EFFECT OF WALL SUBCOLLINGS ON DROPWISE CONDENSATION WITH INVERTED TRAPEZOID NANO-STRUCTURE SURFACE

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ABSTRACT

Effects of inverted trapezoid nano-wires surface (ITWs) and wall subcoolings on dropwise condensation (DWC) are investigated by molecular dynamics simulation with argon fluid. We show that ITWs promote liquid transportation from nano-structure to surface, which helps to keep dry state in the gaps of nanowires. At the wall subcooling of 45 K, three regimes are shown as drop nucleation and growth in nano-structure, drop de-wetting from nano-structure to surface, and dry vapour in nano-structure, noting that the de-wetting process only takes place for one time. At high wall subcooling of 65 K, the three regimes are changed to drop nucleation and growth in nano-structure, double drop de-wetting from nanostructure to surface, and partial-dry-condition in nano-structure. We conclude the stronger capability of ITWs to pull liquid out of nano-wires, even at very high wall subcooling, highlighting the important effect of wall subcoolings on DWC.

Keywords: inverted trapezoid nanowire; wall subcooling; dropwise condensation.

1. INTRODUCTION

Vapor condensation has various applications including water collection from air, power generation, seawater desalination and thermal management [1-3]. Because dropwise condensation (DWC) has higher heat transfer coefficient than filmwise condensation, DWC has received great attention in recent years. The coalescence-induced-jumping was observed during DWC by Rose et al [4]. However, the available studies show that jumping only takes place at low wall subcoolings (ΔT_{sub}). When ΔT_{sub} increases, vapor tends to condense on the surface and move along the surface in sliding or rolling modes, deteriorating condensation performance [5]. Zhu et al. [6] observed the coalescence-induced-jumping at ΔT_{sub}=1.3 K to enhance DWC heat transfer on super-hydrophobic nanowires surface. Based on Wen et al.'s theory [7], densely populated nanostructures suppress drop nucleation in nanostructure gaps, promoting jumping at high wall subcoolings (ΔT_{sub}). The ΔT_{sub} could be 15 K to keep jumping when using 100~140 nm nanowires. When the nanowires spacing decreases to ~100 nm, the maximum ΔT_{sub} could be increased to 20 K for droplet jumping [8].

We note the minimum drop size of ~100 nm that can be observed, below which introduces challenge for measurement [9]. In nanoscale, molecular dynamics (MD) is an effective tool to investigate the related phenomena and mechanisms. Gao et al. [10] simulated DWC, showing that droplets gradually behave Cassise, Partial Wenzle and Wenzel states with decrease of solid structure fraction of nanostructure substrate.

The above literature survey indicates that the DWC related droplet dynamics on nanostructured surface is not well understood. Especially, the de-wetting process from Wenzel state to Cassie state should be further investigated. In this paper, comparative studies were performed with vertical

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nanowires and ITWs (inclined nanowires) as the base substrate materials. Attention was paid to the effect of substrate liquid subcoolings.

2. PHYSICAL MODEL AND SIMULATION DETAILS

To investigate DWC, a vapor-liquid-solid system was established with a 3D-domain of $46.5\sigma \times 46.5\sigma \times 126\sigma$ in x, y, z directions, respectively. Figure 1a shows the simulation box containing both solid structure and argon. At the top of the simulation box, a liquid film with its thickness of H_l=7 nm was set. Then, a bulk vapor region with its height of $H_v=105\sigma$ was arranged in the middle of the simulation box. The top and the bottom of the simulation box function as evaporation and condensation, respectively. Fig. 1b shows the enlarged vapor region and Fig.1c shows the cross-section view of the inverted trapezoid wires (ITWs) above a solid substrate, in which w and h are the width and height of a single inverted trapezoid wire (ITW), and s is the pitch distance of two neighbouring ITWs. Here, $h=7.5\sigma$ and $\varphi=60°$ are used, where φ is the base angle of an ITW with respect to horizontal plane. Under a 3×3 patterned ITWs layer is the solid substrate, having a height of 3σ. Initially, the simulation box is filled with argon atoms, which are arranged in face-centered-cubic (fcc) form. The Lennard-Jones(L-J) potential was applied to argon once simulation starts. A characteristic contact angle of 114.5° between solid and argon is used.

The Newton-equation is solved using the Velocity-Verlet algorithm, with a time step of $\Delta t = 0.002346\tau$, where $\tau = \sqrt{m\sigma^2/\varepsilon}$ is the characteristic time of argon, m, σ and ε are the mass, length scale and energy scale of argon molecule. Our simulations contain three steps. The first step keeps a constant temperature of the fluid domain (not including solid), T_h, by applying NVT. The second step withdraws NVT, instead, applies NVE to reach thermal-equilibrium state between vapor and liquid, in which the heat source and cold source are maintained to have constant temperatures.

