ENERGY AND MOMENTUM TRANSFER IN AN ULTRA-THIN LIQUID FILM UNDER SHEAR BETWEEN SOLID SURFACES

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INTRODUCTION

Liquid in the vicinity of solid surface is featured by a structure consisting of several layers of molecules, which are captured by potential field of solid molecules. At the solid-liquid interface, a temperature jump resulted by a kind of mismatch in molecular motion between solid and liquid has been observed in case heat flux exists at this solid-liquid interface [1,2]. On the other hand, characteristics of thermal energy transfer in the solid-like liquid region close to the solid surface, which are expected to be different from bulk liquid phase, has not been clarified up to now.

This paper presents an analysis of thermal energy and momentum transfer in such solid-like liquid region and at a solid-liquid interface based on molecular dynamics (MD) simulations. Especially, a liquid film of several nanometer thickness under shear between two parallel solid surfaces is investigated. In this case, which has a direct relation to lubrication, momentum transfers between two solid surfaces through the solid-like liquid film and significant heating due to the shear is resulted in the liquid film, which causes heat conduction from the liquid film toward the solid walls. Although some simulations for such system have been reported in literature [3], characteristics and mechanism of the phenomena in the molecular scale, including viscous heating and its dissipation, are not entirely clear. It is expected that the characteristics of thermal energy and momentum transfer in the liquid film are affected by the solid-like structure and biased from the prediction by the continuum theory, which will be clarified in the present study.

SIMULATION METHOD

A MD simulation of thin liquid film between two parallel solid walls has been performed with a system shown in Fig.1. Two atomically structured solid walls were placed in a rectangular cell at each end along the z axis. The space between the solid walls was filled with liquid molecules. Periodic boundary conditions were applied in the x and y directions. In the present study, which investigates basic characteristics common to all the solid-liquid systems, the liquid was assumed as a simple liquid for simplicity and the Lennard-Jones (12-6) potential with parameters for argon was applied for interaction among liquid molecules. The structure of the solid walls was identical to those of the author's previous study [2]. The solid walls had a FCC structure and their (1,1,1) surface contacted the liquid. Each wall had three layers of solid molecules modeled by the harmonic potential with parameters for platinum. Each layer had 20×20 molecules in the x and y directions. Outside the three layers of solid molecules, the phantom molecules [4,5] were installed

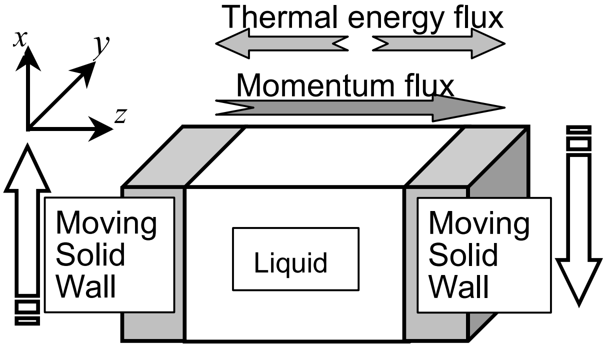

Figure 1 Simulation system

to model a semi-infinite solid having a constant temperature. The temperature of the solid walls was kept constant at 90 K. The interaction between a solid molecule and a liquid molecule was given also by the LJ potential. Dimensions of the simulation cell along the *x*- and *y*-axes were 55.4 Å and 48.0 Å, respectively, which were determined by the alignment of solid molecules. The dimension in the *z* direction, which was defined here as the distance between the equilibrium locations of the two solid surfaces, was determined to be 34.5 Å. The resulted liquid pressure was below 1 MPa, which is sufficiently low not to influence the structure of the liquid phase. Total numbers of molecules were 1620 for the liquid and 2400 for the solid. The simulation was performed for a hundred thousand million steps with a time step of 2.5fs after an equilibration run of one million steps.

The solid wall at each end of the cell moved in the *x* direction with a velocity having the same magnitude, 100 m/s, and in opposite directions. Then, a Couette-type flow was induced in the liquid. This sheared liquid film was analyzed and the results are reported here.

