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Computer simulation of defects interacting with a dislocation in Fe and Ni

E. Kuramoto *, K. Ohsawa, T. Tsutsumi

Research Institute for Applied Mechanics, Kyushu University, 6-1 Kasuga-koen, Kasuga-shi, Fukuoka 816-8580, Japan

Abstract

In order to investigate the fundamental aspects of damage evolution under irradiation computer simulations of the interaction between a dislocation and point defects such as a self-interstitial atom (SIA), a vacancy and interstitial clusters have been performed for various configurations. It is found both in Fe and Ni that a crowdion with axis parallel to the Burgers vector of an edge dislocation interacts more strongly than those with other axis orientations. The same tendency was seen for the dumbbell. The capture range (capture area) within which SIAs are trapped by an edge dislocation is larger for Ni than for Fe, and that for vacancies is much smaller than that for SIAs, suggesting that the bias factor in Ni is larger than that in Fe.

1. Introduction

In order to investigate damage structure evolution in materials used in a neutron irradiation, the atomistic behavior of the interaction between defects, defect clusters and dislocations must be clarified. This process is closely related to the production of the imbalance between vacancy and interstitial fluxes during irradiation, namely, the so-called bias factor. Many theoretical attempts have been made to understand the bias phenomena, such as dislocation bias [1–5], production bias [6,7] and so on. However, atomistic features of the bias factor have not been clearly understood yet. A better understanding of the whole damage generation process, void swelling, radiation embrittlement and so on necessitates more investigation. In the present study, attempts will be made to clarify the atomistic features of the interaction between defects, defect clusters and an edge dislocation in model Fe and Ni lattices, which are typical bcc and fcc metals and are important elements in ferritic and austenitic stainless steels, respectively. A detailed study was made on the interaction between self-interstitial atoms (SIAs) and an edge dislocation under various configurations between them, such as the direction of SIAs and Burgers vector of the dislocation, because the strength of the interaction depends on the configuration.

2. Method of calculation

For the computer simulation of the interaction between defects and an edge dislocation, *N*-body potentials like the embedded atom method (EAM) potential was used. The potentials given by Finnis and Sinclair [8,9] and by Gao et al. [10] were used for Fe and Ni, respectively. An edge dislocation was introduced into the central region of the model lattices shown in Figs. 1(a) and (b) for Fe and Ni, respectively. Sizes of the model lattices are $80b \times 80(2/3)^{1/2}b \times 80(2 \cdot 2^{1/2}/3)b$ and $80b \times 80(2/3)^{1/2}b \times 80(3^{1/2}/2)b$, where b is the magnitude of Burgers vector, for Fe and Ni, respectively, as shown in Fig. 1. The orientation of the model lattices is also shown. The whole lattice with a defect, such as a crowdion, a dumbbell or a vacancy was fully relaxed by the static method (Newton–Raphson method) under a fixed boundary condition. This static

* Corresponding author. Tel.: +81 92 583 7766; fax: +81-92 583 7767.

E-mail address: kuramoto@himiko.riam.kyushu-u.ac.jp (E. Kuramoto).

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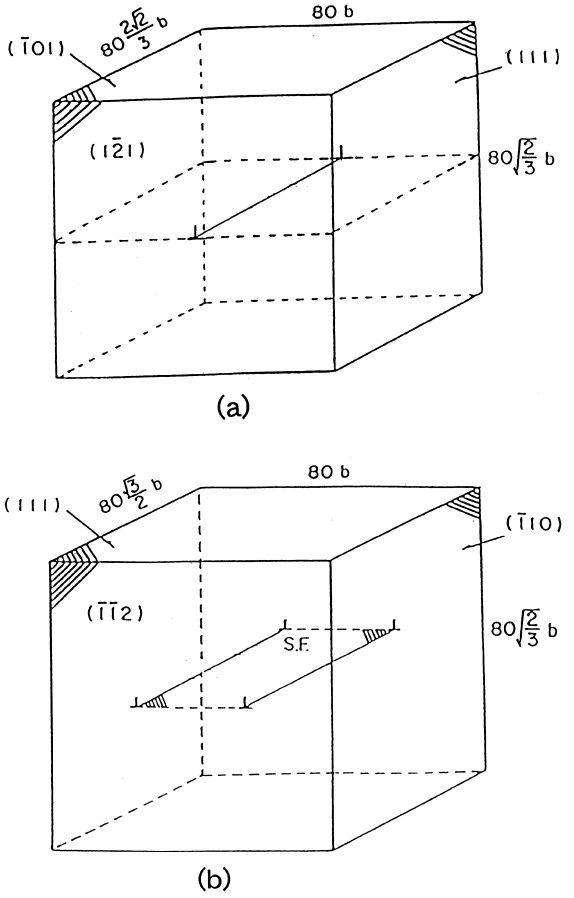