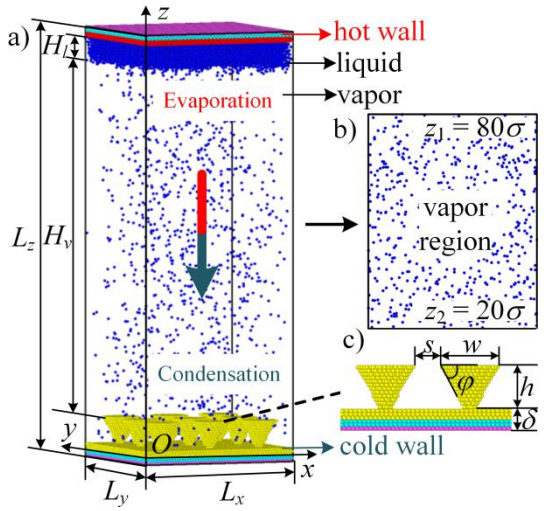

Figure 1: (a) Computation domain; (b) vapor region; (c) nano-structure and geometry parameter.

3. RESULTS AMD DISCUSSION

3.1 Effect Of Nanowire Inclination Angles On Droplet Dynamics

Two base angels of φ=60° (IWT) and 90° (vertical nanowire) are used for comparative investigation. Other parameters are set as T_h=130 K and T_c=85 K and ΔT_{sub}=45 K. Table 1 shows the geometry parameters of nanowires.

Figure 2 plots N_{nano} versus time, where N_{nano} is the number of argon atoms in the vacuum space of nine ITWs or vertical nanowires. ITWs are shown to have a sharp rise of N_{nano} in the early stage to reach a peak value of ~2300 at ~18 ns, identifying easier drop nucleation in the nanostructure gaps. Beyond ~18 ns, N_{nano} decreases sharply to attain a constant value of ~500. In contrast to ITWs, vertical nanowires yield a smooth increase of N_{nano} to reach a constant value of ~1000. Hence, ITWs not only keep easier drop nucleation in nanostructure gaps, but also quickly pulls liquid out of nanostructures to maintain Cassie state. Alternatively, vertical structures do not have the self-propulsion liquid transportation function, preferring to keep Wenzel state. For vertical nanostructures, a short instability regime is observed (see Fig.2b-c). Even though N_{nano} is sharply decreased in a short duration from point 1 to point 3, it quickly recovers to a higher level from point 4 to point 6. Hence, such instability behavior may not influence the overall drop dynamics.

Table 1: Nanostructure parameters

Case	$w+s=15.5\sigma$			
	φ (°)	w (σ)	s (σ)	h (σ)
(a)	60	14.35	1.15	7.50
(b)	90	11.24	4.26	7.50

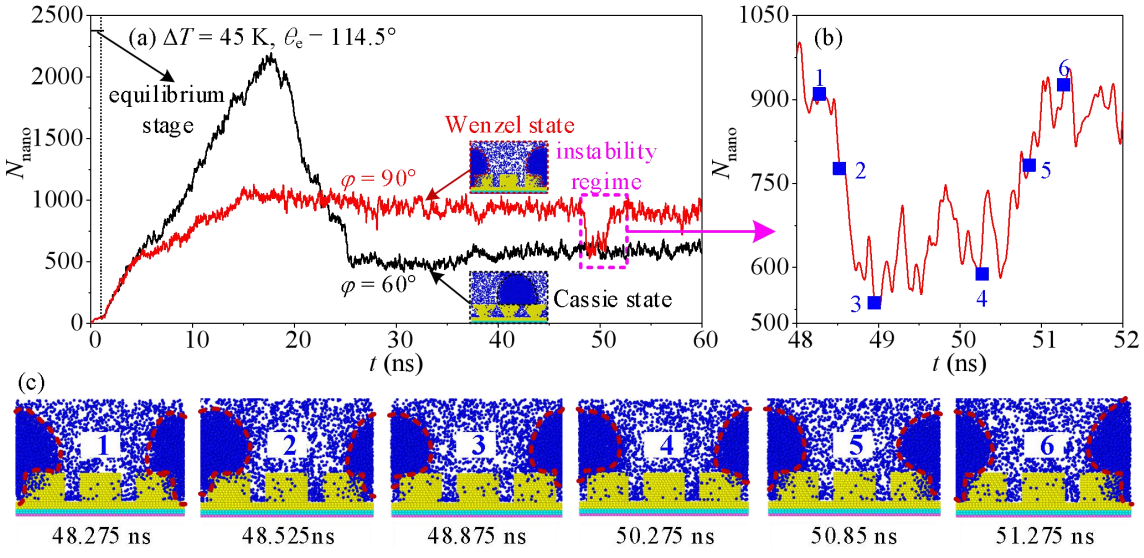

Figure 2: Effect of base angles on the number of atoms in nanostructure gap with ΔT_{sub}=45 K and θ_e=114.5° in (a), (b) and (c) show the behavior at six specific time for vertical nanowire (φ=90°).

