Molecular dynamics simulation on effects of nanostructure on interfacial thermal resistance during condensation

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Received: 17 March 2020; Revised: 11 May 2020; Accepted: 1 June 2020

Abstract
Condensation of fluid molecules on a solid surface with and without a structure at the nanometer scale was simulated by means of the classical molecular dynamics simulations. We investigated effects of the nanostructures and the wettability, on the condensation process and an interfacial thermal resistance on whole surfaces and segments of the surface with the nanostructure. In our calculation system, we employed the fluid system of argon confined between two parallel solid walls, where a cuboid nanostructure was attached to the solid bottom wall. All intermolecular potential functions were the 12-6 Lennard-Jones form. We simulated hydrophobic and hydrophilic conditions by changing the intermolecular strength between the fluid molecules and the solid walls. Our results showed that the droplets tended to be formed at the base of the nanostructure and a droplet formed at the top of the nanostructure, regardless of the interaction strength between the fluid molecules and the solid walls. In addition, the wettability influenced on the contribution of each segment of the nanostructure on heat transfer during condensation. Local interfacial thermal resistance at the top and base of the nanostructure was relatively smaller than those at other segments of the nanostructure at an early stage of the condensation in the case of hydrophobic surface.

Keywords: Condensation, Molecular dynamics, Nanostructure, Interfacial thermal resistance, Heat flux, Nucleation

1. Introduction
Heat transfer with phase change is applied in various industrial fields such as power generation industry, air conditioning systems and cooling of electronic devices. In the above mentioned industrial devices, condensation is one of the important processes, and the enhancement of heat transfer coefficients in condensation processes benefits us from a thermal efficiency point of view. In the case of condensation on a solid surface, it is known that condensation heat transfer coefficients change through the modification of physical and chemical properties of condensation surface, and the enhancements of condensation heat transfer coefficient by designed nano and micro structure pattern on a heat transfer surface have been reported (Chen et al., 2011; Miljikovic et al., 2013; Hou et al., 2015). However, there is limited general knowledge on how the structures influence energy transfer during the condensation. In order to understand the effects of the structures at the nanometer scale (nanostructures) attached to a heat transfer surface in the condensation processes, a molecular dynamics point of view is necessary because the molecular-scale condensation occurs on a surface at the nanometer scale at the initial stage of the condensation heat transfer phenomena.

Before now, a number of studies have been carried out to estimate the heat transfer of molecular scale (Kimura and Maruyama, 2002; Vera and Yildiz, 2015) and the effects of the nanostructures on the heat transfer surface during condensation (Uno et al., 2016, 2018; Gao et al., 2019). However, there were few researches which investigated the effect of the local segment of the nanostructure on the heat transfer surface during condensation. Therefore, we investigated the condensation behavior and heat transfer mechanism in each segment of the surface with the nanostructure, which would be the basis of the detailed design of the heat transfer surface with the optimal nanostructured pattern which realizes high condensation heat transfer coefficient. In this study, we especially focused on the condensation behaviors and the local heat transfer in condensation processes on a solid surface with a cuboid structure. The classical molecular dynamics
simulations were conducted to investigate the effects of the nanostructure and its contribution to the condensation process in terms of the local interfacial thermal resistance.

