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Computer simulation of the dynamical and thermally activated motion of interstitial clusters in Fe

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Abstract

Using the computer simulation technique various properties of interstitial clusters (bundle of crowdions) in Fe has been investigated. The actual shapes of the hexagonal loops were studied in detail and it was found that the direction of each segment of a loop depends upon the loop size; that is, in smaller loops ⟨1 1 1⟩ direction is preferred and in larger loops ⟨1 1 2⟩ direction is realized, resulting in the higher Peierls stress for smaller loops and lower Peierls stress for larger loops. The behavior of the thermally activated motion of loops has been studied by the MD method, showing that the small loop I_{19} moved along ⟨1 1 1⟩ direction at 100 K under the aid of energy deposition 10 eV in a rather uniform way without clear kink formation.

1. Introduction

In materials under irradiation various phenomena such as cascade formation, one dimensional motion of small interstitial clusters, interaction between a dislocation and interstitial clusters, three dimensional motion of radiation induced defects, dislocation bias, production bias occur and finally complicated damage structures are formed, resulting in the degradation of materials [1–7]. The first step of the total understanding of radiation effects on materials is to obtain the information on a cascade; that is, that of vacancies and self interstitial atoms (SIAs) in a cascade. Many computer simulations have so far been made for the cascade formation [8–10]. Vacancies are mainly located inside of a cascade and SIAs are mainly located outside of a cascade. To obtain the information on vacancies in a cascade, low temperature neutron irradiation and low temperature positron annihilation lifetime measurement are suitable. This was already done by the present authors and gave us the distribution of vacancies, which is rather isolated from each other in the case of Fe and Ni [11,12]. But the information of SIAs in a cascade, especially that of a small cluster of SIAs, e.g., a bundle of crowdions moving outwards one dimensionally from the cascade region, cannot be easily obtained from the experiments, suggesting that computer simulation is definitely required. SIAs generated in a cascade play an important role in the damage structure evolution, that is, isolated SIAs migrate three dimensionally to dislocations and contribute to the so-called dislocation bias, and clusters of SIAs, especially bundles of crowdions which can move one dimensionally to sinks such as dislocations contribute to the so-called production bias. These bias effects make the most important contribution to the damage structure evolution in materials under irradiation, and the underlying features of bias effects must be investigated in more detail through computer simulation, especially the dynamic behavior of the bundle of crowdions. In the present paper the studies made in this direction are reported.

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2. Calculations

A model Fe lattice was constructed by using Finnis–Sinclair potential [13] and into a model lattice a straight edge dislocation or bundle of crowdions of $a/2\langle 1\,1\,1\rangle$ Burgers vector was introduced. The size of the model lattice must be large enough to contain the defects with a long range strain field, such as a dislocation, and the size of a simulation box of about $80b$ (b: magnitude of Burgers vector) cubic was used for the static calculation. For the molecular dynamic calculation (MD calculation) usually smaller boxes were used. Relaxed structures were obtained by the static calculation or the MD calculation [15]. The fixed boundary condition or the periodic boundary condition was applied depending on the defects in the model lattice, that is, the former for the bundle of crowdions and the latter for a straight edge dislocation along the dislocation line.

3. Results and discussion

3.1. Interstitial clusters

It is known that interstitial clusters which can make one dimensional motion and arrive at sinks such as dislocations significantly contribute to the production bias, resulting in the formation of voids in materials under irradiation [8–10,14–22]. The interstitial cluster which can make one dimensional motion is a bundle of crowdions, i.e., a dislocation loop of Burgers vector $(a/2)\langle 1\,1\,1\rangle$ in bcc crystals and $(a/2)\langle 1\,1\,0\rangle$ in fcc crystals. Bundle of crowdions $\mathbf{I}_n$ ($n = 7, 19, 37, 61, 91, \ldots$) are of a hexagonal shape consisting of six edge dislocation segments all of which lie on $\{1\,1\,0\}$ slip planes and make slip motion under the shear stress applied symmetrically on each slip plane as shown in the previous work [14,16]. For this configuration important information, such as, the detailed structure of the dislocation segment, the mobility under shear stress and the behavior of small clusters at finite temperatures must be studied, giving rise to the information needed for the understanding of the production bias.