The energy barrier analysis helps us to understand why inclined structures prefer to convert Wenzel state to Cassie state. The energy barrier for such transition is (see Fig.3)

$$G_1 = 2\pi B^2 \gamma_{lv} h \frac{s\cos(\pi-\varphi)+\cos\theta_e}{x\sin(\pi-\varphi)} \tag{1}$$

Where B is the foot print droplet radius on substrate, γ_{lv} is the surface tension, $x=s+w$, where w is the nanowires width.

For vertical structure ($\varphi = 90°$), Bormashenko [11] simplified Eq.1 as

$$G_2 = \frac{2\pi B^2 \gamma_{lv} h\cos\theta_e}{x} \tag{2}$$

Hence, the difference of energy barrier for the two base angles of 60° and 90° is

$$\Delta G = G_1 - G_2 = \frac{2\pi B^2 \gamma_{lv} h}{x}\left[\frac{\cos\theta_e(1-\sin\varphi)+s\cos(\pi-\varphi)}{\sin\varphi}\right] \tag{3}$$

Substituting θ_e = 114.5° and φ = 60° yields $\Delta G < 0$, indicating that the inverted nanostructure prefers to switch Wenzel mode to Cassie mode compared with vertical nanostructure.

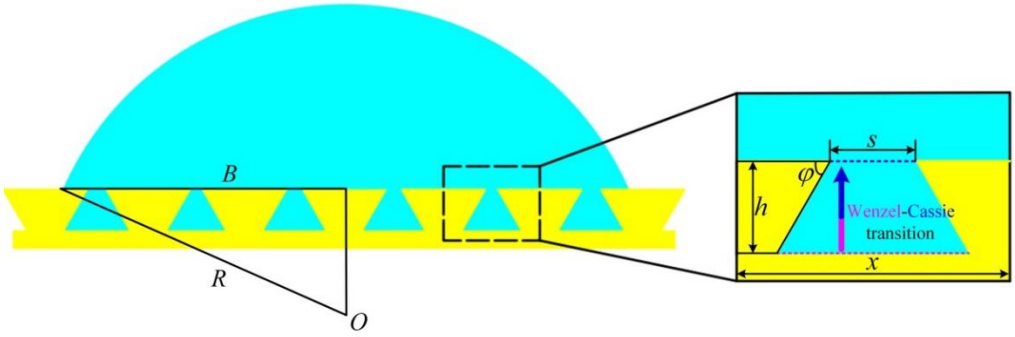

Figure 3: Schematic diagram of ITWs to illustrate transition from Wenzel state to Cassie state.

3.2 EFFECT OF WALL SUBCOOLINGS ON DROPLET DYNAMICS

Here, the bottom substrate temperature equals to 85 K, while the top evaporation surface has a temperature in the range of (100-150) K. Hence, the bottom wall subcooling is in the range of (15-65) K. Effect of wall subcoolings on droplet pattern was investigated. Figure 4a shows N_{nano} versus time, Droplet dynamics was shown in Fig.2b and 2c at moderate wall subcooling of ΔT_{sub}= 45 K and high subcooling of ΔT_{sub} = 65 K, respectively.

DWC with moderate wall subcooling displays three distinct regimes. From the initial time of t=0, the three regimes are identified as drop nucleation and growth in nano-structure (regime I), liquid de-wetting from nano-structure (regime II), and dry nano-structure (regime III), respectively. In regime I, drop nucleation starts in the gaps of ITWs. The nucleated drops are growing to linearly increase N_{nano}, until a peak value is reached at t=17.5 ns to terminate regime I. In regime II, N_{nano} sharply decreases. The corresponding droplet morphology shows that in this regime, larger drop occurs above

the ITWs layer to display hydrophobic to nano-structure surface. Liquid under the ITWS layer are observed to be pulled out of nanostructure, explaining the decreased N_{nano}. Regime III keeps a lower level of N_{nano}. In summary, with a moderate subcooling such as 45 K, ITWs structure keeps a single time liquid de-wetting from nano-structure. ITWs help to keep dry condition in nano-structure gaps.