SIMULATION RESULTS

Figure 2 shows number density distribution of solid and liquid molecules. Some layers of liquid molecules are formed in the vicinity of solid surfaces. The layered structure in the liquid decays

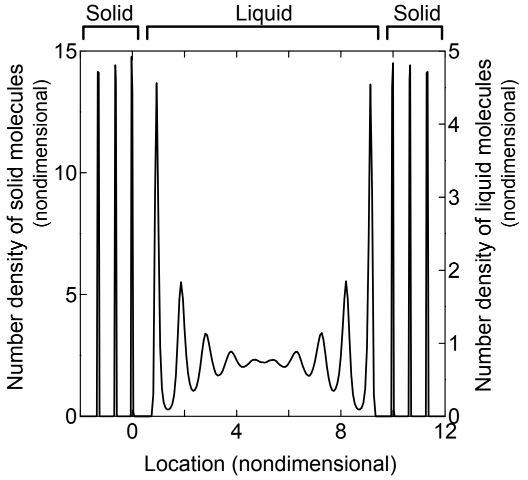

Figure 2 Number density distribution in the solid walls and the liquid layer between them

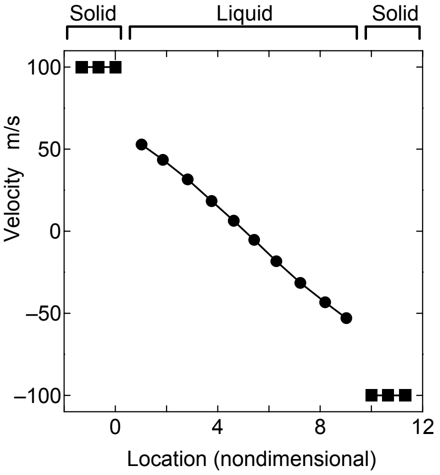

Figure 3 Velocity distribution in the system

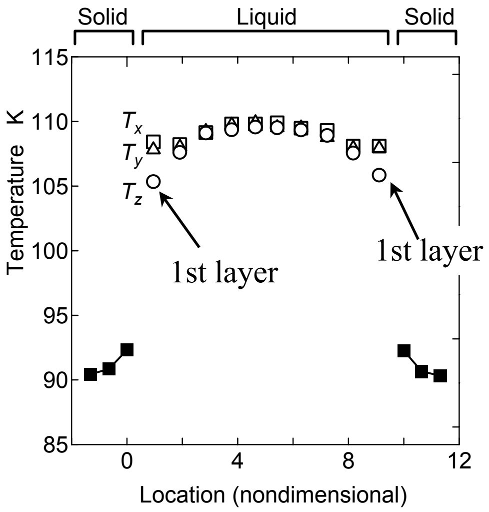

Figure 4 Steady-state temperature distribution in the system

rapidly as location is away from the solid surface. Figure 3 shows distribution of velocity in the z direction, in which left solid wall moves upward and right one downward. Average value over each layer of liquid molecules is plotted by a dot in the figure. While a linear distribution is formed in the liquid, there is a clear velocity jump (slip) at each liquid-solid interface. Magnitude of this jump is approximately 40 m/s in the present case and increases linearly as shear rate of liquid increases.

Figure 4 shows temperature distribution in the liquid film and solid walls. Temperature corresponding to each degree of freedom of molecular motion, which is determined by kinetic energy of molecules for each degree of freedom, is plotted in the figure. Again the plotted temperature is averaged over each layer of molecules. Viscous heating occurs in the sheared liquid film and thermal energy flows from the center of the liquid region to the solid walls. A remarkable feature in this temperature distribution is the difference in the three temperatures in the layer of liquid molecules contacting the solid wall (the first layer). The temperature in the x direction is the highest, which suggests that the first liquid layer is under a highly non-equilibrium condition that kinetic energy is given from the moving solid wall and it has not yet been partitioned equally to other degree of freedom. Balance of energy flux in this highly sheared solid-like liquid structure and mechanism of viscous heating in that structure are now investigated.

REFERENCES

1. S. Maruyama and T. Kimura, A study on thermal resistance over a solid-liquid Interface by the molecular dynamics method, *Thermal Science and Engineering*, vol. 7, no. 1, pp. 63-68, 1999.
2. T. Ohara and D. Suzuki, Intermolecular energy transfer at a solid-liquid interface, *Microscale Thermophysical Engineering*, vol. 4, no. 3, pp. 189-196, 2000.
3. R. Khare et al., Molecular simulation and continuum mechanics study of simple fluids in non-isothermal planar couette flows, *J. Chem. Phys.*, vol. 107, no. 7, pp. 2589-2596, 1997 and references therein.
4. J. C. Tully, Dynamics of gas-surface interactions: 3D generalized Langevin model applied to fcc and bcc surfaces, *J. Chem. Phys.*, vol. 73, pp. 1975-1985, 1980.
5. J. Blomer and A. E. Beylich, MD-simulation of inelastic molecular collision with condensed matter surfaces, *Proc. Int. Symp. on Rarefied Gas Dynamics*, pp. 392-397, 1996.