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Journal of Nuclear Materials 271&272 (1999) 205–208

journal of nuclear materials

MD study of the dynamic behavior of small interstitial clusters in Fe

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Abstract

Dynamic behavior of small interstitial clusters (dislocation loops), such as the interaction with a self-interstitial atom (SIA) in Fe and the interaction between a SIA and an edge dislocation in Fe have been studied by means of molecular dynamics (MD) method in order to clarify their role in the evolution of damage structure during irradiation, especially in the so-called production bias effect through one-dimensional migration to sinks and in the so-called dislocation bias. Model crystal was constructed by using N-body potentials and small interstitial clusters, i.e., bundle of crowdions, a SIA and an edge dislocation were inserted. It was found that a SIA migrates to the edge dislocation core and finally the direction of the crowdion is converted to the direction parallel to the Burgers vector of the edge dislocation. Dynamic behavior of the loop, e.g., the interaction with a crowdion on a central ⟨1 1 1⟩ loop axis was also investigated as a function of time. It was shown that small initial cluster, e.g., I_{19} in Fe is very mobile under the interaction with a crowdion, which shows that this interstitial cluster I_{19} has already property of a dislocation loop of edge character and low Peierls potential for the motion of this loop, which is consistent with the straight edge dislocation in Fe.

1. Introduction

In the study of radiation effects of materials used under high dose and high temperature irradiation, microscopic feature of the evolution of damage structure must be clarified. Radiation induced defects are highly mobile at high temperatures, and some of them that are not mutually annihilated form clusters of vacancy type and interstitial type, causing the change of material characteristics. It has been recognized that various kinds of bias factors are very important for the formation of these clusters. The interaction between self-interstitial atoms (SIAs) and edge dislocations is stronger than that between vacancies and edge dislocations, resulting in the unbalance between the vacancy flow and the interstitial flow in space and time, which makes the formation of each cluster possible (the so-called dislocation bias [1–6]). On the other hand, recently the other bias mechanism, that is, so-called production bias has been proposed, where spontaneous formation and emission of small interstitial clusters from cascade regions may contribute to the bias effect through arrival of them at sinks, such as dislocations, which finally contributes to the resultant evolution of damage structure, namely, void formation, dislocation loops and networks [7,8]. In the present study dynamic behavior of small interstitial clusters interacting with a SIA and the interaction between a SIA and an edge dislocation in Fe will be investigated and described in order to contribute to the study of damage structure evolution.

2. Calculational method

Using the interatomic potential for Fe a model crystal of about 3000 lattice points was constructed and defects were induced as shown in Figs. 1 and 2. A straight edge dislocation on {1 1 0} plane and a SIA were induced in Fig. 1. A cluster of SIAs, i.e., ⟨1 1 1⟩ crowdions I_{19} arranged on {1 1 0} plane and a SIA on a

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0022-3115/99/$ – see front matter
PII: S0022-3115(98)00740-5

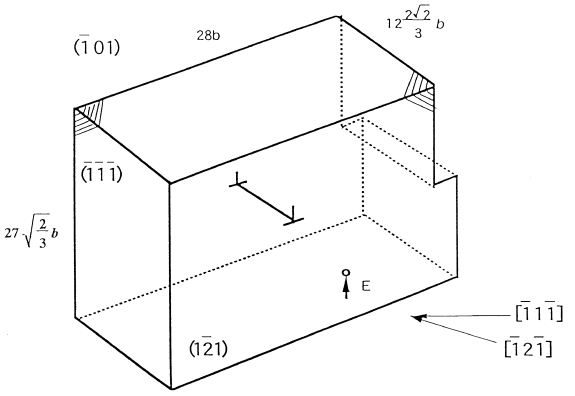

Fig. 1. Model Fe lattice with an straight edge dislocation on {1 1 0} slip plane and a SIA below slip plane interacting each other.