The increased wall subcooling to 65 K has something changed as compared to that of 45 K (see Fig.2). Even though the three regimes are also claimed with ΔT_{sub} = 65 K, regime II is subdivided into two sub-regimes of II_1 and II_2. A major finding with high wall subcooling is that this condition maintains multi-times de-wetting process from nano-structure. As seen from the red curve in Fig.2a, there are two peaks of N_{nano}, with the first peak located at t=11.3 ns and the second peak located at t=36.3 ns. Correspondingly, the first liquid de-wetting process starts at t=11.3 ns and the second liquid de-wetting process starts at t=36.3 ns. We conclude that even at very high wall subcooling, ITWs can keep dropwise condensation above the layer structure. The larger drop above the ITWs layer has the capability to pull the liquid out of nano-structure. Thus, the ITWs layer still keeps partial dry condition.

For DWC, it is a challenge to keep Cassie state over a wide range of parameters. The conventional surface such as nano-pillar structure (cylinder shape) has the difficulties in keeping Cassie state at high wall subcooling, due to difficulties in pulling liquid out of nano-structure. Here, we proposed the inverted trapezoid wires (ITWs). Our MD simulations show that this structure has stronger capability to pull liquid out of nano-structure.

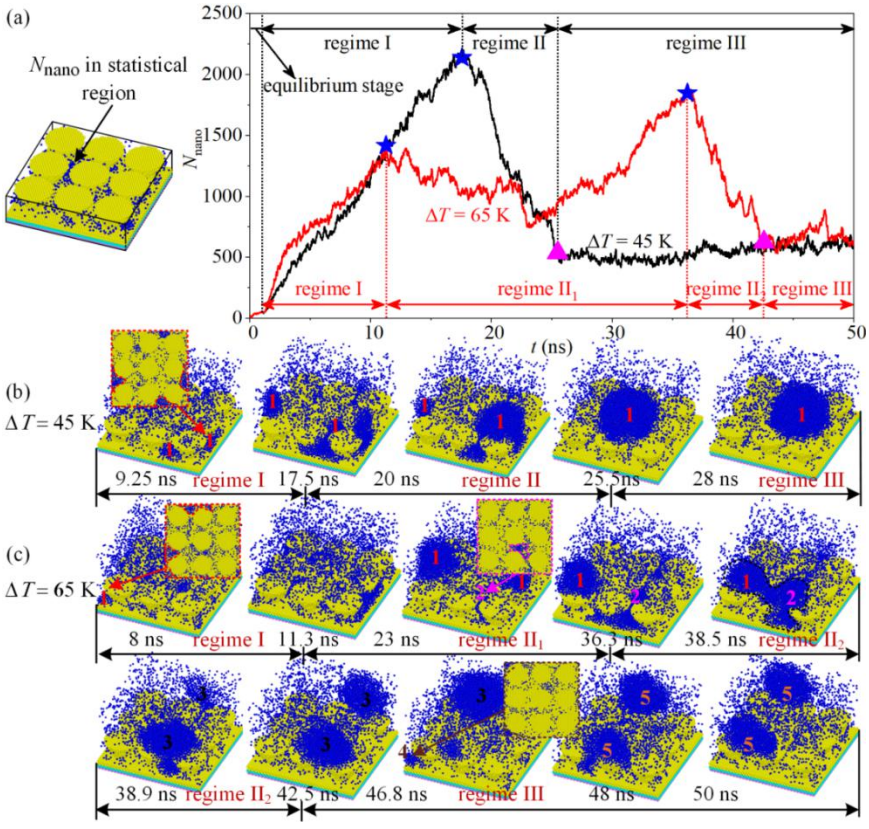

Figure 4: Effect of wall subcoolings on droplet pattern (a: the number of atoms in nanostructure gap with ΔT = 45 K and ΔT = 65 K; b: dynamic droplet patterns with ΔT = 45 K, regimes I, II and III refer to drop nucleation and growth, liquid de-wetting, and dry nano-structure, respectively; c: dynamic droplet patterns with ΔT = 65 K, regimes I, II_1, II_2 and III refer to drop nucleation and growth, first liquid de-wetting from nano-structure, second liquid de-wetting from nanostructure, and partial dry nano-structure, respectively. In (b) and (c), the number in each image represents the number of droplet.

4. CONCLUSION

It is a challenge to keep Cassie state for droplets on condenser surface. Here, we introduced novel concept by using inverted and inclined nanostructures to improve DWC performance. Our MD simulations and theoretical analysis show that ITWS prefer to keep Cassie state, due to the self-propulsion liquid transportation from nanostructure gaps to the top substrate surface. This improved performance even lasts for very high wall subcoolings of 65 K. Future studies are recommended on the underlying mechanism for such phenomenon. The micro/nano fabrication of such structures are also welcome.

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