Molecular Dynamics Simulation of Nanoscale Tribology

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Abstract

A slider-slab sliding model for hard-to-soft and soft-to-soft sliding systems with abrasive and non-abrasive wear conditions is used to investigate atomic-scale friction. The molecular dynamics simulation uses the Morse potential to calculate interatomic forces between atoms. Separation distance between the slider and the slab is changed to simulate repulsive and attractive interactive force fields exerted on interface between two sliding components. Effects of the interaction potential parameters on the sliding friction are investigated. Frictional force, normal force and temperature rise of the slider and the slab are calculated during sliding. Comparison of the hard-to-soft and the soft-to-soft sliding system are carried out and shows different tribological phenomena.

Key Words: Molecular Dynamics, Morse Potential, Friction, Abrasive Wear

1. Introduction

Traditionally, friction in physical systems is studied using macroscopic experiments and theories that consider material bulk properties. However, when the size of a physical system is lower than a characteristic dimension, the macroscopic viewpoint may not be applied. In such physical systems, the interactive forces between atoms govern mechanical behaviors [1]. Theoretically, molecular dynamics (MD) simulation is a good approach for studies of microscopic physical systems if an accurate potential function is selected to calculate interactive forces between atoms [2]. Many MD studies for micromachinings have been conducted [3]. In these studies, a repulsive force field exerted on the interface between a tool and a workpiece was generally used during a cutting process. For MD simulations, the interaction potential depends on materials of two sliding components and interfacial conditions. Therefore, there are studies to investigate effects of various Morse potential used as an interaction potential on chip formation for atomic-scale cutting process [4]. Although investigations of atomic-scale friction and wear by MD simulations have been carried out under different sliding conditions, a more complete and systematic investigation that combines interaction potentials, interactive force fields exerted on interface and wear conditions simultaneously for atomic-scale friction is still needed.

In this study, a slider-slab model was established. Hard-to-soft and soft-to-soft sliding systems (i.e. abrasive and nonabrasive wear conditions) were simulated by MD simulation in slider and slab. The Morse poten-

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tial function was used to calculate interactive forces between atoms.

2. Molecular Dynamics

Figure 1 shows the slider-slab sliding model using in this study. Atomic arrangement is all on the (111) crystal plane of face-centered-cubic (fcc) lattice materials. Three kinds of atoms are used in this model: rigid, thermostat and Newtonian atoms. The rigid atoms form the boundaries of the sliding system and cannot be moved by the interactive forces from surrounding atoms. In order to avoid numerical divergences during sliding simulation, the initial positions of atoms are arranged according to their crystal lattice [5]. The model is composed of a slab of 4279 atoms and a slider of 974 atoms. A sliding distance of 5.252 nm (200,000 time steps) was set for each sliding simulation. An external force is applied on the rigid atoms during sliding simulation to drive the slider with a constant velocity. The pairwise Morse potential [6] used in this study is written as:

$$\phi(r_{ij}) = D\{\exp[-2\alpha(r_{ij} - r_0)] - 2\exp[-\alpha(r_{ij} - r_0)]\} \quad (1)$$

where D and r_0 correspond to dissociation energy and internuclear separation at equilibrium, respectively. In

this study, diamond (C) and copper (Cu) are chosen as hard and soft materials, respectively. Values of the parameters of the Morse potential used in this study are listed in Table 1. In this study, hard-to-soft and soft-to-soft sliding systems were investigated to study atomic-scale friction for sliding components with different hardness.

3. Results and Discussion

3.1 Normal Force and Frictional Force

Figure 2 shows variations of the normal force as the slider moves downward to the slab. Regression analysis was conducted to create the fitting curve shown in Figure 2 and the other similar results shown in this study. As seen, the normal force for separation distances under around 0.2 nm is clearly larger for the sliding system at equivalent separation distances. Here, the normal force changes with separation distance. Based on this force, the atomic interactive forces between the slider and the slab can be divided into three force fields: non-interactive, attractive, and repulsive. These interactive force fields exist in both sliding systems. In addition, Figure 3 illustrates variations of the normal force with sliding distance for different separation distances of the slider. In the current study, five separation distances (0.7 nm, 0.45 nm, 0.2 nm, −0.3 nm and −0.8 nm) are used in the sliding simulations. Based on changes of the normal force during indentation, the relationship between the interactive force field and the separation distance can be described as follows:
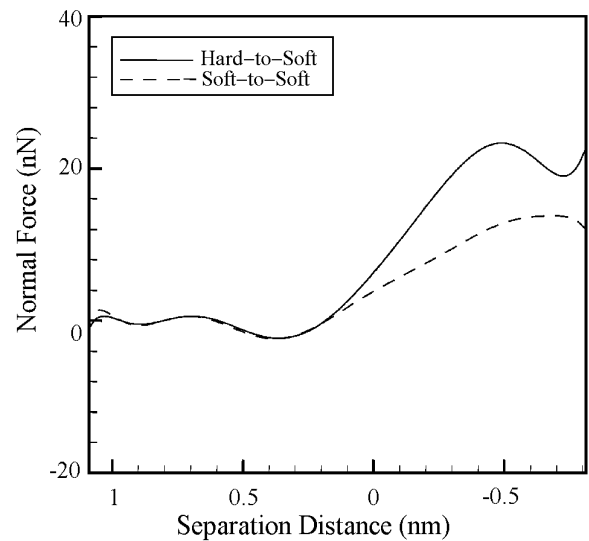
Table 1. Parameters of the Morse potential

