

A molecular dynamics simulation of a bubble nucleation on solid surface

Shigeo Maruyama*¹ and Tatsuto Kimura*²
Computational Science Laboratory

In order to understand the molecular level phenomena related to the phase-change heat transfer, we are performing molecular dynamics simulations of a liquid droplet and a vapor bubble. Since many of practical nucleation phenomena are on the solid surface, we are paying special attention to the effect of a solid surface. In addition to the nucleation phenomena, a microscopic droplet or a vapor are of importance when an extreme condition of heat transfer such as a droplet formation in the chemical vapor deposition process and a bubble formation due to the intense laser heating on the solid surface.

Here, a heterogeneous nucleation of a vapor bubble on a solid surface was simulated by the molecular dynamics method. Liquid argon between parallel solid surfaces was expanded by slowly moving a surface, until a vapor bubble was nucleated. Argon liquid was represented by typically 5000 Lennard-Jones molecules and each surface was represented by three layers of harmonic molecules with the constant temperature heat bath model using the phantom molecules out side of the three-layers. The potential between argon and solid molecule was also expressed by the Lennard-Jones function form with a variable energy scale parameter ϵ . In our previous study on the liquid droplet on the surface,¹⁾ we have found that the depth of the integrated effective surface potential was directly related to the wettability of the surface. Hence, we used a quite wettable potential parameter on the top surface and changed the wettability on the bottom surface.

After the equilibrium of liquid between two solid surfaces at desired temperature was obtained, we slowly expanded the surfaces in the constant temperature condition imposed by the phantom molecules. According to the increase in volume, the decrease of pressure was observed. There appeared patches of liquid where the local potential was considerably high. These patches appeared and disappeared randomly in space and time. Finally, at some point of the decrease of the pressure, one of the patches successfully grew to a vapor bubble on the bottom solid surface where the lower wettability helped to sustain the nucleated bubble. We have always found a single vapor bubble on the surface because of this microscopic system size. Observed pressure showed the minimum at this time of the nucleation. We compared the minimum pressure for various surface potential conditions (wettability) and various temperatures. With the increase in the surface wettability, the minimum pressure approached to the spin-

odal line (the thermodynamic limit of the existence of superheated liquid). When a very high wettability of the surface was employed, the situation was very close to the homogeneous nucleation.

After the stable vapor bubble was formed on the surface, we stopped the expansion and observed the equilibrium structure of the vapor bubble as shown in Fig. 1. After averaging the two-dimensional density and potential distributions, we could define the contact angle. The contact angle was well correlated to the depth of the integrated effective surface potential in excellent agreement with the case of liquid droplet in contact with the surface. With quite wettable conditions, the layered liquid structure near the surface extended to bottom of the vapor bubble.

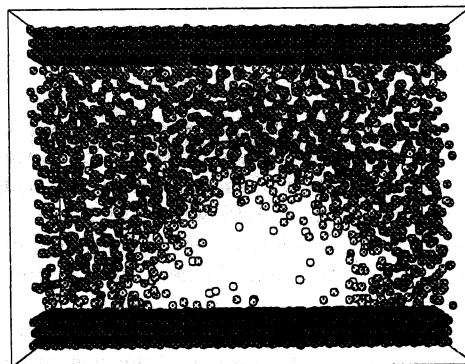


Fig. 1. A sliced snapshot of the vapor bubble on the surface. Only the central 15Å depth is shown.

As a conclusion, we have successfully demonstrated the nucleation of a 3-dimensional vapor bubble on the solid surface using the molecular dynamics method. Furthermore, the characteristics of thermodynamic superheat in the nucleation process and the contact angle were discussed through the potential function (wettability) between surface and liquid molecules.

References

- 1) S. Maruyama et al.: *Microscale Thermophys. Eng.* **2**, 49 (1998).

*¹ Permanent address: University of Tokyo, maruyama@photon.t.u-tokyo.ac.jp

*² University of Tokyo