Fig. 1. Model lattices for Fe (a) and Ni (b), where an edge dislocation is introduced in the central region (in Ni an extended edge dislocation is introduced).

method has no temperature effect, thus all the results obtained correspond to $T = 0$ K. The size of the model lattice was chosen as large as possible to avoid the boundary effect, which was confirmed by calculations made in the model lattices with various sizes. An edge dislocation was placed on a {1 1 0} plane in Fe and an extended edge dislocation was placed on a plane {1 1 1} in Ni. A ⟨1 1 1⟩ crowdion or a ⟨1 1 0⟩ dumbbell was placed around an edge dislocation in Fe and a ⟨1 1 0⟩ crowdion or a ⟨1 0 0⟩ dumbbell was placed around an edge dislocation in Ni.

3. Results and discussion

3.1. Interaction between edge dislocation and point defects in Fe

Variation of the formation energy of a ⟨1 1 1⟩ crowdion around an edge dislocation in Fe was calculated and is shown in Fig. 2. Here, the axis of a crowdion is parallel to the Burgers vector of an edge dislocation as shown in the figure below, and the capture range within which the binding energy (decrease of the formation energy) is larger than 0.067 eV (value of kT, $T = 500$°C) is also plotted in Fig. 3. This region exists below the slip plane of the edge dislocation because of the presence of the tensile strain field. Above the slip plane the crowdion is unstable because of the presence of the compression strain field. The same result for the ⟨1 1 1⟩ crowdion with its axis not parallel but close to the direction perpendicular to the Burgers vector of the edge dislocation (shown in the figure below) is shown in Fig. 4. A big difference is seen between these two results. In the former, the capture range is much larger than the latter, probably because the axial strain of the ⟨1 1 1⟩ crowdion is relaxed to a large extent by the tensile strain field below the slip plane of the edge dislocation. Even when the crowdion is placed just above the slip plane, a decrease in the formation energy is still seen. This is because during a lattice relaxation the crowdion is shifted to just below the slip plane. The same calculation was also made for dumbbells with their axis close to the direction parallel or perpendicular to the Burgers vector of the edge dislocation. The capture range for the former is shown in Fig. 5. Furthermore, the capture range for a vacancy obtained by the same process is shown in Fig. 6. It is much smaller than that for SIAs, because the strain field around a vacancy is smaller than SIAs.

3.2. Interaction between edge dislocation and point defects in Ni

Variation of the formation energy of a ⟨1 1 0⟩ crowdion around an extended edge dislocation in Ni was calculated and is shown in Fig. 7. Here, the axis of the crowdion is parallel to the Burgers vector of an extended edge dislocation, and the capture range within which the binding energy is larger than 0.067 eV ($T = 500$°C) is plotted in Fig. 8. It is seen that this capture range is much larger than that for Fe. Calculations for dumbbells and a vacancy were also made for Ni and the same tendency as that in Fe was obtained. Calculated areas of the capture range for a SIA and a vacancy in Fe and Ni around an edge dislocation are summarized in Fig. 9. This suggests that the area strongly depends on the relative configuration between an SIA and an edge dislocation, and the area of the capture range for an SIA is much larger than that for a vacancy. Values for Ni are much larger than those for Fe, suggesting that the