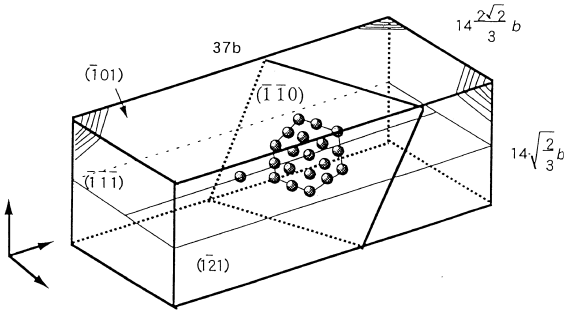

Fig. 2. Model Fe lattice with a cluster of ⟨1 1 1⟩ crowdions I_{19} on {1 1 0} plane and a SIA on a central ⟨1 1 1⟩ atomic row of the cluster.

central ⟨1 1 1⟩ atomic row of the cluster were induced in Fig. 2. The choice of the inter-atomic potential is the most important process in the simulation study, and here the embedded atom method (EAM) type N-body potential by Finnis–Sinclair [9] for Fe (original one) was used. Relaxation of the model lattice with defects was carried out by the molecular dynamics (MD) method with a fixed boundary condition. The MD calculations at finite temperatures were made by the so-called canonical ensemble method developed by Nose [10].

3. Results and discussion

3.1. Interaction between SIA and edge dislocation

To study the dynamic interaction between a SIA and an edge dislocation in Fe the initial kinetic energy 50 eV was given to the lattice point indicated by the arrow in Fig. 3 to generate a SIA in the model Fe lattice. This lattice point is 4 atomic distances below the slip plane of the edge dislocation. The emitted SIA started to move upward in the figure, namely, in the ⟨1 1 0⟩ direction leaving a vacancy behind. In this simulation no external heat is supplied, but the kinetic energy given to the initial lattice point is still conserved even after generation of a SIA and the lattice showed the temperature change as shown in Fig. 4. Numbers denoted in the figure is number of steps (one time step is about 1 fs ($=10^{-15}$ s)). At about step 100 the emitted SIA (⟨1 1 0⟩ dumbbell) recoils into the next lattice point and it keeps moving forward motion until about step 500 and reaches the slip plane of the edge dislocation. By this time the initial kinetic energy of the SIA is nearly gone and the configuration and direction change from ⟨1 1 0⟩ dumbbell to ⟨1 1 1⟩ crowdion. This results in motion toward the dislocation core, namely, motion parallel to the slip plane as a ⟨1 1 1⟩ crowdion until step 2000. Finally it reaches the position just below the dislocation core as a

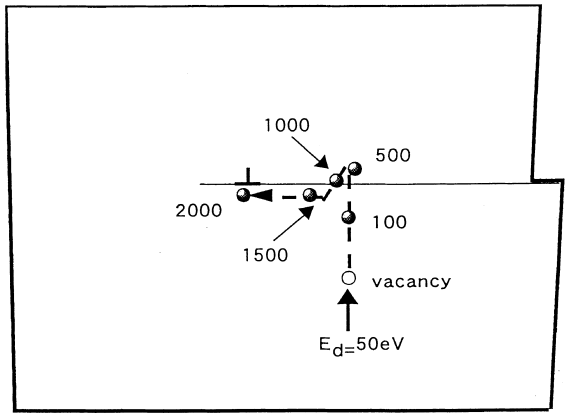

Fig. 3. Time sequence of the dynamic interaction between an edge dislocation on {1 1 0} slip plane and a generated SIA under 50 eV toward the slip plane in Fe.

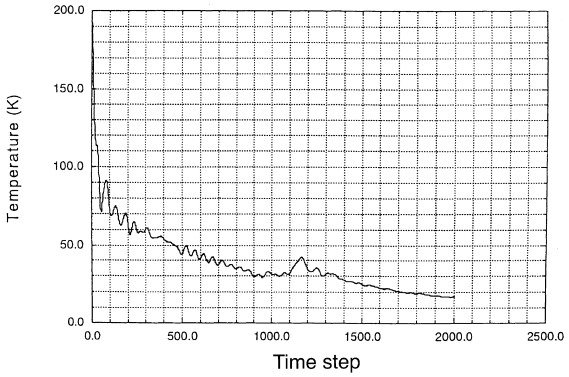

Fig. 4. Temperature change of the lattice during the dynamic interaction between an edge dislocation on {1 1 0} slip plane and a generated SIA shown in Fig. 3.