First of all, the shape of the interstitial clusters (dislocation loops) has been investigated as a function of loop size, where the position of the dislocation center must be determined all through the peripheral region around a hexagonal dislocation loop. The center of a dislocation core was determined as the position where the displacement between two atomic planes just above and below the slip plane becomes $0.5b$ (middle point from zero (negative infinity) to one (positive infinity)) as shown in Fig. 1, where this method is shown for a straight edge dislocation but can be applied for dislocation loops in exactly the same way.

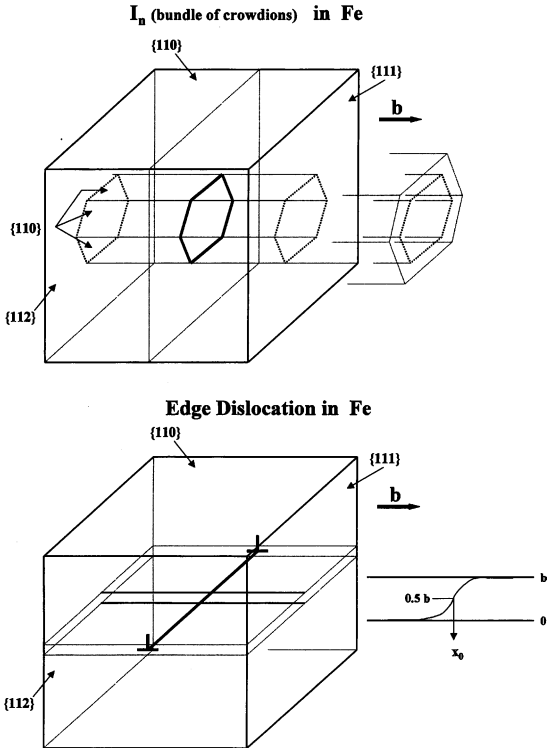

Fig. 1. Schematic drawing for the determination of the center of a dislocation core. (At central position the displacement between two atomic planes just above and below the slip plane becomes $0.5b$.)

There are two possibilities of atomic planes on which dislocation loops, bundle of crowdions in bcc crystals such as Fe, exist, that is, $\{1\,1\,0\}$ plane and $\{1\,1\,1\}$ plane as shown in Fig. 2, where the directions of six segments are also noted. After complete static relaxation of the whole crystal which has a dislocation loop at the central position, however, the actual shapes obtained for dislocation loops are rather complicated depending upon the loop size as shown in Figs. 3 and 4. The dislocation loop of type (b) is formed by bending two segments of $\langle 1\,0\,0\rangle$ direction on that of type (a) towards $\langle 1\,1\,1\rangle$ direction. If this bending is completed, type (a) is converted into type (c), but if bending is stopped half way type (b) is created. It has been observed that for larger loops type (d) is stable, but for smaller ones the type (d) is converted into type (b) and (c) as shown in Fig. 4.

3.2. Stable positions of the dislocation loops

The inherent lattice resistance to the slip motion of dislocation loops of edge character, i.e., Peierls stress, was calculated in the previous paper and the decreasing tendency with increasing loop size was obtained [16]. In