	Slab	Slider	Slider-Slab
D (eV)	0.3429 (Soft)	2.423 (Hard)	0.18
		0.3429 (Soft)	0.26
α (nm)	13.588 (Soft)	25.55 (Hard)	17
		13.588 (Soft)	27
r_0 (nm)	0.2626 (Soft)	0.2626 (Soft)	0.22
		0.2522 (Hard)	0.34

Figure 1. The slider/slab model for MD simulation.

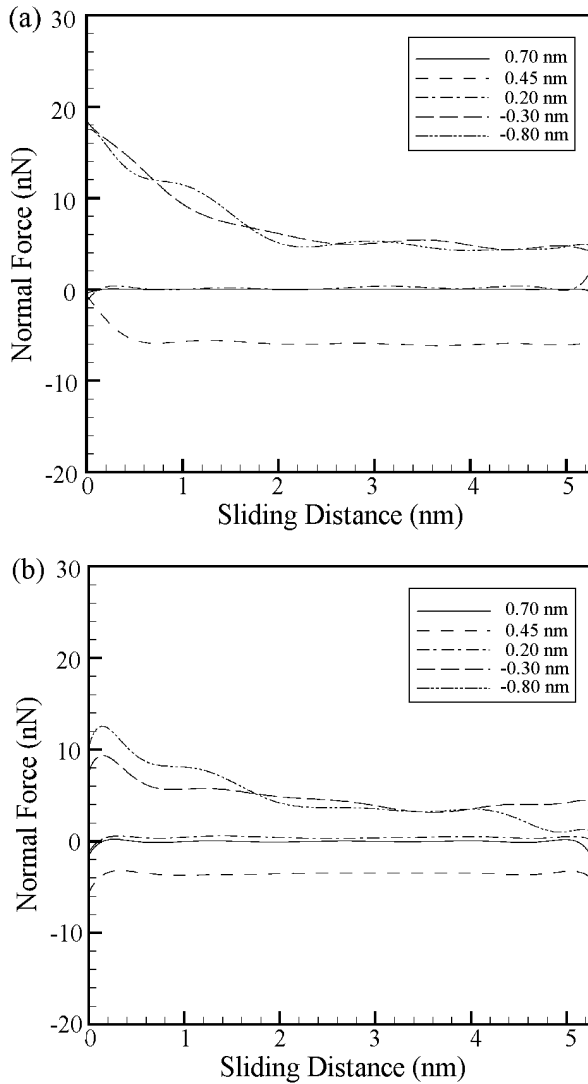**Figure 2.** Variation of normal force with separation distance.

Figure 3. Variation of normal force with sliding distance under different separation distances: (a) hard-to-soft system; (b) soft-to-soft system.

(1) Repulsive force field: 0.2 nm, −0.3 nm, and −0.8 nm.

(2) Attractive force field: 0.45 nm.

(3) Non-interactive force field: 0.7 nm.

In addition, Figures 3 and 4 show that the normal and frictional force rise steeply with increased sliding distance when the slider begins to slide on the surface of the slab under repulsive field conditions (−0.3 nm and −0.8 nm). For the hard-to-soft sliding system, the frictional force approaches zero at separation distances of 0.7 nm and 0.45 nm. For the soft-to-soft sliding system, however, the frictional force for a separation distance of 0.45 nm is larger than that for 0.7 nm, indicating that under attractive force field conditions a larger frictional force is obtained for the soft-to-soft sliding system.

