Molecular Dynamics Simulations of High-speed Nanoscale Sliding with Third Medium

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Abstract. 3D non-equilibrium molecular dynamics simulations are performed to investigate the friction characteristic of Fe-Fe tribopair system under third medium condition. A Fe-Fe sliding simulation model with the soft third medium (Cu nanoparticle) is built. The friction force, evolution of the structure of interface and the temperature profiles of the sliding system are obtained. The influence of the sliding velocity to the temperature and structure change under third medium is investigated. The influence of Cu nanoparticle to the microstructure evolution and change of the friction characteristic is extremely concerned. The results show that the Cu nanoparticle can decrease the friction force and average temperature under the relatively low velocity (25m/s). However, under high velocity (150m/s), the positive effect is not obvious. A Cu nano-film would form on the surface, which is useful for weakening the destruction of the interface, and protecting the sliding blocks. Under high velocity, a mixing layer would be formed in both two cases (with or without Cu nanoparticle).

1. Introduction

High-speed friction is a violent physical process. During the friction process, due to the existence of friction, severe wear occurs between the friction materials, and the matrix material undergoes huge damage, resulting in losses. At the same time, in many fields, in order to overcome friction, a lot of work needs to be done, resulting in huge energy waste. According to statistics, about one third of the world's energy is wasted on friction every year. so how to achieve anti-wear and friction reduction is very important. The interface structure is an important factor that affects friction and wear characteristics. How to obtain and maintain a proper interface structure is the key point to control the friction process.

Nanoparticles have been widely used in friction processes as solid lubricants or lubricant additives. after adding nanoparticles to the friction system, the friction coefficient is reduced and the smoothness of the surface structure is improved. Through the analysis of surface morphology and material composition This is mainly due to the fact that nano-technology particles will deposit on the surface during the friction process and at the same time form a protective film under the influence of frictional heat, thus effectively achieving the effect of anti-wear and anti-friction. Research also found that due to heavy load and high-speed friction, a large amount of plastic deformation on the surface due to direct contact will cause the surface temperature to rise sharply, which promotes the deposition of nano-copper particles to form a soft protective film. Improve friction.

The friction with third medium is quite different from the dry friction [1,2]. There are a wide variety of the third medium, including water [3], oil [4], and solid particles [5-7]. In order to investigate the influence of the third medium, three kind of mechanisms are reported : (a) third body
material [8], (b) surface protective film [9], (c) a self-repair effect [10]. These soft solid mediums have common characteristics in the lubrication mechanisms. Molecular dynamics is a useful simulation method, which can not only simulate macroscopic frictional motion, but also observe changes in microstructure. In light of the above, a model which simulates the Fe-Fe sliding with the third medium of Cu nanoparticle will be built. The mechanism of Cu nanoparticles in changing tribology properties of friction system will be investigated. The direct evidences of the Cu nanoparticle in changing the structure of surface will be obtained. We aim to study the effect of Cu nanoparticle on the temperature rising during friction.

2. Simulation information

Figure 1 shows the simulation model in this paper. Two blocks of Fe atoms are contained in this model. Every block contains three parts. The first part is rigid part. Atoms in these regions are rigid. Atoms in this region move totally the same. The second part is thermostatic part. The Nosé-Hoover thermal bath is carried out on thermostatic region [11]. The third part is Newtonian part. The model B has the same setting with model A except the Cu nanoparticle. The Cu nanoparticle is a metal sphere with radius of 14Å which is placed between the two sliding blocks. The PFF boundary condition are carried out in XYZ directions. The total number of atoms in this model is about 26000. The crystal orientation of the two blocks are [1 0 0], [0 1 0], [0 0 1]. The sliding velocity are imposed in x direction. The normal force is also set to act on each atom in the rigid parts along the y direction, the potential parameter used in this paper is proposed by Bonny et al. [12]. The timestep used in this LAMMPS [13] simulation is 0.025 femtosecond. The cutoff distance is set as 5.6 Å. The open source code Ovito is used to show the movement of all atoms [14]. In this simulation, the normal load F is set to be 8 pN. In order to study the effect of sliding velocity, two velocities are set. The high velocity is 150 m/s and the low velocity is 25 m/s. Due to computational constraints, the time and length scales accessible to MD simulations are limited. So if we want to observe the whole process of the physical phenomenon, the parameters should be enlarged. It is for this reason that a majority of our simulations were conducted at high velocities.

