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MD simulation on nano-scale heat transfer mechanism of sub-cooled boiling on nano-structured surface

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ABSTRACT

In recent years, surfaces with micro/nano-structures were recognized as effective in boiling heat transfer efficiency enhancement. However, macroscopic observations cannot fully clarify the fundamental mechanisms in a nano-scale regime. To understand the mechanism of sub-cooled boiling on the nano-structured surface in nano-scale view, sub-cooled boiling process and its interaction with different nano-structured configurations (cuboid and finger) at different wall superheated temperatures are computed with molecular dynamics. Nanobubbles of gas vapor are observed to be generated and condensed rapidly for nano-scale sub-cooled boiling. With the increasing of wall superheat, the aggregation and coalescence of adjacent nano bubbles become intense, resulting in the formation of a vapor layer separating the heated wall from cooled water liquid. It is found that nano bubbles are easy to be coalesced in horizontal directions in the case of a plain surface, resulting in an earlier formation of the vapor layer, while in the cases of nano-structured surfaces, a kind of nano-scale vertical convection induced by nano cavity is observed, which delays the vapor layer formation and intensifies the initial disturbance causing hydrodynamic instability of the vapor layer significantly. This finding clarifies the difference of heat transfer capacity between the case of nano-structured surfaces and the case of plain surfaces. In view of heat transfer efficiency, cases with nano-structured surfaces manifest a prominent increase of heat flux and critical heat flux values with the increase of wall superheat as compared with cases of plain surfaces, which is in good agreement with available macroscopical experimental results. Therefore, the nano-cavity-induced nano-scale vertical convection mechanism can give a more fundamental explanation to those macroscopic observations.

1. Introduction

Since Jakob and Fritz [1] first used surfaces with sandblasting and machined grooves to enhance boiling heat transfer, there has been a continuous effort to improve boiling processes on heated surfaces in industrial and academic fields [2–4]. With the development of surface manipulation technology in recent years, the surface with micro/nano-structures was recognized as another pathway for boiling efficiency enhancement. Li et al. [5] first reported an unexpected enhancement in boiling performance for a nano-structured copper (Cu) surface compared to a plain surface. Then many researchers reported their works about effects of many kinds of nano-structured surfaces on boiling enhancement such as Chen et al. [6], Betz et al. [7], Yao et al. [8], Weibel et al. [9] and Dong et al. [10] etc. According to those works, there are several points about how micro/nano-surface structures affect boiling heat transfer as Kim et al. [11] summarized in a recent review: (1) increase in active nucleation site density with randomly formed micro/nano-sized roughness; (2) ability of vapor/gas entrapment to enhance cavities by reentrant cavities fabrication and wettability control (increase in liquid contact angle); (3) favorable bubble initiation, growth, and departure on micro-porous layered surfaces; (4) promotion of evaporation mass flux at vapor–liquid interface by micro/nano-structures. However, most these points are concluded from macroscopic observations or some theoretical hypotheses. Researchers have spared no efforts to establish theoretical models that can evaluate the thermal performance and represent all basic mechanisms based on those macroscopic phenomenon and some theoretical hypotheses. For example, the model of Polezhaev and Kovalev [12] was established based on Kelvin–Helmholtz instability wave length change observed in porous surface structure cases, while the model of Park and Bang [13] was based on the

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observation that wire heaters coated with various nanoparticles have different Rayleigh–Taylor wave lengths. The model of Chu et al. [14] incorporates both intrinsic and apparent dynamic contact angle to compute the effect of solid–liquid adhesion force increase with the hypothesis that micropillar structures can enhance the length of the liquid–vapor–solid triple contact line. The model of Zou and Maroo [15] incorporates about 10 parameters to evaluate the effect of additional evaporation of metastable non-evaporating film beneath the vapor bubble which was hypothesized to be fragmented by the microridges vertically arranged on the heating surface. A similar situation exists for other models such as the Kandlikar's model [16], Liter and Kaviany model [17], Kim and Kim model [18], the model of Ahn et al. [19], as well as the model of Quan et al. [20] proposed recently, etc. According to the models addressed above, it is noted that although each model has claimed to have got a relative well agreement with some macroscopic experimental data, hitherto no one has claimed its general applicability. That is, these models are still local and contextual in some conditions. The reason may lie in that there still lacks direct proofs or theories based on nano-scale observations to validate them. In fact, most macroscopic observations are very sensitive to the change of nano-structure configuration as reported in works of Dong et al. [10]. So, are there some special mechanisms related with nano-scale world yet to be clarified? A review of current researches on boiling heat transfer enhancement on micro/nano-structured surfaces seldom involves direct observations in nano-scale view due to instrument application limits (the smallest distinguishable scale in direct observation is about 500 μm according to Ref. [21]) so that the macroscopic conclusions cannot be fundamentally derived from those microscopic results. Besides, as addressed previously, since many theoretical models of nucleate boiling as well as the critical heat flux (CHF) for micro/nano-structured surfaces have been proposed based on some theoretical hypotheses, finding some direct evidence in nano scale view for those hypotheses will be very helpful to further validate those models. Therefore, to study the boiling process and its interaction with nano structures in nano-scale view will be of great significance to fully understand the boiling enhancement mechanism with micro/nano-structured surfaces and help to establish a more universal theoretical model.

