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Molecular Dynamics Simulation of Polycrystalline Metal Under High Velocity Nanoscale Sliding

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Three-dimensional non-equilibrium molecular dynamics simulations are performed to investigate the tribological characteristics of polycrystalline Ni-Ni and Ni-Cu high-speed sliding systems. The grain size distribution, temperature profiles and heat density changes are obtained. Founded on simulation results a correlation between surface grain size and heat conduction is proposed which can help us to fully understand the mechanism of polycrystalline friction behavior and design better friction material. This interaction shows that the sizes of the grains located in the interface decrease and it increases the resistance of friction heat conduction during sliding.

1. Introduction

Friction is a complex process which is accompanied by numerous mechanical and physical phenomenon, such as plastic deformation, frictional heat generating, nanocrystallization and amorphization, wear and material transfer (Cao et al., 2015). Especially at the interface, large changes of the structure and composition of the materials subjected to sliding contact are developed. These changes can greatly influence the friction and wear. In polycrystalline friction, the changes of the size of grains in the interface can greatly affect the tribological characteristics of system. It has been reported and discussed in many numerical and experimental studies. Rigney (2009) did a lot of experiments on studying nanocrystallization occurred in the interface. They found that nanocrystalline can signally influence the mechanical properties of the friction material, such as the Young modulus and hardness. The size of the grains in polycrystal metal also has an impact on its thermal conductivity. Wang (2011) determined an empirical relationship of thermal conductivity as a function of grain size for nanocrystalline Ni films. In their opinion, the thermal conductivity of the nanocrystalline Ni films is in inverse proportion to the size of the grains. Molecular dynamics is a good method to observe the details of friction atomically and it has been used to investigate friction by many researchers. Hu et al. (2014) used MD method to investigate the nano-scale interfacial friction characteristic for different tribopair systems. Sijker et al. (2012) did much work on studying the effect of interface roughness by using MD simulation.
So far, some work had been done on the evolution of crystal grains in the interface during friction. But most of them mainly concentrated on describing its influence on changing the mechanical properties of the friction material. They did not investigate the effect on changing the thermodynamic property of material during friction. A focus on the relationship between the size of the crystal grains and the thermodynamic property of sliding material is needed to draw a whole picture of friction process which is physically reasonable and ultimately useful. Therefore, the aim of this paper is to investigate the mutual influence mechanism between the grains size and the capacity of heat transmission which is helpful for designing better gradient nanostructures friction material.
In this work, the details of the changes of crystal grains are observed. The temperature profiles and heat density distribution are also obtained. The interrelations between the size of the crystal grains in the interface and the thermal conduction are discussed. By performing these studies, the mechanism of how the crystal size changes affect the friction heat conduction can be identified. The results may offer a better understanding of the friction behaviour in polycrystal metal during high-speed sliding.

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2. Simulation model

The 3D simulation model consists of two blocks, as shown in Figure 1. Each of them is 12 x 8 x 8 nm, which consists about 60,000 Ni atoms. In order to simulate different part of sliding system, each block is divided into three parts. The outside layers are rigid atoms, on which the pressure and constant velocity are applied. Beside the rigid layers are thermostat layers. These layers are used to keep the thermal balance of friction system. The rest layers are newton layers, which can move freely due to the force between atoms. The predict boundary conditions is applied on the x and z direction. The positive sliding velocity v/2 is applied on the rigid layers in the upper block, while the negative sliding velocity – v/2 is applied on the rigid layer in the lower block. The Nose-Hover thermal bath (Karthikeyan et al., 1993) is used on the thermostat layers to remove heat generated by friction to maintain the boundary temperature of each block at 300 K. 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 modelled by the EAM potentials. In this paper, the used EAM potential parameter is developed by Foiles et al. (1986). This interatomic potential is capable of accurately molding surface energy and elastic deformation energy. The accurate reproductions of the surface energy and elastic deformation energy are most critical to this work, as it is closely related to the deformation and temperature variation on interfaces. In this study, all simulations are performed by using the code of LAMMPS (Plimpton et al., 1995), which is an open source code developed by Sandia National Laboratories. It has been widely used in molecular dynamics simulation. The visualization work is performed by using OVITO (Stukowski, 2010), which is also an open source code. In the simulations, the time step used to integrate the equations of motion is chosen as 1 fs. The contact simulation is performed by applying the pressure in y direction on the outside rigid atoms in two blocks. After a period of time for system reaching equilibrium, the sliding velocity is added to the rigid atoms to simulate friction process.

