固体壁間の極薄液膜における熱輸送に関する分子動力学的解析
Molecular Dynamics Analysis of Heat Transfer over Ultra-Thin Liquid Films between Solid Surfaces

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Currently, the structure of electronic device has been becoming smaller with the rapid development of nanotechnology. The heat dissipation should be achieved via the interfaces where the ratio of the interface to the volume becomes larger. Now the heat transfer through interfaces between the devices and thermal interface materials, liquids and soft matter in many cases, should be studied, in order to remove efficiently the heat generated in electronic devices. This paper focuses on the heat transfer characteristics over ultra-thin liquid film between solid surfaces, to explain how the thermal resistance between solid surfaces is affected in response to the thickness of the liquid film or the solid surface configurations under the interference from both the solid surfaces simultaneously.

1. Introduction

In recent years, heat dissipation from high performance power modules has become an important problem in the field of electronic packaging. In most cases, power modules are attached with other components such as an insulating plate and heat dissipation devices via thermal interface materials (TIM). As the required thermal conductance between these components is getting higher heat flux with lower temperature difference, the interfacial thermal resistance between the solid components and TIM, typically liquids and soft materials such as grease, becomes a serious problem.

There are a number of studies in the past with molecular dynamics simulations about thermal transport over the solid-liquid interface (1-3), in which heat transfer characteristics of the interface between different face centered cubic (FCC) crystal planes and different species of liquids were explored. The distance between the solid walls on both sides is far and liquids of bulk state exist in between, so the liquid molecules in the vicinity of the interface are almost affected by one side of the solid wall. However, when the solid walls are close enough (typically, less than 2 nm), the liquid molecules in the interface region will be affected by the solid walls on both sides simultaneously. It will have a certain effect on the heat transfer of the interface. Some recent studies have begun to analyze the heat transfer characteristics in this case (4-6). Nevertheless, the heat transfer characteristics in this case should be further explored. In such a case, combination of the two solid walls, symmetrical property for example, should be discussed.

In the present study, with molecular dynamics simulation, the variation of thermal resistance between solid walls was analyzed as a response to the thickness of liquid film between solid walls and the symmetry of surface configuration of the solid surfaces.

2. Molecular Dynamics Simulation

In the present study, as shown in Fig. 1, the simulation system consists of a pair of solid walls (platinum) and liquid film (argon). Periodic boundary conditions are set in the x and y directions. To ensure that the system does not drift during simulation, the outermost layers of solid walls on both sides were fixed. Then, to get a stable heat flux between solid walls, the temperature of the second outmost layer on the left side was set to 135K, and the right one to 105K, so that the average temperature of the liquid film is expected to be 120K, which is close to the medium between the critical temperature and the triple point of argon (7). Here, the non-equilibrium molecular dynamics (NEMD) simulation was established.

As shown in Fig. 2, the solid walls used in the simulation all consist of face-centered cubic (FCC) structure with the surface of (1,1,0) crystal plane. The solid surface configuration is symmetric in the case of parallel surface configuration (PSA), while it is asymmetric in the case of crossed surface
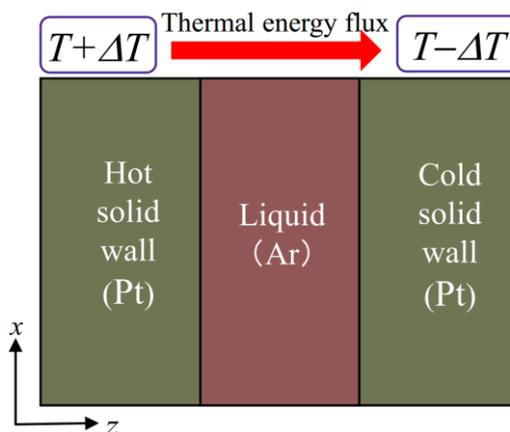
Fig. 1 Simulation system of heat transfer over liquid films between solid walls
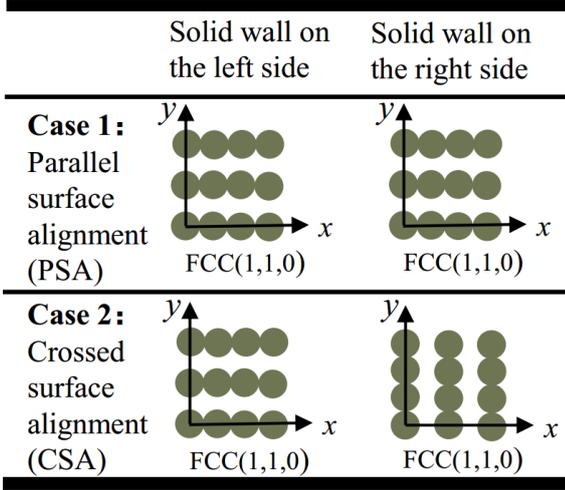
Fig. 2 Solid surfaces used in the simulation

configuration (CSA) where the right solid wall is rotated around z axis by 90°.

