Transactions of the Materials Research Society of Japan 30[3] 905-908 (2005)

Molecular-dynamics Study for the Effects of Stacking Fault Tetrahedron on the Shear Resistance of Cu Crystals

Katsuyuki Kusunoki
Computational Materials Science Division, National Institute for Materials Science, 1-2-1 Sengen Tsukuba-city 305
Fax: 81-298-59-2628, e-mail: kusunoki.katsuyuki@nims.go.jp

Shearing processes of copper crystals containing a stacking fault tetrahedron (SFT) were investigated using molecular-dynamics simulations. Sample crystals were constructed by an EAM potential and were sheared along <110> direction on one of their {111} atomic planes. Edge dislocations generated on the shear plane were observed to be pinned by the SFT which gave rise to the shear resistance of the crystals. The shear stress depended on both the size of SFT and the shearing speed. Smaller SFT was more stable than larger ones against repeated shearing by dislocations.
Key words: copper, stacking fault tetrahedron, shear stress, MD

1. INTRODUCTION

Vacancies and self-interstitial atoms (SIA) in nuclear materials are generated as residues of Frenkel-type defects created by knock-on at irradiation. Most of the SIAs, as having high mobility than that of vacancies, are thought to disappear after migration toward surfaces or interfaces or to make clusters or dislocation loops. Compared to the case of SIAs, a part of vacancies, as having very low migration velocity, make voids or clusters interior of crystal grains. A cluster of vacancies is, under some conditions, transformed into a stacking fault tetrahedron (SFT) and has been thought to affect the mechanical properties of nuclear materials through interactions with dislocations. It will be very difficult to directly observe such interactions by experimental procedures, and the present work was intended to simulate the dynamical process of such interactions between an SFT and dislocations in single crystals of copper using molecular-dynamics calculations.

2. METHOD

An embedding function devised by Oh and Johnson [1] was applied to the calculation of interatomic forces based on the many-body EAM potential [2] that can reproduce various types of crystal properties such as lattice parameter, cohesive energy, elastic constants and the vacancy formation energy in copper crystal. Rectangular parallelepiped samples of copper crystal sized about 14x14x57 in units of lattice parameter without periodic boundaries and containing a triangularly shaped plate of vacancy cluster at the center of the sample were prepared. Each sample had 24 , 33 , and 80 atomic planes along (111), $(1\bar{2}1)$, and $(10\bar{1})$ crystallographic planes. The vacancy cluster spontaneously changed into an SFT very swiftly within the order of pico-seconds. After sufficient time of about 30 pico-seconds for equilibration, atoms on the half of the top plane of the samples were pushed down at constant speed so that the sample is sheared on a (111) atomic plane along $[10\bar{1}]$ direction, the slip system of copper crystal. Every sample was kept at 1K during the simulation.

