

# Influences of velocity slip on the thermal energy transfer at the solid-liquid (S-L) interfaces

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**ABSTRACT** – Thermal energy transfer at solid-liquid (S-L) interfaces play a significant role in determining the performance of lubrication and coating systems. As such, the objective of this study is to investigate the influences of velocity slip at S-L interfaces which is a common application in lubrication and coating systems on the thermal energy transfer at the interfaces. The thermal energy transfer at the S-L interfaces will be evaluated based on thermal boundary resistance (TBR) at the interfaces. It is found that the surface structure of solid influences the velocity slip at the S-L interfaces. The result shows that the velocity slip is correlated with the TBR at the interfaces. Based on the result, it is concluded that the surface structure of solid significantly influence the velocity slip and TBR at the S-L interfaces. Rough surfaces of solid will enhance the chance of thermal energy transfer at the S-L interfaces.

## 1. INTRODUCTION

In lubrication and coating systems, researchers often need to deal with thermal energy transfer at the solid-liquid (S-L) interfaces [1]. In the past there are a significant number of studies that investigate the thermal energy transfer at the S-L interfaces by using thermal boundary resistance (TBR) at the interfaces as a reference. The TBR at the S-L interfaces is contributed by the molecular interaction between the solid and liquid [2]–[6]. Based on MD simulations, it is revealed that the TBR at the S-L interfaces is governed by the wettability of the interfaces or the hydrophilic level of the surfaces [7]–[9]. As such, it is understood that the knowledge of TBR at the S-L interfaces is an important phenomenon that needed complete understanding to design and optimize systems.

Although in the past there are quite sums of publications [2]–[9] that look into the TBR at the S-L interfaces, the influences of the slip length due to the surface structure is less numerous. Therefore, the objective of this study is to investigate the influences of the velocity slip on the TBR at the S-L interfaces. The influences of the velocity slip at the S-L interfaces will be evaluated based on the surface structure of solid.

## 2. SIMULATION SYSTEM AND MODEL

### 2.1 The simulation model

The present simulation system consists of liquid confined between two parallel solid walls as shown in **Figure 2.1**. The two parallel solid walls consist of three types of face-centered cubic (FCC) crystal planes with the surfaces of (100), (110) and (111) facing the liquid on both sides of the simulation system. The surface structure of (100), (110) and (111) crystal planes is shown in Figure 2.2. The liquid confined between the two parallel solid walls consists of a simple liquid. The contacts interfaces of solid and liquid as shown as per Figure 2.1 is referred here as the S-L interfaces. The size of the simulation system for  $L_x$ ,  $L_y$  and  $L_z$  are approximately  $40 \times 40 \times 120$  Å, respectively. The  $L_x$ ,  $L_y$  and  $L_z$  referred to the length of the simulation system in  $x$ -,  $y$ - and  $z$ -axis. The distance between the two parallel solid walls where the simple liquid is filled is approximately 60 Å.

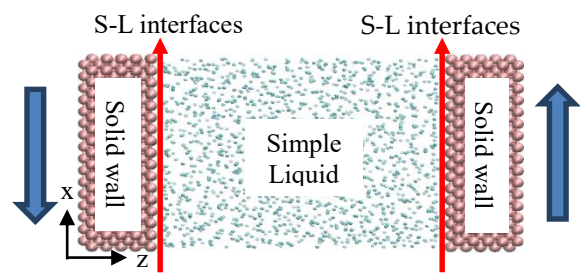


Figure 2.1 Liquid confined between two parallel solid walls

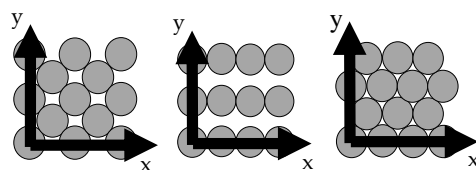


Figure 2.2 Liquid confined between two parallel solid walls

## 2.2 Potential functions

In this study the simple liquid and the two parallel solid walls is modelled by using potential functions. The simple liquid is modelled by using Lennard Jones 12-6 (LJ) with liquid methane interaction force where the details can be found elsewhere [10]. The same potential functions have been utilized in the authors previous report [11], [12]. As for the two parallel solid walls, the Morse potential have been utilized with Gold interaction force. The details of the potential functions is given in ref [5], [13]. The interactions between solid and liquid molecules is calculated using LJ potentials and the interaction parameter is calculated by using Lorent-Bertholet combining rules which is given in ref [14]. In this study the all of the potential functions is cut beyond the radius of 12.0 Å. A periodic boundary condition is applied in the  $x$ - and  $y$ -axes, whereas  $z$ -axis the solid atoms is restricted at its on lattice.

