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Elementary processes in channeling deformation in FCC copper: a molecular dynamics study

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Abstract

To understand the channeling deformation mechanism in irradiation-damaged materials, the interaction processes between dislocations and radiation induced defect clusters was investigated by molecular dynamics simulation. Small interstitial Frank loops can be easily eliminated by dislocation, but larger ones can stay at original sites after intersection. Vacancy Frank loops are weaker obstacle to dislocation compared with the interstitial ones and they cannot be absorbed by dislocation at low temperature.

1. Introduction

FCC metals like stainless steel and copper alloys were widely used as structural and functional components in fission and fusion reactors. After irradiation by high-energy neutron, their microstructures were manifested in the form of matrix defects such as Frank loops, SFTs and voids. They made the deformation localize in narrow bands. The defect density decreases sharply in the bands while keeps almost unchanged in between. These narrow deformation bands, which were termed as dislocation channels, are important due to their connection with the premature failure of reactor structure. To understand the mechanism, interaction between dislocation and defect clusters must be well understood at atomistic level. Recently Rodney and Martin [1] investigated the interaction between dislocation and glissile interstitial clusters in Ni by molecular dynamics simulation and found the clusters can be dragged away by dislocation after a change in Burgers vector. While being dragged, they travel along the dislocation line, and are eliminated either by coalescence with other absorbed clusters or by absorption at unit or superjogs. Based on that, the dislocation was though to be a center of dynamic recombination, coalescence, and elimination of vacancy and interstitial defect clusters. In the MD simulation by Wirth et al. [2], SFTs in Cu was found to be very stable, they can remain intact after being sheared by the dislocation, only truncated SFT can be absorbed by the passage of an edge dislocation. Above information reminds us to be careful in modeling the elimination mechanism of different type. However, the elimination of defect clusters upon intersection with dislocation has been widely used as an assumption on the short-range interaction in dislocation dynamics simulations [3–6]. This should be doubted, because during the in situ TEM observations [7] of deformation in proton-irradiated stainless steel, the Frank loops survived even after substantial intersection by dislocations. The contradiction comes from the wrong generalization of our knowledge on the interaction between dislocation and defect clusters of various types and sizes. To the authors, it is very strange that though Frank loops are the main defect type in irradiated stainless steel, MD simulation on Frank loops are rare except our recent investigations [8,9], in which the sessile Frank loops were discovered to change into glissile dislocations under high stress level. In this study, we will present our new results for the size effect on the intersection between dislocation and Frank loops.

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2. Simulation method

Copper was taken as the simulation material because of its similarity with stainless steel in both crystal structure and low SFE character. A well-testified long-range EAM potential [10] were used in this study. Constant simulation temperature of 10^{-6} K was achieved by using velocity-scaling method at every integration step. The detail description could be found in previous papers [8,9]. Here we give a short explanation on the simulation model. It consisted of about 120 000 atoms and had a size of $30\times33\times30\ a_0^3$. Fixed boundary condition was applied to the surfaces where external load was applied while free boundary condition was applied for other surfaces. Compression was carried out in displacement-controlled manner up to a strain of 5% by 50 load steps. After insertion of Frank loops and dislocation, the lattice was relaxed to generate the correct configuration with minimum energy.

3. Results

3.1. Intersection between an edge dislocation and 7-SIAs or 7-vacancies Frank loops

Fig. 1 shows the compression process of a lattice with two interstitial Frank loops and one edge dislocation. The upper and bottom loops were arranged to inhabit on $(\bar{1}11)$ and $(11\bar{1})$ planes, respectively. The dislocation was inserted to slip on (111) plane and has a Burgers vector of $\frac{a_0}{2}[10\bar{1}]$. During the preliminary relaxation before loading, the dislocation dissociated into two Shockley partial dislocations of $\frac{a_0}{2}[11\bar{2}]$ (heading) and $\frac{a_0}{2}[2\bar{1}1]$ (trailing). The heading partial approached the upper loop during preliminary relaxation and changed it into one-dimensional crowdion bundle along $[10\bar{1}]$ direction. Due to a larger distance from the heading partial, the bottom loop kept its configuration as Frank loop. But in the following deformation process, the heading partial approached and transformed the bottom loop into crowdion bundle along the same $[10\bar{1}]$ direction at No. 2 and No. 3 stage, respectively. We should note that the transformation occurred just upon the contact between loops and dislocation. During deformation from No. 2 to No. 3 stage, the heading partial bowed out between the two crowdion bundles. At the same time, the trailing partial caught up with the heading one at the site of the bottom loop. From No. 3 to No. 5 stage, driven by the dislocations the bottom crowdion bundle began to move along its Burgers vector. But that movement is still slow until a No. 5, at which dissociation of the bundles occurred and a single vacancy was left at the original site while the rest of the bundle move faster with the dislocation. This also applies for the upper crowdion bundle, but at later stage of No. 7.