⟨1 1 1⟩ crowdion parallel to the Burgers vector of the edge dislocation. This conversion from dumbbell to crowdion was also observed in the MD simulation made by Kamiyama et al. [6] in V. In the temperature change in Fig. 4 the small increase at about step 1200 is probably due to the generation of binding energy between the crowdion and the edge dislocation. Almost the same result was obtained in the case where the initial SIA was generated on the opposite side of the slip plane, that is, 4 atomic distances above the slip plane in Fig. 3.

3.2. Dynamic behavior of small interstitial loops

It is known that small interstitial loops are mobile in a one-dimensional way during irradiation [11] and contribute to the production bias when the cascade formation of damage occurs. It is, however, not known under what kind of stress small interstitial loops move one-dimensionally. Dislocations usually move under uniform shear stress, but for dislocation loops with Burgers vector perpendicular to a loop plane the shear stress with axial symmetry (symmetrical around a loop axis) is considered to activate one-dimensional motion. As an example a crowdion is placed on the central ⟨1 1 1⟩ atomic row of the loop, because this crowdion supplies the axial shear stress to the loop. In the actual irradiation situation at high temperatures there are many opportunities of a crowdion being on the ⟨1 1 1⟩ atomic row of the loop axis. To study the dynamic interaction between a loop and a crowdion, a molar dynamics calculation was performed in the Fe model lattice as shown in Fig. 2. The top views of the model lattice (see through all the atomic layers ($\bar{1}$ 0 1) from the top to the bottom) are shown in Fig. 5, where the location of both a 19-interstitial dislocation loop I_{19} and a crowdion is seen as a function of the time step (one time step is about 1 fs ($=10^{-15}$ s)) at $T=0$ K. The configuration at step 0 is the initial configuration, initial distance between them is 4b, and at step 3000 both crowdion and dislocation loop I_{19} show the movement of some atomic distances (2–3 atomic distances for the loop and more than 10 atomic distances for the crowdion), but of the opposite direction as the result of the repulsive interaction between them. Namely, the crowdion supplies the repulsive force

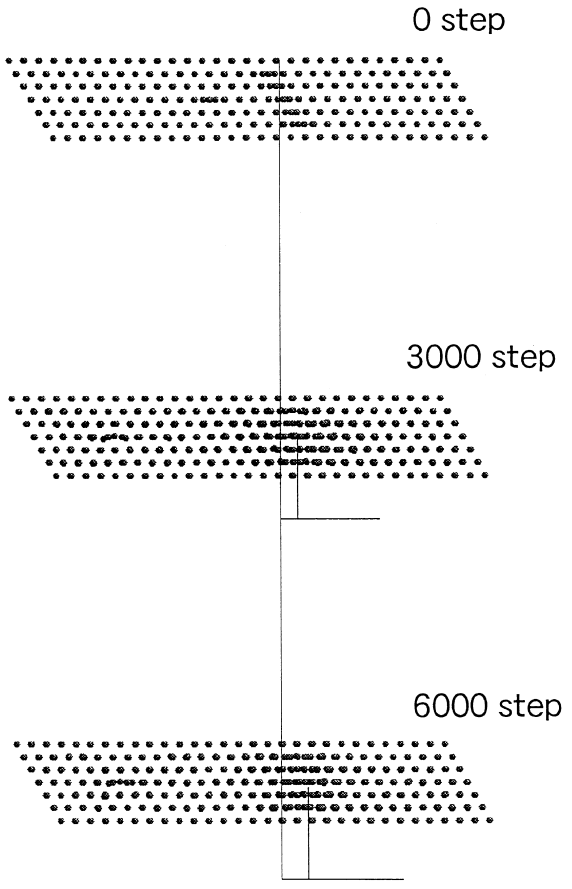

Fig. 5. Dynamic interaction between an interstitial cluster I_{19} and a crowdion as a function of time step at $T=0$ K.