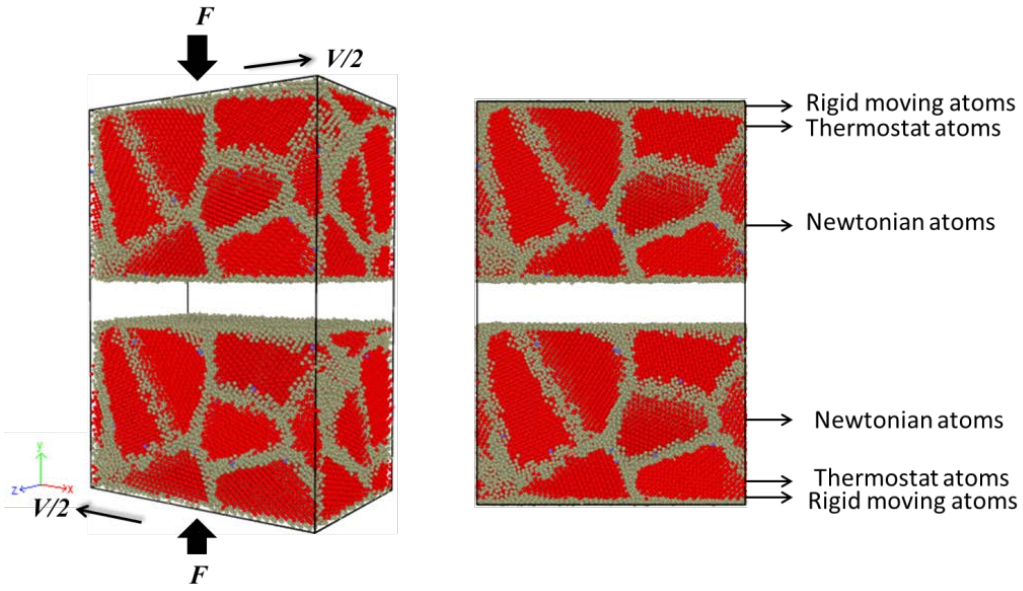

Figure 1: Schematic views of the tribopair system set-up shown in 3D and 2D. The initial information is shown in the right, and different layers are introduced in the left

3. Results and discussion

3.1 The evolution of the gains

The results of polycrystalline simulations for Ni-Ni and Ni-Cu interfaces are presented in this section. Figure 2 shows the configurations at 5, 25, 75 picosecond (ps) for the Ni - Ni simulations with the relative velocity v = 3 Å/ps, pressure p = 500 MPa. Different colours correspond to different structures. The FCC atoms are coloured green, HCP atoms are coloured red and the amorphous atoms are coloured white. At the primary stage of friction, as shown in Figure 1(a), the gains are distinct and uniform. As sliding going, a plenty of dislocations occurred in grains near the interface, shown in Figure 1(b). At longer times, it can be found that grains near the interface are teared into several smaller grains (Figure 1(c)). The sizes of grains decrease.

Figure 3 shows the snapshots of the Ni–Cu simulation. Just like in the case of Ni-Ni, the dislocations occurred near the interface. It should be noted that fragmentation of the grains is easier to happen in Cu block, which is the softer material.