2. Calculation methods

The calculation Models A and B employed in the present study are shown in Fig. 1. The fluid region was confined between the top and bottom parallel solid walls, and a cuboid nanostructure was attached to the bottom wall in the case of Model B. The size of the fluid molecular region was 25.1 - 25.1 - 80.0 nm³, and the periodic boundary conditions were employed in the x- and y-directions. Each solid wall consisted of three layers, and the temperature of the middle layer of each wall was controlled at a certain constant value by the Langevin method with the outermost layers fixed. The solid atoms were arrayed in a fcc lattice structure with (100) surface. The nanostructure was modeled as the square-pillar, and the side length of the structure was 12.6 nm. Numbers of fluid atoms, solid atoms at the upper wall (solid atoms of the bottom wall in the case of the flat surface) and solid atoms at the bottom wall in the case of the surface with a nanostructure were 192000, 24576 and 48000, respectively. All the potential functions employed in the present study were in the 12-6 Lennard-Jones (LJ) forms. The values of the LJ parameters σ and ε are summarized in Table 1 (Zhu and Philpott, 1994; Fujiwara and Shibahara, 2013). The length and energy parameters between the solid atoms and fluid molecules were determined by the Lorentz-Berthelot combining rule. The Lennard-Jones potential function multiplied by the interaction potential parameter α between the solid walls and the fluid molecules was used to control the fluid-solid interaction intensity, as follows:

$$\phi_{Ar-Pt}(r_{ij}) = 4\alpha\varepsilon_{Ar-Pt}\left(\frac{\sigma_{Ar-Pt}}{r_{ij}}\right)^{12} - \left(\frac{\sigma_{Ar-Pt}}{r_{ij}}\right)^{6}$$ \hspace{1cm} (1)

In this study, the interaction strength parameter α was changed as 0.045, 0.065 and 0.085, where the contact angle of a liquid droplet on a solid surface, calculated by molecular dynamics simulation, was 103°, 88° and 68° at 100 K, respectively (Bo and Vijay, 2009). The LAMMPS (Plimpton, 1995) package was used to conduct the simulations. The calculation model and interaction strength parameter α in each case are shown in Table 2. The cutoff distance was 10 Å, and the time step was 5.0 fs, respectively.

The procedure of the calculation is as follows. First, the velocity-scaling was used to control the temperature of fluid molecules at 115 K for 15 ns. Then, without the velocity-scaling, the simulation was run for 5 ns with the temperature control of the solid walls at 115 K by the Langevin method with a damping factor of 200 fs. By setting the initial arrangement of the fluid molecules near the upper wall surface, we made a calculation system in which the liquid film exists only near the upper wall surface in the initial equilibrium state. The density of the liquid film at z = 70.0 nm and the wall were approximately 1.13 g cm⁻³ and 19.7 g cm⁻³, respectively. After equilibrating at 115 K, the temperature of the solid bottom wall was changed to 85 K by the Langevin method. In the results shown below, we defined the time when the solid bottom wall was changed to 85 K as 0 ns. Then, the fluid molecules were cooled, and the condensation occurred near the solid bottom wall. We obtained various physical values until 25 ns.

To evaluate energy transfer during the condensation process, we calculated the total energy transfer Q at the bottom wall with or without the nanostructure, and obtained the heat flux q by using the following equation where S and t are the surface area and time, respectively.

$$q = \frac{1}{S} \frac{dQ}{dt} = \frac{1}{S} \sum_{i \in L} \langle F_i \cdot v_i \rangle$$ \hspace{1cm} (2)

Here $F_i$ and $v_i$ were the force and the velocity, respectively and L represents the atoms of which temperature were controlled by the Langevin method. In addition, $\langle \rangle$ represents the time average. We can calculate Q from the energy increase in the temperature control layer of the bottom wall and the nanostructure. By measuring argon temperature in the neighboring region of each face of the nanostructure and bottom wall temperature, we calculated the temperature difference ∆T at the fluid-solid interface. We calculated the temperature of the fluid molecules using the fluid molecules contained in the control volume 0.37 nm apart from the wall surface for the calculation of the temperature distribution of
the fluid molecules around the surface with the nanostructure. The interfacial thermal resistance \( R \) is expressed by the following equation using the temperature difference \( \Delta T \) and the heat flux \( q \).

\[
R = \frac{\Delta T}{q}
\]  

We calculated time evolution and time average of \( Q, q, \Delta T \) and \( R \) on the whole surface as well as surface segments, as shown in Fig. 2, and investigated the effects of the nanostructure and wettability on these values.