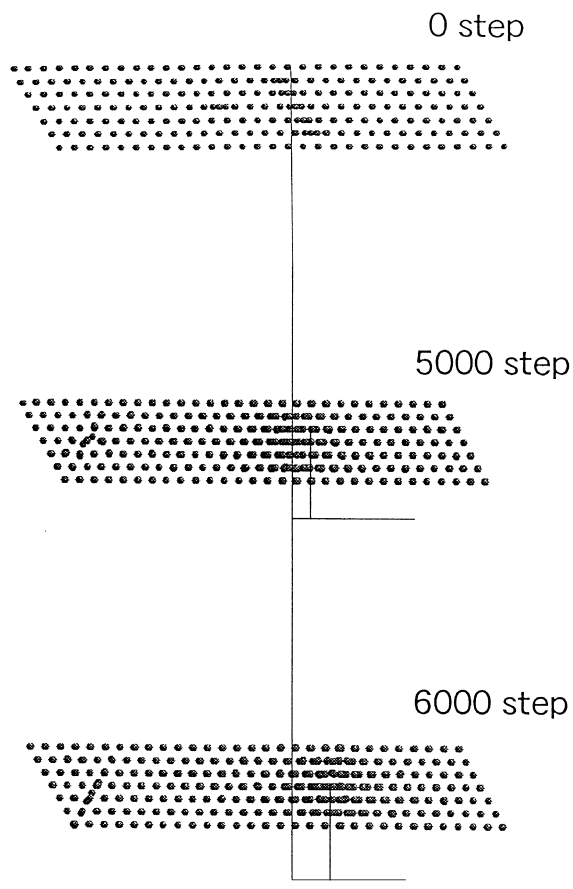

Fig. 6. Dynamic interaction between an interstitial cluster I_{19} and a crowdion as a function of time step at $T=300$ K.

through ⟨1 1 1⟩ atomic row to the central potion of the loop I_{19}, resulting in the axial shear stress on the loop I_{19}. Further movements are seen at 6000 step, and the crowdion shows larger moving distance than the loop I_{19}, which means the crowdion has lower migration resistance than the loop I_{19}. The result at $T = 300$ K is shown in Fig. 6, where until step 5000 there is not much movement. After this, a remarkable movement of the loop is seen by step 6000. This is considered to be thermally activated motion of the dislocation loop I_{19} under the axial shear stress. If it is assumed that one atomic jump occurred during 1000 step ($= 1000$ fs) at $T = 300$ K, the activation energy $U = 0.1$ eV is obtained, which is reasonable from the viewpoint of the low Peierls stress for the edge dislocation in Fe, and is similar to the result obtained by Stoller et al. [12]. It is also seen that the loop I_{19} sits on the inclined $(\bar{1}\ \bar{1}\ 0)$ plane at the initial time, but as time increases, it is turned to the vertical plane $(\bar{1}\ \bar{1}\ \bar{1})$ perpendicular to ⟨1 1 1⟩ axis, probably due to the decrement of the loop energy. Another point to be noted is the SIA conversion from the crowdion to the dumb bell structure at $T = 300$ K. This is also a thermally activated process, and is consistent with the formation energies of 3.94 eV for a crowdion and 3.89 eV for a dumbbell in Fe model lattice (present investigation).

4. Conclusions

Dynamic behavior of the interaction between an edge dislocation and a SIA was investigated by MD method in the iron model crystal. A SIA migrated to the dislocation core and finally the dislocation of the crowdion was converted to the direction parallel to the Burgers vector of the edge dislocation. It was also shown that a small interstitial cluster, e.g., I_{19} in Fe is very mobile under the interaction with a crowdion, which shows that this small dislocation loop has a very low Peierls potential.

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