Contents lists available at ScienceDirect



International Journal of Heat and Mass Transfer

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

Enhancement of boiling heat transfer of thin water film on an electrified solid surface



HEAT and M

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ARTICLE INFO

Article history: Received 27 October 2016 Received in revised form 7 February 2017 Accepted 9 February 2017

Keywords: Boiling Liquid film Surface electric charge Molecular dynamics

ABSTRACT

Rapid boiling of liquid film appears on solid surfaces with ultrahigh temperatures or heat fluxes, where a vapor layer is rapidly formed between the liquid film and the surface, leading to the film detachment from the surface and hence significantly reducing the heat transfer rate. In this work, a new idea, solid surface is charged with surface charges, is proposed to suppress the formation of vapor layer and prevent the liquid film detachment. To examine the effectiveness of the idea, the boiling behaviors of water films on gold (100) surfaces with various wettability conditions as well as with or without surface charges are investigated by molecular dynamics simulations. The results show that the electric field induced by the surface charges leads to an increased attractive interaction between the water film and the gold surface. Meanwhile, it is very interesting that a cone-shaped liquid column moves upward from the free surface of the water film due to the directional arrangement of water molecules along the electric field direction, which helps the nucleation bubble to break through the water film. Thus, the formation of vapor layer is suppressed and the water film detachment is never observed during the whole phase-change process of water film. The results also reveal that the electric field significantly increases the collision rate between water molecules and gold atoms, and hence enhances heat transfer from the gold surface to the water film.

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1. Introduction

Boiling heat transfer is an important and challenging topic in the areas of heat and mass transfer. Boiling of thin liquid films on a solid wall can be categorized into normal boiling and rapid boiling depending on surface superheat [1]. Rapid boiling always occurs when the liquid film is superheated to a degree far beyond its normal boiling point. In this process, phase change of the liquid near the wall region proceeds very rapidly, leading to that the wall is completely covered by a vapor layer and the liquid film detaches from the wall as the vapor layer expands [1–3]. The rapid boiling of liquid films is analogous to the well-known Leidenfrost phenomenon where a liquid droplet is separated from the wall due to the formation of a vapor layer between them when the wall temperature is higher than the Leidenfrost temperature [4]. The insulating vapor layer has a very high thermal resistance and hence dramatically degrades heat transfer, which may cause wall dryout or even burnout. It is therefore undesirable for heat transfer applications.

Molecular dynamics (MD) simulations are powerful tools for understanding the mechanisms of boiling at the atomic scale, and have been widely used to study the complex rapid boiling behaviors [1-3,5-8]. Some MD studies focused on the effects of wall superheat and wettability on the rapid boiling [3,5]. For example, Hens et al. [3] studied the bubble nucleation and the rapid boiling of argon films on a platinum surface. Their results showed that the rapid boiling can take place more easily on hydrophilic surfaces or/and at high degree of superheats. Several MD simulations have studied the boiling of liquid films on nanostructured surfaces [1-2,6-8]. The results demonstrated that the heat transfer rate can be drastically increased by properly designing the nanostructure, while the rapid boiling is always observed when the wall temperature is higher than a specific threshold value depending on the pattern and size of nanostructure.

Recently, a few experimental works [9,10] devoted their efforts to suppress the Leidenfrost phenomenon by applying an external

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electric field to liquid droplets. In these works, a voltage was applied between the drop and the heated wall. Celestini and Kistetter [9] found that increasing the voltage leads to a decrease of the vapor layer thickness; the Leidenfrost state is completely suppressed and the water droplet starts boiling when the voltage exceeds a certain critical value. Shahriari et al. [10] presented that by means of an external electric field, the Leidenfrost state suppression is observed for a variety of liquids, ranging from low electrical conductivity organic solvents to electrically conducting salt solutions. Their measurement showed that elimination of the vapor layer can improve heat dissipation capacity by more than one order of magnitude. The mechanism behind suppression of vapor layer formation was explained by the analogy of aparallelplate capacitor [9,10], in which two plates with opposite charges attract each other. Thus, interfacial electric field in the vapor laver can attract liquid toward the surface and promote wetting. However, the explanation has not been supported by direct microscopic evidences because it was proposed only based on the phenomenological analysis.

Inspired by the results from Refs. [9,10], we propose a method using electrified solid surfaces to suppress the formation of vapor layer under the condition of ultrahigh wall temperatures. Considering that in the previous experiments, the wall is charged and an opposite electrode is plugged into the liquid droplet, electrical shorting easily takes place for electrically conducting liquids. Meanwhile, this arrangement of electrodes may also cause unwanted electrolysis and chemical reactions in the droplet [10]. Therefore, an approach, the solid wall is charged with surface electric charge, is put forward to generate the external electric field. MD simulations are performed to examine the effectiveness of applying the electric field to enhance the boiling heat transfer of thin water film on ultrahigh temperature walls. Furthermore, the simulations are also expected to provide an atomic-scale insight into the vapor layer suppression by electric field.