![Fig. 1 Calculation models A and B.](image)

| Table 1 Lennard-Jones potential parameters. | \( \sigma \) Å | \( \epsilon \) \( 10^{-21} \) J |
|--------------------------------------------|----------------|----------------|
| Ar-Ar                                      | 3.40           | 1.67           |
| Pt-Pt                                      | 2.54           | 109            |
| Ar-Pt                                      | 2.97           | 13.5           |

| Table 2 Calculation condition in Case 1-6. | \( \alpha \) and contact angle | hydrophobic | hydrophilic |
|-------------------------------------------|--------------------------------|-------------|-------------|
| Model A                                   | 0.045, 103°                  | Case1       | Case5       |
| Model B                                   | 0.065, 88°                   | Case2       | Case4       |

To evaluate the contribution of each surface segment with a cuboid nanostructure on heat transfer during condensation, we divided the surface with a nanostructure into the segments (1)-(5), as shown in Fig. 2. We defined the five segments of the surface with the nanostructure as (1) flat segment at the bottom wall, (2) base segment, (3) sidewall, (4) top corner and (5) top flat segment of the structure, respectively. We calculated the time average of local energy transfer \( Q \), local heat flux \( q \), local temperature difference \( \Delta T \) and local interfacial thermal resistance \( R \) at each surface part of the bottom wall with the nanostructure. The calculation method for the local interfacial thermal resistance was similar to that for the total interfacial thermal resistance, but separating the surface with the nanostructure into five segments.
3. Results and Discussion

3.1 Effects of nanostructure and interaction parameter $\alpha$ on condensation phenomena

Figure 3 shows the time evolutions of condensation behavior in Case 1 and 2. It is found that droplets were generated at 5 ns, at the early stage of condensation in Case 1, as shown in Fig. 3 (a). These droplets kept growing and coalesced, and eventually became one large droplet as shown in Fig. 3 (c). On the other hand, in Case 2, multiple droplets were generated on the top, the side and the base of the nanostructure at 5 ns as shown in Fig. 3 (d). It was reported that droplets tended to be formed just near the sides of the nanostructure when the size of the structure was less than 10 nm (Uno et al., 2016, 2018). We can observe that there was a difference in the droplets on the base and sidewalls of the nanostructure which was more than 10 nm. At 15 ns, some of the droplets coalesced and the others grew on the top and the base of the nanostructure as shown in Fig. 3 (e). Finally, the droplet on the top and the base of the nanostructure kept growing and the height of the droplet reached about 6 nm on the top of the nanostructure as shown in Fig. 3 (f).

The time evolutions of condensation behavior in Case 3 and 4 are shown in Fig. 4. The liquid film with a non-uniform thickness was generated at 5 ns in Case 3 as shown in Fig. 4 (a). After that, a uniform liquid film was formed at 15 ns and kept growing until 25 ns as shown in Figs. 4 (b) and (c), respectively. In Case 4, the liquid film grew at the base of the nanostructure and a hemispherical droplet was formed on the top of the nanostructure at 15 ns as shown in Fig. 4 (e). At the same time, the number of the fluid molecules between the nanostructures increased and the droplet on the top of the nanostructure kept growing. Finally, the height of the droplet reached about 8 nm on the top of the nanostructure at 25 ns as shown in Fig. 4 (f).

Figure 5 shows the time evolutions of condensation behavior in Case 5 and 6. In Case 5, a liquid film with a uniform thickness was generated at 5 ns, and it continued to grow uniformly in the film thickness as shown in Figs. 5 (a), (b) and (c). On the other hand, the liquid film grew from the base of the nanostructure, and a droplet was formed on the top of the nanostructure at 5 ns in Case 6 as shown in Fig. 5 (d). At 15 ns, the fluid molecules on the top of the nanostructure flowed down into the nanostructure gap, as shown in Fig. 5 (e). The region between the nanostructures was flooded at 25 ns as shown in Fig. 5 (f).

