The paper was presented at the Tenth Meeting
"New Trends in Fatigue and Fracture" (NT2F10)
Metz, France, 30 August–1 September, 2010

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MOLECULAR DYNAMIC STUDY OF MICROSTRUCTURE EVOLUTION OF CRYSTALLINE MATERIAL DURING CONTACT SLIDING

MOLEKULARNA DINAMIČKA STUDIJA RAZVOJA MIKROSTRUKTURE KRISTALNOG MATERIJALA PRI KONTAKTNOM KLIZANJU

Original scientific paper
UDC: 539.374
Paper received: 31.01.2011

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Keywords
- molecular dynamics
- plastic deformation
- microstructure
- crystalline material
- velocity profile

Ključne reči
- molekularna dinamika
- plastična deformacija
- mikrostruktura
- kristalni materijal
- profil brzina

Abstract

The focus of this paper is on the plastic deformation and microstructure evolution of crystalline material during sliding. Molecular dynamic simulations of Cu/Fe contact blocks have been performed under a pressure of 500 MPa and velocities ranging from 20 m/s to 1300 m/s. The results show that severe plastic deformation occurs in the Cu block while the Fe block does not deform plastically during the sliding. Accompanied with the occurrence of plastic deformation, the mixing of Fe atoms into the Cu block and growth of bcc Cu layer on the Fe surface are observed at the sliding interface. By investigating the mean square displacement of different regions of Fe block and velocity profiles along the cross section of the two blocks, the diffusion process of Fe atoms and the fluid-like behaviour of Cu atoms are also analysed.

Izvod

Ovaj rad se fokusira na plastičnoj deformaciji i razvoju mikrostrukture kristalnog materijala pri klizanju slojeva u dodiru. Simulacije molekularne dinamike kontaktnih blokova Cu/Fe su izvedene pod pritiskom od 500 MPa i pri brzinama u rasponu od 20 m/s do 1300 m/s. Rezultati pokazuju da se naglašena plastična deformacija javlja u Cu bloku, dok se Fe blok ne deformiše plastično tokom klizanja. Uz pojavu plastične deformacije, na granicama klizanja primećuje se i pojava mešanja Fe atoma unutar Cu bloka i rast Cu sloja u prostorno centriranoj kubnoj rešetki (bcc) na površini Fe. Istraživanjem srednjeg kvadrata pomeranja različitih oblasti Fe bloka i profila brzina duž poprečnog preseka oba bloka, takođe je analiziran i difuzioni proces Fe atoma kao i fluidno ponašanje (tečenje) Cu atoma.

INTRODUCTION

It is now widely recognised that sliding dramatically changes the material near the sliding interface. The changed materials, which have been given many names like transfer layer, third body and mechanical mixing layer, would greatly influence both friction and wear properties of a sliding system. It has been reported that development of a stable transfer layer would result in decreases in the wear rate and coefficient of friction for the unlubricated sliding of metals /1, 2/. Therefore, understanding of the microstructural evolution and material diffusion during the formation of transfer layers is important in order to have a complete picture of sliding friction phenomenon. However, due to the difficulty of *in situ* observation of transfer layers formation, the understanding of structural changes is limited. To overcome this limitation, molecular dynamics (MD) simulations provide a strong substitute tool. With the development of computer speed and parallel simulation technology, MD simulations have provided substantial information and insight into dynamics of sliding contacts. Hammerberg et al. /3/ used MD simulation to investigate the frictional behaviours of two material pairs of ductile metals, Ta/Al and Ag/Cu. Kim et al. /4/ have studied interfacial sliding behaviour of model crystalline materials and verified the similarities between fluid flow and atomic flow at the sliding interface. Although MD simulation is simpler than the real sliding and has the difficulty to attain larger enough system sizes and simulation times for physically relevant results, it helps to reveal the dynamic characters of sliding interfaces. Therefore, in this paper, 3D MD simulations of dynamic friction at metal block-block interface are carried out to investigate the friction characteristics of soft-to-hard (Cu/Fe) tribopairs. The microstructural evolution and velocity profiles of the tribopairs are analysed at different sliding speeds.