2. Model and method

As shown in Fig. 1, the simulation cell employed is a cuboid box with dimension of $6.12 \times 80 \times 2.4 \text{ nm}^3$. The cell can be divided into three regions, namely vapor, liquid and solid regions. Both the vapor and liquid regions are filled with water molecules, and the solid is a gold plate. Periodic boundary conditions are applied in the *x*- and *z*-directions, while a fixed boundary condition is assumed in the *y*-direction. The gold plate with 1.06 nm thickness (1080 gold atoms) is placed on the bottom of the box and its lower



Fig. 1. Model of initial simulation system.

surface is located at y = 0 nm. A 10.34 nm thickness water film (4480 water molecules) is placed on the upper surface of the gold plate. The gold (100) surface is modeled by face-centered cubic crystals with lattice constant of 4.08 Å. The gold plate consists of six layers, the bottom layer is fixed to prevent the plate deformation [3] and other five layers are modeled as thermostat.

Water molecules are characterized by the rigid SPC/E model with an O—H bond distance of 0.1 nm and an H—O—H angle of 109.47° [11]. The SPC/E model is used for water molecule in this work because it has been proven to adequately capture a broad swath of liquid water's properties [12]. Moreover, in our previous work [13], we employed different water models to investigate evaporation of water and aqueous droplets in the presence of electric field. The results showed that although there were quantitative differences among the different models, the same conclusions were obtained qualitatively by these models. The embedded atom model (EAM) [14] is adopted for simulating the interaction between gold atoms. The interaction of water molecules consist of the Coulombic and Lennard-Jones 12–6 potentials [15] expressed as:

$$U_{ij} = \frac{q_i q_j}{r_{ij}} + 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right]$$
(1)

where U_{ij} is the potential energy between particles, and q_i , r_{ij} , σ_i and ε_i denote the charge of the *i*th particle, the distance between the *i*th and the *j*th particle, the zero energy separation distance and the minimum energy, respectively. The interaction between the water and gold molecules is modeled by the Lennard-Jones 12–6 potentials. The values of parameters for the water-water and gold-water interactions are shown in Table 1. A spherical truncated length for short-range forces is taken as 1 nm, and the long-range electrostatic interaction is solved by PPPM (particle-particle particle-mesh) method [16] with an accuracy of 10^{-4} . The SHAKE algorithm [17] is applied for water molecule to maintain its bond length and angle.

To generate an external electric field, the upper surface (the first layer) of the gold plate is charged with electric charge [18,19], as shown in Fig. 2. Each atom in the first layer bears a discrete positive charge of 0.03 e, which corresponds to a surface charge density of 0.06 C m⁻². For the purpose of comparison, the boiling of water film on gold plates without surface electric charge is also simulated. For each kind of gold plate, the wettability between liquid and solid surface is controlled by changing the plate-liquid energy parameter [20,21], with $\varepsilon_{O-Au} = 0.0554 \text{ eV}$ for surface A and ε_{O-Au} = 0.0114 eV for surface B, as listed in Table 1. To determine the wettability of the surfaces, MD simulations are performed to measure the static contact angles of a droplet with 4480 water molecules on surfaces A and B, respectively. After running of 1000 ps under NVT ensemble at 298 K, the droplet reaches its equilibrium state, as shown in Fig. 3. The value of contact angle is determined to be 28.2° for surface A and 85.6° for surface B, which suggests that surface A is hydrophilic while surface B is a nonwetting surface. From the physical point of view, the wettability is relevant to the interactions between liquids and substrates. Liquids can easily wet the substrates if the solid-liquid interactions

| Table 1 | |
|---------------------|-------------|
| Values of potential | parameters. |

| Particles <i>i</i> , <i>j</i> | $\sigma_{i,j}(extsf{A})$ | $\varepsilon_{i,j}(eV)$ | <i>q</i> (e) |
|-------------------------------|---------------------------|-------------------------|--------------|
| 0—0 | 3.1660 | 0.0067 | -0.8476 |
| H—H | 0.0000 | 0.0000 | +0.4238 |
| 0—Н | 0.0000 | 0.0000 | - |
| O—Au (A) | 2.8675 | 0.0554 | - |
| O—Au (B) | 2.8675 | 0.0114 | - |
| H—Au (A) (B) | 0.0000 | 0.0000 | - |
| | | | |

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