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Molecular dynamics simulation of microstructure evolution and heat dissipation of nanoscale friction

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ABSTRACT

The atomic scale interfacial microstructure evolution and heat dissipation process in nanoscale friction are investigated by 3D non-equilibrium molecular dynamics (MD) simulations. Two Ni blocks of different orientations are built to simulate the self-mate friction. The embedded atom (EAM) potentials are employed in these simulations. The microstructure evolution is observed. The temperature and velocity profiles along the height direction, which is perpendicular to the direction of motion, are calculated under sliding velocity. The heat dissipation process is studied. The effect of sliding velocity is also obtained. The results show that extensive plastic deformation and temperature rise occur in the interface. Atomic scale mechanical mixing and generation of mixing layer are observed in the regions near the contact interface. The sliding velocity has great impact on temperature rise. The study of the growth dynamics of mixing layer also sheds light on the formation process of mixing layer.

1. Introduction

When two solids sliding against each other or have the tendency of relative motion, wear and energy conversion, which are the results of contacting physical resistance, will happen in the interface. These phenomena are called friction. Many studies show that during this process, energy will dissipate in a complex way, which is accompanied by numerous mechanical and physical phenomena, such as plastic deformation [1], heat generation [2], nanocrystallization and amorphization [3,4], wear and material transfer [5–7]. Among these changes are material transfer and amorphization in the interface and the formation of a mixing layer. It has been reported that the mixing layer has great impact on friction. For example, Rigney's [8] studies showed that the formation and development of the mixing layer can greatly affect both friction coefficient and average temperature. The simulation work of Hammerberg [9] also showed that a stable mixing layer helps to decrease the wear rate and friction coefficient. Meanwhile, the mixing layer is also the source of friction heat and the bridge of heat exchange. In Lacroix's [10] studies, the Reynolds number of the mixing layer were studied by a series of experiments. It showed that the mixing layer plays an important role in heat transfer in friction and melt. It is well known that friction heat generated in the interface will strongly influence the friction characteristics. It can affect coefficient of friction and structure of objects [11]. Obtaining the temperature distribution is helpful for explaining the mechanical of heat dissipation. Therefore, a complete understanding of the temperature variation, microstructure evolution and the relations between them is quite important for investigating the friction mechanism under high velocity and high pressure.

However, since the difficulty of measuring the temperature variation and in situ observation of the mixing layer formation by experimentation, the understanding of friction is not complete, especially friction under high velocity. Thus various theoretical models and numerical methods are proposed to investigate the mechanism of friction. Such as the adhesion theory by Bowden and Tabor [12], the adhesion theory indicates that when two surfaces are brought into contact, adhesion between the molecules at the touching high points of the surfaces provides the majority of the friction. When sliding begins, these high point bonds are continually broken and then reformed as new high points. The independent oscillator (IO) model proposed by Tomlinson [13], which had been widely accepted, suggests that friction is a form of energy which changes base on the relative position of atoms. It has good agreement with some experiment results. Kuciej [14–16] and his team also did a lot of work on obtaining temperature field of tribosystem by using analytical method. In their researches,

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Nomenclature

$(E_k)_{tot}$	total kinetic energy, J
$(E_k)_{cm}$	average kinetic energy, J
$(E_k)_j$	kinetic energy of an atom, J
F_i	embedding energy, J
h	thickness of mixing layer, m
i,j	atom indices
k	number of calculated atoms
k_B	Boltzmann constant, $J{\cdot}K^{-1}$
M	mass of an atom, kg
N	number of atoms
r_{ij}	distance between atoms, m
T_j	temperature, K
v_{ix}, v_{iy}, v_{iz}	velocities in different directions, $m{\cdot}s^{-1}$
$\bar{v}_x, \bar{v}_y, \bar{v}_z$	average velocities in different directions, $m{\cdot}s^{-1}$
v	sliding velocity, $m{\cdot}s^{-1}$
F	normal force, pN

Greek Symbols

ϕ_{ij}	pair potential between atom i and atom j, J
μ	dynamic viscosity, $N{\cdot}s{\cdot}m^{-2}$
ρ_i	electron density, m^{-3}
τ	shear force, N
δ_0	yield stress, N