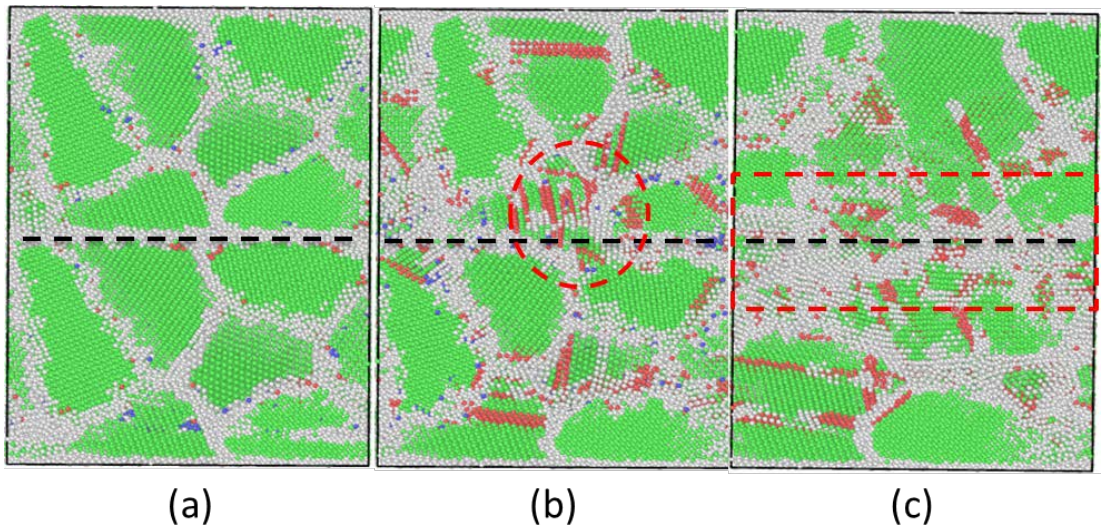

Figure 2: Still images of friction state at different sliding times for Ni-Ni friction system. (a) t = 5 ps; (b) t = 25 ps;(c) t = 75 ps. The velocity is 3 Å/ps; the pressure is 500 MPa

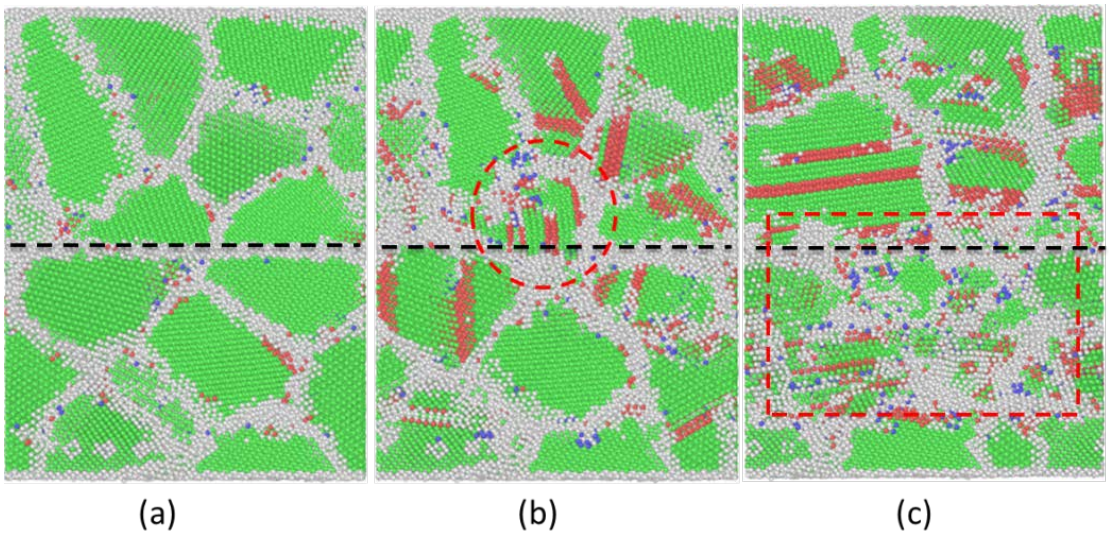

Figure 3: Still images of friction state at different sliding times for Ni-Cu friction system. (a) t = 5 ps; (b) t = 25 ps;(c) t = 75 ps. The velocity is 3 Å/ps; the pressure is 500 MPa

In order to investigate the grains quantificationally, the crystal size distribution at different sliding time is calculated, as shown in Figure 4. The black histograms show the initial crystal size distribution. The red and blue histograms show the crystal size distribution at time t = 25 and 75 ps. At the beginning of sliding, the sizes of grains are mainly concentrated in 1.5 - 2.7 nm. After a period of time for sliding, the crystal size distribution of the grains becomes more dispersed. It suggests that some grains are broken up into small grains during this time. After sliding for a longer time, the crystal size distribution of the grains has an interesting change. The number of small grains keeps increasing; the number of large grains also increases. Combining with Figure 2(c), it can be found that at the place which is far away from the interface, some crystal grains grow and elongate. Figure 5 shows that the average size of the crystal grains decreases as friction going. These phenomena are found not only in the simulations, but also in many experiments.

The change of the crystal grains in the surface is an important phenomenon in friction. It is necessary to find out its effect on friction behaviour.