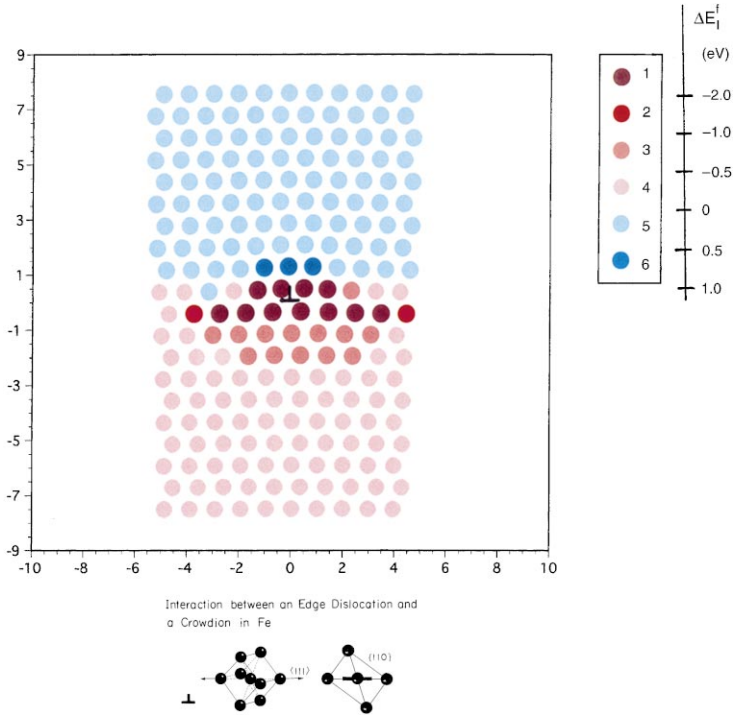

Fig. 2. Calculated formation energy of a ⟨1 1 1⟩ crowdion around an edge dislocation in Fe, where the axis of a crowdion is parallel to the Burgers vector of an edge dislocation.

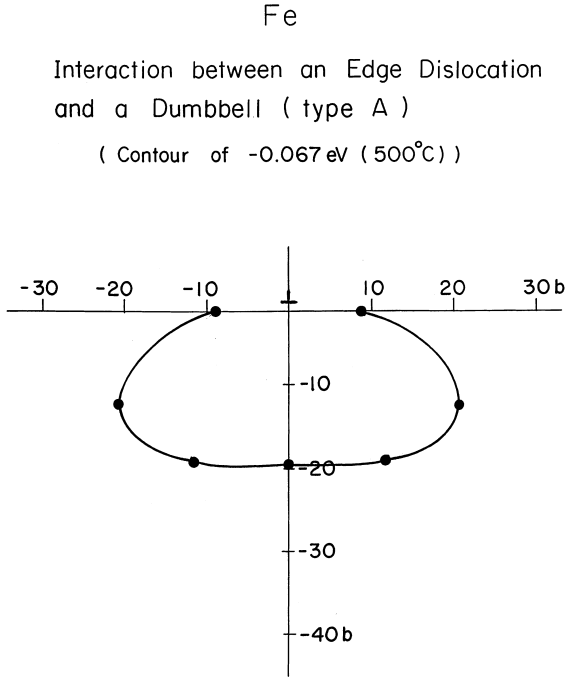

Fig. 3. Capture range within which the binding energy (decrease of the formation energy) is larger than 0.067 eV (value of kT, $T = 500°C$) for a ⟨1 1 1⟩ crowdion around an edge dislocation in Fe, where the axis of a crowdion is parallel to the Burgers vector of an edge dislocation.

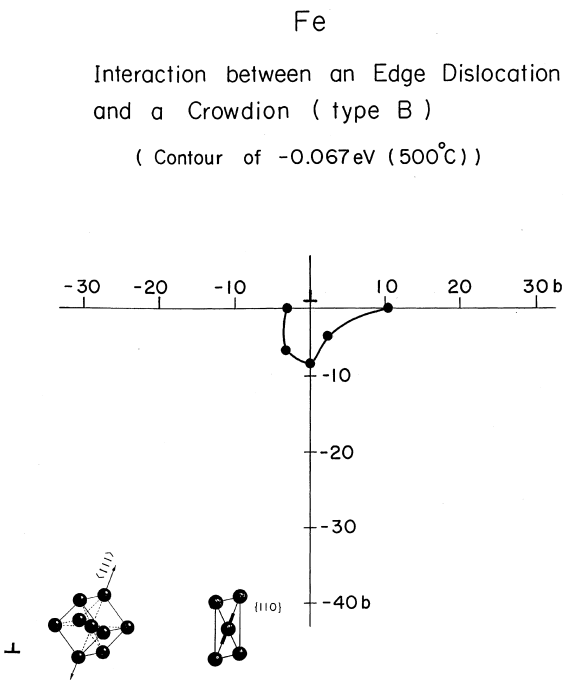

Fig. 4. Capture range within which the binding energy (decrease of the formation energy) is larger than 0.067 eV (value of kT, $T = 500$°C) for a $\langle 1\,1\,1 \rangle$ crowdion around an edge dislocation in Fe, where the axis of a crowdion is not parallel but close to the direction perpendicular to the Burgers vector of an edge dislocation shown in the figure below.