In the present simulation, the interaction among solid molecules is modeled by Morse potential given by (8):

$$\Phi(r_{ij}) = D\left[e^{-2\alpha(r_{ij}-r_0)} - 2e^{-\alpha(r_{ij}-r_0)}\right], \qquad (1)$$

where $D = 6.617\times10^{-20}$ J, $\alpha = 1.85\times10^{10}$ m, and $r_0 = 2.774\times10^{-10}$ m.

The interaction among liquid molecules is modeled by Lennard Jones(LJ) potential given by:

$$\Phi_{LJ}(r_{i,j}) = 4\varepsilon\left[\left(\frac{\sigma}{r_{ij}}\right)^{12} - \left(\frac{\sigma}{r_{ij}}\right)^{6}\right], \qquad (2)$$

where $\varepsilon = 1.6533\times10^{-21}$ J, $\sigma = 3.4236\times10^{-10}$ m.

The interaction between solid and liquid molecules is also calculated by LJ potential, where $\varepsilon = 1.0927\times10^{-21}$ J, $\sigma = 2.94\times10^{-10}$ m.

Since it is known that the pressure of the system has an effect on the result, before the data production run, the pressure in the z direction was controlled with the method proposed by Lupkowski (9). With the target pressure of 10 MPa, and the system volume was determined.

After the pressure control, the heat flux of the system was measured. In the measurement, the control surfaces which parallel to the xy plane were set. The thermal energy flux J_z passing through the control surfaces was calculated by the equation given as follows (10):

$$J_z S_{xy} = \sum_i\left[\left(\frac{1}{2}m\boldsymbol{v}_i^2 + \frac{1}{2}\sum_j\Phi_{ij}\right)/\Delta t\right]\frac{v_{i,z}}{|v_{i,z}|}$$

$$+ \frac{1}{2}\sum_i\sum_{j>i}[\boldsymbol{F}_{ij}\cdot(\boldsymbol{v}_i + \boldsymbol{v}_j)]\frac{z_{ij}}{|z_{ij}|}, \qquad (3)$$

where the first term on the right side is the energy transport by molecules passing through the inspection surfaces, and the second term is energy propagation between molecules by the intermolecular forces between a pair of molecules sandwiching the inspection surface. $\boldsymbol{F}$ and $\boldsymbol{v}$ are the intermolecular force and the molecular velocity vector, m and z are the mass of molecule and the distance in the z direction, and Φ is potential. In addition, ij are the molecules i and j. The second term was decomposed into x, y, z directions by following manner and each term was evaluated (2):

$$\boldsymbol{F}_{ij}\cdot\boldsymbol{v}_i = F_{ij,x}\cdot v_{i,x} + F_{ij,y}\cdot v_{i,y} + F_{ij,z}\cdot v_{i,z}. \qquad (4)$$

3. Simulation results

In the stage of pressure control, by adjusting the number of liquid molecules, different systems with different number of layers of the liquid molecules were obtained. Two typical number density distributions are shown in Fig. 3. As compared under the same pressure, when there is only 1 liquid layer between solid walls, the peak value of liquid density will become very high. In addition, the distance between the solid surfaces, which has not been shown here, is almost specific to the number of the layers of the liquid molecules. It increases stepwise to the number of the layers of the liquid molecules.

A typical distribution of temperature is shown in Fig. 4. Temperature jump (temperature difference between the solid and liquid over the interface) is defined on the midpoint between the surface layers of solid and liquid by extrapolation, and it is decomposed according to the degrees of freedom of molecular motion as T_x, T_y and T_z. In the case displayed here, there is a large temperature jump at the solid-liquid interface. In the case, the temperature jump in x direction is the largest. When there is only 1 layer in the liquid film, its distribution is very special, although is not shown here.

The thermal resistance between the solid surfaces on both sides R_{total} consists of 2 parts: the thermal resistance of liquid R_{liquid}, and the interfacial thermal resistance R_i. Furthermore, R_i consists of the interfacial thermal resistance of the left side $R_{i,l}$ and the interfacial thermal resistance of the right side $R_{i,r}$.