Abbreviations

EAM	embedded atom potential
MD	molecular dynamics
FCC	face center cubic
MSD	mean square displacement
RDF	radial distribution function

the influence of pressure and thermal resistance are studied. They also developed a numerical analysis method to solve the problem of nonuniform distribution of friction heat. Nosko [17] studied the heat partition by considering two relatively moving objects as the friction source. However, most of these analyses are macroscopic, simplified and lack of details on transient variation. The complexity of friction makes it difficult to calculate the temperature distribution and the mechanism of energy dissipation. To overcome these difficulties, the molecular dynamics (MD) simulation is supposed to be an effective method. Many studies of friction were proposed by MD simulations. For example, Li et al. [2] used MD to investigate the frictional behaviors between single crystal Al, Ni and its co-crystal. In their work, the relationship between temperature rise and deformation is studied with embedded atom (EAM) potential. It is found that plastic deformation is the major source of heat dissipation. Rigney et al. [18] studied plastic deformation and microstructure evolution in Fe-Cu crystalline tribopair system by using MD simulation. The effects of sliding velocity and crystal orientation were concluded. It showed that the extent of plastic deformation increases with sliding velocity. So far most MD simulations focus on the changes of friction coefficient and local deformation [19–21]. Temperature distribution, energy dissipation and observation of the mixing layer are rarely mentioned in recent literatures. In this work, the nanoscale friction model on the nickel based coating is built. The evolution of microstructure of interface is observed. Molecular dynamical simulation conclusions of temperature and velocity profiles along the height direction both in the substrate and sliding block are presented. The influence of the temperature is studied. The growth dynamic model of mixing layer is also built to investigate the mechanism of formation of mixing layer theoretically.

2. Simulation

2.1. Geometry and boundary information

The MD simulations model performed in this work is shown in Fig. 1. This model contains two blocks of Ni atoms, which are both arranged with face center cubic (FCC) structure. Each block can be divided into three parts. Two outmost parts, three layers wide, are created for standing for the farthest region from the sliding interface. Atoms in these regions are rigid, which means all the atoms will move as a single entity.

The parts next to them are thermostatic regions. Atoms in this region are maintained at a constant temperature (300 K) to dissipate the heat generated during sliding. This is done by using Nosé-Hoover thermal bath [22]. All the other atoms in the model are Newtonian atoms, which can move freely due to force generated by the potential between atoms. Adiabatic thermal conditions are enforced on this tribopair system, meaning that no heat exchange will occur between system and environment. Periodic boundary condition is imposed in the x direction while free surface boundary conditions are enforced in y and z directions.

2.2. Establishment of initial conditions

For molecular dynamics simulations, once the system size, boundary conditions and initial velocity (normally comply with a Maxwell-Boltzmann distribution at the desired temperature) are decided, the system to be simulated is defined. The sizes of two blocks are both 7.04 nm in x direction, 7.04 nm in y direction and 2.816 nm in z direction. In the 2D model, we just concern the x direction and y direction. The total number of atoms in this model is about 53,000. To avoid interlocking of two blocks when they are pressed together, those two blocks are set to have different crystal orientation. The crystal orientation of the upper block is [100], [011], [0−11], while the crystal orientation of the lower one is [100], [010], [001]. In order to simulate dynamical friction, the rigid part of the upper block is maintained a sliding velocity v in the positive x direction, ranging from 1 to 5 Å/ps.

2.3. Interaction potentials

It is important to adopt a realistic force potential for the tribology faces in the current system, because the friction process involves plastic deformation, which depends on a proper force field. The interactions between atoms are modeled by the EAM potentials. The EAM potential is

$$U_{EAM} = \sum_{i=1}^{N}\left[F_i(\rho_i) + \frac{1}{2}\sum_{j=1,j\neq i}^{N}\phi_{ij}(r_{ij})\right] \tag{1}$$

Here, the index i and j indicate the elemental types of atoms i and j respectively, r_{ij} is the scalar distance between atoms i and j, ϕ is a pairwise interaction potential, and ρ_i is the electron density at atomic site i due to all its neighbors,

$$\rho_i = \sum_{j=1,j\neq i}^{N}\rho_j(r_{ij}) \tag{2}$$