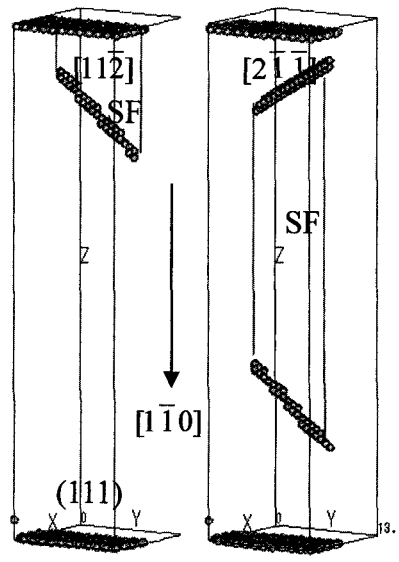
3. RESULTS AND DISCUSSION

3.1 Effect of shearing speed on the deformation of crystals with no SFT

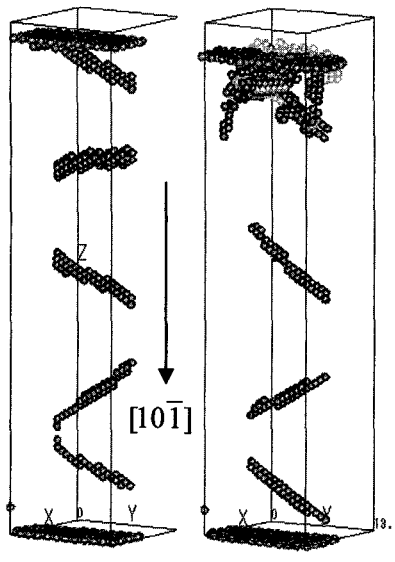
Firstly we investigated into the effect of shearing speed on the deformation behavior of samples for the case that SFT does not exist. The results showed that when the shearing speed exceeds some critical value, higher shearing speed increases dislocation density in the sample and consequently raises the deformation resistance of the samples. Too high shearing speed caused the collapse of samples (see Fig.1(b)). However, as far as the shearing speed does not exceed the critical value, the effect of shearing speed on the shear stress is expected to be small. In case when the shearing speed was $2x10^8$/s the maximal resolved shear stress (MRSS) in the present system was 2.2GPa, which value is close to 0.86GPa, an experimental value of MRSS for the yield stress of a whisker crystal along <111> extension [3]. Although slower shearing speeds, which will greatly raise the cost of computation, may lower the MRSS, we applied the above speed to every simulation for the samples with an SFT. The shearing process is well illustrated in Fig. 1(a), where dislocated atoms aligned along $[1\bar{1}2]$ direction appeared on (111) atomic plane when the shear stress exceeds the yield stress of the crystal making a stacking fault (SF) on the (111) atomic plane. When the shearing proceeds to some extent and the first dislocation runs some distance, the second partial dislocation, with its axis parallel to $[2\bar{1}1]$ direction and being conjugate to the first one, appeared to relax the accumulated stress on the (111) atomic plane. The second dislocation swept the (111) atomic plane so that it erases the SF created by the first dislocation. The stress-strain curve is shown in Fig. 2(a). Every peak in this figure indicates the generation of a new partial dislocation at the top of the shearing plane.

3.2 Effect of SFT on the shear properties of Cu

Secondary, we investigated into the cases when a sample with a preliminarily introduced SFT is sheared. Figure 2(b) shows the stress-strain curve for a crystal containing an SFT consisting of three-atoms-length stair rods.

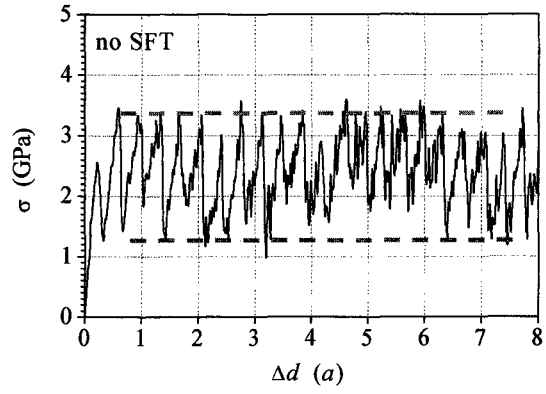


(a) $\dot{\varepsilon} = 2x10^8 / s$

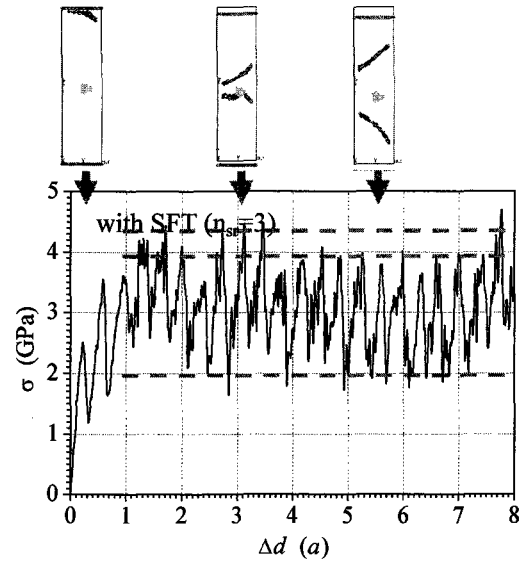


(b) $\dot{\varepsilon} = 1x10^9 / s$

Fig. 1 Shearing process along (111) plane toward [10$\bar{1}$] direction. Force is applied to the half of the uppermost atoms. Lines show the partial dislocations migrating on the (111) shear plane.



