Interrelation between Dislocation Loops and an Edge Dislocation

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Since it has recently become an important subject to study the interrelation between a dislocation loop and a straight edge dislocation because of dynamic behaviors of small dislocation loops under irradiation condition, the simulation studies were made in model Fe lattice. It was found that dislocation cores both for a loop and a dislocation can be expressed by the regular array of three types of crowdions and have stable positions of b/3 periodicity, but this regularity and periodicity are disturbed as the decrease of the loop size. The relation between a dislocation core and crowdion types are also studied. Furthermore, this change gives rise to the increase of the inherent lattice resistance (Peierls stress) for the dislocation loops.

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1. Introduction

It is well-known that dislocation loops are produced in crystals through the condensation process of supersaturated point defects such as vacancies and self-interstitial atoms (SIAs) and also produced as punched-out loops from oversized precipitates in the matrix, furthermore it is recently known that they are produced through the direct formation (SIA loops) from cascades induced by the irradiation which produces high energy primary knock-on atoms (PKAs). In the last one it is recognized that emitted small SIA clusters (SIA loops) make one dimensional motion and disappear at sinks such as dislocations and grain boundaries, resulting in the void swelling due to the so-called production bias (an important bias in the matrix under irradiation together with the dislocation bias) (an important bias in the matrix under irradiation together with the dislocation bias). SIA loops which make one dimensional motion are bundles of crowdions, that is, dislocation loops of the edge character with Burgers vector a/2(111) in bcc metals. Easy one dimensional motion of small SIA loops to sinks gives rise to excess vacancies in the matrix which cause void swelling of the material under irradiation. Consequently the detailed studies of the structure and the dynamic motion of small SIA clusters (loops) are required to have the comprehensive understanding for this void swelling phenomenon which plays a key role for the material development in the irradiation environments such as fission reactors and fusion reactors. In this paper the interrelation between dislocation loops and an edge dislocation will be investigated on the standpoint of both point defects (crowdions) and a dislocation.

2. Calculations

In order to investigate fundamental characters of dislocation loops and a straight edge dislocation, model Fe lattice was constructed by using Finnis-Sinclair potential and into a model lattice a straight edge dislocation or a bundle of crowdions of a/2(111) 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 a size of simulation box is about 80b (b: magnitude of Burgers vector) cubic was used for the static calculation, but for the molecular dynamic calculation (MD calculation) usually smaller boxes were used. Relaxed structures were obtained by the static calculation or the MD calculation. The fixed boundary condition or the periodic boundary condition was applied depending on the defects in the model lattice, that is, the former for a bundle of crowdions and the latter for a straight edge dislocation along the dislocation line. The present positions of a dislocation line and a dislocation loop (variable along a loop periphery) were determined by a conventional way, that is, as a position where the displace-
ment between two atomic planes just above and below a slip plane becomes \( b/2 \) as shown in Fig. 1. Each crowdion constituting a loop, especially ones existing on a loop periphery was characterized as a deviation from the isolated crowdion, that is, the change of a distribution of the interatomic distance between adjacent two atoms along the crowdion axis. The core structures of an edge dislocation and a dislocation loop were also obtained by drawing the atomic configurations obtained after full relaxation of a whole lattice. Dynamical properties were studied under the condition of the shear stress application, which was made by a conventional way for a straight edge dislocation, but for a dislocation loop was made axial symmetrically as shown in Fig. 2. Behaviors of small loops at finite temperatures were studied by using MD calculations.\(^6\)–\(^{11}\)

3. Results and Discussion

3.1 Crowdions (isolated and bundled) and edge dislocation

It is well known that a crowdion has a structure which has an extra atom on the crowdion axis and has a strain field extending along this axis, i.e., \( (111) \) direction in the case of bcc metals. To characterize this crowdion the distribution of the interatomic distance between adjacent two atoms along a crowdion axis, that is, along \( (111) \) direction was obtained after full relaxation of a whole crystal which has a crowdion at a central position. Two kinds of distribution were obtained as shown in Fig. 3, where two patterns are shown, namely, one shortest distance exist (type 1), and two shortest distances exist (type 2) in the central position of a crowdion. In the other words, the center of the strain distribution is located between two atoms in the former, but that is located on an atom in the latter. These two have almost equal energies as shown in this figure, where a slightly higher energy is seen for the type 2 than the type 1.