Due to the length limitation, the intersection between two vacancy loops and an edge dislocation cannot be shown here. Though the setup of the simulation is the same except that the loops were inserted by deleting atomic plate of 7 atoms on $(\bar{1}11)$ and $(11\bar{1})$, respectively. As previous case, the dislocation dissociated after preliminary relaxation. During deformation, the heading partial approached the loops and then cut through them before the trailing partial approach the loops. The trailing partial also cut through in the same way at later stage of deformation. It should be noted that the dislocation segment between the two loops only showed very limited bow-out. Those phenomena mean that the vacancy loops cannot exert strong pinning on the dislocation's slipping. However, after intersection, both the two loops stayed at their original sites but with a sheared configuration. Detailed analysis [11] showed the number of vacancies after intersection was also 7, but two vacancies had been sheared into the neighboring layer. That raises a doubt on the local rules used in recent multi-scale modeling of deformation in irradiated materials [3–6], in which the incorporation of defect clusters had been assumed.

3.2. Intersection between an edge dislocation and small interstitial Frank loops containing 61-SIAs

The setup in Fig. 2 is just the same as that in Fig. 1 except that the Frank loops have 61 interstitials. The configuration after preliminary relaxation is quite similar as the case for 7-SIAs loops, but the loops here were not transformed into crowdion bundles. During all the intersection process, the two loops stayed at their original sites while the two partial dislocations contact, then bowed out between and finally unpinned from them at No. 7 stage. Compared with the case of 7-SIAs loops, the intersection stress was increased from 1.3 to 1.8 GPa due to the increase in size of the loops. This qualitatively agrees with the hardening law $\Delta\tau = \alpha Gb(Nd)^{-0.5}$. Detailed analysis [11] showed that, the two loops still kept their extrinsic stacking faults after intersection process.

3.3. Intersection between an edge dislocation and small vacancy Frank loops containing 61 vacancies

The set up shown in Fig. 3 was just the same with that in Fig. 2 except that the loops had 61 vacancies. Obviously, different from the smaller ones, the two loops took a three-dimensional configuration due to the dissociation at periphery. Such configuration actually is an intermediate configuration between Frank loop and SFT, the segments on prismatic planes were just partial dislocations. Serra et al. [11] has reported similar configuration. The dissociation proved that the vacancy Frank loops become unstable when their sizes increase. During deformation from No.1 to No.5 stage, the