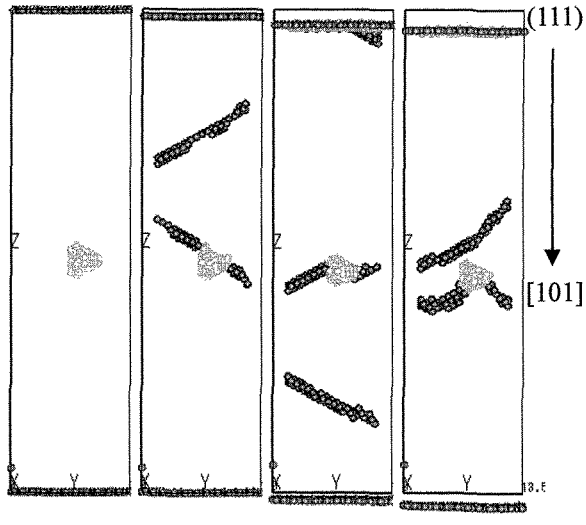
(a)



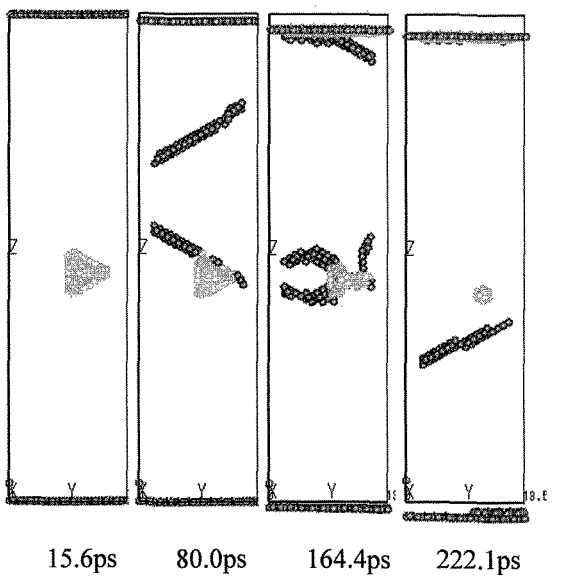
(b)

Fig. 2 Stress-strain curves of the present (111)/ [10$\bar{1}$] slip system; (a) for a crystal with no SFT, and (b) for a crystal with an SFT having three-atoms-length stair- rods. The first peak corresponds to the first generation of a partial dislocation, which gives the value of MRSS.

It is remarkable that the stress minima of the samples with an SFT are higher by about 0.8GPa than that of crystals with no SFT (see the dashed lines in Fig. 2(a) and (b)). This phenomenon indicates that the residual stress of a crystal is raised by the existence an SFT. Two levels are recognized for the maxima of stresses (see the broken lines in Fig. 2(b)). Among them, the lower one corresponds to the accumulated elastic stress shortly before the relaxation by the generation of a new partial dislocation, and the higher one indicates the raise in the shear stress, which is caused by the interaction between the dislocation and the SFT.



(a)



(b)

Fig. 3 Side views of the interaction between an SFT and moving dislocations for cases when the stair-rod is composed of (a) three-atoms and (b) five-atoms. Thin triangular plates indicate SFTs and thick lines indicate dislocations. In case when the stair-rod length is short the SFT is stable against repeated cutting by dislocations and moves toward the shear direction. On the contrary, in case when the stair-rod length is long, the SFT become unstable owing to the accumulation of pinned dislocations at around the SFT.

In case when the stair-rod of an SFT had three-atom length (n_{sr}=3), overall gain in the maximal shear stress was about 1GPa, which was caused by both the increase in the residual stress and the interaction between the SFT and a pinned dislocation. Figure 3(a) shows the shearing process, viewed from [111] direction, of the sample containing the SFT which had three-atom length stair-rods.

The SFT-size dependence of the shear stress is shown in Fig. 4, where the shear stress becomes highest when the stair-rod of an SFT contains about five-atoms (n_{sr}=5).

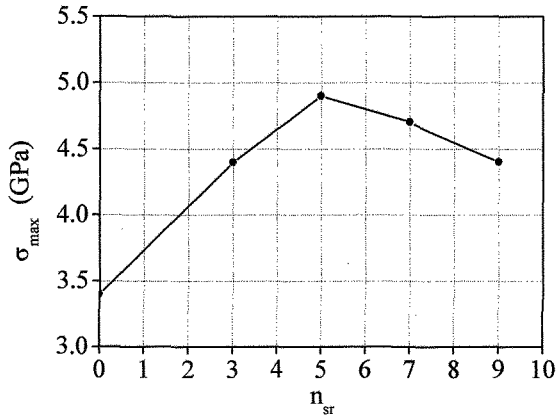


Fig. 4 SFT-size dependence of maximal shear stress.