These distributions for isolated crowdions are, however, changed when crowdions are bundled, that is, in dislocation

**Formation Energy of a Crowdion in Fe**

- **type-1**: 3.938903 eV
- **type-2**: 3.947848 eV

Fig. 2 The method to apply the axially symmetrical shear stress on a dislocation loop of a hexagonal shape.

Fig. 3 Two types of crowdions in Fe: type 1 and type 2 with their formation energies.
loops and in a straight edge dislocation. The most typical case is for a straight edge dislocation of $a/2(111)$ Burgers vector lying on a $[110]$ plane extending along $(112)$ direction, and the distribution of the atomic distance for a crowdion existing on the atomic plane just above a slip plane of a dislocation is shown in Fig. 4, where three types of crowdions are seen, that is, type 1 and type $2^+$ and type $2^-$. The type 1 is essentially same as that for an isolated crowdion but strain localization is
rather low. Type $2^+$ and $2^-$ are slightly deformed structures to plus (one direction along (111) crowdion axis) or minus (the opposite) direction of the type 2 for an isolated crowdion and the strain localization is again low compared with that for the isolated one.

The reason why three types are needed comes from the crystal structure itself, that is, as shown in Fig. 4 (inserted figure), (112) direction of a straight edge dislocation has a periodic structure of three atomic distances on (110) plane. There exist three types of core structures corresponding to these three types of crowdions as shown in this figure, but schematically. The ones obtained from the real simulation are shown in Fig. 5, the cross sectional view of a straight edge dislocation line, where type 1 crowdion corresponds to the dislocation core structure with its center on the boundary of two adjacent triangles, type $2^+$ corresponds to that with its center in the downward triangle and type $2^-$ corresponds to that with its center in the upward triangle.

The actual array of these three types of crowdions along a straight edge dislocation line is shown in Fig. 6, where periodic array of type 1, $2^+$, $2^-$ expressed by dots are shown. The position of these dots representing crowdion types are placed at the positions of the dislocation core as shown in Figs. 4 and 5, almost on a straight line.
3.2 Stable positions of edge dislocation and dislocation loops

In Fig. 6 not only as grown stable position of a straight edge dislocation, but also other stable positions obtained by stressing (shear stress) and unstressing processes are also shown, suggesting unexpected results that stable positions of a straight edge dislocation are distributed with a periodicity of \( b/3 \) and every \( b/3 \) periodicity crowdion types are regularly changed, that is, shifting one atomic distance along a dislocation line as shown schematically in Fig. 7, and every \( b \) periodicity the same configuration of the crowdion type are realized. This is the peculiar property of a straight edge dislocation lying along \( \langle 112 \rangle \) direction, but a dislocation along \( \langle 111 \rangle \) direction, i.e., 70° dislocation has not this property, but has only one type of crowndions and a periodicity of \( b \) as shown in Fig. 8.

It is then the most important subject that the situation observed here for a straight edge dislocation remains or not for dislocation loops. In order to investigate this point, the same analysis as that for a straight edge dislocation was made for dislocation loops of pure edge character which have \( a/2 \langle 111 \rangle \) Burgers vector and a hexagonal loop shape as shown in Fig. 1. The result for a segment of a hexagonal loop \( I_{547} \), a dislocation loop consisting of 547 SIAs (a bundle of crowndions), is shown in Fig. 9 (for a bottom segment of a hexagonal loop). The direction of the edge segment of this loop is almost \( \langle 112 \rangle \), just like a straight edge dislocation, but not exactly, especially at both end parts. The other stable positions obtained by the same way as that for a straight edge dislocation are similar to that for the edge case, but exactly speaking the \( b/3 \) periodicity is clearly disturbed by the segment end effect. This end effect is considered to be the very essential one for a dislocation loop. The schematic view of this hexagonal dislocation loop \( I_{547} \) with three types of crowndions is shown in Fig. 10.