Comparing Fig. 3 (c) with Fig. 4 (c) and Fig. 5 (c), it was confirmed that the dropwise condensation occurred in the case of $\alpha = 0.045$ and the filmwise condensation occurred in the cases of $\alpha = 0.065$ and 0.085, on the flat surface, respectively. We also observed that the droplets on the top of the nanostructure kept growing in the cases of $\alpha = 0.045$ and 0.065 as shown in Figs. 3 (d)-(f) and Figs. 4 (d)-(f). On the other hand, as shown in Fig. 5 (f), the droplet on the nanostructure top was merged with the liquid film in between the nanostructure at 25 ns. These results show that the combinations of the surfaces wettability and the presence or absence of the nanostructure affect condensation behaviors at the initial stage of the condensation.
Fig. 3 Time evolutions of condensation behaviors of $\alpha = 0.045$; (a) 5 ns in Case 1, (b) 15 ns, (c) 25 ns, (d) 5 ns in Case 2, (e) 15 ns, and (f) 25 ns.

Fig. 4 Time evolutions of condensation behaviors of $\alpha = 0.065$; (a) 5 ns in Case 3, (b) 15 ns, (c) 25 ns, (d) 5 ns in Case 4, (e) 15 ns, and (f) 25 ns.
3.2 Effects of nanostructure and interaction parameter $\alpha$ on total heat transfer

The time evolutions of the total energy transfer at the bottom wall $Q$ are shown in Fig. 6. It was found that with the increase in $\alpha$ from 0.045 to 0.085, $Q$ increased in both cases of Model A and B. $Q$ was larger in the case of Model B compared to that in the case of Model A regardless of $\alpha$. This is because the surface area was enlarged in the case of Model B compared with that in the case of Model A by attachment of the nanostructure. In the case of $\alpha = 0.045$, the droplets had been formed and kept growing gradually as shown in Fig. 3 and $Q$ increased linearly with the droplets growing. On the other hand, the liquid films had been formed as shown in Fig. 4 and Fig. 5, and $Q$ increased largely in the cases of $\alpha = 0.065$ and 0.085 at the early stage of the condensations. From these results, it’s found that the liquid films at the early stage of condensation affected the energy transfer enhancement at the bottom walls regardless of the surface with and without the nanostructure.

![Fig. 6 Time evolutions of total heat transfer $Q$ at bottom wall; (a) $\alpha = 0.045$, (b) $\alpha = 0.065$, and (c) $\alpha = 0.085$.](image)

The time evolutions of the heat flux $q$ are shown in Fig. 7. In the case of $\alpha = 0.045$, we found little difference in $q$ in the cases of Model A and B, and $q$ increased slightly with time. On the other hand, $q$ of Model A was larger than that of Model B in the cases of $\alpha = 0.065$ and 0.085, and $q$ decreased with time. There was a difference in whether or
not the fluid molecules had been flooded on the heat transfer surfaces including the nanostructure, as shown in Fig. 3, Fig. 4 and Fig. 5. As a result, \( q \) was much smaller in the case of \( \alpha = 0.045 \) than those in the cases of \( \alpha = 0.065 \) and \( 0.085 \).

The time evolutions of the temperature difference \( \Delta T \) are shown in Fig. 8. \( \Delta T \) decreased with the increase in \( \alpha \) regardless of Model A and B. \( \Delta T \) was more likely to decrease in the case of Model B than that of Model A in all the cases. This is because the droplets and the liquid film on the surface grew easily and cooled quickly by the enlargement of the surface area in the case of Model B.

