



# Explosive boiling of nano-liquid argon films on high temperature platinum walls: Effects of surface wettability and film thickness

Yan-Hong Wang<sup>a,b,c</sup>, Shao-Yu Wang<sup>a,b,c</sup>, Gui Lu<sup>a,b,c,\*</sup>, Xiao-Dong Wang<sup>a,b,c,\*\*</sup>

<sup>a</sup> State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources, North China Electric Power University, Beijing, 102206, China

<sup>b</sup> Research Center of Engineering Thermophysics, North China Electric Power University, Beijing, 102206, China

<sup>c</sup> Key Laboratory of Condition Monitoring and Control for Power Plant Equipment of Ministry of Education, North China Electric Power University, Beijing, 102206, China

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## ABSTRACT

Because of scaling effect, phase change behaviors of nano-liquid films on solid surfaces display distinct features from macroscale pool boiling. In this work, evaporation and explosive boiling of nano-liquid argon films with various film thicknesses on hydrophilic or hydrophobic platinum surfaces are investigated via molecular dynamics simulations. The simulations show that the onset of explosive boiling closely depends on the film initial thickness on both the hydrophilic and hydrophobic surfaces, and the onset temperature for explosive boiling significantly reduces with the increase of the film thickness. In addition, the simulations also demonstrate that, with the same film thickness and the same wall superheat, explosive boiling is triggered on the hydrophilic surface, while only evaporation is observed on the hydrophobic surface, indicating that a high surface wettability reduces the onset temperature, which is opposite to the prediction by classical nucleation theory and the observation in pool boiling experiments. For a thicker film and a higher surface wettability, it is found that a larger temperature gradient is generated along the film thickness direction due to the heat accumulation effect, which leads to a very high temperature occurring at the film bottom and thereby is responsible for the lower onset temperature for explosive boiling on these circumstances.

## 1. Introduction

The explosive boiling is a violent gas-liquid phase change process that takes place under a transient extra-high heat flux in a very short time [1,2]. The huge shock waves generated by explosive boiling often leads to some catastrophic events, such as the explosion accidents in nuclear reactors, metallurgy, superconductors, and liquefied natural gas [3]. Recently, with the rapid development of high-tech industries, explosive boiling has also found many new applications in cooling of microelectronic devices [4], microelectronic heat transfer devices [5,6], laser surgery [7], inkjet printing [8], laser cleaning [9], and so forth. For example, the main mechanism of laser cleaning is that the surface of a cleaned material is first covered with a liquid film, and then a laser is used to irradiate it. When the laser energy is absorbed by the liquid film, it will cause a violent explosion of the liquid film and leads to an energy transport from the liquid film to the cleaned surface. The high transient explosive force is sufficient to remove the surface dirt, thus achieving the cleaning purpose [9].

The study of explosive boiling is of great significance for the prevention and control of explosion accidents in traditional industries and

for the development of new technologies in modern high-tech industries. Since explosive boiling commonly occurs in the order of microseconds, it is very difficult to observe a series of complex dynamics by common visualization experiments, such as the bubble nucleation, growth, coalescence, and detachment. Thus, it is a very challenging task to reveal the microscopic mechanism of explosive boiling. Recently, some efforts have been devoted to studying evaporation and explosive boiling of nano-liquid films via molecular dynamics simulations [10–21].

In these studies [10–21], a nano-liquid film was commonly placed on a solid surface with a constant wall temperature. Hasan et al. [10] investigated the evaporation characteristics for a 3.01 nm liquid argon film over a solid surface with different surface materials and different wetting conditions at a constant wall temperature of 130 K. Their results showed that both the surface wettability and surface material have a significant effect on evaporation. Moreover, they presented that macroscopic thermodynamics approach can predict the evaporation characteristics of nanoscale thin liquid film. It has been demonstrated that explosive boiling of nano-liquid films depends not only on the surface wettability [11–15] and surface nanostructure [12,16–19], but

\* Corresponding author. State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources, North China Electric Power University, Beijing, 102206, China.

