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Molecular Dynamics Study of Boiling Heat Transfer on Hydrophilic Rectangular Nano Groove Surfaces

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Extended Abstract

Using nanostructured surfaces to enhance boiling heat transfer is an important way to solve thermal management problems in high-power electronic devices. In this paper, molecular dynamic research methods are used to investigate the bubble nucleation and boiling heat transfer properties of rectangular nano-grooves on two types of hydrophilic surfaces. The first type of groove is a conventional rectangular groove structure (CRGS) with a size of 3 nm (x) × 5 nm (y) × 1 nm (z) and a small rectangular groove with a size of 1 nm (x) × 5 nm (y) × 1 nm (z) is added to the CRGS to form the second type of groove, which is named overlapping rectangular groove structure (ORGS). The simulation domain is 14.7 nm (x) × 5 nm (y) × 80 nm (z). The face-centered cubic (FCC) copper atom with a lattice constant of 3.6149Å is used to construct the groove structure. The TIP4P water model is used to describe the phase transition behavior of water. The potential function uses the standard Lennard-Jones 12-6 (L-J) potential and the long-range Coulomb potential. The contact angle of water on the hydrophilic wall is 13 degrees.

The boiling heat transfer process of the CRGS and ORGS was investigated by bubble volume, evaporation rate, heat flux, potential energy, etc. at the temperature of 605K. Bubble generation and collapse are observed during bubble nucleation, and it is also seen that the bubbles tend to form above the grooves owing to the nucleation sites provided by the groove structures. The differences in nucleation time, bubble volume, and heat flux between the CRGS and the ORGS are compared. It is found that the nucleation time of bubbles on the CRGS surface, is 406ps earlier than that on the ORGS surface, and the evaporation rate of water molecules on the CRGS surface is higher than that on the ORGS surface. It is also found that the variations of the average temperature, total potential energy, total kinetic energy, and total energy of the water molecules with time in the CRGS surface and ORGS surface are the same, and the reason for this trend might be that the number of water molecules in the small rectangular groove on the ORGS surface is only 0.83% of the total number of water molecules, which has little influence on the average temperatures, total potential energy, etc. of the water. Compared to the CRGS surface, the water molecules in the small rectangular groove of the ORGS surface are constrained by strong potential energy from the hydrophilic groove walls and the water molecules. Thus, the water molecules above the small rectangular groove on the ORGS surface gain heat by liquid-liquid heat transfer, while the water molecules in the same position on the CRGS surface absorb heat directly from the wall by solid-liquid heat transfer. The solid-liquid atom-to-atom interactions are stronger than liquid-liquid atom-to-atom interactions[1,2], therefore the water molecules that directly contact with the wall in the case with the CRGS surface can gain energy sooner than liquid-liquid heat transfer mode in the case of the ORGS surface, leading to earlier nucleation in the case with CRGS surface. In a word, based on the results of the present study, the CRGS surface has a better boiling heat transfer performance than the ORGS surface. Further study on boiling heat transfer on the groove structure with a large solid-liquid contact area is currently underway. These results in this study can provide a guidance for the structural design of boiling heat transfer surfaces.

References

[1]Wenbin Zhou , Dongmei Han, Hualin Ma , Yanke Hu , Guodong Xia， Microscopic mechanisms behind nucleate boiling heat transfer enhancement on large-aspect-ratio concave nanostructured surfaces for two-phase thermal management， International Journal of Heat and Mass Transfer 195 (2022) 123136.

[2]Yu-Jie Chen, Xue-Jiao Chen, Bo Yu, Wen-Jing Zhou , Qun Cao , Wen-Quan Tao,Investigation of water bubble nucleation by using molecular dynamics simulation,Journal of Molecular Liquids 334 (2021) 116037.