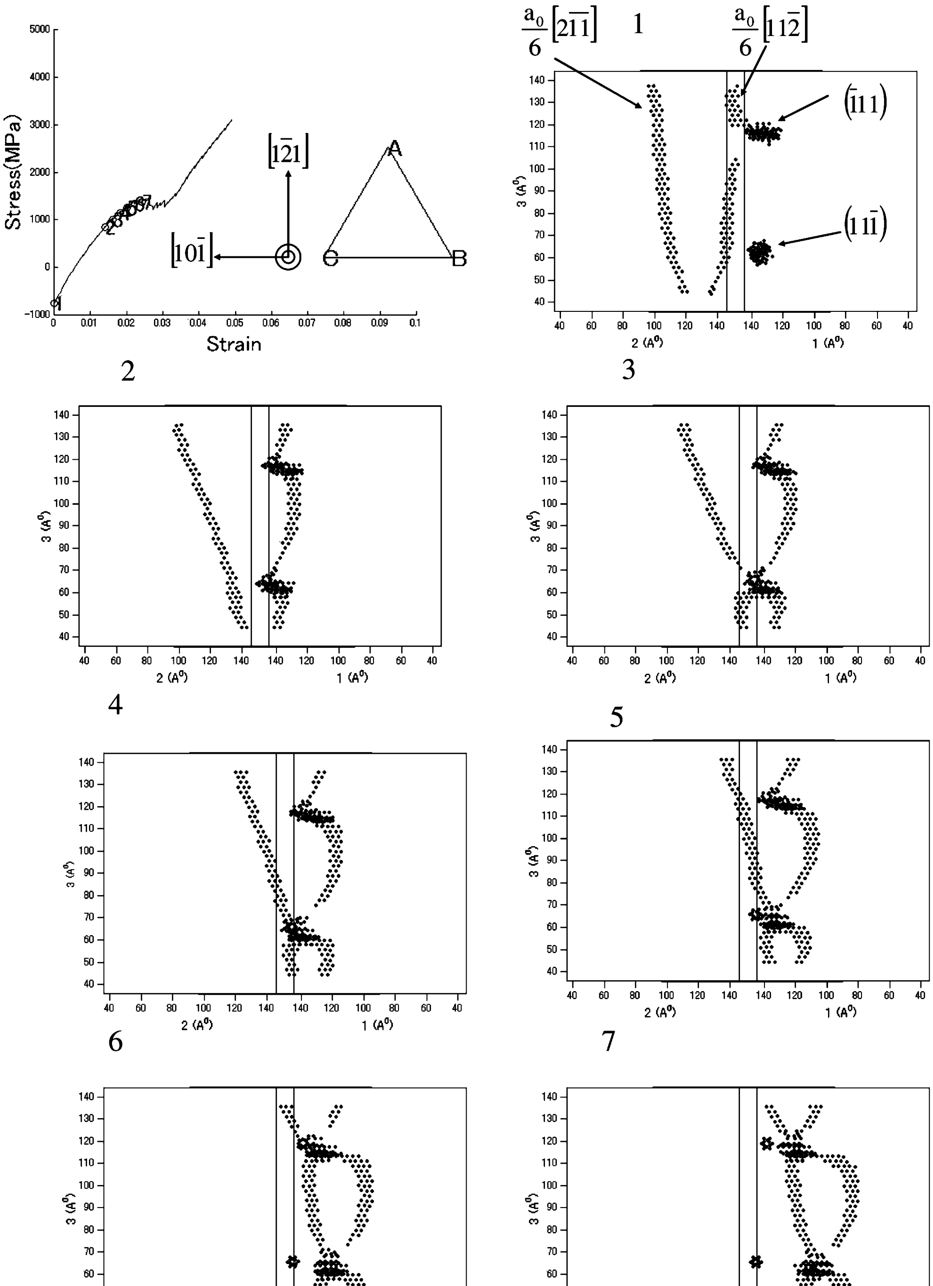

Fig. 1. Interaction between dislocation and 7-SIAs Frank loops. Upper and bottom loops were inserted on $(\bar{1}11)$ and $(11\bar{1})$, respectively. The inserted edge dislocation was $a_0/2[10\bar{1}]$, but it dissociated into two partial dislocations as shown in the figure.

dissociated heading partial approached and bowed out between the two loops, while the trailing partial is caught up. From No. 6 to No. 7 stage, the dislocations finally cut through and induced observable changes to the two loops. However, main parts of the loops stay at their original sites after intersection. Detailed analysis [12] showed that the loop had the same number of vacancies after intersection. The upper loop also follows the same mechanism but not shown here to avoid repeating. Comparing the stress response and the bow-