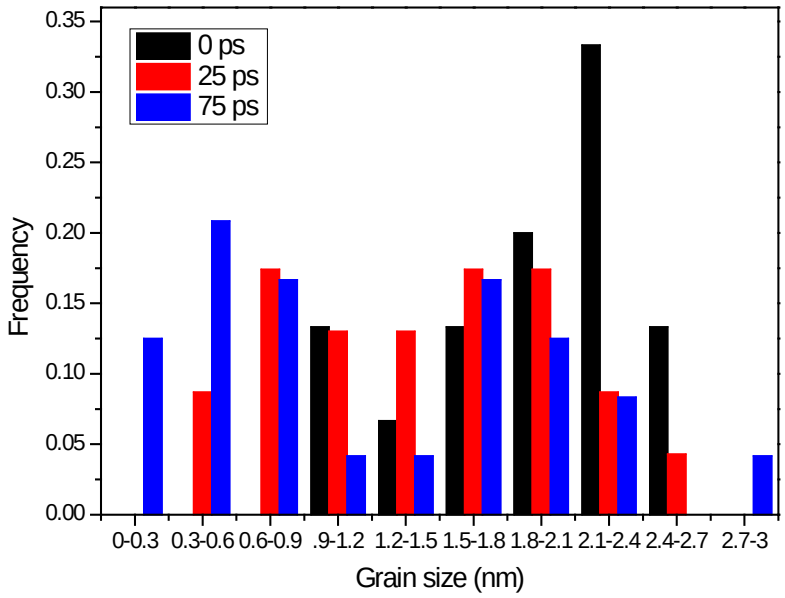

Figure 4: The crystal size distribution at different sliding time. The black histograms show the initial crystal size distribution. The red and blue histograms show the crystal size distribution at time t = 25 and 75 ps

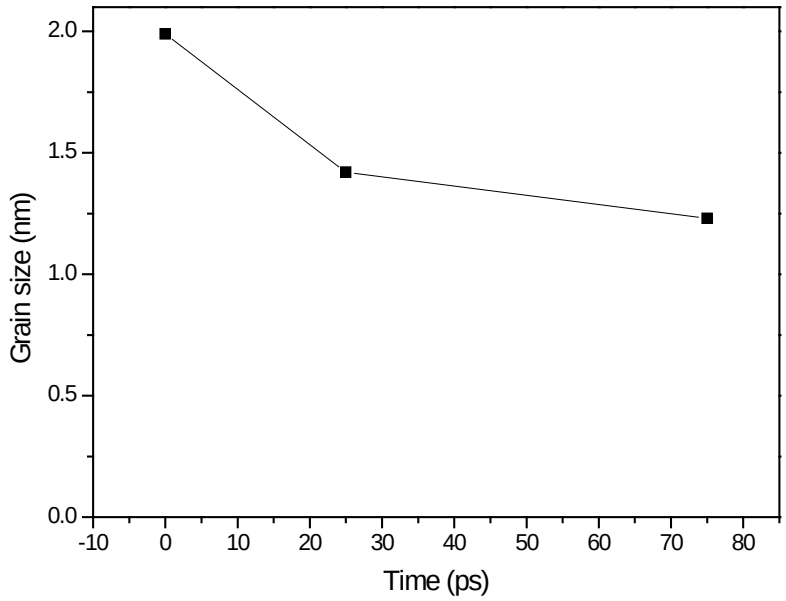

Figure 5: The average size of crystal grains at different sliding time

3.2 The changes of friction heat dissipation

Figure 6 shows temperature distribution of the system at different time. The temperature increases as the friction continues, especially the temperature of interface. It has the largest temperature rise. It can be seen that at the preliminary stage of sliding, the temperature distribution is relatively flat. This suggests that the friction heat transport fast. The friction heat generated in the interface can be dissipated in time. However, at longer times the temperature of the interface rises quickly and dramatically, it means that a mass of friction heat builds up in the interface. The heat density distribution, shown in the Figure 7, also indicates that a plenty

of heat is accumulated in the interface. It can be seen that the friction heat is well-distributed in y-direction in the primary period of sliding. As friction continues, the heat density in the interface rises obviously. It suggests that, due to the destruction of structure of the interface, the thermal conductivity has been affected and a large quantity of friction heat accumulated near the interface.

