Molecular Dynamics Simulation of Microscale Phase Transfer

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Abstract: Microheat pipes occupy smaller volume than traditional heat sinks, and can be directly fitted with electronic components, which can ensure good heat dissipation effect. Because the size of liquid film in micro heat pipe is only a few nanometers, it is difficult to estimate the time of phase transformation equilibrium by experimental method, and the existing dangerous devices can not carry out phase transformation heat transfer experiments under micro-scale conditions. Therefore, the simulation of liquid phase transformation under micro-scale conditions by molecular dynamics method can achieve good experimental results. This paper will discuss the content of this aspect.

With the continuous progress of manufacturing technology, electronic components are developing towards miniaturization and integration. However, the heat dissipation of electronic components has attracted wide attention. Microscale liquid film can absorb or release a lot of heat energy during phase transition, which can be well applied to the heat dissipation of electronic components. Microheat pipes can achieve good heat transfer effect by using liquid phase change in micro-scale channels. Therefore, it is of great practical value to analyze and study the phase change characteristics of working medium in micro-heat pipes. The liquid film which plays a key role in phase change heat transfer has only a few nanometers thickness. Molecular dynamics can be used to understand in-depth the specific composition of atomic level. It is not suitable for nano-scale scientific research.

1. Selection of Water Model

Water can be used as working medium in micro heat pipes. Because there are many models adopted, the micro-scale phase change heat transfer model with strong applicability should be chosen. TIP4P model has been improved by using three particles. The diagonal line of hydrogen and oxygen bonds in the middle of the three atoms is filled with the fourth atom with no sanction and only charge. The atom shows Lennard-Jones morphology, as shown in Figure 1.

![Fig. 1 TIP4P water model structures](image)

Using the four charged particles of IPT4P water model for molecular dynamics simulation, we
can obtain more accurate results. However, there are many interactions between particles, so the amount of mathematical calculation will become larger. If the computer does not have good performance, the computational efficiency will not be guaranteed, and the calculation will fail. Therefore, the selected model should satisfy the computer performance and the required physical quantities, while the TIP4P model can satisfy the requirements of molecular dynamics simulation of micro-scale phase change heat transfer.

2. Study on Evaporation Rate of Liquid Vapor Phase Transition in Water Film

2.1 Modeling

In order to improve the heat transfer ability and efficiency, it is necessary to study the liquid evaporation rate deeply. The liquid vapor phase transition of water film with the same thickness should be simulated, and the liquid vapor phase should be simulated at the same system temperature. In the simulation system, there are two different substances, liquid water and silicon. Three different stages are used to simulate the evaporation of liquid film. The first stage is to control the temperature. The method of speed calibration can be used to reflect the temperature by the speed of atoms. When the atoms run one step, the running speed of silicon atoms on water molecules and substrates will be again. The temperature of the system is controlled at 275 K. Secondly, the control stage is called relaxation stage, and the temperature of the substrate is controlled at 275k by the method of velocity calibration. The temperature control on the water molecule is removed without human interference. Therefore, the water molecule can move randomly in the simulated region, thus realizing the purpose of relaxation. The final stage is called heating stage, which further increases the temperature of silicon atoms on the substrate to 400 K, and monitors the molecular trajectory. In this stage, the liquid film begins to produce phase transition, and water molecules evaporate to the vacuum region without the restriction of the liquid film. After a period of time, the liquid does not evaporate any more, thus forming phase transition equilibrium.

2.2 Influencing factors of evaporation rate

2.2.1 Effect of System Temperature on Evaporation Rate

The thickness of the water film in the molecular dynamics simulation system reaches 2 nm, and the temperature is raised from 375 K to 425 K. Phase transition is simulated in five intervals of 12 K. By calculating the evaporation rate in each case, the relationship curve between the evaporation rate and time under different temperature conditions is determined (as shown in Figure 2). From this, we can know that although the thickness of liquid film is the same, the evaporation rate has a great difference. The evaporation rate will increase continuously with the increase of temperature. When the system temperature rises to 425 K, the evaporation rate will be the highest. Big value.