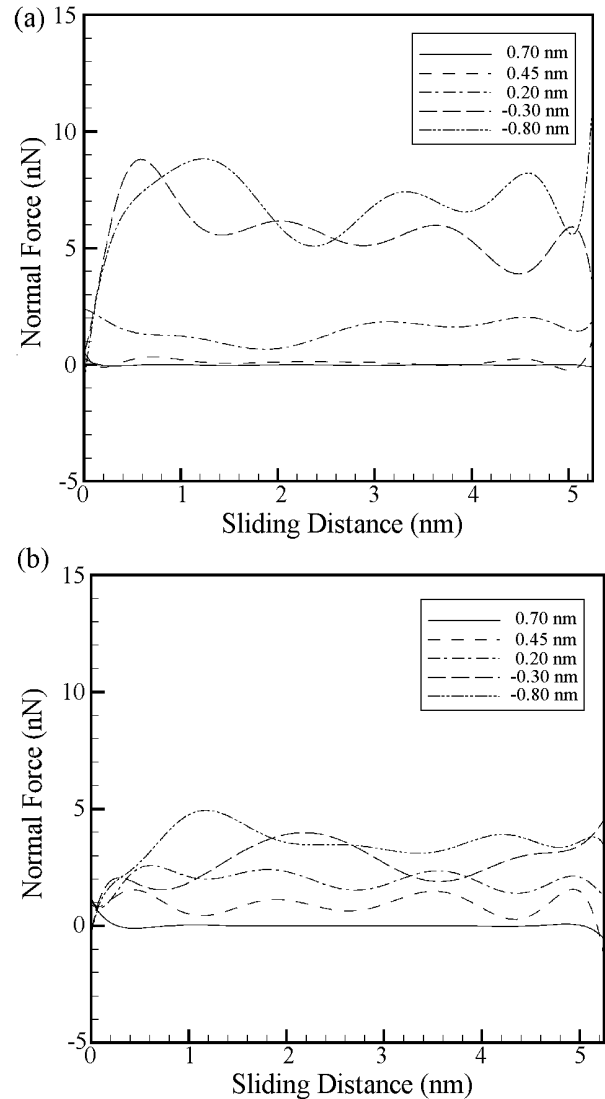As shown in Figure 4, the frictional force oscillates

Figure 4. Variation of frictional force with sliding distance under different separation distances: (a) hard-to-soft system; (b) soft-to-soft system.

during sliding. This is an indication of stick-slip conditions. The stick-slip phenomenon during atomic-scale sliding was also observed in other studies. Under the repulsive force field, at the same separation distance, and the frictional force for hard-to-soft sliding system is larger than that for the soft-to-soft sliding system. It means that an atomic-scale abrasive wear process leads to a larger frictional force when a positive normal force is produced during sliding. Under the attractive force field, there is no contact between the slider and the slab, hence the frictional force is small for both sliding systems under the attractive force field.

3.2 Temperature of the Slider/Slab Interface

Figure 5 illustrates slab temperature variations with separation distance. It indicates that at the same separation
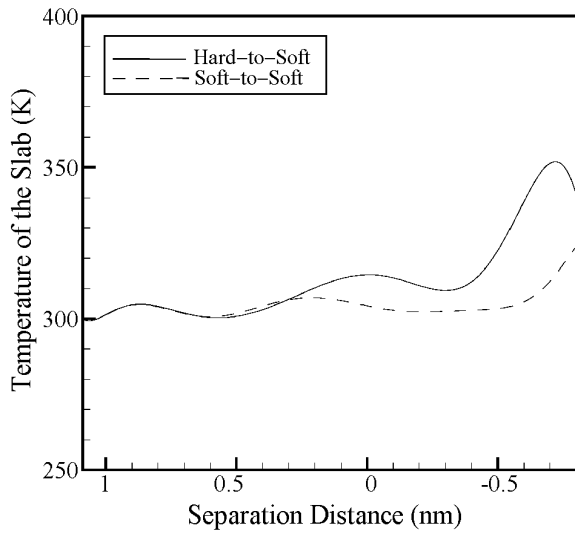
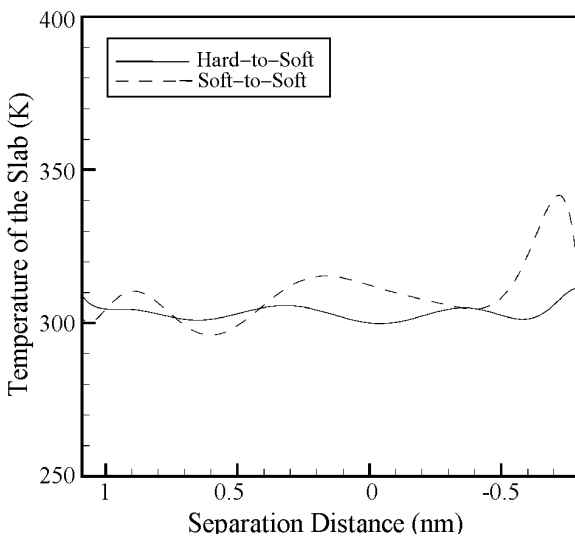**Figure 5.** Variation of slab temperature with separation distance.

