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Study of fundamental features of bias effect in metals under irradiation

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Abstract

Studies on bias mechanisms, such as the dislocation bias and production bias have so far been made in the Fe and Ni model crystals. In the present work the interaction between an edge dislocation and interstitial clusters has been mainly studied by computer simulation from the viewpoint of the production bias for Fe and Ni. Capture zones for interstitial clusters I_n (bundles of n crowdions, $n = 1, 2, 3, 5$) to an edge dislocation line have been obtained, with the definition of the capture zone as the region where the binding energy is larger than $kT = 0.067$ eV ($T = 500$ °C). This shows increasing capture areas on the expansion side of the edge dislocation line with increasing size of interstitial clusters both in Fe and Ni. The energy change from the as-trapped state of the interstitial cluster to the absorbed state into the edge dislocation core was also calculated. This showed that the final stable configuration is a jogged state in Fe. This is also correct in Ni but only when the size of the interstitial cluster is larger than a certain value. These results give a confirmed basis to the production bias mechanism.
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1. Introduction

In the damage structure evolution in materials used in neutron irradiation environment the so-called bias effect plays an important role because the formation of defect clusters are usually caused by this bias effect. Many theoretical attempts have been performed to understand various bias mechanisms, such as dislocation bias [1–7], production bias [8–10] and so on. The origin of the dislocation bias is based on the very fundamental feature of the irradiation-induced defects, namely, inherent properties of self-interstitial atoms (SIAs) and vacancies. Clustering of SIAs generates only planar type clusters, that is, dislocation loops and not three dimensional clusters. On the other hand, clustering of vacancies generates clusters of various types, planar clusters and three dimensional clusters like voids and stacking fault tetrahedra. Planar clusters of SIAs (interstitial type dislocation loops: *I*-loops) have preferential absorption for SIAs relative to vacancies, that is, a bias effect. This is due to larger binding energy of SIAs to *I*-loops than vacancies, which basically originates from the larger formation energy of SIAs than vacancies in ordinary metals. The limit of the size of *I*-loops (exactly speaking a bundle of crowdions) is a straight edge dislocation, because the edge dislocation can be considered to be a semi-infinite stacking of crowdions. Then the bias effect must work in the same way for both *I*-loops and an edge dislocation, being called 'dislocation bias'. On the other hand, so-called production bias comes from the one dimensional motion of small interstitial clusters emitted from the cascade region toward the sinks such as dislocations and grain boundaries.

In previous papers the detailed features of dislocation bias have been noted [4–6], and the dynamic motion of small interstitial clusters have been described [11–15]. Hence in the present paper the interaction of small interstitial clusters with edge dislocations are studied.

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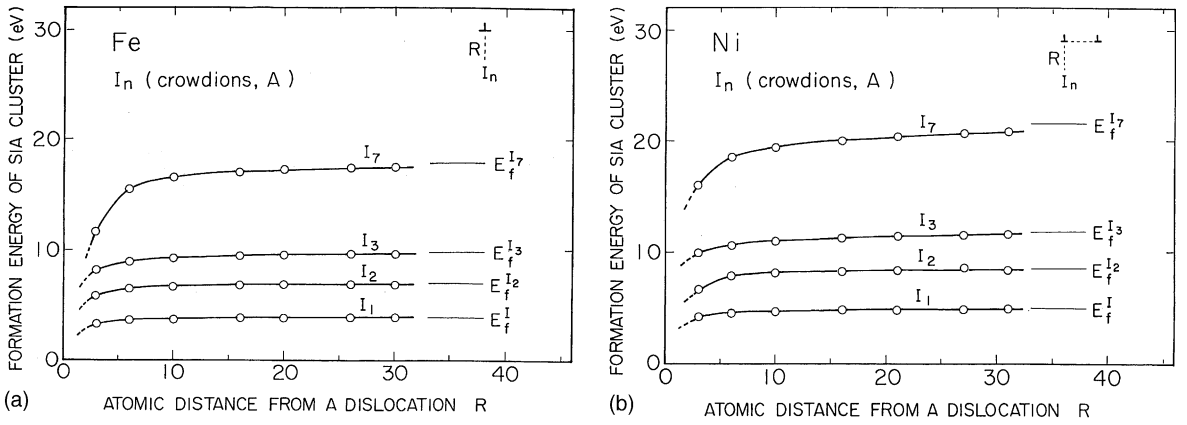

Fig. 1. Calculated values of the formation energy (binding energy) of the interstitial clusters I_n (bundles of n crowdions, $n = 1, 2, 3, 7$, where the axis of each crowdion is parallel to the Burgers vector of an edge dislocation) as a function of the distance R from the edge dislocation core for Fe (left) and for Ni (right).

