International Journal of Heat and Mass Transfer 95 (2016) 278–287

Contents lists available at ScienceDirect

International Journal of Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ijhmt

Bubble formation on solid surface with a cavity based on molecular dynamics simulation

Xiaohui She [a,b], Timothy A. Shedd [c], Brett Lindeman [c], Yonggao Yin [a,b,*], Xiaosong Zhang [a,b]

[a] School of Energy and Environment, Southeast University, Nanjing 210096, China
[b] Ministry of Education of Key Laboratory of Energy Thermal Conversion and Control, Southeast University, Nanjing 210096, China
[c] Department of Mechanical Engineering, University of Wisconsin-Madison, Madison 53706, USA

ARTICLE INFO

Article history:
Received 10 July 2015
Received in revised form 20 November 2015
Accepted 23 November 2015
Available online 21 December 2015

Keywords:
Molecular dynamics simulation
Bubble formation
Cavity surface
Platinum
Argon

ABSTRACT

In this paper, molecular dynamics simulations are conducted to analyze the bubble formation in liquid argon on a platinum surface with a cavity. Comparisons are made between the channels with and without the cavity on the lower wall; varying argon densities and surface wettabilities are also examined. The cavity on the surface can significantly enhance the growth of the bubble. The argon atoms in the cavity experience large repulsive forces, repulsive force gradients, density gradients and potential energy along the *z* axis, which are much larger than those near the plane surface. The argon atoms at the bottom of the cavity seem to be crystallized with all the hydrophilic surfaces, while for the argon atoms near the plane surface, they are solid-like with the strong hydrophilic surface and fluid-like with the weak hydrophilic surface. For the hydrophobic surfaces, there are few atoms in the cavity, and large fluctuations of density are observed near the surface. The plane surface shows almost the same density distributions as the cavity surface, and the surface feature seems to be irrelevant to the bubble formation.

1. Introduction

Nucleate boiling has attracted considerable attention in fundamental research over the past several decades [1,2], primarily due to its highly-efficient heat transfer characteristics. Classical theory predicts extremely large superheats (the order of hundreds degrees in some situations) for nucleation on smooth surfaces [3]. However, most experimental works have reported that nucleate boiling is observed to occur at much smaller superheats [4,5]. One popular explanation for this controversial problem is that the smooth solid surface is not perfectly smooth and micro- or nano-scale cavities may exist on the surface [6–8]. What's more, there may be pre-existing gas in the cavities, which enhances the bubble formation.

A better understanding of the nucleation mechanism can enhance energy efficiency in engineering processes. Molecular dynamics simulation is a powerful method to study nanoscale bubble behavior. Extensive work has been done from a molecular scale for bubble nucleation on a solid surface [9–18]. Hens et al. [9] conducted molecular dynamics simulations to understand the mechanism for bubble formation on a platinum substrate with particular emphasis on the surface texture. Results showed that the hydrophilic surfaces provided favorable conditions for bubble nucleation and formation of vapor films. Yamamoto and Matsumoto [10] investigated the initial stage of nucleate boiling on an ideally smooth surface with a molecular dynamics simulation, where the entire surface was heated at first, and then one part of the surface was heated, the other part was cooled. Maroo and Chung [11,12] simulated a nanoscale evaporating meniscus constructed by a thin liquid argon film on a heated platinum surface. The heat and mass transfer characteristics and pressure variation in the meniscus were studied, and a novel thermal equilibrium model for the wall-fluid heat transfer boundary condition was developed. Nagayama et al. [13] and Nagayama and Cheng [14] used molecular dynamics simulations to examine the bubble nucleation behavior confined in a nanochannel; effects of interface wettability on microscale flow in the nanochannel were also studied. The phase transition of a simple liquid bounded between two parallel walls, a few nanometers apart, was investigated with molecular dynamics simulations by Schoen et al. [15]. Maruyama et al. [16,17] compared the contact structure of liquid droplet on a solid surface for a simple Lennard-Jones fluid system and a practical water-on-platinum system. They also simulated the heterogeneous nucleation of a vapor bubble on a solid surface using molecular dynamics. Hens et al. [18] analyzed the effect of an external electric field on the spreading and evaporation of a nano-scale water droplet on a solid platinum surface.

