Molecular dynamics simulation of a nanoscale sliding layer system

Min Kyu Yeo, Yong Hoon Jang

School of Mechanical Engineering, Yonsei University, 262 Seongsanno, Seodaemun-gu, Seoul 120-749, Republic of Korea

A B S T R A C T

A molecular dynamic simulation result is obtained for a nanoscale sliding layer system, with an emphasis on lattice structural changes and temperature variation induced by friction. A model for a stationary and moving layer of aluminum is analyzed at different sliding speeds. The model shows that the average temperature of the molecular structure increases rapidly during the transient period. The change of the FCC structure to an amorphous structure in the stationary layer is observed when the temperature rapidly increases. The characteristics of the frictional effects are revealed by a change of the frictional force and the coefficient of friction. A negative frictional force can be seen after an abrupt drop of the frictional force at a certain sliding speed.

1. Introduction

Nanoscale sliding systems have been attracting great interest in the field of nanoscale engineering. Nanoscale devices based on the movement of molecules have been applied to energy storage, drug delivery, electronics, data storage and chemical manufacturing [1]; the development of this technology has improved these state of the art technologies. However, since the movement of molecules is unpredictable, limitations exist in analytic study and experiments regarding nanoscale sliding friction.

Early investigations on macro- and microfriction performed by Tomlinson [2] and Bowden and Tabor [3] led to the development of experimental and analytical methods for the nanoscale frictional system but it was necessarily limited to analyze the behavior of the atomistic system due to a lack of deeper understanding of that system. The limitations of the classical analytical method have been overcome by molecular dynamic (MD) simulations and estimating the behavior of an atom or molecule based on statistical mechanics.

Sliding friction takes place between two surfaces in the absence of a lubricant. Such friction is known as dry friction even if the process occurs in an ambient environment. Results from these models reveal how elastic deformation of the substrate from the sliding atoms affects energy dissipation and how the average frictional force varies with changes in the force constant of the substrate in the direction normal to the direction of motion. Specifically, MD simulations have been used to study the sliding of metal tips across a clean metal surface by numerous groups [4–14]. Harrison et al. [5] have investigated the friction of diamond surfaces in sliding contact and have explored the behavior of the frictional coefficient according to the applied load, temperature, and sliding velocity. Oligschleger and Schon [6] estimate the thermal conductivity in nanoscale heat transfer and propose the mechanism of the heat transfer between the crystal and glass structure due to friction, based on the heat transfer characteristics that they described. Through such methodologies, the MD simulation has been applied to the problem of nanoscale friction in the hard disk system [7]. Jeng et al. [8] have studied the nanotribological characteristics of the nanosliding system for two different materials. For a copper tip sliding across a copper surface [9], adhesion and wear occur when the attractive force between the atoms on the tip and the atoms at the surface becomes greater than the attractive force within the tip itself. They also provided data on how the characteristic ‘stick-slip’ friction motion can depend on the area of contact, the rate of sliding, and the sliding direction. Additional studies of stick-slip in the sliding of much larger, square-shaped metal tips across a metal surface was performed by Li et al. [14]. This study predicted that the collective elastic deformation of the surface layers in the response to sliding is the main cause of the stick-slip behavior, and stick-slip produces phonons that propagate through the surface layer. In addition, they also found a temperature distribution in the regions near the contact interface, showing that plastic deformation in the near-surface regions accounts for most of the friction heat and the temperature increase [15].

Several sliding systems in MD simulations focus on the elastic deformation of the substrate from the sliding atom affecting energy dissipation and the average frictional force varying with changes in

© 2010 Elsevier B.V. All rights reserved.
the force of the substrate. These results are caused by a low sliding speed, which does not cause severe deformation of the substrate. In a real system, however, a significant deformation of the substrate occurs due to sliding friction, even if the sliding speed is low, leading to a change of the lattice structure. This change of lattice structure is usually accompanied by severe temperature variations of the substrate.

This paper attempts to provide insight into the mechanistic features of mechanically induced lattice structural changes by focusing on the transient thermal phenomena taking place during sliding and the subsequent generation of amorphous structures and thermal changes, connected with the sliding of atomic planes. The microscopic dynamical features of sliding interfaces – the friction phenomena, the atomic structure changes induced by the mechanical deformation, and the related processes – were investigated by means of molecular dynamic (MD) simulations.

2. Simulation model

The model for the simulation performed in the present work is shown in Fig. 1 in which the lengths of x, y, and z direction are each 6.075 nm. The model is arranged with the faced centered cubic (FCC) structure. Since the model has a specific thickness in the z direction, the stationary part is considered as a geometrical layer structure.