\*\* Corresponding author. State Key Laboratory of Alternate Electrical Power System with Renewable Energy Sources, North China Electric Power University, Beijing, 102206, China.

E-mail addresses: [lugui02@gmail.com](mailto:lugui02@gmail.com) (G. Lu), [wangxd99@gmail.com](mailto:wangxd99@gmail.com) (X.-D. Wang).

also on the film thickness [20,21]. Hens et al. [11] simulated the phase change process of liquid argon films with a 2 nm thickness on smooth platinum substrates. Their results showed that at a constant wall temperature of 250 K, explosive boiling occurs on the hydrophilic surface, while only evaporation appears on the hydrophobic surface. Apparently, a higher wall temperature is required to trigger explosive boiling on the hydrophobic surface. It should be noted that, the onset temperature for nucleate pool boiling is commonly defined as a critical wall temperature above which a nucleated bubble can generate on a heated surface, while below which nucleation cannot take place. Similarly, the onset temperature for explosive boiling of liquid films can be defined. When the wall temperature is lower than the onset temperature, the only evaporation of liquid films occurs, while the wall temperature is higher than the onset temperature, the liquid film will depart from the wall such that explosive boiling takes place. Thus, from Hens et al.'s results it can be concluded that the onset temperature for explosive boiling is lower on the hydrophilic surface than that on the hydrophobic surface. In Hasan et al.'s [12] and Shavik et al.'s [13] simulations, the thickness of liquid argon films was increased to 3 and 3.01 nm, respectively. Their results further confirmed that the onset temperature for explosive boiling on a hydrophilic surface is lower than that on a hydrophobic surface. Zhang et al. [14,15] investigated phase change behavior of a thin liquid argon film (11 argon liquid layers) on solid aluminum substrates with a constant wall temperature of 150 or 350 K. Their results showed that at the low wall temperature of 150 K only evaporation is observed for the hydrophobic, neutral, and hydrophilic substrates; when the wall temperature increases to 300 K, explosive boiling is triggered for the hydrophilic and neutral substrates, while evaporation still maintains on the hydrophobic substrate. The results again support that the onset temperature for explosive boiling increases with the reduction in surface wettability. Zhang et al. [14,15] also pointed out that how to improve heat transfer rate for hydrophobic surfaces needs more simulations or experiments. It should be noted that pool boiling experiments [22], numerical simulations [23] and classical nucleation theory all show that the onset temperature for nucleate pool boiling is lower on a hydrophobic surface than on a hydrophilic surface. Apparently, the surface wettability exhibits a completely opposite effect on the onset temperature of boiling for macroscale (pool boiling) and nanoscale (explosive boiling) phase change behaviors.

Recently, many studies have focused on phase change behaviors of nano-liquid films on nanostructured substrate [12,16–19]. For example, Seyf et al. [16–18] investigated the phase change characteristics of a thin liquid argon film on metal substrates with different nanostructures. When the surface was structured by an array of nanoscale spherical particles [16,17], the results showed that the nanostructures significantly affect evaporation/boiling of the liquid film and the degrees of superheat and size of nanoparticles have significant effects on the trajectories of argon atoms and the net evaporation rate. Subsequently, they changed substrate material from copper to silver and aluminum as well as nanostructures from array of spherical particles to cone array [18]. They found that the cone-like nanostructures also enhance the heat transfer from substrate to film; however, the evaporation rate does not change significantly with the size of nanostructure when it is less or equal to the film initial thickness. Furthermore, the separation temperature associated with separation of liquid film from solid surface strongly depends on the size of nanostructure, but it is not sensitive to the type of material. Wang et al. [19] investigated evaporation and explosive boiling of a thin liquid argon film on an aluminum substrate decorated by cubic nanostructures with different heights at a constant temperature of 150 or 310 K. Their simulations indicated that the heat transfer efficiency is significantly improved by nanostructures and evaporation rate increases with the increase in height of nanostructures.