The same analysis was made for a segment of a hexagonal loop \( I_{127} \), a dislocation loop consisting of 127 SIAs (a bundle of crowndions) and the result is shown in Fig. 11, where the direction of the segment is not \( \langle 112 \rangle \), but is about 20 degree rotated to \( \langle 111 \rangle \) and consists of only one type of crowndions, just like a 70° dislocation mentioned above. The loop of this configuration has \( b \) periodicity as a 70° dislocation. The schematic view of this hexagonal dislocation loop \( I_{127} \) with three types of crowndions is again shown in Fig. 12.

The change of the dislocation loop shape and the habit plane on which loops lie are obtained after full relaxation of a model lattice which has a loop and are shown in Figs. 13 and 14, where larger loops have \( \{ 111 \} \) habit planes and each segment of a loop has \( \langle 112 \rangle \) direction, but a habit plane for smaller loops has tendency to fall down to \( \{ 110 \} \) plane, and the segment direction has \( \langle 111 \rangle \) direction. These changes are considered to be responsible for the increase of lattice resistance of dislocation loops with decreasing loop size.

3.3 Peierls stress for edge dislocation and dislocation loops

As the decrease of the size of a dislocation loop the regularity of an edge dislocation core structure is gradually disturbed, which results in the increase of the inherent lattice resistance (Peierls potential and Peierls force) for the
dislocation loops as shown in Fig. 15 obtained from the stressing simulation shown in Fig. 2. It is considered that the regular structure of the periodicity of $b/3$ in a straight edge dislocation gives the lowest Peierls stress, and the disturbance of this situation in dislocation loops results in the increase of Peierls stress.

3.4 Thermally activated motion of small dislocation loops

In actual crystals small dislocation loops make one dimensional motion via thermally activated process. In this process the most important subject is if the kink pair formation occurs or not on a dislocation loop line. This has been studied by classical string model and the kink pair formation can be expected on a dislocation loop beyond a certain size, and the details of this study will be published on the other paper. MD simulations were also made for small dislocation loops $I_{19}$, $I_{37}$ at 100 K, 300 K for 3 ps, and a clear kink pair formation has not been observed, but fluctuation of a dislocation loop line has been observed as shown in Fig. 16, where the result of MD simulation of $I_{37}$ in Fe at 300 K, 3 ps is shown. The color change from blue to red shows the shift ($2b$) to the right direction in this figure. (At $t = 0$ ps 10 eV is given to the central atom of the loop to the right direction)

This simulation must be extended to larger dislocation loops which is the future work.

4. Summary

It is nowadays a very noticeable subject to study the interrelation between a dislocation loop and a straight edge dislocation, because in the field of radiation damage one dimensional motion of small interstitial clusters, dislocation loops is considered to be one of the origin of the bias effect which causes the void swelling of the materials used in the irradiation environments. Simulation studies were made in model Fe lattice to clarify the basic properties of dislocation loops on the viewpoint of the interrelation between a dislocation and a dislocation loop. It was found that dislocation cores both for a loop and a dislocation can be expressed by the regular array of three types of crowdions and have stable positions of $b/3$ periodicity, but this regularity and periodicity are disturbed as the decrease of the loop size. Furthermore, this change gives rise to the increase of the inherent lattice resistance (Peierls stress) for
the dislocation loops. Thermally activated motion of small loops has been studied by both classical string model and MD simulation, and kink pair formation on a dislocation loop has been discussed.

REFERENCES