2.1. Simulation algorithm

The simulation algorithm is divided into three main parts: the first part is to select information for the simulation model, the second is to establish the initial conditions of atoms, and the final part is to extract the new location and velocity of atoms according to the constant time interval due to the loading and boundary conditions of the model. Through these steps, the phenomenon of nanoscale friction is focused on the thermal and mechanical deformation of molecules.

2.2. Selection of initial information

An intermolecular function should be specified for the MD simulation because it is needed to calculate the intermolecular force. The interactions between atoms are modeled using the potential of the embedded-atom-method (EAM) form [16], which is currently the method of choice for metals in classical atomistic simulations. In this simulation, we select aluminum as a material for the layer in the sliding system, and the corresponding parameters of the EAM potential are chosen. We also select the lattice constant of aluminum, a key factor to determine the structure of a metal, such as the FCC structure. The lattice constant is the distance of a unit cell for the crystal molecule structure. After constructing a unit cell of a given lattice constant, the shape of the structure can be designed. We specify cells to use the linked-cell method, time interval, total simulation time, and the sliding speed of the moving layer.

The sliding speed of the moving part is specified from 10 to 100 m/s in the x-direction. The total sliding time is 50 ps and the time interval is 0.05 fs. It is important to select a proper time interval in the MD simulation because the atoms, not having absolute zero temperature, vibrate with a high speed. The time interval is selected, based on the calculation time and accuracy to search the appropriate trajectories of molecules according to time interval.

2.3. Establishment of initial and boundary conditions

After the potential of the material for the simulation model is defined, initial conditions and boundary conditions are established. The initial speed of the model is prescribed to the individual molecule using the initial temperature. This temperature is statistically converted to the speed of individual particle by the Maxwell–Boltzmann distribution. The speeds of distributed particles are all different, but the model has the equivalent kinetic energy of 300 K. We use the linked-cell method technique to approximately evaluate the forces and energy for rapidly decaying potentials. It is easy to find the atoms which can affect each other if the model is divided into cells whose lengths are close to the cutoff radius.

As shown in Fig. 1, the two main parts of the model are the moving body and the stationary layer. In the current analysis, since we focus on the thermal and mechanical deformation of the stationary layer due to sliding, the moving part does not experience the internal change in structure during the simulation, except for the rigid body translation of the moving part. To calculate the forces easily at the sliding interface, we maintain the top two layers of atoms in the stationary layer as the atoms situated within the cutoff radius. The stationary layer is divided into Newtonian atoms, thermostat atoms and fixed atoms. In the Newtonian atom, the atoms move freely due to forces between molecules, which enable us to investigate the thermal and mechanical behavior due to sliding. The thermostat atoms are maintained at a speed corresponding to a constant temperature of 300 K, although their positions are changed with speed due to the initial temperature. The fixed atom, used for fixing the position of the stationary layer, maintains the position during simulation. Periodic boundary conditions are enforced in the x and y direction of the model, as shown in Fig. 1.

2.4. Simulation procedure

In this MD simulation program, the time integration algorithm is implemented by using the velocity Verlet method. To improve the computation performance, a new neighbor list algorithm using cell decomposition is employed. For each simulation case, the model is allowed to run for $5 \times 10^4$ steps using the velocity rescaling technique [17], is then maintained for $5 \times 10^4$ steps in order to raise the average system temperature to 300 K and then is allowed to reach thermal equilibrium. The heat flux and temperature are calculated and collected for every time step. In order to investigate the frictional behavior, the temperature induced by frictional heat is statistically calculated by the kinetic energy, defined as

$$E_{avg} = \frac{1}{2} m \bar{v}^2 = \frac{3}{2} k_B T_{avg}$$

where $k_B$ is the Boltzmann constant, $m$ and $v$ are the mass and velocity of the atoms, and $T_{avg}$ is the average temperature.

3. Results and discussion

3.1. Average temperature according to sliding speed

The stationary layer of the model is investigated to measure the average temperature. Fig. 2 shows the transient average temper-
ature with respect to time according to the sliding speed, which ranges between 10 and 100 m/s.

Time evolves up to 50 ps. According to Fig. 2, an abrupt increase of temperature at a specific time, $t_c$, can be noticed. In addition, a similar trend of temperature variation occurs before an abrupt increase of temperature. As sliding speed increases, the time, $t_c$, at which an abrupt increase of temperature occurs, decreases and may converge. After an increase in temperature, the system undergoes temperature fluctuation and then reached another stable state. At the sliding speed of 10 m/s, we extend the time evolution of the analysis so that we can notice an abrupt increase of temperature, as shown in Fig. 3. However, temperature decreases and approaches the previous state after the sudden increase of temperature.