## 2.3 Simulation details

Reversible references propagator algorithm (r-RESPA) have been utilized for the time integration time steps [15], [16]. At first the temperature of the simulation systems was raised slowly to the targeted temperature at  $0.7 T_c$  (critical temperature) of the liquid for 1 to 2 million time steps. Then the simulation systems were equilibrated for 3 to 4 million time steps until a uniform temperature is acquired throughout the simulation systems. Then, an opposite directions of motion with 100 m/s of velocity is applied to the two parallel solid walls as shown in Figure 2.1. Such setup is run for 5 to 8 million time steps. The motion creates shears to the liquid and flow energy. The flow energy is converted into thermal energy and is transferred via heat conduction to the two parallel solid walls. In this study since the (110) crystal plane have asymmetrical surface structure two directions of shears is applied to the system in  $x$ - and  $y$ -directions. Then data acquisition time steps were run for 10 -20 million time steps.

## 3. RESULTS AND DISCUSSION

### 3.1 Velocity distributions

Firstly, the velocity distributions of the simulation system are measured. Figure 3.1 shows the velocity distributions for (100), (110) $x$ , (110) $y$  and (111) crystal planes. In the figure, the (110) $x$  and (110) $y$ , is referred to the (110) sheared in  $x$ - and  $y$ -directions, respectively.

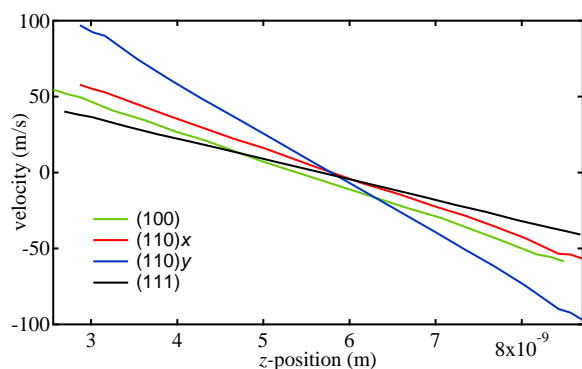


Figure 3.1 Velocity distributions of (100), (110) $x$ , (110) $y$  and (111)

Based on the velocity distributions it is found that there exists velocity slip at the S-L interfaces for (100), (110) $x$  and (111) crystal planes but none is observed for (110) $y$  crystal planes. The velocity slip is defined here as the velocity discontinuity at the S-L interfaces. The order of the velocity slip is (111), (100) (110) $x$  and (110) $y$  start from the highest to the lowest. Based on Figure 2.2, it is understood that (110) $y$  has the highest roughness of surfaces as compared to (100), (111) and (110) $x$  crystal planes. As such, the results suggest that for the case of (110) $y$  crystal plane the surface structure traps liquid molecules near the S-L interfaces and eliminate the velocity slips at the S-L interfaces.

### 3.2 Thermal boundary resistance

The details regarding the thermal boundary resistance (TBR) can be found in ref [11], [14], [17]. Table 3.1 shows the TBR for the cases of (100), (110) $x$ , (110) $y$  and (111) crystal planes. Based on the table, the TBR is in the order of (111), (100), (110) $x$ , and (110) $y$  start from the highest to the lowest. The same order can be observed in the velocity slip. As such, the results suggest that the velocity slip is correlated with the TBR at the S-L interfaces. For the case of (110) $y$ , the surface structure traps liquid molecules at the vicinity of S-L interfaces that increase the chance of thermal energy transfer at the S-L interfaces. As for the case of (111) since the surface structure is smoother as compared to other cases of crystal planes. As such, the liquid molecules easily slipped that reduces the chance of thermal energy transfer at the S-L interfaces for the case of (111) crystal plane.

Table 3.1 Thermal boundary resistance for (100), (110) $x$ , (110) $y$  and (111) crystal planes

Crystal Plane	TBR ( $\text{m}^2\text{K}/\text{W} \times 10^{-6}$ )
100	0.1503
110 $x$	0.1288
110 $y$	0.0963
111	0.1551

## 4. SUMMARY

This study examined the thermal energy transfer at S-L interfaces by considering the influences of velocity slip at the interfaces. It is found that, rough surfaces of solid enhance the thermal energy transfer at the S-L interfaces and smooth surface of solid reduces the thermal energy transfer. The rough surface of solid traps liquid molecules at the S-L interfaces that enhance the thermal energy transfer. The current results suggest that the velocity slip at the S-L interfaces influences significantly the thermal energy transfer at the interfaces.

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