Effect of Solid Properties on the Process of Bubble Nucleation: a Molecular Dynamics Study

Yang Li[1], Wenjing Zhou[1,*], Yonghai Zhang[1], Baojin Qi[1] and Jinjia Wei[1, 2, *]

[1]School of Chemical Engineering and Technology, Xi'an Jiaotong University, Xi'an, Shaanxi, 710049, China

[2]Key Laboratory of Multiphase Flow in Power Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi, 710049, China

[*]Corresponding Author: Wenjing Zhou. Email: wj.zhou@mail.xjtu.edu.cn.

Abstract: Nucleation boiling is used in a wide range of engineering and science fields, such as electronics cooling, new energy and the microelectromechanical systems (MEMS) technology. Besides, a better understanding of the nucleation is fundmental significance for the application and enchcement of nucleation boiling in the traditional and modern high-tech industries. Unfortunately, due to the complexity of physical mechanisms in nanoscale and the limit of small scale, accurate experimentation of nucleation cannot be accomplished. Therefore, it is important to study the influence of solid properties on nucleation despite its general importance by performing molecular dynamics simulation researches. In present work, we succeed in simulating the nanoscale boiling of liquid argon film on the solid surface, and the solid properties are varied to test their effects on bubble nucleation. The simulation results show that the bonding strength between solid atoms and the solid atomic mass has a radically different effect on nucleation while they have little effect on the contact angle between liquid and solid atoms. If the value of the bonding strength is too large, the liquid and solid phases will hardly interact with each other and too little heat will be transferred to form a bubble nuclear. On the other hand, if the value of the bonding strength is too small, it will be easy to appear explosive boiling and be hard to form a stable vapor bubble. For the solid atomic mass, the result is the opposite of the bonding strength. The smaller the value of the solid atomic mass, the harder nucleation on the solid surface. Due to the variations of the solid atomic mass and the bonding strength between solid atoms leads to a difference in the vibrational density of state (VDOS) of the solid atoms, meaning a difference in the thermal vibrational coupling between solid and liquid atoms, and thus appearing the different boiling phenomenon.

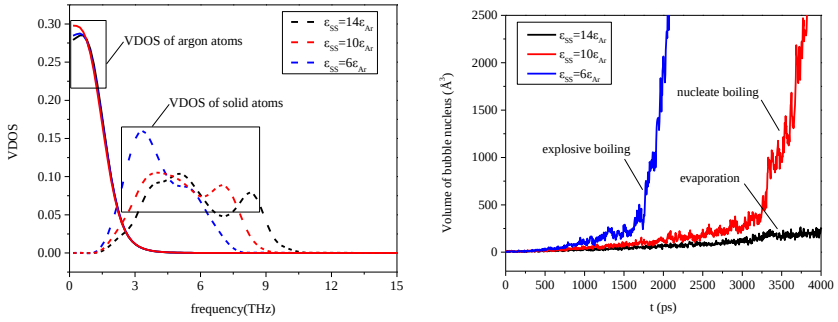

Figure 1: (a) VDOS of argon atoms and solid atoms located at the liquid-solid interfaces, (b) Volume curves of bubble nucleus with time of different cases