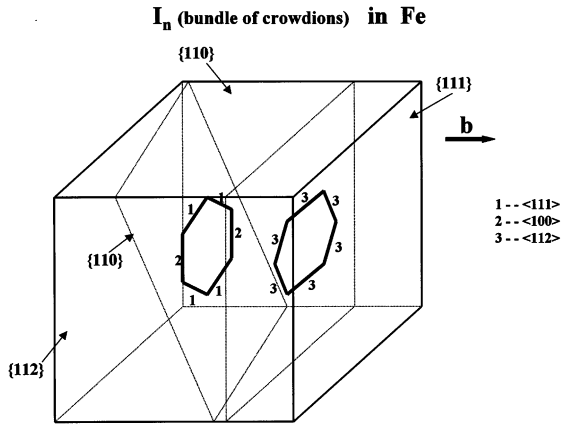

Fig. 2. Dislocation loops on two atomic planes, {1 1 0} plane and {1 1 1} plane in Fe. (The directions of six segments are also denoted.)

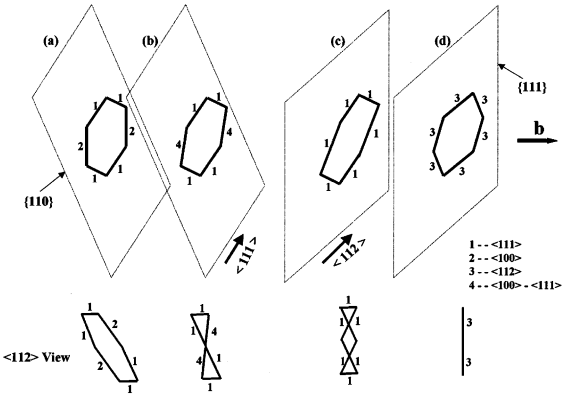

Fig. 3. Types of dislocation loop shapes (a–d) in Fe obtained after relaxation.

I_n (bundle of crowdions) in Fe

I_n	I_7	I_{19}	I_{37}	I_{61}	I_{91}	I_{127}	I_{169}	I_{217}	I_{331}	I_{547}	I_{817}
type	c	c	b	b	b	b	d	d	d	d	d

Fig. 4. Calculated size dependence of the type of the dislocation loops in Fe.

the present paper the stable positions of the dislocation loops were investigated in order to obtain information on the Peierls potential. Stable positions of the cores of the dislocation loops were obtained for hexagonal shaped dislocation loops of various sizes, i.e., I_{19}, I_{217}, I_{817}, I_{1951}, and also for a straight edge dislocation. Basically, the stable position of the dislocation core is usually distributed with a period of b (magnitude of Burgers vector) along $\langle 1\,1\,1\rangle$ direction on the slip plane $\{1\,1\,0\}$, but the edge dislocation line has a special character, i.e., a periodicity of $b/3$ as shown in the inserted figure in Fig. 5, and actually the calculated values of Peierls energy at these points distributed with a periodicity $b/3$ are exactly equal as shown in Fig. 5. In this figure the values of stable points are calculated ones, but the potential shape is schematic because of the difficulty of the calculation of Peierls potential.

On the other hand, in the case of dislocation loops these stable positions are split into two opposite directions as shown in Fig. 5 by a dotted line, that is, the value of x decreases with decreasing loop size. This decreasing behavior of x is shown in Fig. 6, suggesting that through the decrease of a loop size, dislocation

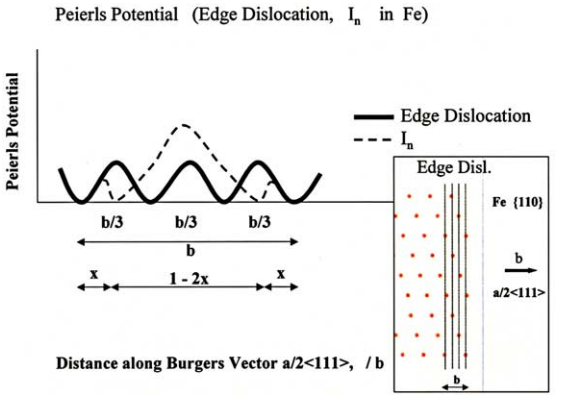

Fig. 5. Calculated stable positions of dislocation loops in Fe (designated by x) together with that for a straight edge dislocation. (In the inserted figure the origin of the periodicity $b/3$ for the edge dislocation is illustrated.)