Figure 9 shows the time evolutions of the interfacial thermal resistance \( R \) on the whole surface. The interfacial thermal resistance calculated in the case of the hydrophilic surface was in the order of \( 10^{-7} \) K m\(^2\)/W, which corresponds to those shown in the previous study (Kimura and Maruyama, 2002). Model A was larger than that of Model B in the case of \( \alpha = 0.045 \). On the other hand, we can find little difference in \( R \) between the cases of Model A and B in the cases of \( \alpha = 0.065 \) and \( 0.085 \). Thus, the interfacial thermal resistance changed corresponding to the condensation behavior, and the change of that was large in the case of \( \alpha = 0.045 \) because of the motion of droplets and liquid films.
3.3 Effects of attached structure and interaction parameter $\alpha$ on interfacial thermal resistance averaged over whole surface

In this section, we discuss clearly the effects of the nanostructure and interaction parameter $\alpha$ on the heat transfer mechanism by using the physical value averaged during the whole calculation time. The effects of the interaction parameter $\alpha$ on the heat flux $q$, the temperature difference $\Delta T$ and the interfacial thermal resistance $R$ over the whole surface during 25 ns are summarized in Fig. 10. $q$ of Model B was smaller than that of Model A in the cases of $\alpha = 0.065$ and 0.085. In Fig. 10 (b) $\Delta T$ was larger in the case of Model A than in the case of Model B regardless of $\alpha$. The results showed that $q$ increased, while $\Delta T$ decreased with the increase in $\alpha$ regardless of Model A and B. It is considered that the temperature gradient in Model B was smaller than that in Model A because the heat transfer at the surface was increased by attaching the nanostructure on the bottom wall. In Fig. 10 (c) $R$ of Model A was larger than that of Model B regardless of $\alpha$. However, $R$ of Model A was slightly smaller than that of Model B in the case of $\alpha = 0.065$. We can also confirm that $R$ of Model A and B was almost the same value in the case of $\alpha = 0.085$. The interfacial thermal resistance $R$ of Model B decreased in the case of the hydrophilic surface, although it slightly increased or did not change in the cases of the hydrophilic surfaces.

Thus, the heat transfer surface with and without the nanostructure as well as the wettability affected the heat flux $q$, the temperature difference $\Delta T$ and the interfacial thermal resistance $R$ averaged over the whole surfaces.
3.4 Effects of interaction parameter $\alpha$ on local interfacial thermal resistance in the case of the surface with nanostructure

In the case of the calculations for the local heat transfer, the droplets and the liquid films formed with the similar trend as those for the total heat transfer. Figure 11 shows the effects of the interaction parameter $\alpha$ on (a) the heat flux $q$, (b) the temperature difference $\Delta T$ and (c) the interfacial thermal resistance $R$ at the surface segments (1)-(5) in Fig. 2. In Fig. 11 (c), the interfacial thermal resistance of Model A averaged over the whole surface is also plotted for comparison with the local interfacial thermal resistance at the surface segments (1)-(5) of Model B.

In the case of $\alpha = 0.045$, condensation was promoted around the base and top of the nanostructure and segment at the bottom wall as shown in Fig. 3 (f) and a large amount of heat was transferred by the condensation of the droplets. As a result, $q$ was relatively large at surface segments (2) and (5). It was reported that the absolute value of the potential energy was the highest at the base of the nanostructure (Shan et al., 2019), so the kinetic energy of the fluid molecules was easily deprived at the surface segments (2). It might lead the result of the droplets formation and high value of $q$ at the base of the nanostructure. The heat flux $q$ showed a high value at the top of the nanostructure, because the droplet on the top of the nanostructure continued to grow without contact with other droplets. On the other hand, it was difficult for the fluid molecules to adhere to the surface segment (4) because of the low absolute value of potential energy, and $q$ was relatively small at the surface segment (4). As a result, $q$ at the surface segment (5) was approximately 4 times as large as that at the surface segment (2). In the case of $\alpha = 0.065$, the condensation was promoted around the base and the top of the nanostructure as shown in Fig. 4 (d) and $q$ was large at the surface segments (2) and (5). In the case of $\alpha = 0.085$, $q$ was large at the surface segments (4) and (5). This is because the energy was efficiently transferred by the thin liquid film at the surface segments (4) and (5) as shown in Fig. 5 (e). On the other hand, $q$ was relatively small at the surface segments (1) and (2). The temperature of the fluid molecules rapidly decreased, and it might reduce the amount of heat transfer at the flat and the base segments of the bottom wall.

