



An investigation on vapor condensation on nanopillar array surfaces by molecular dynamics simulation

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ABSTRACT

Molecular dynamics simulation is used to investigate condensation of Argon vapor on nanopillar array surfaces made of copper. It is shown that condensation in the pillar array is nonuniform with respect to height. Effects of pillar height, pitch distance of nanopillars, wall subcooling and wettability on condensation of Argon vapor are discussed. It is found that higher pillars, denser pillars and stronger wall surface wettability can suppress vapor condensation at the bottom of a nanopillar array, making vapor more likely to condense in the upper section of the array. It is also shown that the condensation peak in the nanopillar array can be shift from bottom to top with the increasing wall subcooling. The formation of Cassie state droplets is observed and discussed.

1. Introduction

Vapor condensation is an omnipresent phenomenon in nature [1]. For example, the formation of fog in the atmosphere [2] and breath figures on a glass surface [3]. Compared with convective heat transfer, condensation heat transfer usually possesses higher heat transfer coefficient and thus has wide practical applications in heat pipes [4], power plants [5] and air conditioners [6].

In recent years, with rapid developments in nanofabrication technology, nanostructured surfaces have been used to enhance condensation heat transfer. In 2009, Boreyko and Chen [7] observed self-propelled dropwise condensation on superhydrophobic surfaces with micro and nano two-tier roughness. Subsequently, Miljkovic et al. [8] reported that jumping condensation on nanostructured superhydrophobic surfaces has a higher heat transfer coefficient than dropwise condensation on smooth hydrophobic surfaces. Meanwhile, a number of nanostructured surfaces [9–15] were designed and manufactured to produce jumping condensation for condensation heat transfer enhancement.

However, one of the major problems of nanostructured surfaces is that jumping condensation on these surfaces is not stable [15]. The droplets on condensation surface could appear in a highly pinned Wenzel state [8] under some circumstances, making droplets hard to be removed by coalescence. In the experiment by Miljkovic et al. [8], jumping condensation was found to be replaced by flooded condensation, which had a lower heat transfer coefficient than dropwise condensation on smooth surfaces under high supersaturation. Wen et al. [15] also reported that jumping condensation could turn into ordinary dropwise condensation when the wall subcooling was high.

As the initial steps of condensation, nucleation and early-stage growth of droplets play an important role in the appearance of Wenzel state droplets. According to Enright et al. [16], a relatively low nucleation density is another necessary condition for the emerge of Cassie state droplet in addition to relatively hydrophobic wettability. When the nucleation density is high enough (produced by high supersaturation or high wall subcooling) to bring multiple droplets in a single unit cell of the pillar array, the consequence of growth and merging of droplets is producing Wenzel state droplets. Another viewpoint [15] is that different droplet wetting states are the result of nucleation position. Droplets cannot nucleate inside a nanostructure when wall subcooling is low due to the low vapor density and high nucleation barrier. Thus, the nucleation occurs on the tips of the nanostructure and produce Cassie droplets. But, when wall subcooling is high, nucleation is easier and droplets can also nucleate inside a nanostructure. In this case, the growth of droplets would bring Wenzel droplets. However, it is difficult to investigate droplets nucleation and its subsequent growth on nanostructured surfaces experimentally because the magnitude of the critical droplets diameter in experiments is about 10 nm [15,16] and the magnitude of droplet size could be observed in-situ in experiments is about 100 nm [17]. Thus, other research methods suitable for smaller scale are needed to study nucleation and early-stage growth of droplets on nanostructured surfaces.

As a powerful research tool at the nanoscale, molecular dynamics simulation has been widely used to investigate droplet nucleation and early-stage growth on smooth surfaces [18–24], as well as condensation on nanostructured surfaces [25]. Xu et al. [21] investigated droplet nucleation on smooth solid surfaces with different solid-liquid interaction strengths. Li et al. [25] studied vapor condensation on

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nanostructured surfaces and found nanostructures could facilitate condensation. However, few molecular dynamics studies have been carried out for droplets nucleation and its subsequent growth on a nanopillar array having a high aspect ratio.

In this paper, nucleation and early stage of droplet condensation of Argon vapor on nanopillar array surfaces made of copper are investigated by molecular dynamics simulation. The condensation intensity distribution is analyzed and effects of subcooling, height and pitch distance of nanopillars, and wall wettability on condensation of Argon vapor are discussed. Finally, the formation of Cassie state droplets is also discussed.