METHODOLOGY

Simulation Model

The model for the simulation performed in the present work is shown in Fig. 1a which consists of approximately 60,000 atoms. Three kinds of atoms are used in the model: rigid moving, thermostat and Newtonian atoms. The outermost three layers in each block are rigid moving atoms, which were only allowed to move in the sliding x direction. The next eleven layers next to rigid atoms are thermostat atoms, where Nose-Hover thermal baths are attached to remove the heat produced by the sliding and to maintain the boundary of each block at 0 K. All the other atoms are Newtonian atoms which are unconstrained and can move freely due to forces between molecules. Periodic boundary conditions are applied in the x and y direction. In the z direction, two boundary conditions are applied to the rigid atoms in both sliding blocks: (1) A constant normal force, F_n, is applied first in order to press both blocks together with P_n = 500 MPa. After the contact system has reached equilibrium, the rigid atoms are set fixed and only allowed to move in x direction. (2) To keep a constant sliding speed, the velocities u_u of the upper and u_l of the lower block, are kept constant: $u_u = -u_l = V_x/2$. The interactions between atoms are modelled using the potential of the embedded-atom-method (EAM) form, and the one developed by Bonny et al. /5/ for the Cu/Fe alloy is employed in the current simulation. The opening MD code LAMMPS /6/ is used for the current investigation and the atom visualisation is done by using the VMD programme /7/.

Simulation Steps

The simulation process involves following two steps: contact and sliding. During the contact process, the initial separated Cu and Fe blocks are made joined within the simulation box by applying an opposite normal forces F_n to the rigid moving atoms and by keeping the temperature of the whole system at 0 K. The normal force is chosen such that the resulting normal compressive stress has a magnitude of ~500 MPa. After the system is equilibrated with the applied load, the two boundary conditions mentioned above are applied on the rigid moving atoms to start sliding.

During the sliding, evolution of friction is tracked by monitoring the x-direction tangential force of the Cu rigid moving layer. The diffusion of Fe atoms is measured by the mean square displacement (MSD), which is defined as

$$MSD = \frac{1}{N}\sum_{i=1}^{N}\left|r_i(t) - r_i(0)\right|^2 . \quad (1)$$

Where $r_i(t)$ is the displacement component of atom i in the respective dimension x, y or z at time t. Using the Einstein expression, the diffusion coefficient, D, is obtained from the MSD by

$$D = \lim_{t\to\infty}\left(\frac{1}{2t}MSD\right). \quad (2)$$

To obtain the velocity profile, the simulation domain is divided along the z direction into layers consisting of approximately 800 to 1000 atoms for both Cu and Fe blocks, and the velocities of each layer is computed every 100 time steps and averaged over 100 samples.