To explore the variation of temperature according to sliding speed in more detail, a series of phase portrait are shown in Fig. 4.

![Phase portrait for different sliding speeds.](image)

Fig. 4. Phase portrait for different sliding speeds.

A phase portrait, representing the two dimensional relationships between temperature $T$ and its time derivatives $\dot{T}$, is used to investigate the stability of the system. The result shows that the temperature at a sliding speed of 30 m/s converges to 500 K and temperature at sliding speeds of 100 m/s converges to above 525 K. When the sliding speed is faster, the state trajectories converge to a point, meaning that the system approaches a different state, which is stable. A more definite explanation of these features is followed by a change in the lattice structure of the system.

### 3.2. Change of lattice structure according to sliding speed

During sliding, we have found the change of atomic structure through local bond order parameters. The local bond order parameters are often used to determine crystal structures in molecular simulations. This method estimates whether the lattice structure deforms or not, based on the fact that the lattice structure of regular shapes have their own location parameters and that the difference of parameters from the crystal structure can be calculated.

We prescribe the lattice structure as an amorphous structure which deviates from the average bond order parameter of the FCC structure. Fig. 5 shows the ratio of FCC and amorphous structure at different sliding speeds.

![Ratio of FCC and amorphous structure at different sliding speeds.](image)

Fig. 5. Ratio of FCC and amorphous structure at different sliding speeds.

When the sliding speed is 30 m/s, FCC structure changes monotonically to an amorphous structure before an abrupt increase of temperature, approaching 10% of the FCC structure. After an abrupt increase of temperature, the ratio of the FCC increases up to 40% and then continuously diminishes. If the sliding speed increases to 100 m/s, the ratio change of FCC and amorphous structure occurs rapidly after the immediate engagement of sliding. Later the ratio of the FCC and amorphous structure stays at 25% and 75%, respectively. Notably, after the system undergoes an abrupt change of temperature due to friction, the lattice structure also changes significantly and then maintains a different state.
3.3. Growth rate of temperature

Fig. 6 shows the growth rate of temperature at different sliding speeds. The growth rate of temperature is defined as a slope of the exponential growth of temperature. This definition is based on the fact that a perturbation in the temperature fields can increase exponentially with time. The mathematical form of growth rate in temperature variation is

\[ T = T_0 + \Theta e^{bt} \]  

where \( T_0 \) and \( b \) represent the unperturbed temperature and the growth rate, respectively. Specifically, the growth rate of temperature in the transient regime is calculated in the region of an abrupt increase of temperature.

In Fig. 6, the growth rate is dependent on sliding speed and varies dramatically as speed increases. At low sliding speed, a linear growth rate is seen; at high speed, the growth rate increase severely. In the meantime, there is a plateau region of growth rate which can be considered as no change of growth rate. This results explicitly shows the dependence of sliding speed on growth rate of temperature of the system. The linear line is intentionally plotted to represent the linear behavior of growth rate in the low sliding speed.

3.4. Friction coefficient according to sliding speed

In order to calculate the coefficient of friction in the sliding system, the tangential force and normal force of the moving layer are obtained in the \( x \) and \( z \) coordinates, respectively. Fig. 7 shows the coefficient of friction according to several sliding speeds. This coefficient increases before an abrupt increase of temperature, compared to Fig. 2. As the sliding speed increases, the friction coefficient increases even more, and the decreasing amount of friction coefficient at an abrupt increase of temperature is larger.

For typical transient behavior of the coefficient of friction when the sliding speed is 30 m/s, the coefficient gradually increases in a similar trend of temperature in Fig. 2, before an abrupt decrease. When the coefficient of friction decreases rapidly, the system undergoes a sudden increase in temperature, after which the friction coefficient increases again. If we compare the transient variation of the friction coefficient with the change of the lattice structure, shown in Fig. 5(a), the friction coefficient follows a trend similar to that of the ratio of amorphous structures in the system.

On the other hand, the coefficient of friction occasionally reaches a negative value when the sliding speed is 100 m/s because the tangential force exhibits a negative value. Thus, the atomistic structure of the moving layer and its contacting stationary body is subjected to loading which applies to the sliding direction of a moving body. If we explore the lattice structure when a negative friction coefficient occurs, such as in Fig. 5(b), the ratio of the FCC structure decreases to 5%, which means that, conversely, the amorphous structure increases up to 95%. When the system is stabilized after an abrupt increase in temperature, the temperature converges to a constant value and the coefficient of friction is determined to be between 0.2 and 0.4.