![Simulation models](image)

Figure 1. Simulation models. (A) Dry sliding. (B) With nanoparticle

3. Results and discussion

3.1. Verification of simulation model

The unit cell volume is calculated under different equilibrium temperature. Figure 2 shows the W.B. Person’s [15] experiment data. The comparison shows that the simulation data basically agree well with the experiment data. The maximum error is 1.68%. It gives us the confidence that the simulation model is well enough for obtaining correct results.
Figure 2. The result of the comparison between the present simulation data and W.B. Pearson’s experiment data.

3.2. Friction force

Figure 3 and Figure 4 show friction force evolution with sliding time for two sliding velocity (25 and 150 m/s). Figure 3 shows that the friction force changes with sliding time at relatively low sliding velocity (25m/s). In the dry sliding case, the friction force increases sharply at first, and then fell. At last, the friction force fluctuates near the stable value. But in the case with Cu nanoparticle, the friction force change more smoothly and continuously. It may be due to the reason that the Cu nanoparticle can effectively decrease the energy barrier of the transition of static friction to kinetic friction. Figure 3 also indicates that the nanoparticle can decrease the friction force. However, in the case with the relatively high sliding velocity (150m/s), which is shown in Figure 4, the difference of the evolution of friction force is not so obviously. But the friction force of the case with Cu nanoparticle is still smaller than the case without nanoparticle. Thus we can get the conclusion that the Cu nanoparticle is helpful for friction reduction.

Figure 3. Friction force change with time at relatively low velocity. $v=25\text{m/s}$. $P=8pN$
Figure 4. Friction force with respect to sliding time. \( \nu = 150 \text{m/s}. \) \( F = 8 \text{pN} \)

3.3. Temperature

Figure 5 and Figure 6 show temperature evolution with sliding time for two sliding velocity (25 and 150 m/s). Figure 5 shows the evolution of temperature with the relatively low sliding velocity (25 m/s). In the dry sliding case, the temperature increased sharply at first, and then fell. Finally, the temperature fluctuates around 450K. But in the case with Cu nanoparticle, the temperature changes more gently. Figure 5 also suggests that the Cu nanoparticle can decrease the average temperature of friction system. In addition, an interesting phenomenon should be noted that, in the case without Cu nanoparticle, the temperature is more fluctuant. It is because that the Cu nanoparticle can decrease energy barrier of atomic stick-slip movement of the atoms on the surface. Figure 6 shows the temperature evolution with the relatively high sliding velocity (150 m/s). In these two cases (with or without Cu), the temperature rapidly increase at first, and then reach the steady value. The Cu nanoparticle can make the rise of temperature smoother.

Under low sliding velocity conditions, the Cu nanoparticle is helpful for friction reduction and temperature decreasing, but this positive role is not clear under high sliding velocity conditions. This may be due to the difference of the structure of the interface under different velocity.

Figure 5. The average temperature with respect to sliding time. \( \nu = 25 \text{m/s}. \) \( F = 8 \text{pN} \)
3.4. Structure

Figure 7 and Figure 8 show the evolution of microstructure with sliding time for two sliding velocity (25 and 150 m/s). Figure 7 shows the evolution of microstructure with the relatively low sliding velocity (25m/s). For the case without Cu nanoparticle, the two blocks are joined directly by applying the opposite normal load. The initially smooth interface is roughened. As friction continues, more plastic deformation occurred on the interface. The material mixing is also observed. For the case with Cu nanoparticle, the evolution of microstructure is different. No deformation is observed in the two sliding blocks. The nano-film is very effect in weakening the friction process and reducing the deformation of sliding blocks. Figure 8 shows that, in both of the two cases, a region formed at the interface. In this region, atoms mix obviously. It was reported by Rigney et al. According to their study, the physical property of this region is quite different. The deformation rate is very high. The basic structure changes a lot. It is the source of friction heat. It is useful for heat dissipating and friction reducing. This is why the case under high sliding velocity has lower friction force and higher temperature.

