

# Momentum and energy transfer characteristics in nanoscale Couette flow and at solid-liquid boundaries

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## ABSTRACT

A Couette flow in an ultra-thin liquid film confined between solid plates has been studied by molecular dynamics simulations. Water was assumed for the liquid film, to which a shear is given by the relative motion of two solid walls. Thermal energy is generated by so-called ‘viscous heating’, resulting in a heat conduction as well as a transfer of momentum in the system. It was revealed that there is little velocity slip at the boundary even the shear stress is as high as the order of  $10^2$  MPa, which is contrary to the case with monatomic or linear molecules that showed a large velocity jump.

Key Words: Nanoscale flow, Solid-liquid boundary, Energy transfer, Momentum transfer

## 1. Introduction

Analysis of solid-liquid interfaces to clarify their characteristics of thermal energy transfer and momentum transfer is important not only for basic research on nonequilibrium microscopic thermal and fluid phenomena, but also for practical applications, such as lubrication control under extreme conditions, fabrication of low friction surfaces, and the development of new lubricants.

We have been working on molecular dynamics simulation of sheared liquid films confined by solid surfaces, where both energy and momentum transfer are present simultaneously. Monatomic and linear molecules were employed as liquid and various interesting findings were reported by the previous study.<sup>1,2</sup> In the present report, liquid water film is analyzed and the characteristics of the energy and momentum transfer at the solid-liquid interfaces are examined by employing four different solid surfaces, whose configuration have been found to have great influences on those characteristics in cases of monatomic and diatomic liquid films.<sup>3</sup>

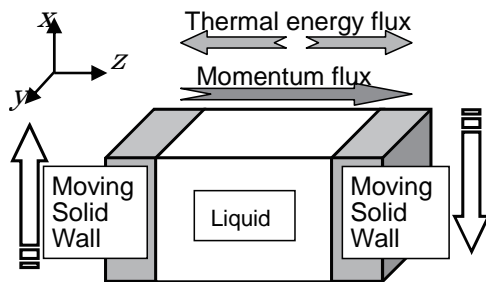


Fig. 1 Simulation system

## 2. Molecular Dynamics Simulation

The simulation system employed in the present study is shown in Fig. 1. The system consists of two parallel solid walls and a liquid film between them. The solid walls at each end of the cell moved in the  $x$  direction with velocities of the same magnitude and in opposite directions. As a result, the momentum flux is generated in the liquid film, liquid temperature being raised by the viscous heating, and the generated thermal energy is transferred to the solid walls. The velocity of solid wall was selected to be  $\pm 100$  m/s. The thickness of the liquid film was set to

Table 1 Solid walls employed in the simulation

	Surface molecular number density	Surface crystal plane	Surface molecular configuration	Numbers of atoms in $x$ and $y$ directions
A	Largest	FCC (1,1,1)		20×20
B	↑ ↓	FCC (1,0,0)		20×17
C	Small	FCC (1,1,0)		20×12
D				12×20

be  $5\sigma_{OO}$  (a few nanometer). Periodic boundary conditions were applied in the  $x$  and  $y$  directions.

The four solid walls used in the simulation are shown in Table 1. Interaction between the solid molecules is modeled by the harmonic potential with parameters for platinum. The spring constant, equilibrium distance, and mass of molecules are 46.8 N/m,  $2.77 \times 10^{-10}$  m, and  $3.24 \times 10^{-25}$  kg, respectively. Outside the solid molecules, the phantom molecules<sup>4</sup> are installed to model a semi-infinite solid at a constant temperature of 300 K.

For water, the SPC/E potential, which is the most successful potential model that reproduces various thermophysical properties and equation of state of real water, was applied. For the potential between a water molecule and a solid molecule, the work of Kimura and Maruyama<sup>5</sup> has guided us and the SH potential<sup>6</sup> was applied.

### 3. Simulation Results

For the case with wall B, the macroscopic flow distribution and the temperature distribution are shown in Fig. 2. A Couette-like flow is observed in the liquid film and there is almost no slip at the solid-liquid interfaces, which is contrast to the fact

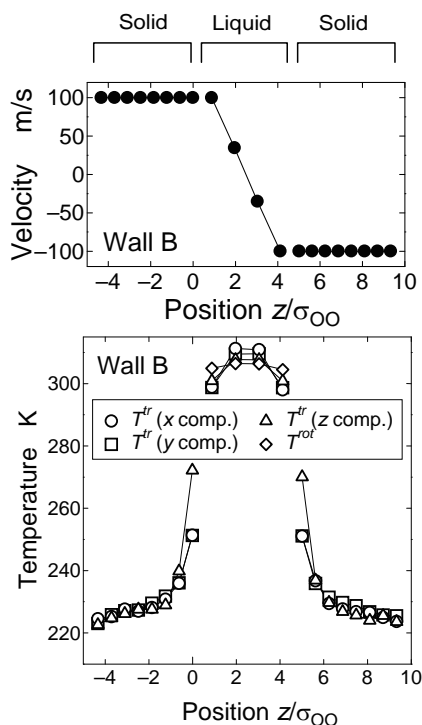


Fig. 2 Velocity (upper panel) and temperature (lower panel) distribution in liquid water film and platinum solid walls. The temperature shown here corresponds to kinetic energy of molecules in each degree of freedom.

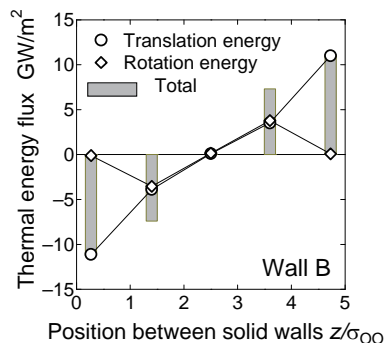


Fig. 3 Thermal energy flux in the liquid water film and at the solid-liquid interfaces for the case of solid wall B: Contribution of translational energy transfer and rotational energy transfer.

that large velocity jump was observed in most cases of linear molecules. The temperature difference between  $T^r$  and  $T^{rot}$  is remarkable, which shows that the system is in nonequilibrium state.

Thermal energy flux measured at the control surfaces in the film and at solid-liquid interfaces is plotted in Fig. 3. In bulk liquid, the contribution of the rotational motion to the total thermal energy flux is assumed to be around 70%.<sup>7</sup> Strongly influenced by the solid wall, the contribution observed in the present simulation is reduced to 60-40% in the center region of the liquid film, while no contribution is made at the solid-liquid interfaces.

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