Figure 6. Variation of slider temperature with separation distance.

Figure 7. Variation of slab temperature with sliding distance under different separation distances: (a) hard-to-soft system; (b) soft-to-soft system.

distance a hard-to-soft sliding system leads to a higher temperature rise of the slab. For the hard-to-soft sliding system, the temperature of the slab begins to increase when the slider enters the attractive force field. The soft-to-soft sliding system does not have such a trend. In addition, the plot of slider temperature variation with separation distance, as shown in Figure 6. It shows that during indentation the temperature of the slider remains an almost constant 300 K for the hard-to-soft sliding system, whereas the soft-to-soft sliding system shows a significant temperature rise with large fluctuations.

Figure 7 shows slab temperature variation with sliding distance for different separation distances. The instan-
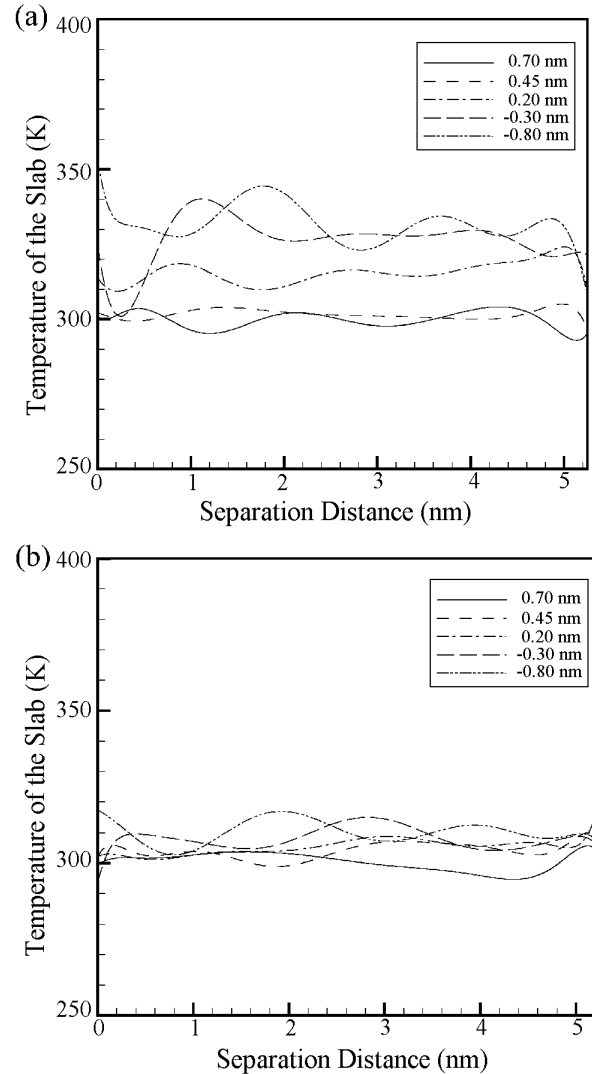
taneous temperature of the slab oscillates during sliding for both sliding systems. As shown in Figure 7(a), the hard-to-soft sliding system has an increasing slab temperature as the separation distance decreases, although the slab temperature remains at approximately 300 K (attractive force field). As shown in Figure 7(b), effects of the separation distance on the temperature rise of the slab are insignificant for the soft-to-soft sliding system.

4. Conclusions

This study establishes hard-to-soft and soft-to-soft sliding systems to simulate abrasive and non-abrasive sliding conditions. Separation distance between two sliding components was changed to simulate different

interactive force fields between the two sliding components. When we increase the separation distance between the slider and the slab, the deformation and the wear in the sliding components are observed to be greater under the repulsive force field for both sliding systems. Under the attractive force field, the attractive normal force and the frictional force are not large enough to result in a permanent deformation in the sliding components except for large dissociation energy at the interface. The sliding component with larger dissociation energy undergoes lower temperature rise because atoms of such components possess a larger bonding force and absorb only reluctantly the kinetic energy from external energies during sliding. Also, it is difficult to increase the total kinetic energy of atoms when the atomic motions are restricted by fixed boundary geometrical constraints. Therefore, the sliding components with more fixed boundary constraints undergo a lower temperature rise.

A larger dissociation energy (D) for the slider/slab interface leads to larger frictional force, temperature rise, deformation and the wear during sliding for both sliding systems. The effect of Morse potential parameter α between the slider and the slab on the frictional force, normal force and the temperature rise of the sliding components is not clear, a result attributable to the small influence of parameter α on the interatomic bonding energy. Additionally, a larger parameter r_0 results in a lower temperature rise of the sliding components during sliding for both sliding systems.

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