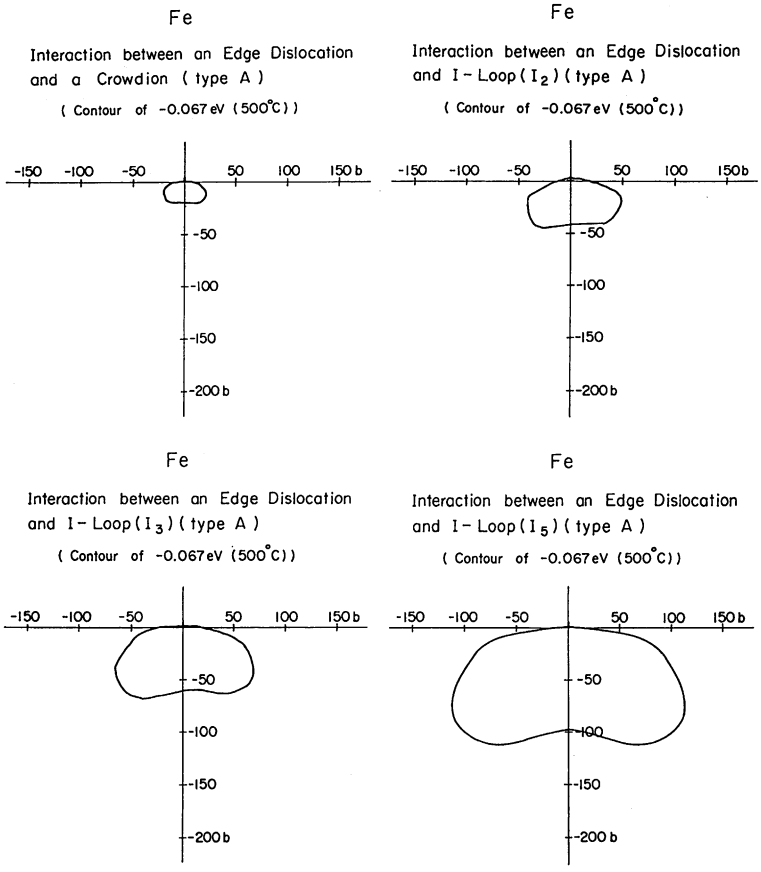

Fig. 2. Calculated capture zones for interstitial clusters I_n ($n = 1, 2, 3, 5$) to an edge dislocation line in Fe where the binding energy is larger than $kT = 0.067$ eV ($T = 500$ °C).

2. Calculational method

Model crystals of Fe and Ni were constructed by using EAM type potentials, that is, Finnis–Sinclair potential for Fe [16] and that developed by Gao, Bacon and Ackland for Ni [17]. The size of the model crystals must be large enough to accommodate the defect strain field, especially a dislocation, which has a long range strain field around it. Typical sizes of the model crystals are $80b \times 80(2 \times 2^{1/2}/3)b \times 80(2/3)^{1/2}b$ and $80b \times 80(3^{1/2}/2)b \times 80(2/3)^{1/2}b$ (where b is the magnitude of the Burgers vector) for Fe and Ni, respectively. But sometimes larger model crystals were needed to obtain the interaction range between an edge dislocation and interstitial clusters. The whole crystal with defects was completely relaxed in the static way.