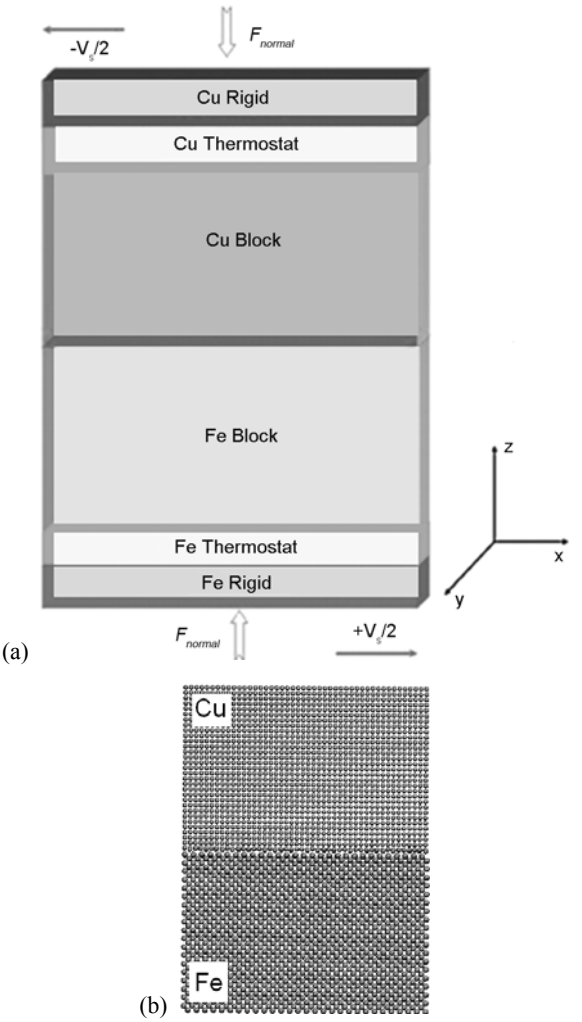


Figure 1. (a) MD simulation model, three kinds of atoms are indicated by different colours (shades), and (b) visualization of the initial contact interface of Cu/Fe tribopairs.
Slika 1. (a) MD model simulacije, tri vrste atoma su predstavljeni različitim nijansama, i (b) vizuelizacija početnom kontakta granice Cu/Fe tribološkog para.

SIMULATION RESULTS

This section analyses the results obtained by the MD simulation. Figure 2 is a plot of friction force evolution during a computer simulation process with a sliding velocity of 600 m/s for Cu/Fe tribopairs. It is obvious that after an initial transient, the friction force reaches a steady-state value, which can be obtained by averaging the friction force over time. In other simulations with different velocities, the friction behaviours are all similar to those shown in Fig. 2. Their differences are laid in the different steady-state friction values and the amplitudes that fluctuated around the values. Figure 3 shows the steady-state friction force value evolutions as a function of sliding velocity for all simulation models for Cu/Fe tribopairs. In the low velocity regime, the friction force increases almost linearly with the increasing of velocity. As the velocity increases further, the increase of the friction force slows down and reaches a peak value at critical speed of 300 m/s. When the increasing velocity exceeds the critical value, the friction force decreases gradually with the increasing velocity and finally

reaches a plateau. As friction is an energy dissipative process that converts the kinetic energy of the sliding materials into heat and increases the temperature near the interface, therefore, the interface materials may be softened by the increasing temperature which may lead to the drop of friction force at high velocity. This phenomenon is known as velocity weakening of the friction force and is reported by early experimental work of Bowden /8/ and by recent MD simulation work of Hammerberg /3/.

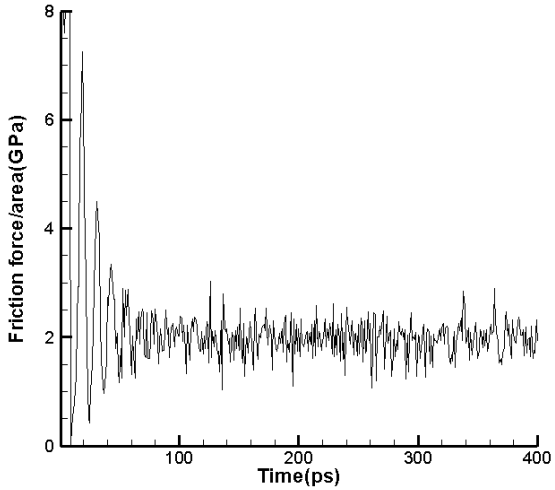


Figure 2. Friction force with respect to sliding time for Cu/Fe system with a sliding velocity of 600 m/s.
Slika 2. Sila trenja i vreme klizanja za sistem Cu/Fe sa brzinom klizanja od 600 m/s.

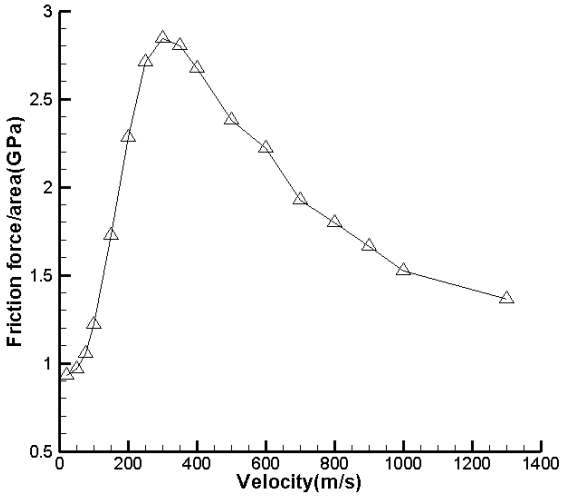


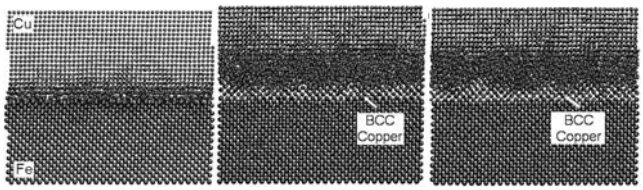
Figure 3. Velocity weakening phenomenon of the friction force for Cu/Fe system.
Slika 3. Fenomen slabljenja brzine sile trenja za sistem Cu/Fe.