One may argue that the predicted friction coefficients of 0.2–0.4 are relatively low for metal–metal sliding. We find that it depends on sliding speed. As shown in Fig. 7, the coefficients of friction according to sliding speed are seen. At low speed of sliding speed, the coefficient of friction ranges up to 0.8 before abrupt change of temperature. As the sliding speed increases, the coefficient of friction before the abrupt change of temperature increases too and approaches over 1.0. After the abrupt change of temperature, it decreases severely and reach the frictional coefficient of 0.4. However, the lattice structure is already changed to amorphous dominant structure. It is hard to say that the coefficient of friction for the amorphous structure may have a low value, but we may conjecture that the frictional behavior of the amorphous lattice structure is different from that of the FCC structure.

The coefficient of friction is explored just before the abrupt decrease. The value of the coefficient of friction just before the abrupt decrease is termed the “critical friction coefficient.” This denotes the frictional coefficient just prior to an abrupt change of lattice structure or an abrupt increase of temperature. Fig. 8 shows the critical frictional coefficient, which tends to vary linearly between a sliding speed of 10 and 50 m/s, according to several sliding speeds. After a sliding speed of 50 m/s, the critical friction
Fig. 7. Coefficient of friction according to different sliding speeds.
Fig. 8. Critical coefficient of friction for different sliding speeds.

speed varies little but tends to approach a constant value. If the sliding speed is fast, then the system has a large critical friction coefficient.

Some features related to the friction coefficient is explored regarding variations in the frictional force according to the sliding speed as shown in Fig. 9. When the sliding speed is 30 m/s, the frictional force increases linearly and then drops abruptly. Sorensen et al. [8] already showed a similar result for the friction force variation. For the sliding speed of 100 m/s, a similar trend can be seen but the slope of the frictional force with respect to time is steeper than the sliding speed of 30 m/s. One exception, is that a negative frictional force can be seen after an abrupt drop of the friction force at a sliding speed of 100 m/s. The negative sign of the frictional force indicates that the frictional force is applied to the direction of sliding. It is described in detail that when the rigid part is moving at a sliding speed of 100 m/s, the atoms are aligned to the direction of sliding direction. Specifically, there is no displacement to the direction of sliding direction for the bottom atoms, but the upper atoms of stationary part are displaced a little to the direction of sliding direction. As shown in Fig. 10, angle $\theta_1$ is represented to measure the tangential displacement of atoms and assumed to be clockwise direction. After some instants, the internal atoms of stationary part undergoes severe deformation of lattice structure. This interrupts the previous aligned motion of atoms. Angle $\theta_2$ is shown as a counterclockwise direction. At this instant, the frictional force is calculated as negative value.

Fig. 9. Frictional forces according to two different sliding speeds (a) 30 and (b) 100 m/s.

Fig. 10. Snapshots showing the layer at a sliding speed of 100 m/s (a) for positive coefficient of friction (b) for negative coefficient of friction.

Fig. 11. Average vertical displacement of a stationary body at a sliding speed of 100 m/s.
Finally, whether the instability at the sliding interface could induce the total instability of the system is investigated. Fig. 11 shows the average displacement in the direction of the z coordinate for the stationary body when the sliding speed is 100 m/s. According to this result, when the frictional force and the corresponding coefficient of friction undergo an abrupt decrease, the average displacement varies severely. Thus, it can be speculated that, if there is a considerable change of the friction force or friction coefficient, the atoms of the stationary body are oscillated such that the kinetic energy of the atoms increases, resulting in an increase of temperature.

4. Conclusion

We have presented MD simulation results for the nano-scale sliding layer problem with a particular focus on lattice structure changes and temperature variation induced by friction. To achieve the results for this research, the modeling of a stationary and moving layer of aluminum is performed at different sliding speeds. We have calculated forces between atoms through EAM potential modeling and integrated the force using a predictor corrector algorithm. Through the analysis performed, we have found that the average temperature of the molecular structure increases rapidly during the transient period. The rapid variation of temperature is analyzed using the growth rate of temperature. We have also shown changes of the atomic lattice structure in the stationary layer from FCC to an amorphous structure. The characteristics of frictional effect are revealed by changes in the frictional force and the coefficient of friction. A negative sign after an abrupt decrease in the force indicates that the frictional force changes to the direction of sliding.

References