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Computer simulation of the interaction between an edge dislocation and interstitial clusters in Fe and Ni

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Abstract

Atomic structures of interstitial type dislocation loops and the interaction between these loops and an edge dislocation have been investigated for Fe and Ni by means of computer simulation in order to understand the basic feature of the damage structure evolution during irradiation which provides cascade formation of defects. Clusters of crowdions or dumbbells were placed in the model lattices and final structures were observed after full relaxation. It is found that in the case of clusters of crowdions, relaxation of the structure, namely, split of strain concentration for each crowdion in the cluster occurs with increasing the number of crowdions in one cluster, i.e., beyond about ten, and this split structure indicates the transition to dislocation loops, because a straight edge dislocation has the same split nature both in Fe and Ni. In the study of the interaction between an initial cluster and an edge dislocation it is found that a stacking fault of an extended edge dislocation is heavily deformed by the presence of an interstitial cluster just below the slip plane. Finally the critical stress for the motion of an interstitial loop, that is, Peierls stress, for the dislocation loop was investigated and it is found that as the loop size increases, Peierls stress decreases and approaches the level for a straight edge dislocation.

1. Introduction

Structures and dynamic behaviors of interstitial clusters and interaction between these clusters and an edge dislocation have recently become very important in the study of damage evolution in the materials under high temperature and high dose irradiation. It is well known that the bias effect is very important in the evolution of damage structure during irradiation. Recently, not only dislocation bias [1–5] but also production bias has become important, where small interstitial clusters play key roles as shown in the computer simulation [6,7]. However, detailed structures of small interstitial clusters and dynamic behavior, such as response to the applied stress have not been clarified yet. Recent progress in the atomic potential models and the computer techniques have made it possible to calculate detailed structures of defect clusters and interaction between them in the model lattices of acceptable size. In the present study structures and interaction behaviors between small interstitial clusters and an edge dislocation, and the response to the applied stress are investigated by embedded atom method (EAM) type potentials for Fe (bcc) and Ni (fcc).

2. Calculation method

To study the interaction between small interstitial clusters and an edge dislocation the model crystals of Fe and Ni which have large enough size to place these defects were constructed by using *N*-body potentials, that is, Finnis–Sinclair potential for Fe [8] and that given by Gao et al. [9] for Ni and were completely relaxed by the static method. Interstitial clusters were formed by placing crowdions (⟨1 1 1⟩ for Fe and ⟨1 1 0⟩ for Ni) or dumbbells (⟨1 1 0⟩ for Fe and ⟨1 0 0⟩ for Ni) on {1 1 0} plane in Fe and on {1 1 1} plane in Ni. Edge dislocations

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were also inserted on these planes and in the case of Ni an extended dislocation was finally obtained.

3. Results and discussion

3.1. Interaction between dislocation loop and edge dislocation

Formation energies of a crowdion and a dumbbell were obtained for Fe and Ni as shown in Table 1 together with energies for vacancies. Before the study of the interaction between a dislocation loop and an edge dislocation characters of interstitial clusters consisting of crowdions were investigated and results are shown in Fig. 1 for Fe. Large interstitial clusters are considered to be dislocation loops because it was found from the present calculation that concentrated strain of each crowdion begins to be split into two parts on the crowdion axis in the clusters of more than ten crowdions as shown in Fig. 1 (for a dislocation loop I_{91}), where the ordinate shows the distance between two adjacent atoms on the $\langle 1\ 1\ 1\rangle$ crowdion axis, i.e., $z_{k+1} - z_k - 1$ (difference of z-coordinate (parallel to $\langle 1\ 1\ 1\rangle$ crowdion axis) in unit of b) expressed as the difference from the interatomic distance of the perfect lattice b. This splitting tendency is also seen in a straight edge dislocation if atomic rows parallel to Burgers vector above a slip plane are considered to be stacking of infinite numbers of crowdions. The same tendency was obtained in clusters of $\langle 1\ 1\ 0\rangle$ crowdions in Ni.