3. Results and discussion

In Fig. 1 calculated values of the formation energy (binding energy) of the interstitial clusters I_n (bundles of n crowdions, $n = 1, 2, 3, 7$, where the axis of each crowdion is parallel to the Burgers vector of an edge dislocation) as a function of the distance R from the edge dislocation core (R is the perpendicular distance from the slip plane toward the expansion side of the edge dislocation as shown in the figure) are shown both in Fe and Ni. The axis of a crowdion in Fe is the $\langle 1\,1\,1 \rangle$ direction, and in Ni it is the $\langle 1\,1\,0 \rangle$ direction. For all cases of I_n, the formation energy decreases from the values in the isolated states shown in the figure with decreasing of R; that is, the binding energy increases for decreasing R with larger values for larger n.

No significant difference was observed between Fe and Ni in the binding behavior of interstitial clusters to an edge dislocation. However, this is only in the direction perpendicular to the slip plane of the edge dislocation toward the expansion side. Hence the binding behavior for the interstitial clusters I_n to the edge dislocation must be calculated for all the directions around an edge dislocation line and the capture zone where the binding energy is larger than kT must be determined.

In Fig. 2 the calculated capture zones for interstitial clusters I_n ($n = 1, 2, 3, 5$) to an edge dislocation line are shown in the case of Fe where the binding energy is

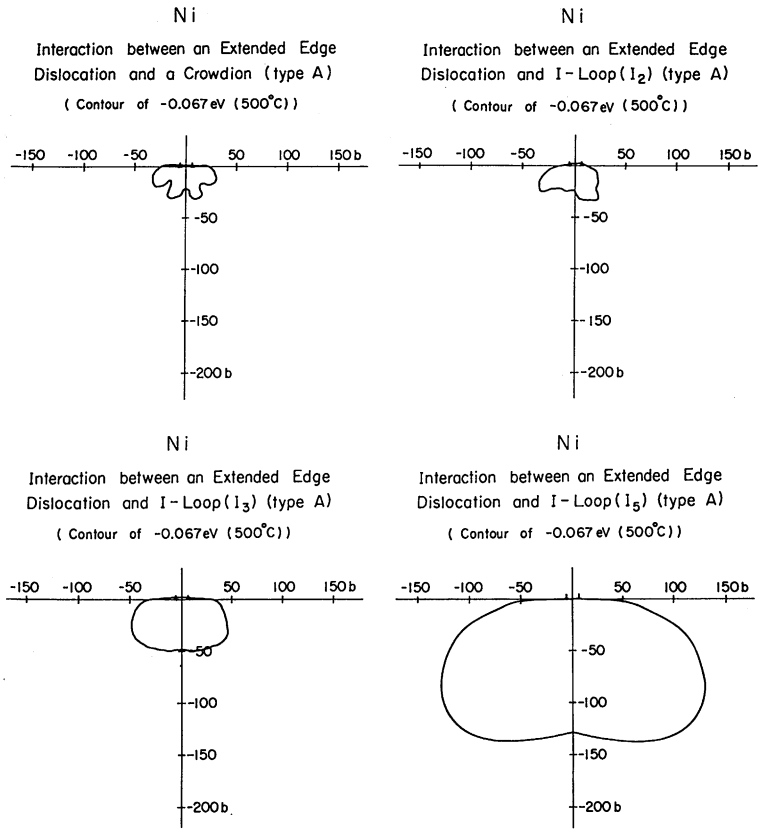

Fig. 3. Calculated capture zones for interstitial clusters I_n ($n = 1, 2, 3, 5$) to an extended edge dislocation line in Ni where the binding energy is larger than $kT = 0.067$ eV ($T = 500$ °C).

larger than $kT = 0.067$ eV ($T = 500$ °C). This shows increasing capture areas on the expansion side of the edge dislocation line with increasing interstitial cluster size. In Fig. 3 similar results for Ni are shown. The non-smooth shape of the capture area for $n = 1$ in Ni comes from the reorientation of a crowdion during relaxation, resulting in a more stable configuration depending upon the initial position of the crowdion.

In Fig. 4, a comparison of calculated capture areas for interstitial clusters I_n ($n = 1, 2, 3, 4, 5$) between Fe and Ni is shown, indicating an increase in area with interstitial cluster size for both Fe and Ni. For sizes of $n = 4$ and 5 capture areas are larger in Ni than Fe. This result shows that interstitial clusters emitted from cascades which are moving one dimensionally can be trapped around edge dislocation lines, a basic requirement in the production bias model.