Some studies have also reported the effect of liquid film thickness on boiling nucleation behaviors. Dou et al. [20] studied the explosive boiling of water films with various thicknesses on a hydrophilic surface

under laser irradiation. Their simulations indicated that at a constant wall temperature of 1000 K, evaporation occurs for the film with thickness of 1.38 nm, while explosive boiling takes place for the films with thicknesses of 2.76 and 5.52 nm. This result implies that for the 1.38 nm thick liquid film, a higher wall temperature needs to be applied to trigger its explosive boiling. Thus, the onset temperature for explosive boiling is higher for a thinner liquid film. Rabbi et al. [21] investigated boiling heat transfer behaviors of argon films with thickness ranging 3–6 nm on a hydrophilic platinum surface. They found that at the same wall temperature of 250 K, evaporation is observed for the films with thicknesses of 3 and 4 nm, while explosive boiling occurs for the films with thicknesses of 5 and 6 nm. These works clearly demonstrated that, on hydrophilic surfaces the onset of explosive boiling for nano-liquid films depends on the film thickness, and the onset temperature reduces with the increase in the film thickness.

Regardless of macroscale pool boiling [22,23], or explosive boiling of nanoscale liquid films [11–21], the phase change behaviors and the onset temperature strongly depend on the surface wettability and they display distinct features on hydrophilic and hydrophobic surfaces. So far, the effect of liquid film thickness on explosive boiling is studied only on hydrophilic surfaces; nevertheless, there has not yet been paid enough attention to that on hydrophobic surfaces. Based on the above reasons, in this work molecular dynamics simulations are employed to compare the phase change behaviors of nano-liquid films with various thicknesses on the hydrophilic and hydrophobic surfaces. The main goal of this paper is to answer two questions. One is that whether the film thickness influences the onset temperature of explosive boiling on hydrophobic surfaces. The other is to reveal the microscopic mechanism on why the film thickness influences the onset temperature.

## 2. Simulation method

Fig. 1 shows the initial configuration of the simulated system, which is a cuboid box with dimensions of 7.4 nm × 7.4 nm × 80.0 nm ( $x \times y \times z$ ) and composed of solid, liquid, and vapor regions. The solid platinum plate is placed at the bottom of the box, it consists of 4332 platinum atoms arranged in the face-centered cubic lattice structure with a lattice constant of 3.92 Å. The plate includes 6 layers atoms and has a 1.2 nm thickness. To prevent the plate deformation, its bottom layer is kept fixed. The nano-liquid argon film is placed over the solid plate, and the thickness is taken to be 1, 3, and 6 nm, respectively, which consists of 1568, 4704, and 9016 argon atoms. The rest of the box is filled with vapor argon atoms. Periodic boundary conditions are employed in the  $x$ - and  $y$ -directions, and fix boundary conditions are applied to the  $z$ -direction. A reflect wall is assigned to the top of the box in the  $z$ -direction. When argon atoms collide with the reflect wall, they will bounce back to the box and remain their original velocity without any losses of momentum and kinetic energy.

The interactions between Ar-Ar, Pt-Pt, and Ar-Pt atoms are modeled by the Lennard-Jones (L-J) potential functions [24],

$$\phi(r) = 4\epsilon \left[ \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \right] \quad (1)$$

where  $r_{ij}$  is the distance between particles  $i$  and  $j$ ,  $\sigma$  and  $\epsilon$  denote the zero-energy separation distance and the minimum value of L-J potential, respectively. To balance the computational speed and accuracy, all the potentials were truncated at  $3.5\sigma_{\text{Ar-Ar}}$ . Different surface wettabilities can be modeled by varying parameter  $\epsilon_{\text{Ar-Pt}}$  [10]. Our simulations indicate that with  $\epsilon_{ij} = 0.0650$  eV, the contact angle of argon droplet on the platinum plate is 43° (hydrophilic surface); while with  $\epsilon_{ij} = 0.0050$  eV, the contact angle is 132° (hydrophobic surface), as shown in Fig. 2. The values of  $\sigma$  and  $\epsilon$  for the Ar-Ar, Pt-Pt, and Ar-Pt interactions are listed in Table 1.

After a reasonable initial simulated system is constructed, the energy minimization of the system is first implemented. During the

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