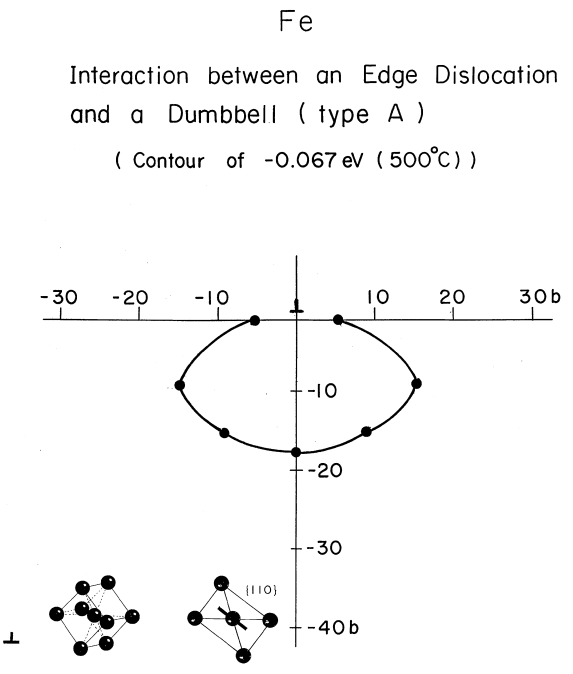

Fig. 5. Capture range within which the binding energy (decrease of the formation energy) is larger than 0.067 eV (value of kT, $T = 500$°C) for a $\langle 1\,1\,0 \rangle$ dumbbell around an edge dislocation in Fe, where the axis of a dumbbell is close to the direction parallel to the Burgers vector of an edge dislocation.

bias factor for Ni (fcc) is larger than that for Fe (bcc). This is consistent with experimental observations so far obtained [11–15].

4. Conclusion

Calculations for the interaction between an edge dislocation and an SIA, a vacancy and interstitial clusters have been performed for various configurations. It is found both in Fe and Ni that crowdions with their axis parallel to the Burgers vector of an edge dislocation interact more strongly than those with other axis orientations. The same tendency was seen for the dumbbell. The capture range (capture area) within which SIAs are trapped by an edge dislocation (binding energy, the decrease of the formation energy is larger than kT) is larger for Ni than for Fe, and the capture range for vacancies is much smaller than that for SIAs. This suggests that the bias factor in Ni is larger than that in Fe.

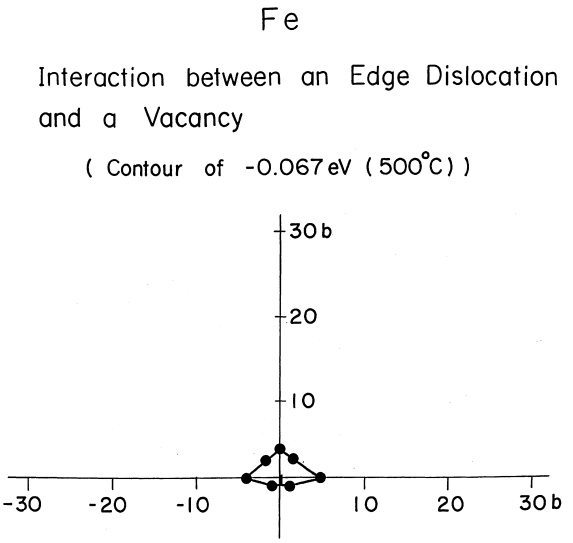

Fig. 6. Capture range within which the binding energy (decrease of the formation energy) is larger than 0.067 eV (value of kT, $T = 500$°C) for a vacancy around an edge dislocation in Fe.