* Corresponding author at: School of Energy and Environment, Southeast University, Nanjing 210096, China.
E-mail address: y.yin@seu.edu.cn (Y. Yin).

http://dx.doi.org/10.1016/j.ijheatmasstransfer.2015.11.082
0017-9310/

Nomenclature

Ar	argon
E	energy (kcal/mol)
f	force (kcal/mol Å)
H	height of the argon channel (Å)
h	height of the cavity (Å)
k_B	Boltzmann constant (1.38×10^{-23} J/K)
ke	kinetic energy (kcal/mol)
L	length of the channel (Å)
l	length of the cavity (Å)
m	mass (kg)
N	number of atoms
pe	potential energy (kcal/mol)
Pt	platinum
R	ratio of actual density to the saturated density
T	temperature (K)
W	width of the channel (Å)
w	width of the cavity (Å)

Greek symbols

α	potential energy factor to adjust the strength of hydrophilic interaction
β	potential energy factor to adjust the attraction for hydrophobic interaction
σ	length parameter of LJ potential (Å)
ε	energy parameter of LJ potential (J)
ρ	density (g/cm^3)
ϕ	potential energy (J)

Subscripts

Ar	argon
Pt	platinum
s	saturation

Even though the above studies have simulated the bubble formation on a solid surface using molecular dynamics and provided significant insight in the formation of nano-bubbles, most of the research has been conducted on a smooth surface and studies of the bubble formation on a surface with a cavity are lacking. In this paper, molecular dynamics simulations are carried out to analyze the bubble formation behaviors of liquid argon on a platinum surface with and without a cavity. Comparisons of bubble formation phenomena are made between the cavity surface and smooth surface based on different argon densities under a given surface wettability, and the temperature, density, force and energy profiles are obtained. Several mechanisms by which cavities can enhance the bubble formation are then discussed. In addition, bubble formations on the cavity surface and smooth surface are observed using different hydrophilic and hydrophobic surfaces.

2. Simulation methods

Heterogeneous nucleation of a vapor bubble on a solid cavity surface is simulated using the molecular dynamics method in the

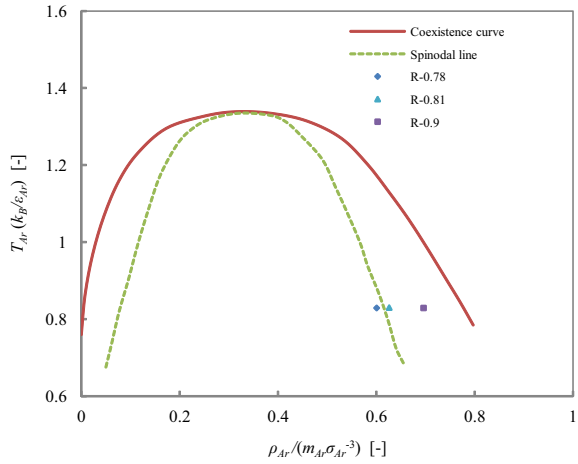

Fig. 2. Simulation points and phase diagram with coexistence curve and spinodal line.

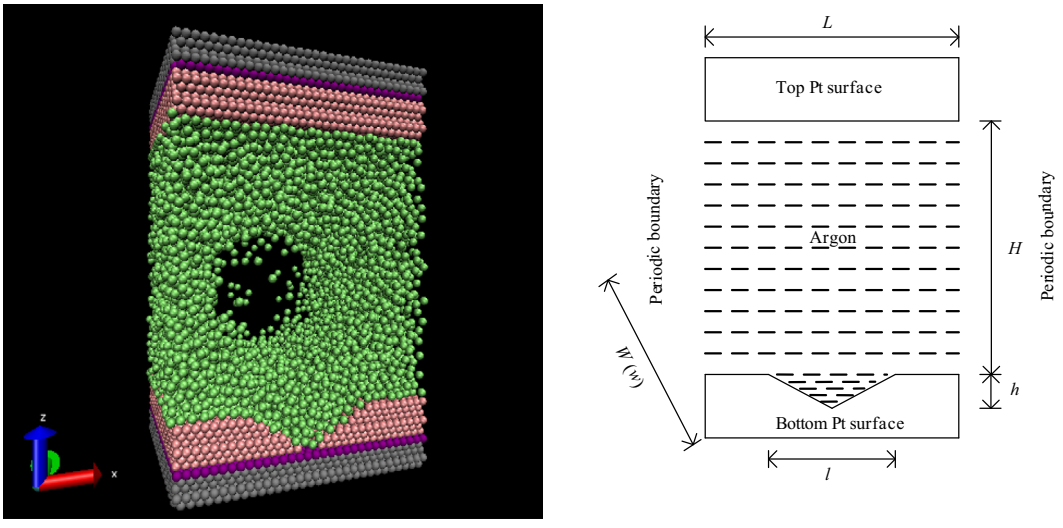

Fig. 1. A snapshot of liquid argon between parallel solid walls (a) and system geometry (b).