3.3 Shearing process of SFT

It was ascertained that, compared to larger SFT, smaller SFT is, in spite of its weaker pinning effect on moving dislocations, fairly stable against cutting by dislocations. This is shown in Fig. 3(a), where an SFT is observed to gradually move toward $[10\bar{1}]$ direction, retaining its initial form unchanged and being little damaged against repeated cutting by dislocations. Although the details are not given here, the mechanism of such "self-repairing" process seems to be very interesting and is worthy of further investigation.

Contrary to the case of smaller SFT, larger SFT has stronger pinning effect on moving dislocations retarding their migration speed, and consequently, causing pilings and collisions of dislocations around the SFT, which gave raise to the local stress and then caused the collapse of SFT. In this case, as the birth of an SFT is originated to a vacancy cluster, the collapse of an SFT generated single vacancies or vacancy clusters (see Fig. 3(b)). Also, the collision and consolidation of dislocations gave birth to interstitials or their clusters, which were observed to move toward the surfaces or interfaces of the sample leaving a debris at there (see Fig. 5).

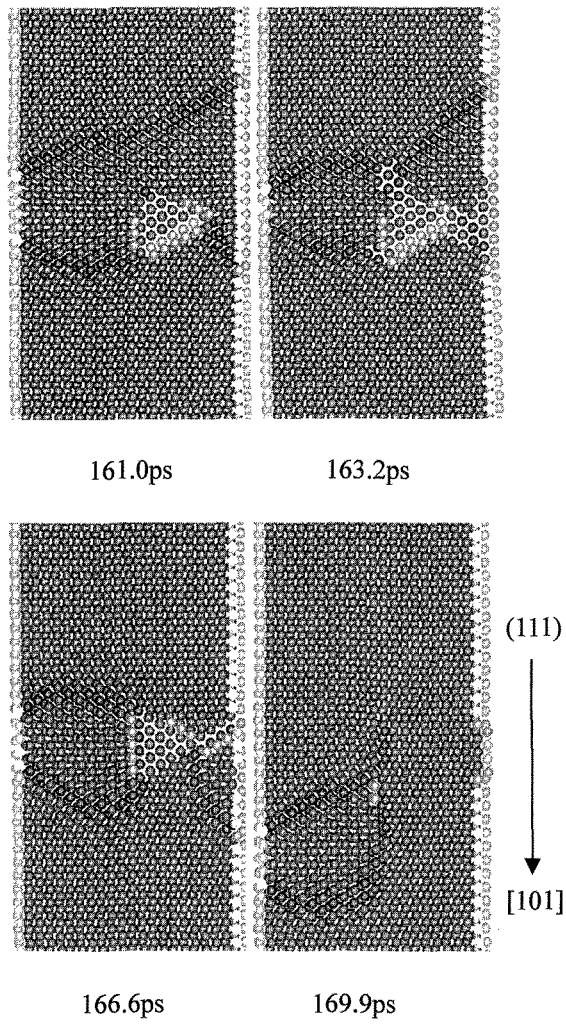


Fig. 5 Side views of interaction among an SFT and moving dislocations for a case of n_{sr}=5. Dislocations are indicated as thick curved lines around the SFT (thin triangular regions). Only three adjacent (111) atomic planes are shown. The upper figures show the accumulation of dislocations at an SFT. The lower figures show the consolidation of the dislocations, where the collapse of the SFT took place leaving vacancies. The lower right figure shows the debris of atoms, which were emitted as an interstitial cluster at the consolidation of dislocations and migrated very swiftly to the surface of the sample.

4. CONCLUSION

Molecular-dynamics simulations were carried out to study the shearing process of perfect and defected copper crystals with a stacking fault tetrahedron (SFT). Results show that for perfect crystals the present simulation could reproduce virtually the same order of yield stress of real copper crystal. An increment in the shear stress was observed for crystals with an SFT, which can have responsibility for irradiation-induced hardening of nuclear materials.

References

[1] M. S. Daw and M. I. Baskes, *Phys. Rev.* **B29**, 6443 (1984)

[2] D. J. Oh and R. A. Johnson, *J. Mat. Res.* **3**, 471 (1988)

[3] S. S. Brenner, "Growth and Perfection of Crystals", Ed. by R. H. Doremus, B. W. Roberts, and D. Turnbull, Wiley, New York, (1958).

(Received December 23, 2004; Accepted April 28, 2005)