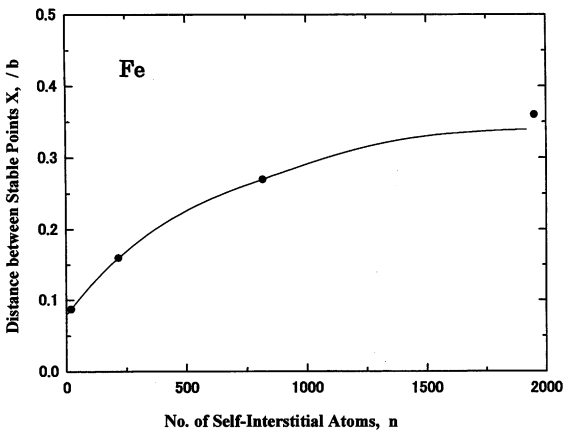

Fig. 6. Calculated values of x as a function of loop size in Fe.

loops tend to have a periodicity nearly b. The important point of this feature is that Peierls potentials which dislocation loops must overcome depend upon the loop size, and smaller Peierls stress can be expected for larger loops and an edge dislocation line probably because of finer periodicity $b/3$. The periodicity of $b/3$ comes from the fact that dislocation segments of a loop have the direction $\langle 1\,1\,2\rangle$, but the periodicity b comes from the direction $\langle 1\,1\,1\rangle$ of a segment. The former is seen for larger dislocation loops and a straight edge dislocation, and the latter is seen for smaller loops as shown in the results in Figs. 3 and 4. The calculated result of decreasing tendency of Peierls stress with the increase of a loop size was previously obtained [16]. In order to confirm this situation in more detail, Peierls stress was obtained in the calculation for two straight dislocation lines, i.e., a pure edge dislocation of $\langle 1\,1\,2\rangle$ direction in Fig. 3 and a dislocation of $\langle 1\,1\,1\rangle$ direction (also in Fig. 3, about 20° from $\langle 1\,1\,2\rangle$) both of which have the same Burgers vector, $(a/2)\langle 1\,1\,1\rangle$ in Fig. 3. The result is that for the former Peierls stress is 0.0004μ (μ: shear modulus) and for the latter 0.0006μ, which supports the consideration above.

3.3. Behavior of dislocation loops at finite temperatures

Since a straight dislocation slips by the aid of the thermally activated kink pair formation, it is reasonable to consider that the same mechanism might occur for the case of motion of dislocation loops. But in the case of smaller limit of dislocation loops some change might occur for this mechanism, because the ratio ($R = D/b$), where D is the diameter of a loop and b is the periodic distance of the motion, the magnitude of Burgers vector, might probably become an important parameter which determines the behavior of motion. By the analytic calculation for this problem using a conventional string model [23], it predicts that in the case of the ratio R smaller than a critical value no meta-stable configuration (such as a kink pair) exists, suggesting that in this case of smaller dislocation loops the motion might be regarded as motion of a cluster of crowdions just like diffusion [21,22,24]. The total concept mentioned here is schematically drawn in Fig. 7, where the value of E/kT is an important parameter determining the character of the thermally activated motion of a dislocation and dislocation loops. For larger value of E/kT the conventional character of kink pair formation can be expected, but for smaller E/kT fast motion in a totally activated fashion will be expected.