Evolution of microstructure

Based on the velocity-weakening phenomenon shown in Fig. 3, the sliding deformations under three sliding velocities 300 m/s, 600 m/s and 1000 m/s were investigated. Figures 4-6 show the microstructural changes at different times and sliding distance for those three velocities. In all three cases, there is obvious plastic deformation occurring in the upper copper block while there is negligible plastic deformation in the lower iron block. The largest plastic strain of copper block is near the sliding interface and little deformation can be observed far from the interface. By comparing Figs. 4(a) and 5(a), it is obvious that the extent of plastic deformation in copper becomes greater with the increasing of velocity for the same sliding distance. And for the same sliding time, Figs. 4(b) and 5(b), it is also clear that the plastic deformation of copper is more severe with higher velocity. However, when one compares the longer sliding time images, Figs. 4(c), 5(c) and 6(c), it can be seen that several shear bands appear in the copper block along the <110> close packed directions at the velocity 300 m/s. This is due to the largest shear stress in the copper block at the velocity of 300 m/s, which is consistent with the velocity weakening of friction force shown in Fig. 3.

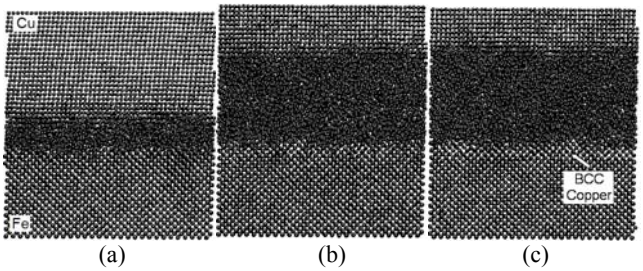
(a) (b) (c)

Figure 4. The still image of Cu/Fe tribopairs after sliding under velocity of 300 m/s. (a) time = 10 ps, distance = 3 nm, (b) time = 100 ps, distance = 30 nm, (c) time = 200 ps, distance = 60 nm.
Slika 4. Snimak tribološkog para Cu/Fe posle klizanja pri brzini 300 m/s. (a) vreme = 10 ps, rastojanje = 3 nm, (b) vreme = 100 ps, rastojanje = 30 nm, (c) vreme = 200 ps, rastojanje = 60 nm.



(a) (b) (c)

Figure 5. The still image of Cu/Fe tribopairs after sliding under velocity of 600 m/s. (a) time = 5 ps, distance = 3 nm, (b) time = 100 ps, distance = 60 nm, (c) time = 168 ps, distance = 100.8 nm.
Slika 5. Snimak tribološkog para Cu/Fe posle klizanja pri brzini 600 m/s. (a) vreme = 5 ps, rastojanje = 3 nm, (b) vreme = 100 ps, rastojanje = 60 nm, (c) vreme = 168 ps, rastojanje = 100.8 nm.



(a) (b) (c)

Figure 6. The still image of Cu/Fe tribopairs after sliding under velocity of 1000 m/s. (a) time = 12 ps, distance = 12 nm, (b) time = 55 ps, distance = 55 nm, (c) time = 160 ps, distance = 160 nm.
Slika 6. Snimak tribološkog para Cu/Fe posle klizanja pri brzini 1000 m/s. (a) vreme = 12 ps, rastojanje = 12 nm, (b) vreme = 55 ps, rastojanje = 55 nm, (c) vreme = 160 ps, rastojanje = 160 nm.