![Figure 6. The average temperature with respect to sliding time. \( \nu = 150 \text{m/s}, F = 8 \text{pN} \)](image)

**Figure 6.** The average temperature with respect to sliding time. \( \nu = 150 \text{m/s}, F = 8 \text{pN} \)

**Figure 7.** The snapshots of friction system at different time. The velocity \( \nu = 25 \text{m/s}, \) pressure \( F = 8 \text{pN} \).

| Time  | 0ps       | 50ps   | 250ps  |
|-------|-----------|--------|--------|
|       | Without Cu|        |        |
| Time  | 0ps       | 50ps   | 250ps  |
|       | With Cu   |        |        |

**Figure 7.** The snapshots of friction system at different time. The velocity \( \nu = 25 \text{m/s}, \) pressure \( F = 8 \text{pN} \).
Figure 8. The snapshots of friction system at different time. The velocity $v=150$ m/s, pressure $F=8$ pN.

Figure 9 and Figure 10 show the evolution of the structure factor. In order to obtain the local structure information, the friction blocks have 6 layers in the Y direction. 1-3 layers are belonging to the upper block; 4-6 layers are belonging to the lower block. The Mean Square Displacement (MSD) and Radial Distribution Functions (RDF) of each layer are studied. Figure 9 shows the MSD of the case with Cu nanoparticle under different velocity (25 and 150 m/s). In the case with relatively low velocity (25 m/s), as shown in Figure 9(a), the MSD of most layers are almost zero, which means that the structures of the two blocks are undamaged. It indicates that the Cu nanoparticle can effectively protect the sliding blocks. In the case with relatively high velocity (150 m/s), the MSD of 3 and 4 layers, the region nearest the interface, increases with sliding time. It suggests that plastic deformation occurs in those layers. It is consistent with the conclusions observed above.

Figure 9. The MSD of different layers with respect to sliding time of the case with Cu. $P=8$ pN. (a) $v=25$ m/s; (b) $v=150$ m/s

Figure 10 shows the RDF of the case with Cu nanoparticle under different sliding velocity (25 and 150 m/s). Under the low velocity, the RDF of each layer has several distinctive peaks, which means that all layers keep short range regular arrangement. As shown in Figure 10(a). Figure 10(b) shows the...
RDF of each layer under high velocity (150m/s). It can be seen that the peaks of RDF curve of layer 3 and 4 are undistinguished. It suggests that the initial crystal structure of layer 3 and 4 have been destroyed. This further illustrates that the Cu nanoparticle can effectively decrease the plastic deformation and defect structure with low velocity.

![Figure 10](image)

Figure 10. The RDF of different layers of the case with Cu nanoparticle. P=8pN. (a) \( \nu = 25 \text{m/s} \); (b) \( \nu = 150 \text{m/s} \)

3.5. Discussion
Two kinds of friction (with or without Cu nanoparticle) under different sliding velocity are studied by MD simulations. The results show that the Cu nanoparticle can decrease the friction force and average temperature significantly when the sliding velocity is relatively low. Just as shown in Figure 3 and Figure 5. But this positive role of Cu nanoparticle is not so obviously when the sliding velocity is relatively high. This interesting phenomenon makes us to find out what is happening during friction under different velocity. So we obtained the snapshots of system at different time. It can be observed that a Cu lubricate layer formed on the interface when the sliding velocity is low. The Cu lubricate layer good lubrication effect, the friction force and temperature are decreased. Not only the friction characteristics are improved, the structure of sliding blocks is also protected. According to Figure 9 and Figure 10, when the sliding velocity is low, the crystal structure is more intact, the plastic deformation is less compared with the case without Cu nanoparticle. Therefore, we can find that the Cu nanoparticle is an effective solid lubricant for with low velocity friction.

4. Conclusions
The friction characteristic of Cu nanoparticle is investigated by using the Molecular dynamic simulation. The friction force, temperature and structure changes are analyzed. The observations and conclusions from this study are:

1. The improvement in friction properties due to Cu nanoparticle is more obvious at low velocity than at high velocity.

2. At relatively low velocity (25m/s), the Cu nanoparticle formed a nano-film on the surface. It is responsible for the decrease of the friction force and average temperature. Due to the Cu nano-film, the sliding blocks have less plastic deformation and structure defect.

3. At relatively high velocity (150m/s), a mixing layer formed on the interface in both two cases (with or without Cu). Atoms in this layer have good mobility, and the structure is short range disordered. It is the reason why the friction force decreases with the increase of velocity.

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