2. Methodology

All simulations in this paper were conducted using LAMMPS software [26,27]. Fig. 1 (a) shows the simulation domain under consideration. The simulation domain is a cuboid with fixed edge lengths of L_x, L_y, L_z in x, y, z directions, respectively. The subcooled surface made of copper is placed at the bottom of the simulation domain (at $z \approx 0$), comprising a slab base with a thickness of h_B and with an array of nanopillars with a height of h on the top. As shown in Fig. 1 (b), nanopillars of circular cross sections with a diameter of D are arranged at a pitch distance P . Fig. 2 is a cross-sectional view of the A-A plane in Fig. 1 (b). At the top of the simulation domain, there is a Monte Carlo (MC) region with a thickness of h_M , where Grand Canonical Monte Carlo (GCMC) is performed every 100 molecular dynamics (MD) simulation time-steps to supply vapor molecules (Argon) and maintain the vapor density. The temperature in MC region is maintained at T_{bulk} in both GCMC and MD, and the density of vapor is maintained as ρ_{bulk} , which is the saturated vapor density corresponding to the temperature T_{bulk} , in the process of GCMC. Boundary conditions of the computation domain are periodic in x and y directions, and reflected in z direction. There are two stages for each simulation: equilibrium stage and cooling stage. In the equilibrium stage, the temperature of the condensation surface T_w is set to be equal to T_{bulk} (saturated temperature) and simulation is conducted until the system reaches an equilibrium state which is reflected by a stable number of molecules inside simulation box and uniform temperature and bulk vapor density. After the equilibrium state is reached, the simulation entered the cooling stage, where T_w is set at a value lower than T_{bulk} ($T_w < T_{sat}$) and condensation process begins.

Table 1 lists geometric parameters used in the simulation. Since effects of height and pitch distance of nanopillars are investigated in this paper, different pillar heights ($H = 3.7$ nm, 10 nm, 20 nm, 30 nm)

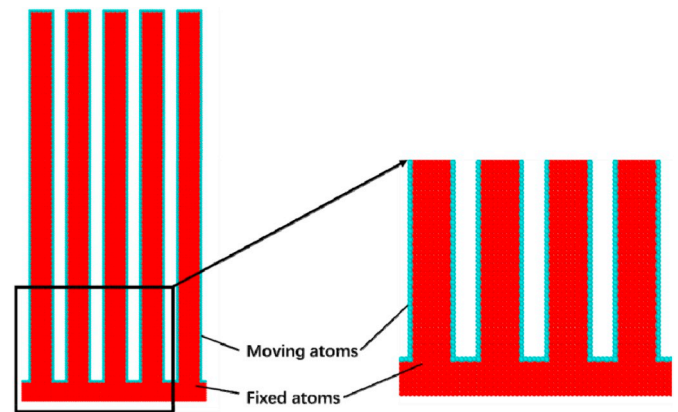


Fig. 2. Cross-sectional view (section A-A in Fig. 1 (b)) of condensation surface in a dense array with 5×5 nanopillars.

Table 1
Geometric parameters in simulation domain.

L_x, L_y	15.0 nm
h_B	1.5 nm
H	3.7 nm, 10.0 nm, 20.0 nm, 30.0 nm
h_M	3.0 nm
D	2.0 nm (dense array), 5.0 nm (sparse array)
P	3.0 nm (dense array), 7.5 nm (sparse array)
L_z	$h_B + H + h_M + 25.5$ nm

and pitch distances ($P = 3$ nm and 7.5 nm representing dense and sparse arrays respectively) are chosen for study. With L_x and L_y fixed, the number of nanopillars is 5×5 and 2×2 for dense array and sparse array respectively. The values of P and D are chosen to make the ratio P/D to be the same for both dense array and sparse array.

The condensation surface in the simulation is obtained by cutting face centered cubic crystal with a lattice constant of 3.7416 Å into desired shape. Fig. 2 illustrates the cross-sectional view (section A-A in Fig. 1 (b)) of atomic condensation surface in a dense array. In order to reduce the cost of calculation, only the outmost one layer of solid atoms (atoms in light blue) are allowed to move during the MD simulation, and the rest atoms inside solid (atoms in red) are fixed. Considering the focus of this paper is on the vapor-liquid phase change behavior in the fluid side rather than heat transfer inside solid, this treatment is reasonable.

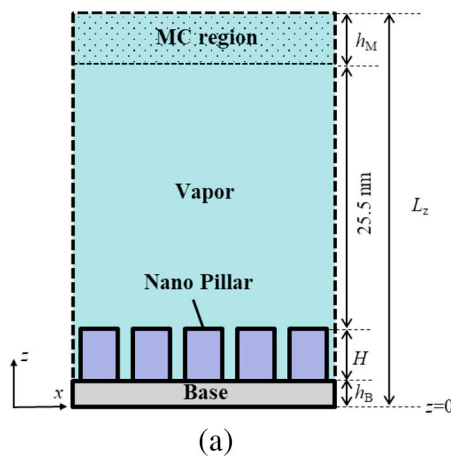


Fig. 1. Sketch of simulation domain (dense array with 5×5 nanopillars). (a) Front view of simulation system (b) Top view of nanopillar array.

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