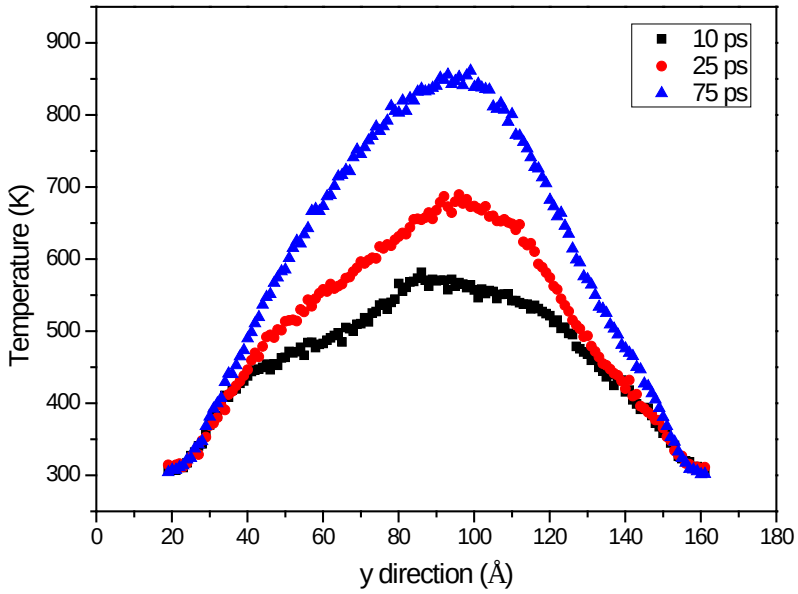

Figure 6: The temperature distribution at different sliding time

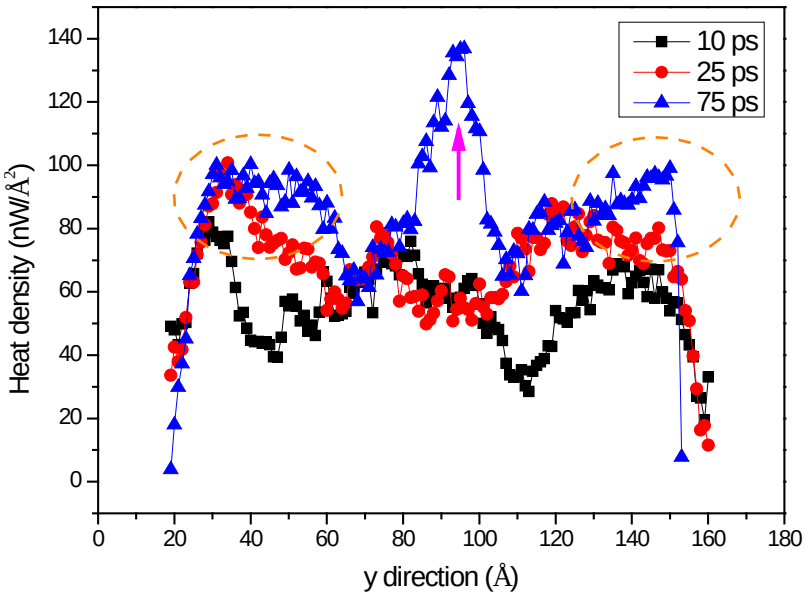

Figure 7: The heat density at different sliding time

3.3 Discussions

As it is known that the structure determines the characteristics. The change of structure of the materials may influence their capacity of heat transmission. Based on Figure 2 and 5, the grain sizes near the interface decrease. According to Figure 6 and 7, friction heat accumulated near the interface. Combining with the results of changes of grain size mentioned above, it can be found that the fragmentation of the grain in the interface has a strong relationship with the friction heat accumulation. Since the grains in the interface are broken into small grains, the size of the grains become small, the grain boundary density increases. The

probability of the electron (or phonon) collision scattering is greatly increased. The scattering phenomenon is enhanced, which leads to the increase of the grain boundary thermal resistance. It has a negative influence on heat conduction in metals. The heat generated in the interface will be more difficult to be dissipated. The local temperature will rise rapidly.

4. Conclusions

Molecular dynamics simulations of high-speed friction are conducted using an embedded atom potential. The changes of size of the grains, temperature profiles and heat density distribution are the main parameters considered in this simulation. The interactions among them were investigated. The conclusions are as follows:

1. As sliding going, the size of grains in the interface decrease. In self-mated case(Ni-Ni), big grains near the interface are broken into small ones. In soft-hard case, (Ni-Cu), grains sizes decrease mostly happen in the soft material.
2. The grain refinement increases the resistance of heat conduction near the interface. It makes the friction heat accumulate quickly in the interface which may increases the local temperature and changes the thermal conduction properties of the material.
3. A interaction between the evolution of grain size and change of thermal properties during friction is proposed. It is helpful for understanding the heat dissipation process. It can be used to design and optimize the structure of the gradient nanograined friction material, which shows excellent performance in reducing the friction force, from the view of heat transfer. These relationships could be of practical importance when designing the gradient nanograined coating, which can transfer the friction heat effectively during friction and protect the substrate material. The experiment work on observing the grain size changing and temperature distribution during friction will be carried out in follow-on work. A measurable optimal scheme on designing new structure of the friction material will be proposed and practiced.

Acknowledgments

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