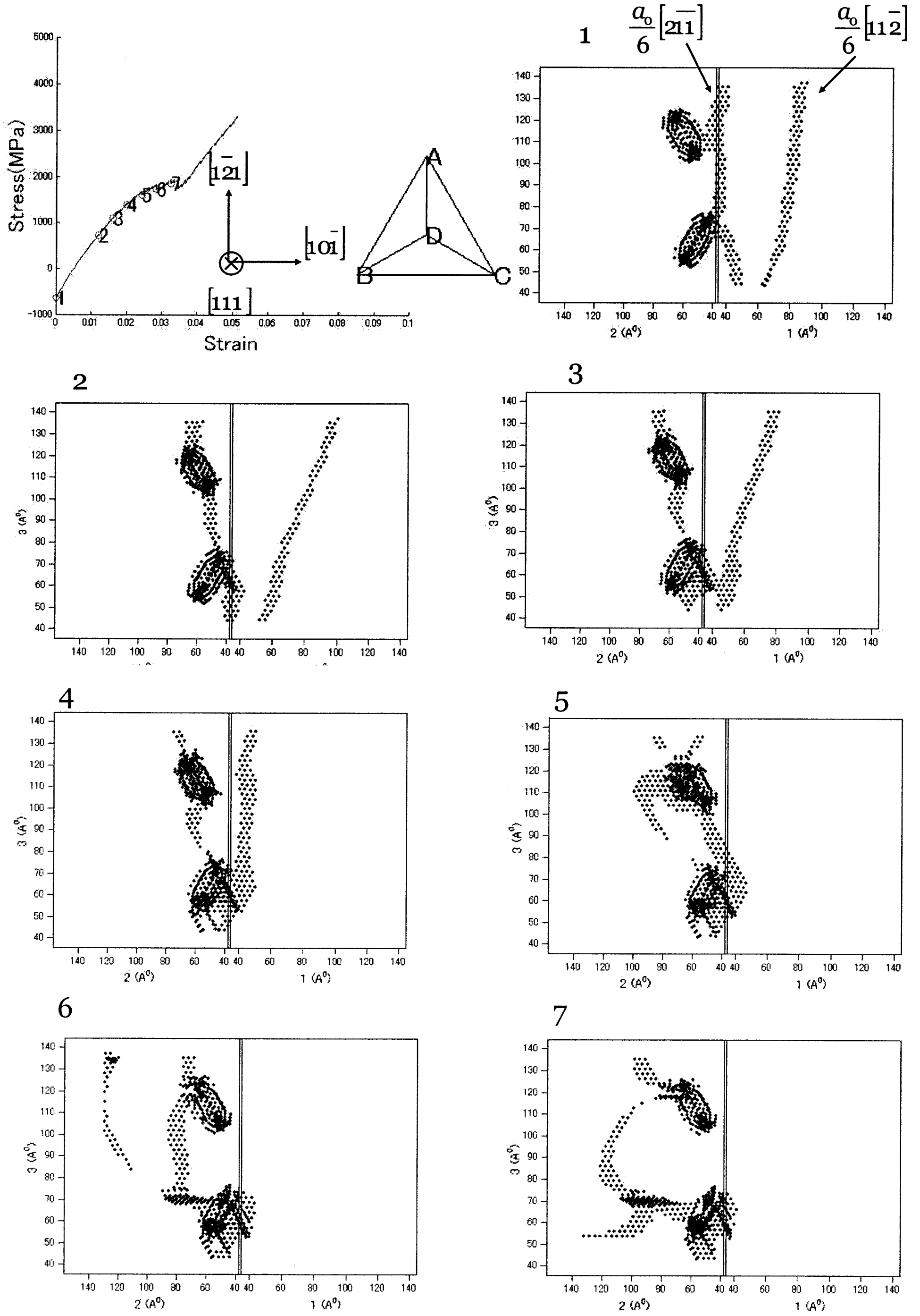

Fig. 2. Interaction between dislocation and 61-SIAs Frank loops. Upper and bottom loops were inserted on $(\bar{1}11)$ and $(11\bar{1})$, respectively. The inserted edge dislocation was $a_0/2[10\bar{1}]$, but it dissociated into two partial dislocations as shown in the figure.

out phenomenon at previous case for smaller loops, larger loops need higher stress level to cut through. This increase is about 100 MPa, which is much smaller than the 600 MPa for comparable interstitial Frank loop cases. Therefore, vacancy Frank loops are weaker obstacles to dislocations compared with interstitial ones.