Slip planes of dislocation loops are not loop planes but tube surface planes surrounding the loops and Burgers vectors $a/2\langle 1\ 1\ 0\rangle$ for Ni and $a/2\langle 1\ 1\ 1\rangle$ for Fe lie in the hexagonal tube planes, that is, four $\{1\ 1\ 1\}$ planes and two $\{1\ 0\ 0\}$ planes in Ni and six $\{1\ 1\ 0\}$ planes in Fe. It is clearly seen that $a/2\langle 1\ 1\ 0\rangle$ dislocation loop in Ni is extended on four $\{1\ 1\ 1\}$ planes into two partial dislocations with stacking fault regions between them, but is not extended on two $\{1\ 0\ 0\}$ planes. If this loop in Ni contacts with an extended straight edge dislocation, a big change of structure occurs for both a loop and an edge dislocation as shown in Fig. 2. In Fe a dislocation loop is not extended on the hexagonal slip plane, but on contact with a straight edge dislocation both a loop and an edge dislocation are heavily deformed. These calculational results show the strong interaction between a dislocation loop and a straight edge dislocation both in fcc and bcc metals.

Table 1
Formation energies of self-interstitial atoms in Fe and Ni

	Fe	Ni
Crowdion	$\langle 1\ 1\ 1\rangle$ crowdion 3.94 eV	$\langle 1\ 1\ 0\rangle$ crowdion 5.11 eV
Dumbbell	$\langle 1\ 1\ 0\rangle$ dumbbell 3.89 eV	$\langle 1\ 0\ 0\rangle$ dumbbell 4.86 eV
Vacancy	1.83 eV	1.42 eV

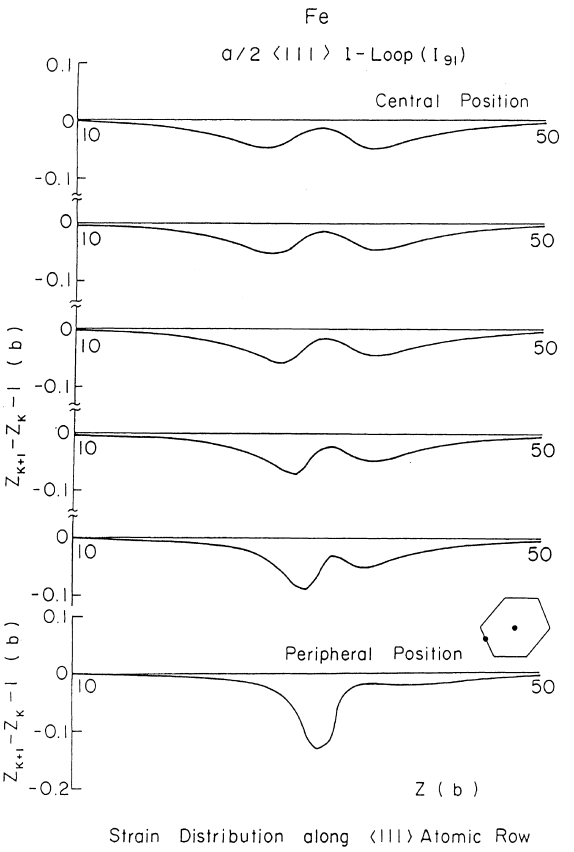

Fig. 1. Distribution of the interatomic distance between two adjacent atoms on each $\langle 1\ 1\ 1\rangle$ crowdion axis in an interstitial cluster (dislocation loop I_{91}) in Fe.

In Fig. 3 formation energies of interstitial clusters I_7 and I_{19} are shown as a function of distance from the dislocation (exactly speaking, from the slip plane of an edge dislocation) for Fe. Interstitial clusters slide on the hexagonal tube drawn above. It is seen that the formation energy rapidly increases in the vicinity of the dislocation core, especially on the hexagonal tube b, that is, binding energy rapidly increases, but its behavior depends on the relative position a, b and c. It is reasonable that on tube b the decrease of formation energy is larger than the other two tubes a and c because interstitial clusters are mainly located in the expansive strain field of an edge dislocation. I_7 on the tube a shows rapid decrease of formation energy because of structural relaxation of I_7, that is, change of the crowdion direction occurs for three of seven crowdions in the cluster, that is, from the original direction to that parallel to the Burgers vector of an edge dislocation by the strong interaction force from the dislocation. I_{19} on the tube a shows rather