With such motivations, molecular dynamics (MD) is used in the present paper to simulate the nano-scale sub-cooled boiling process of water on nano-structured surfaces at different conditions. The physical sub-processes of nucleate boiling and interaction between micro-bubbles and nano structures are numerically analyzed.

It should be noted that with the advantages of describing physical process at atomic level, MD simulation is widely applied to study micro/nano-scale heat and mass transfer problems in recent years. For example, Dou et al. [22] conducted a MD simulation on rapid boiling of water films adjacent to a heated gold surface and the results clearly show that the water layers nearest the surface overheat and undergo explosive boiling. Gu and Urbassek [23] performed a MD simulation on rapid boiling of liquid-argon films irradiated by an ultrafast laser, in which a detailed microscopic view of the explosive boiling process is obtained by monitoring the space and time dependence of the hydrodynamic variables as well as the local thermodynamic state. Zou et al. [24] simulated a homogeneous nucleation of water and liquid nitrogen explosive boiling induced by laser heating, in which the velocity scaling method is applied to realize the heating process and three influencing factors, including the initial equilibrium temperature, the area of the heating zone and the heat quantity are analyzed. Hens et al. [25] simulated nano bubble formation in liquid Argon film on a superheated platinum substrate surface to understand its formation mechanism under different degrees of superheat and surface conditions with particular emphasis on the surface texture. Other MD works include those of Maroo and Chung [26], Yi et al. [27], Nagayama et al. [28] etc. In summary, although all addressed MD works are very meaningful and helpful to clarify more insight of physical process in boiling process, few works are focused on sub-cooled boiling processes on micro/nano structured surfaces.

To understand the mechanism of sub-cooled boiling of water (a common industrial coolant) on metal copper surfaces (a common industrial heat sink) in nano-scale view, sub-cooled boiling process and its interaction with different nano-structured configurations (cuboid and finger) at different wall superheated temperatures are computed with molecular dynamics in the present investigation. For comparison, cases with plain surfaces are also included. Nano-bubble formation process and its effect on heat transfer performance at wall superheated degrees ranging from (2–152 K) under standard atmospheric pressure conditions will be discussed. Heat transfer effects and its difference in mechanism are analyzed based on simulation results.

2. Numerical methods and models

2.1. Basic governing equations and potential models

The basic governing equations of MD are based on Newton's second law, as listed in Eq. (1), where F_i is the sum of the forces exerted on molecule i by other molecules in the system, which is obtained from a gradient of the potential function U between molecules. Once the force exerted on molecule i is obtained, its acceleration rate a_i, velocity V_i and position r_i can also be determined according to mechanical laws. Then the macroscopic physical properties of the substance, like volume, temperature, pressure, etc. can subsequently be obtained via statistical methods.

$$\begin{cases} \vec{F}_i = -\nabla_i U = -\left(\frac{\partial}{\partial x_i}\vec{i} + \frac{\partial}{\partial y_i}\vec{j} + \frac{\partial}{\partial z_i}\vec{k}\right)U \\ \vec{F}_i = m_i\vec{a}_i \\ \vec{v}_i = \vec{v}_i^0 + \vec{a}_i t \\ \vec{r}_i = \vec{r}_i^0 + \vec{v}_i^0 t + \frac{1}{2}\vec{a}_i t^2 \end{cases} \tag{1}$$

The general formula of potential function U is defined in Eq. (2), where $\vec{r}_i$ are the coordinates of the i-th atoms.

$$U = U(\vec{r}_1, \vec{r}_2, \cdots, \vec{r}_i, \cdots, \vec{r}_n) \tag{2}$$

In the present investigation, the heat transfer process of water and copper plate will be simulated with MD and thus three kinds of atoms: copper, oxygen, and hydrogen are involved. For interactions of atoms such as Cu–O, Cu–H, and Cu–Cu, Lennard–Jones (L–J) interaction is applied as

$$U_{ij} = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right], \quad r < r_c \tag{3}$$

where i, j correspond to interacting atoms and ε, σ are parameters for L–J potential function, and r_c is the cutoff distance. For different kinds of atoms, the ε, σ can be determined by a mixture rule as

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \cdot \varepsilon_j}, \quad \sigma_{ij} = \frac{\sigma_i + \sigma_j}{2} \tag{4}$$

For water molecule, a rigid planar four-site interaction potential model for water (TIP4P) proposed by Jorgensen et al. [29] is used, which is very suitable in description of water's dynamic and thermal properties. Then the intermolecular interaction between water molecules is described by a potential function U_{ab},

$$U_{ab} = \overbrace{\sum_i^a \sum_j^b \frac{k_c q_{a_i} q_{b_j}}{r_{a_i b_j}}}^{U_C} + \overbrace{\sum_i^a \sum_j^b 4\varepsilon_{a_i b_j}\left[\left(\frac{\sigma_{a_i b_j}}{r_{a_i b_j}}\right)^{12} - \left(\frac{\sigma_{a_i b_j}}{r_{a_i b_j}}\right)^{6}\right]}^{U_{LJ}} \tag{5}$$