Figures 4 to 6 also show other three interesting and important phenomena occurring just above the original interface for Cu/Fe tribopairs. The first one is the extensive mechanical mixing of Fe atoms into the Cu block. By

comparing Figs. 4(c), 5(c) and 6(c), it is obvious that more Fe atoms are mixed into the Cu block with higher velocity. The possible explanation for this mixing phenomenon would be analysed in the following section by investigating the mean square displacement (MSD) and velocity profiles of the sliding system. The second interesting phenomenon is the shift of deformed region and sliding interface to an upper position in the copper block. This shift of the sliding interface demonstrates that sliding actually occurs in the soft material when the sliding pairs are the soft material in contact with hard material. The highly deformed soft material under the shift sliding interface would more likely have a role as a lubricant between those two sliding pairs which would significantly reduce the friction effect. Another important phenomenon worth noting is that the amorphous copper is observed to transfer to *bcc* structure on the epilayer of the iron surface. This structural change corresponds to the material property transformation: from soft material to hard material, which results in that the actual sliding would happen in the interior of the softer copper.

Mean Square Displacement (MSD) and velocity profiles

As Fe atoms are observed to mix into the Cu block during sliding, therefore, the diffusion coefficient of Fe atoms under different speeds would be discussed in this section. The diffusion coefficient is measured by calculating the mean square displacement (MSD) in *y*-dimension, as *x* and *z*-dimensions are biased due to the simulation setup. Figure 7 shows the MSD of Fe atoms at the interface under different speeds, in which it can be seen that the diffusion of Fe atoms increases for higher relative speeds. This is consistent with the microstructural evolution results shown in Fig. 5 and Fig. 6, where under higher sliding speed condition, more Fe atoms can be seen to mix into Cu block. Furthermore, three different groups of Newtonian atoms are defined within the Fe block according to the geometrical regions in Table 1 to investigate the MSD at a different distance from the interface. The upper region directly starts at the interface, which is located at $z = 100$ and the lower region starts from the beginning of Newtonian atoms in the Fe block at $y = 30$. From Fig. 8, it is clear that the diffusion in the upper region is much higher than that in the middle and in the lower region. And nearly zero value of MSD can be obtained in both middle and lower regions, which indicates that the diffusion of Fe atoms only occurs near the interface (the upper region).

The velocity profiles along the *z*-direction are analysed at different sliding time for relative speeds of 300 m/s and 1000 m/s. In both figures, the interfaces, defined as a position that has 0 average velocities, all are located in the upper Cu block. At low speed of 300 m/s, the velocity profile spreads quickly and reaches a steady state after 20 ps. At high speed of 1000 m/s, the velocity profile keeps spreading with a slow down spread rate after 20 ps. And the shift of sliding interface position can be obviously observed from those velocity profiles. This is consistent with the evolution of microstructure shown in Fig. 6 and indicates that sliding actually occurs in the interior of the softer material.

Table 1. Geometrical regions of Fe blocks for calculating MSD.
Tabela 1. Geometrijske oblasti Fe blokova za proračun MSD.

Region	x_{lo}, x_{hi} (A)	y_{lo}, y_{hi} (A)	z_{lo}, z_{hi} (A)
Lower	0 , 83	0, 28.7	30, 34
Middle	0 , 83	0, 28.7	60, 64
Upper	0 , 83	0, 28.7	100, 104

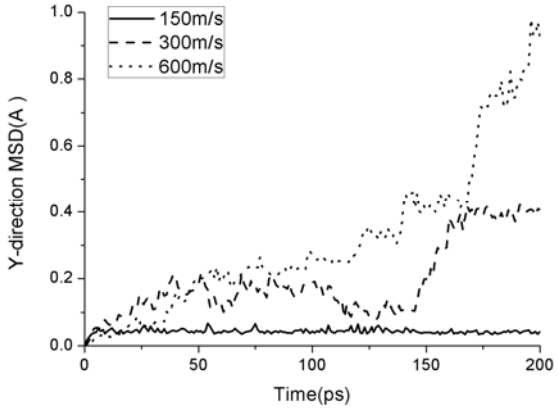


Figure 7. *Y*-direction MSD (A^2) of Fe atoms at the interface under relative speeds of 150, 300 and 600 m/s.
Slika 7. *Y*-pravac MSD (A^2) za Fe atome na granici pri relativnim brzinama 150, 300 i 600 m/s.