In Fig. 11 (b) $\Delta T$ was small at the surface segment (4) in the case of $\alpha = 0.045$. On the other hand, $\Delta T$ was small at the surface segment (2) in the case of $\alpha = 0.065$ and 0.085. It depends on the balance of temperature change of the fluid molecules due to the phase change and cooling rate of fluid molecules in each segment.

In Fig. 11 (c), the local interfacial thermal resistance $R$ was relatively small at the surface segments (2) and (5) in the case of $\alpha = 0.045$ and 0.065. On the other hand, $R$ was relatively large at the surface segment (4). This implies that energy transfer was prompted at the surface segment, where the droplets were likely to grow in the cases of $\alpha = 0.045$ and 0.065. As a result, $R$ at the surface segment (4) was approximately 4 times as large as that at the surface segment (5) in the case of $\alpha = 0.045$. We can observe that, in the case of $\alpha = 0.045$, the local interfacial thermal resistances at the surface segments (1), (2), (3) and (5) were smaller than the interfacial thermal resistance averaged over the whole surface in the case of Model A, and it leads to the smaller interfacial thermal resistance averaged over the whole surface in the case of Model B as shown in Fig. 10 (c). It was found that the efficient heat transfer with the effect of the nanostructure on accelerating condensation at the surface segments (1), (2), (3) and (5) reduced the interfacial thermal resistance averaged over the whole surface of Model B during condensation. On the other hand, in the case of $\alpha = 0.085$, $R$ was almost the same value on each surface segment. Detailed observation revealed that $R$ was relatively small at the surface segment (4) because of the efficient energy transfer through the thin liquid film as shown in Fig. 5 (e). We also confirmed that $R$ was relatively large at the surface segments (1) and (2) because a liquid film was formed and kept growing between the nanostructures, which increased the interfacial thermal resistance. Additionally, it was found that the variation of $R$ on each surface segment became smaller with the increase in $\alpha$.

These results show that the influence and the role of each segment of the nanostructure for the heat transfer are dependent on the wettability of the surface. Even if the size or shape of the nanostructure changes, it is considered that the condensation behavior affects the heat transfer, and the local heat transfer also changes significantly as shown in the result of this study.
4. Conclusions

The condensation of the fluid molecules on the solid surface with and without the cuboid nanostructure was simulated by the classical molecular dynamics simulations. The effects of the nanostructure, on the condensation process and the interfacial thermal resistance during the condensation, were numerically investigated. Main findings in the present study are summarized as follows:

1. The condensation progressed favorably from the base of the cuboid nanostructure and a droplet formed at the top of the nanostructure at the early stage of condensation. On the other hand, the fluid molecules difficultly condensed at the top corner of the nanostructure.

2. The interfacial thermal resistance averaged over the whole surface decreased with the increase in the interaction parameter between the fluid molecules and the solid wall in the cases of the surface with and without the nanostructure. The interfacial thermal resistance averaged over the whole surface decreased in the case of the hydrophobic surface with the nanostructure, although it slightly increased or did not change in the cases of the hydrophilic surfaces in comparison with those of the flat surface.

3. The contribution of the segments of the surface with the nanostructure on the condensation heat transfer changed greatly depending on the wettability of the surface. In the case of the hydrophobic surface with the nanostructure, the interfacial thermal resistance at the top corner of the nanostructure was approximately 4 times as large as that at the top of the nanostructure. On the other hand, the interfacial thermal resistance at the top corner of the nanostructure was relatively small in the case of the largest interaction parameter between the fluid molecules and the solid wall.