![Fig. 2 The relationship between evaporation rate and time at different temperatures](image)

The evaporation rate of liquid film decreases with the increase of temperature. When the
temperature is less than 400 k, the evaporation rate will increase rapidly with the increase of system temperature. If the temperature is higher than 400k, the evaporation rate will continue to increase, but with the increase of temperature, the increase will decrease. It can be shown that it is not practical to treat saturated state with evaporation rate at high temperature and further increase evaporation rate by increasing temperature, which can be accomplished by other ways.

By observing the planar projection maps of the above five different temperatures, it can be found that not all liquids have phase transitions, and there are liquid films with a certain thickness without evaporation. Because of the change of temperature, the thickness of the liquid film left behind is different, and the thickness of the liquid film without evaporation is smaller when the temperature is high. The reason for the absence of evaporative liquid film is that the surface of silicon substrate has a certain tension, which plays a small role under macro conditions and can be neglected. However, in the micro-scale case, the effect of surface tension is obvious, which will make it difficult for water on the silicon surface to evaporate from the constraint of gravity, so a certain thickness of liquid film without evaporation will be retained around the substrate. With the increase of temperature, the thermal operation of water molecule will be more intense, the kinetic energy obtained will become larger and larger, and the separation ability will be stronger. It will be easier to get rid of the substrate and turn into vapor molecules. Therefore, in the case of a lot of temperature, the thickness of the liquid film without evaporation is smaller.

### 2.2.2 Effect of Liquid Film Thickness on Evaporation Rate

The phase transition of thin films with thickness of 2, 3 and 4 nm is simulated by the above method. There are 250, 380 and 504 water molecules in the simulation system, respectively. The temperature is set to 400 K. The evaporation rate under three thickness conditions is calculated. The evaporation rate under different liquid film thickness conditions is shown in figure 3.

![Fig. 3 The relationship between evaporation rate and time under different liquid film thickness](image)

It is found that the evaporation rate decreases exponentially with time regardless of the thickness of the liquid film. The evaporation rate increases with the increase of film thickness, while the attenuation rate decreases with the increase of film thickness. Therefore, the greater the thickness of the liquid film, the more time it takes to reach equilibrium. However, under the three thicknesses, no evaporation liquid film with a certain thickness is formed, and the thickness values are basically the same, which indicates that van der Waals force will only exert a greater binding force on molecules in a fixed range.

It is generally believed that evaporation can only take place on the surface of liquid, and the higher the temperature, the higher the rate of evaporation. Under macroscopic conditions, compared with the thinner liquid film, the higher the liquid film temperature is, the slower the temperature increases. When the phase transformation occurs, the temperature of the film thickness on the
surface is relatively low, and the evaporation rate is very small. From the simulation results, it can be found that the higher the thickness of liquid film, the higher the evaporation rate. It shows that there is a great difference between the micro-scale and macro-scale conditions. The surface temperature of liquid film under three thickness conditions is analyzed by mathematical statistics, and the reasons are analyzed one by one.

Fig. 4 shows that the temperature of liquid-gas interface varies with time under different thickness conditions. It can be seen that even though the temperature of liquid-gas interface fluctuates greatly, the rising speed of temperature is not affected by thickness, and the increasing speed of liquid film temperature of each thickness is similar. Moreover, the thick liquid film can supply more water molecules for evaporation, so it has a higher evaporation rate. It can be explained that not only the water molecules at the surface position produce phase transition, but also the internal molecules participate in the phase transition process. Therefore, if you want to improve the heat transfer efficiency of micro heat pipe, you can use the method of increasing temperature and thickness.

3. Conclusion

In order to analyze and understand the influence factors of phase change evaporation rate under micro-scale conditions, molecular dynamics simulations of phase change phenomena under different liquid film thickness and different simulated system temperature conditions were carried out. From the simulation results, it can be found that the evaporation rate of the liquid film decreases exponentially with the time going on. The temperature value of the simulation system and the thickness of the liquid film are the main factors affecting the evaporation rate. With the increase of the temperature of the system and the thickness of the film, the corresponding evaporation rate will increase significantly. If the temperature value is more than 400k, the evaporation rate will not be affected by the increase of temperature. The method of increasing the thickness of liquid film can be used to improve the evaporation rate. In either case, there will be a liquid film with a certain thickness without evaporation, which is due to the Van der Waals force formed between the substrate silicon and the liquid. Because of this force, the phase transition of water molecules around the substrate will be restricted. With the increase of temperature, the thickness of the evaporated liquid film will become smaller and smaller.

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References