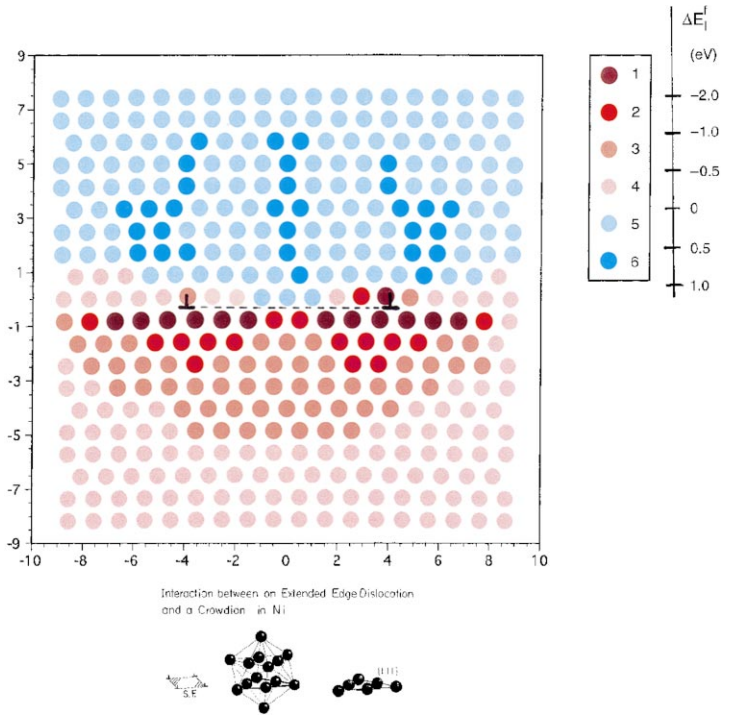

Fig. 7. Calculated formation energy of a ⟨1 1 0⟩ crowdion around an extended edge dislocation in Ni, where the axis of a crowdion is parallel to the Burgers vector of an extended edge dislocation.

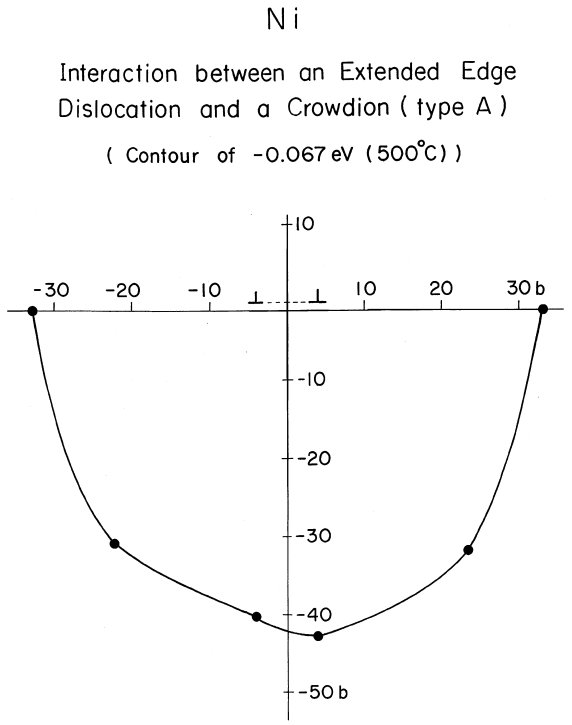

Fig. 8. Capture range within which the binding energy (decrease of the formation energy) is larger than 0.067 eV (value of kT, $T = 500$°C) for a ⟨1 1 0⟩ crowdion around an extended edge dislocation in Ni, where the axis of a crowdion is parallel to the Burgers vector of an extended edge dislocation.

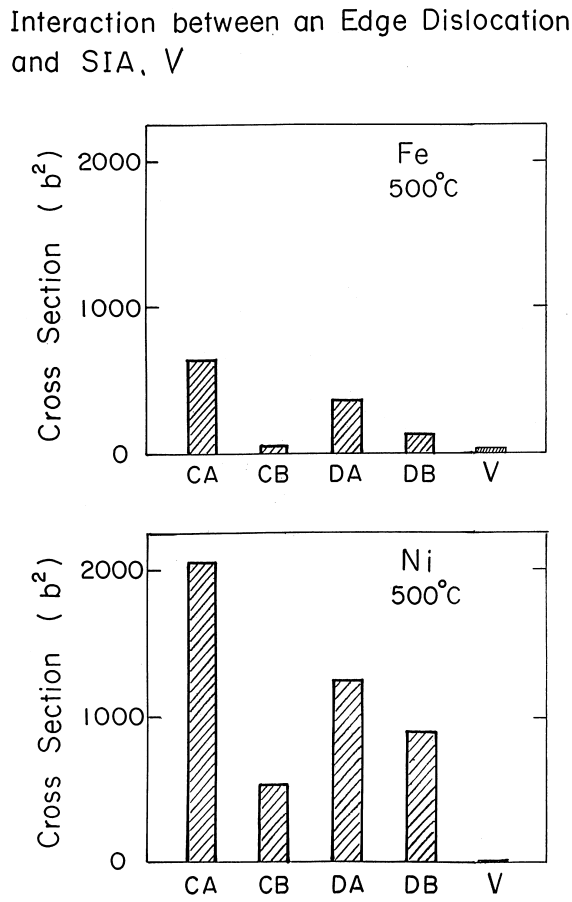

Fig. 9. Calculated areas of the capture range for an SIA and a vacancy around an edge dislocation in Fe and Ni.

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