4. The variation of local interfacial thermal resistance on each surface segment became smaller with the increase in the interaction parameter between the fluid molecules and the solid wall.

We believe our basic insight of local heat transfer on the surface with the nanostructure would be useful for designing the optimal nanostructure pattern surfaces to control heat transfer during condensation and for developments of industrial applications. In the future, we should check three points. Firstly, we would like to investigate the effects of the size of the nanostructure on condensation behavior and heat transfer to confirm the relation between local heat transfer in this study and the size of the nanostructure. Secondly, we would like to investigate the effects of condensation behavior on condensation rate and heat transfer. Thirdly, we would like to check the influence of the upper wall geometry on the interfacial thermal resistance at the bottom wall.

Acknowledgment

This work has been supported by the Japan Society for the Promotion of Science (JSPS), “Grant-in-Aid for Science Research (B) No. 18H0382”.

Fig. 11 Effects of interaction parameter \( \alpha \) on (a) heat flux \( q \), (b) temperature difference \( \Delta T \), and (c) thermal resistance \( R \) at the surface segments (1)-(5).
References

Bo, S. and Vijay, K., Molecular dynamics simulation of the contact angle of liquid on solid surfaces, The Journal of Chemical Physics, Vol. 130, 034705, (2009).

Chen, X., Wu, J., Ma, R., Hua, M., Koratkar, N., Yao, S. and Wang, Z., Nanograzed micropyramidal architectures for continuous dropwise condensation, Advanced Functional Materials, Vol. 21 (2011), pp. 4617-4623.

Fujiwara, K. and Shibahara, M., A Molecular dynamics study on wetting phenomena at a solid surface with a nanometer-scale slit pore, Nanoscale and Microscale Thermophysical Engineering, Vol. 17 (2013), pp. 1-9.

Gao, S., Liu, W. and Liu, Z., Turning nanostructured surfaces with hybrid wettability areas to enhance condensation, Nanoscale, Vol. 11, No.2 (2019), pp. 459-466.

Hou, Y., Yu, M., Chen, X., Wang, Z. and Yao, S., Recurrent filmwise and dropwise condensation on a beetle mimetic surface, ASC Nano, Vol. 9, No.1 (2015), pp. 71-81.

Kimura, T. and Maruyama, S., Molecular dynamics simulation of heterogeneous nucleation of a liquid droplet on a solid surface, Microscale Thermophysical Engineering, Vol. 6, No.1 (2002), pp. 3-13.

Miljikovic, N., Enright, R., Nam, Y., Lopez, K., Dou, N., Sack, J., and Wang, N., E., Jumping-droplet-enhanced condensation on scalable superhydrophobic nanostructured surfaces, Nano Letters, Vol. 13 (2013), pp. 179-187.

Plimpton, S., Fast parallel algorithms for short-range molecular dynamics, Journal of Computational Physics, Vol. 117 (1995), pp. 1-19.

Uno, G., Shibahara, M. and Ueki, Y., Molecular dynamics study on influences of nanostructured surface on heterogeneous nucleation of liquid droplets, Proceedings of the 27th International Symposium on Transport Phenomena (2016), ISTP27-015.

Uno, G., Fujiwara, K., Ueki, Y. and Shibahara M., Molecular dynamics study on effects of nanostructured surfaces on heterogeneous nucleation of liquid droplets, Transactions of the JSME (in Japanese), Vol. 84, No. 858, (2018).

Vera, J. and Yildiz, B., Temperature and heat flux dependence of thermal resistance of water/metal nanoparticle interfaces at sub-boiling temperatures, International Journal of Heat and Mass Transfer, Vol. 86 (2015), pp. 433-442.

Zhu, S. and Philpott, M. R., Interaction of water with metal surfaces, The Journal of Chemical Physics, Vol. 100 (1994), pp. 6961-6968.