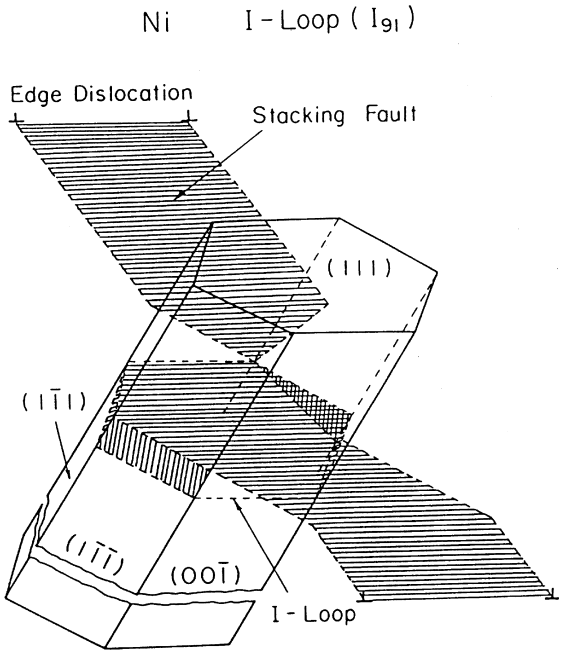

Fig. 2. $a/2\langle 1\ 1\ 0\rangle$ dislocation loop I_{91} and an extended edge dislocation interacting with each other in Ni.

complicated behavior, i.e., decrease and increase of formation energy in the neighborhood of a dislocation core, where the increase comes from the bowing out of an edge dislocation line. Almost the same tendency is seen for the case of Ni, where the interaction between interstitial clusters and one of two partial dislocations of an extended edge dislocation is calculated.

3.2. Peierls stress for interstitial dislocation loop

Motion of small interstitial dislocation loops plays a very important role in the production bias mechanism [6,7] and the experimental evidences are also obtained [10]. It is well known that a dislocation line makes slip motion on a slip plane under applied shear stress, and it is reasonable to apply the cylindrical (axial symmetrical) shear stress to the dislocation loop as shown in Fig. 4. The critical shear stress under which the loop starts to move on the hexagonal tube shaped slip plane, that is, the Peierls stress for the dislocation loop, was obtained as a function of loop size, i.e., number of $\langle 1\ 1\ 1\rangle$ crowdions in the loop for Fe. The result for $a/2\langle 1\ 1\ 1\rangle$ dislocation loops in Fe is shown in Fig. 5, where Peierls stress decreases as the loop size increases and reaches the value for the straight edge dislocation. It is not so easy to explain this tendency. One thing which must be discussed is that in smaller dislocation loops character of each $\langle 1\ 1\ 1\rangle$ crowdion still remains because the