In order to clarify this feature the molecular dynamics calculation was made for a small dislocation loop I_{19} at 100 K. Fig. 8 shows a snap shot of thermally activated motion of the cluster I_{19} (type (c) in Fig. 3) expressed by each position of a dislocation core of a hexagonal loop I_{19} mentioned above, where 10 eV is

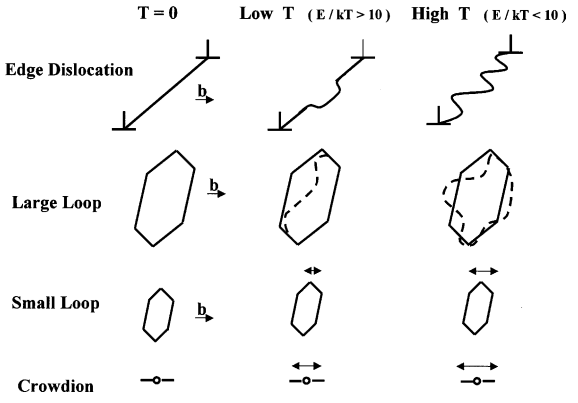

Fig. 7. Schematic drawing of thermally activated motion of a dislocation and dislocation loops as a function of loop size and temperature.

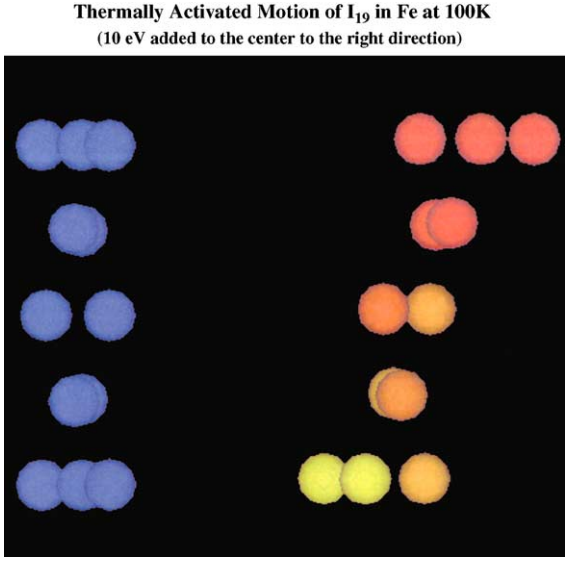

Fig. 8. Result of the MD calculation of the behavior of I_{19} in Fe at 100 K.

added to the central atom in the cluster toward the right direction ($\langle 1\,1\,1\rangle$ direction) at the initial moment so that the activated motion might be caused easily. Within 3 ps the I_{19} loop moved along $\langle 1\,1\,1\rangle$ direction over about 4 atomic distances from the initial position (left) to the final position (right), suggesting that the activation energy is very low, ~0.013 eV. It is very important to establish whether the motion is caused by the formation of a kink pair or not. The sequential observation of the loop motion during 3 ps shows no clear formation of a kink pair, but rather uniform motion of a whole cluster. This means that the motion of I_{19} at 100 K aided by 10 eV addition is rather caused through a total diffusion manner not by a kink pair formation. More detailed

studies will be required for the thermally activated motion of dislocation loops of various sizes over a wide temperature range in order to clarify the intercorrelation between a motion with kink pair formation and that of a total diffusion of a cluster. This will be done in the near future.

4. Summary

In the materials under irradiation the damage structure evolution is determined by bias mechanisms, such as dislocation bias, production bias, etc. In the present paper, some investigations for these two subjects have been performed. Using the computer simulation technique various properties of interstitial clusters (bundle of crowdions) in Fe has been investigated. The actual shapes of the hexagonal loops were studied in detail and it was found that the direction of each segment of a loop depends upon the loop size, that is, in smaller loops $\langle 1\,1\,1\rangle$ direction is preferred and in larger loops $\langle 1\,1\,2\rangle$ direction is realized, resulting in the higher Peierls stress for smaller loops and lower Peierls stress for larger loops. This is due to the periodicity change from $b/3$ to b as the decrease of loop size. The behavior of thermally activated motion of loops has been studied by the MD method, showing that the small loop I_{19} moved along $\langle 1\,1\,1\rangle$ direction at 100 K under the aid of energy deposition 10 eV in a rather uniform way without clear kink formation.

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