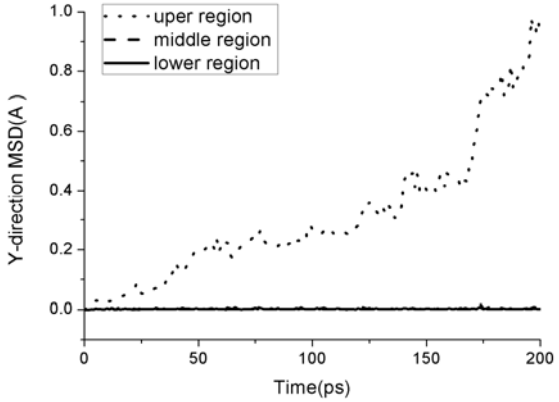


Figure 8. *Y*-direction MSD (A^2) of Fe lower, middle and upper groups under relative speeds of 600 m/s.
Slika 8. *Y*-pravac MSD (A^2) za Fe atome u donjim, srednjim i gornjim grupama pri relativnim brzinama od 600 m/s.

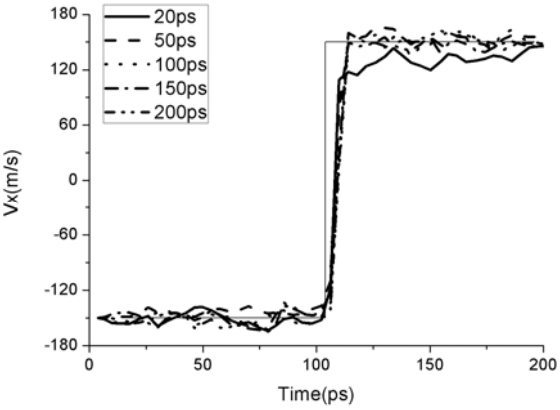


Figure 9. Velocity profiles along *z*-direction of Cu/Fe tribopairs at different time for speed of 300 m/s. The initial contact interface is indicated by dashed line.
Slika 9. Profili brzina duž *z*-pravca tribološkog para Cu/Fe za različita vremena i brzinu 300 m/s. Početna kontakt granica je označena isprekidanom linijom.

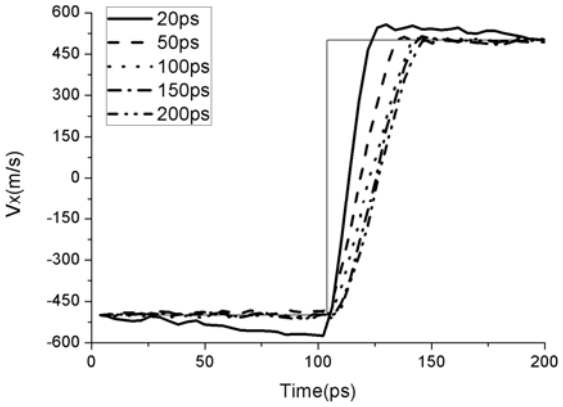


Figure 10. Velocity profiles along *z*-direction of Cu/Fe tribopairs at different time for speed of 1000 m/s. The initial contact interface is indicated by the light-slide line.
Slika 10. Profili brzina duž *z*-pravca tribološkog para Cu/Fe za različita vremena i brzinu od 1000 m/s. Početna kontaktna granica je označena svetlom punom linijom.

CONCLUSIONS

Molecular dynamics simulations are performed for the Cu/Fe soft to hard contact sliding metal-pairs with the velocity ranging from 20 m/s to 1000 m/s. Extensive plastic deformation and amorphization of Cu block, while negligible deformation of Fe block are observed at all ranges of the sliding. In addition, dynamic recrystallization of amorphous copper to *bcc* crystal structure on iron surface and the mixing of iron atoms into copper block can also be seen in the simulation. The MSD results show that the mixed iron atoms are all from the surface region of Fe block. The velocity profiles results indicate that real sliding actually occurs in the interior of the softer Cu block.

ACKNOWLEDGEMENT

The current work is funded by the National Basic Research Program of China through Grant No. 2010CB631005 and Chinese National Natural Science Foundation No. 10672086 and 10776019.

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