the cooling regions with blue color on both sides of the surface. In Fig. 1, the periodic boundary condition is applied in the x- and y-directions, and the upper boundary of z direction is the reflecting wall. If an atom moves outside the wall on a time step by a distance delta, then it is put back inside the wall by the same delta, and the sign of the corresponding component of its velocity is flipped. The two layers at the bottom of surface act as heat source. Spring force is exerted on each platinum atom to ensure platinum atoms vibrate around their own initial position during the process of simulations. At each time step, the magnitude of the force on each

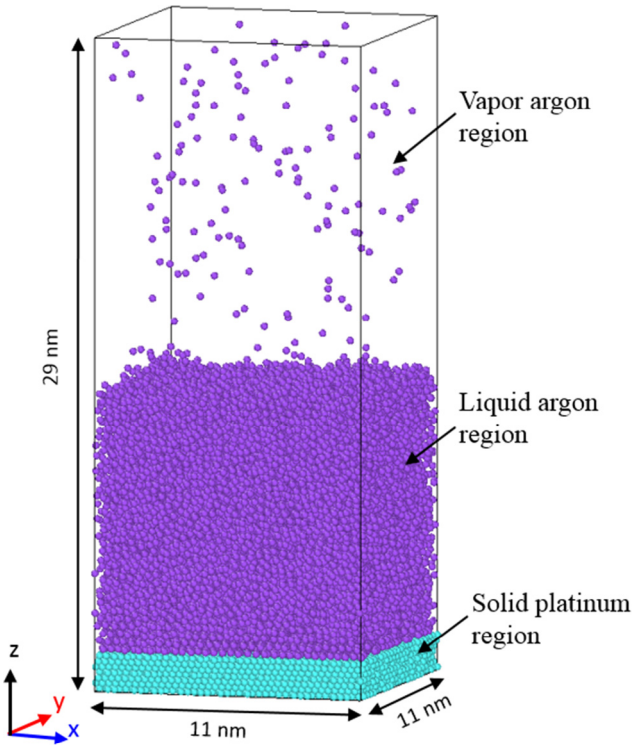

Fig. 1. Simulation system.

atom is −Kr, where r is the displacement of the atom from its current position to its initial position. K is the coefficient factor of spring, and the magnitude is 6.817 eV/Å.

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [16] is employed to simulate the processes of bubble nucleation. Simulations are carried out with the time step of 5 fs and the cutoff distance r_c is set as 3.5 σ_{Ar}. The Velocity Verlet algorithm [17] is adopted to integrate the motion equations at each time step. The simulation process includes two stages: preparation and data acquisition. In the preparation stage, 2.5 ns simulation is performed to achieve equilibrium at the temperature of 85 K. The Langevin thermostat is adopted to control system temperature. During the data acquisition stage, the temperature of cool regions are kept unchanged, while the temperature of heat region is risen to 350 K to run another 5 ns for a data acquisition and the simula-

[1] For interpretation of color in Fig. 2, the reader is referred to the web version of this article.