

# 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. 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

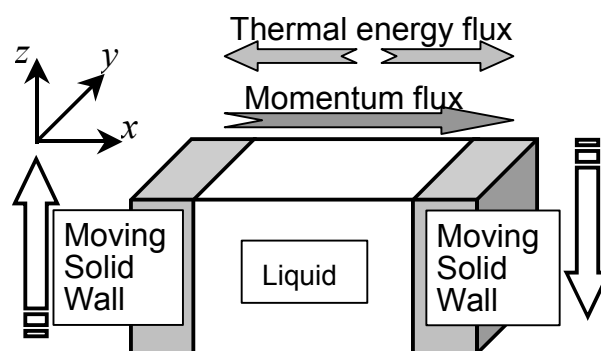


Figure 1 Simulation system

each end along the  $z$  axis. The space between the solid walls was filled with liquid molecules. The temperature of the solid walls was kept constant at 90 K. Periodic boundary conditions were applied in the  $x$  and  $y$  directions. For the liquid molecules, the Lennard-Jones (12-6) potential was applied with parameters for argon. 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 a harmonic potential with parameters for platinum. Each layer had  $20 \times 20$  molecules in the  $x$  and  $y$  directions. Outside the three layers of solid molecules, the phantom molecules [3,4] were installed to model a semi-infinite solid having a constant temperature. The walls were kept at 90K. 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 two million steps.

The solid wall at each end of the cell moved in the  $z$  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 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

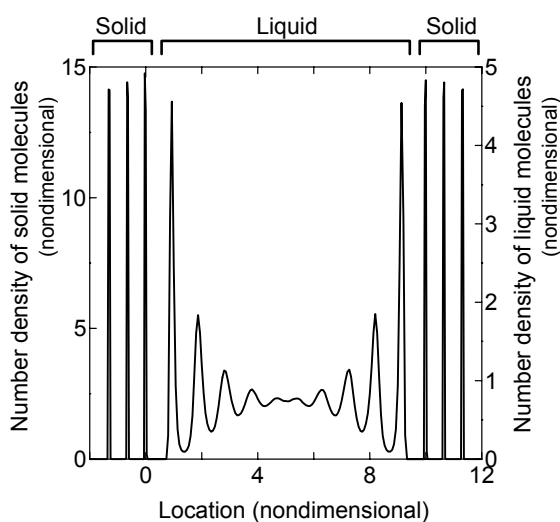


Figure 2 Number density distribution in the solid walls and the liquid layer between them

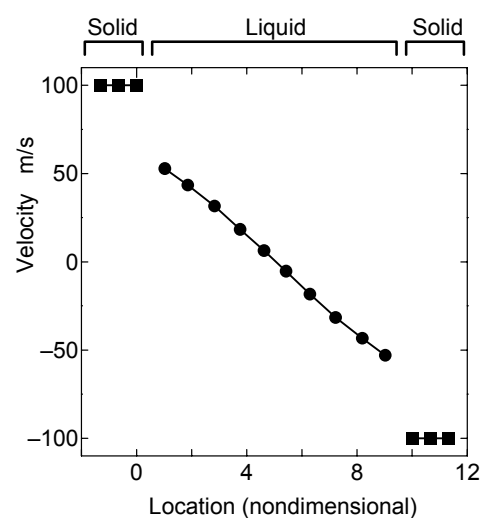


Figure 3 Velocity distribution in the system

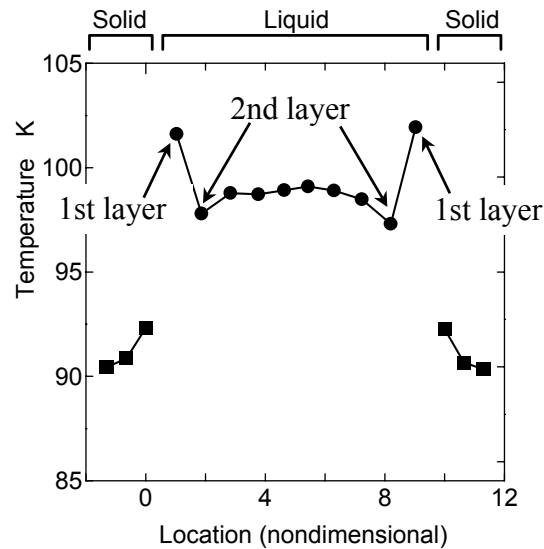


Figure 4 Steady-state temperature distribution in the system

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 liquid film and solid walls. 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 local peak in the layer of liquid molecules contacting the solid wall (the first layer). Such local peak cannot be observed in macroscopic continuum at steady state. In fact, thermal energy flows from the second layer of liquid molecules to the first layer, in spite that temperature of the first layer is higher than that of the second layer. This suggests that thermal energy flow in this molecular liquid is not governed by the average temperature of the molecular layers. Balance of thermal energy flux in this highly sheared solid-like liquid structure and mechanism of viscous heating in that structure are now investigated.

## REFERENCES

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