The relationship between R_{liquid} and the distance between solid surfaces is shown in Fig. 5. For the cases where there is only 1 layer in the liquid film, the thermal resistance within the liquid is treated as zero. Obviously, R_{liquid}
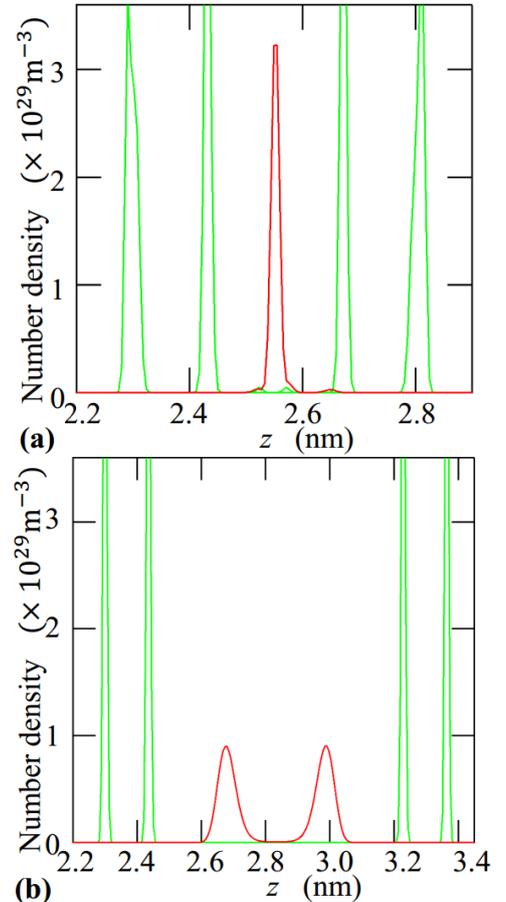
Fig. 3 The number density distribution of solid and liquid molecules (The green lines represent solid molecules, and the red lines represent liquid molecules).
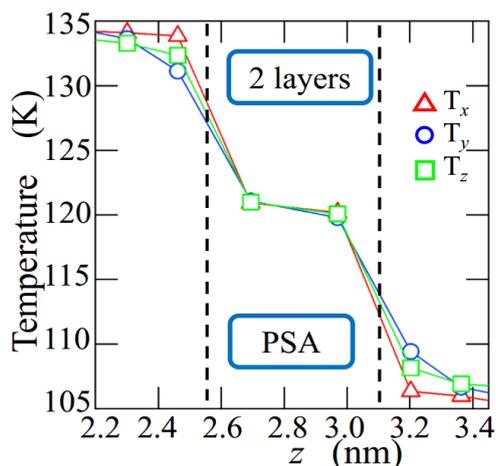
Fig. 4 Temperature distributions (The black dotted lines represent the solid-liquid interfaces).
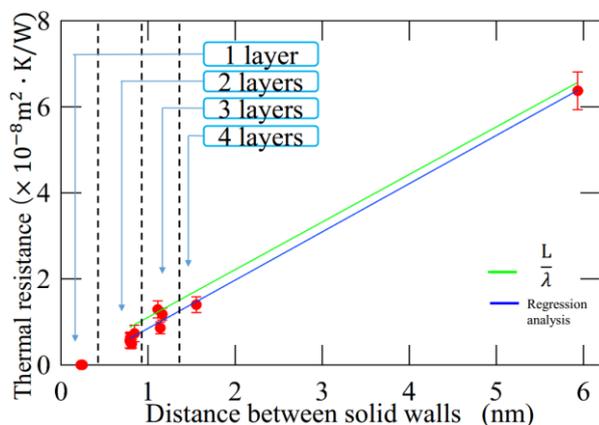
Fig. 5 Relationship between the thermal resistance of liquid and the distance between solid surfaces.

is generally proportional to the distance between the walls and the value is close to the well-known macroscopic thermal resistance of materials according to their thermal conductivity. As for The solid-liquid interfacial thermal resistance, which is not shown here, it shows a response to number of layers of liquid molecules and density of the layers in a complicated manner in the cases with two or more liquid layers. It is extremely low in the cases with one liquid layer, mechanism of which is being examined now.

The results of CSA, which are not shown here, shows that the heat flux is degraded by the asymmetry introduced to the system, and the mechanism is clarified by the decomposition of heat flux into x, y and z components.

4. Summary

Molecular dynamics simulations of heat transfer over an ultra-thin liquid film between solid walls have been performed. Surface configurations of the solid, the symmetry of the system introduced by the solid wall, and amount of the liquid between the solid wall were the parameters of the system and their influences on heat transfer and interfacial thermal resistance were examined.

It was found that the thermal resistance at the solid-liquid interface is significantly influenced by the amount of the liquid between the solid surface and the symmetry of the system introduced by the molecular alignment of the solid surfaces. To obtain detailed view of the phenomena in real applications of TIM and solid materials, behavior of complex liquid molecules should be taken into account, which is our next work. The results of these studies will lead not only to demonstration of the physical phenomena in such molecular thermofluid system but also to finding some theoretical references for the design of TIM and heat dissipation system.

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