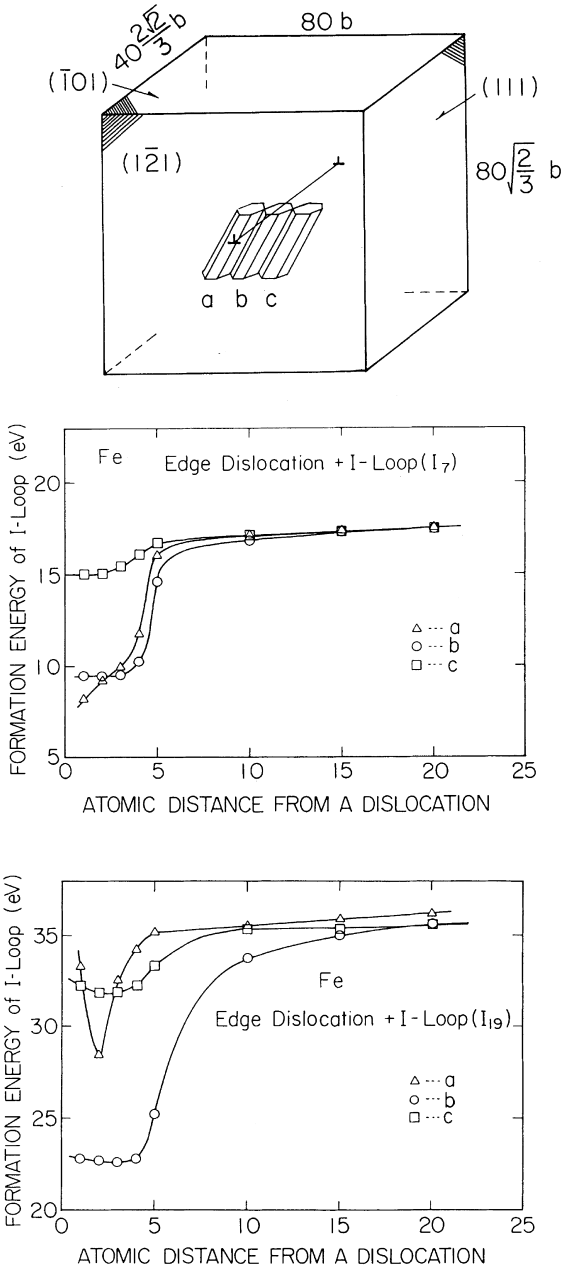

Fig. 3. Relation between formation energies of I_7 and I_{19} and the distance from the edge dislocation line on three different paths a, b and c as drawn above for Fe.

distribution of Burgers vector along the slip plane is not smooth which is contrary to the smooth distribution in a straight edge dislocation and this might give the resistance force to the motion of the total dislocation loop. More detailed investigations will be required to obtain further understanding.

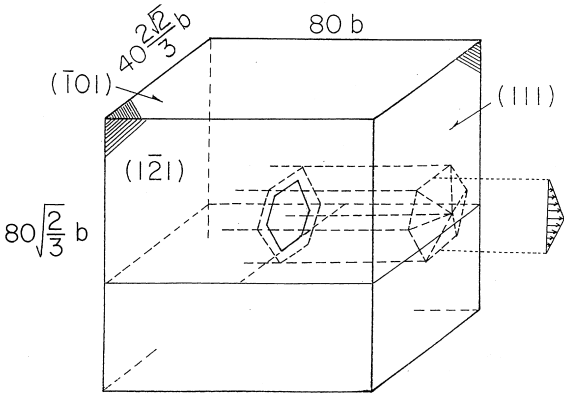

Fig. 4. $a/2\langle 1\ 1\ 1\rangle$ dislocation loop and cylindrical (axial symmetrical) shear stress applied on the loop in Fe.

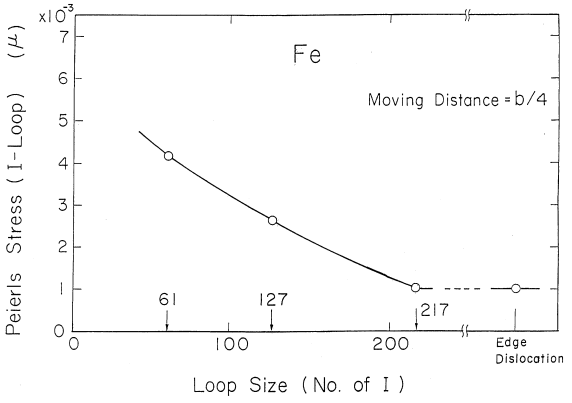

Fig. 5. Relation between the Peierls stress for the $a/2\langle 1\ 1\ 1\rangle$ dislocation loop and the loop size, i.e., number of $\langle 1\ 1\ 1\rangle$ crowdions in the loop for Fe.

4. Conclusion

Clusters of self-interstitial atoms in Fe and Ni were formed in the model lattice and it was found that increasing the number of crowdions in the cluster splitting of the localized strain, i.e., relaxation occurs along the $\langle 1\ 1\ 1\rangle$ crowdion axis especially in the central part of the loop, which suggests that clusters have tendency to convert to dislocation loops, because a straight edge dislocation has the same behavior as this. The interaction between a dislocation loop and a straight edge dislocation was investigated and it was found that for both Fe and Ni the binding between these two is very strong and sometimes morphology changes occur for both of them. Dynamic behavior of a dislocation loop was investigated under the cylindrical shear stress and it was found that Peierls stress for a dislocation loop decreases with increasing loop size probably due to the loss of strain localization of constituting crowdions.

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