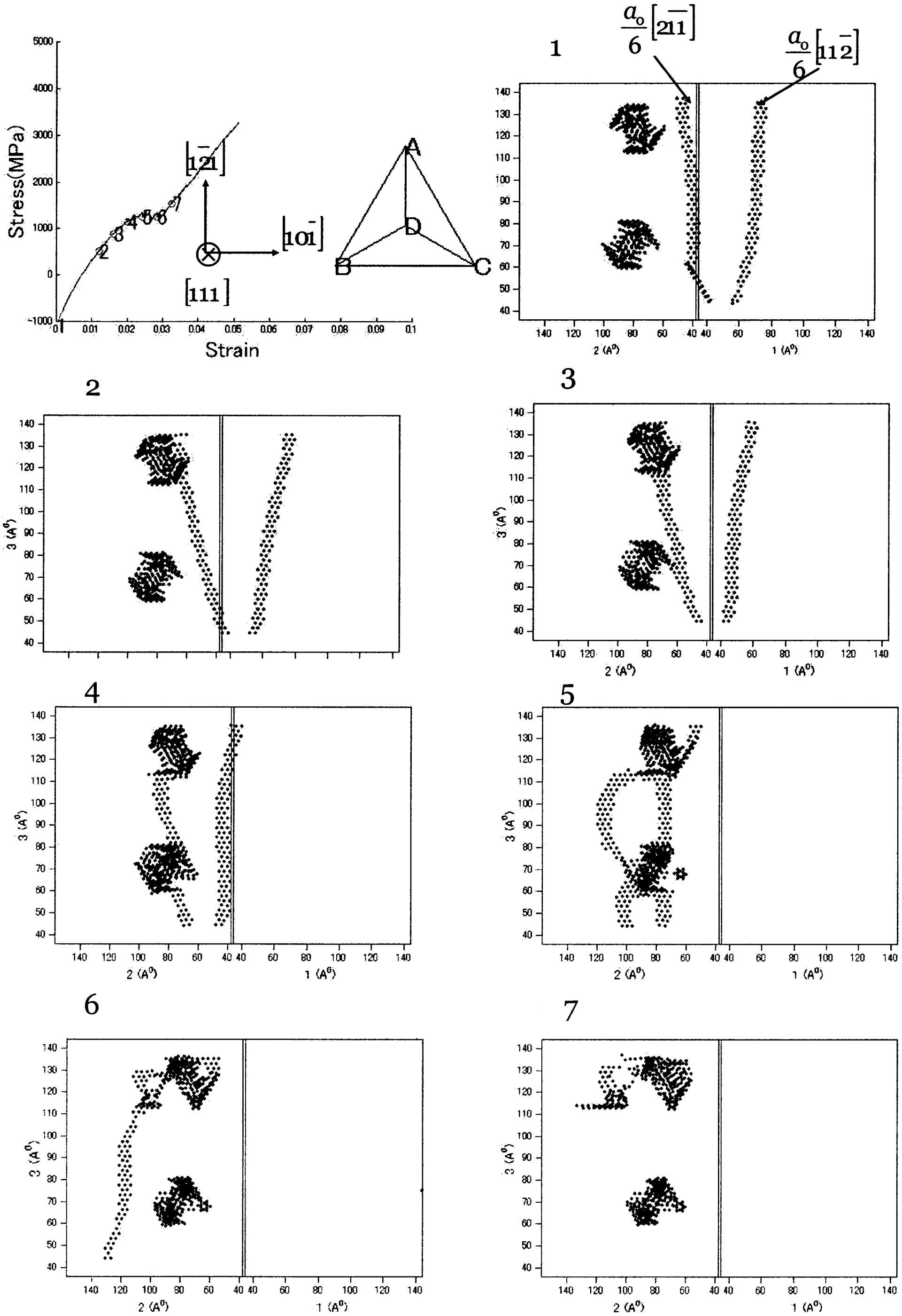

Fig. 3. Interaction between dislocation and 61-vacancies Frank loops. Upper and bottom loops were inserted on $(\bar{1}11)$ and $(11\bar{1})$, respectively. The inserted edge dislocation was $a_0/2[10\bar{1}]$, but it dissociated into two partial dislocations as shown in the figure.

4. Conclusion and discussion

Intersection process between Frank loop and edge dislocation was investigated using molecular dynamics simulation. Interstitial Frank loops were found to be stronger obstacle to dislocation than vacancy ones. Small interstitial Frank loops can be easily swept away by dislocation, but when the size increases they become stable. They can neither be unfaulted nor eliminated by dislocation. Vacancy Frank loops were not stable when their size increase and they cannot be absorbed by dislocation at the temperature in this study.

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