Successive trapping of interstitial clusters at an edge dislocation line forms an atmosphere of interstitial clusters around the dislocation line if the temperature is not too high. This causes the so-called cascade induced source hardening. But if the temperature is high enough for interstitial clusters to be resolved and absorbed into a dislocation core, the climb motion of the edge dislocation line must occur just like the absorption of single interstitial atoms migrating three dimensionally in the case of dislocation bias. In order to clarify this discussion point, the energy change from the as-trapped state of the interstitial cluster to the absorbed state into the edge dislocation core, i.e., the jogged state, must be calculated.

In Fig. 5 the calculated result for the decrease of the formation energy for I_3 is shown during the absorption process into an edge dislocation core in the case of Fe, suggesting that the formation energy decreases significantly with final formation of a jogged configuration. In Fig. 6 similar calculated results for I_n ($n = 3, 5, 7$) both

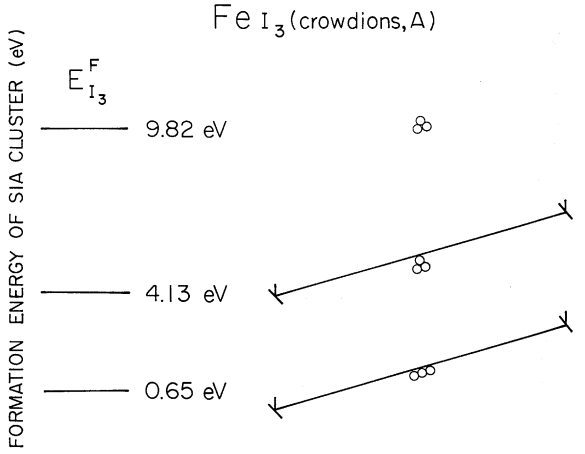

Fig. 5. Calculated result for the decrease of the formation energy for I_3 during the absorption process into an edge dislocation core in Fe.

in Fe and Ni are shown, where in the case of Ni the absorption occurs on one of the two partial dislocations of an extended edge dislocation. In this latter case the final absorption is not that shown in the figure, but the absorption of an interstitial cluster into an extended dislocation core must be fulfilled as shown in Fig. 7, where both partial dislocation lines climb, forming an extended jog. The exact shape of the extended jog can be drawn by tracing the region of the stacking fault, where the climbed region has a stacking fault just one atomic distance lower from the original atomic plane. The energy change in this process of formation of the fully extended jog in Ni was calculated and is shown in Fig. 8, where the extended jog state becomes more stable when the number of crowdions in an interstitial cluster is larger than 10.

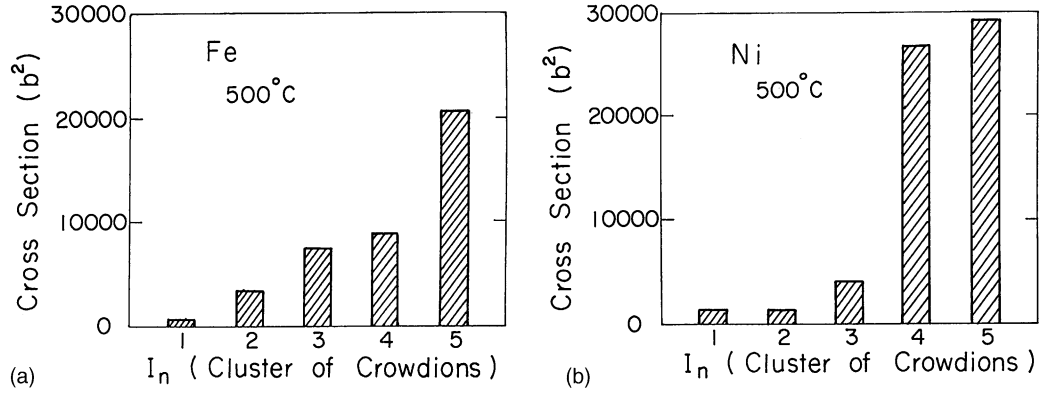

Fig. 4. Comparison of calculated capture areas for interstitial clusters I_n ($n = 1, 2, 3, 4, 5$) between Fe and Ni (interaction between an edge dislocation and I_n).

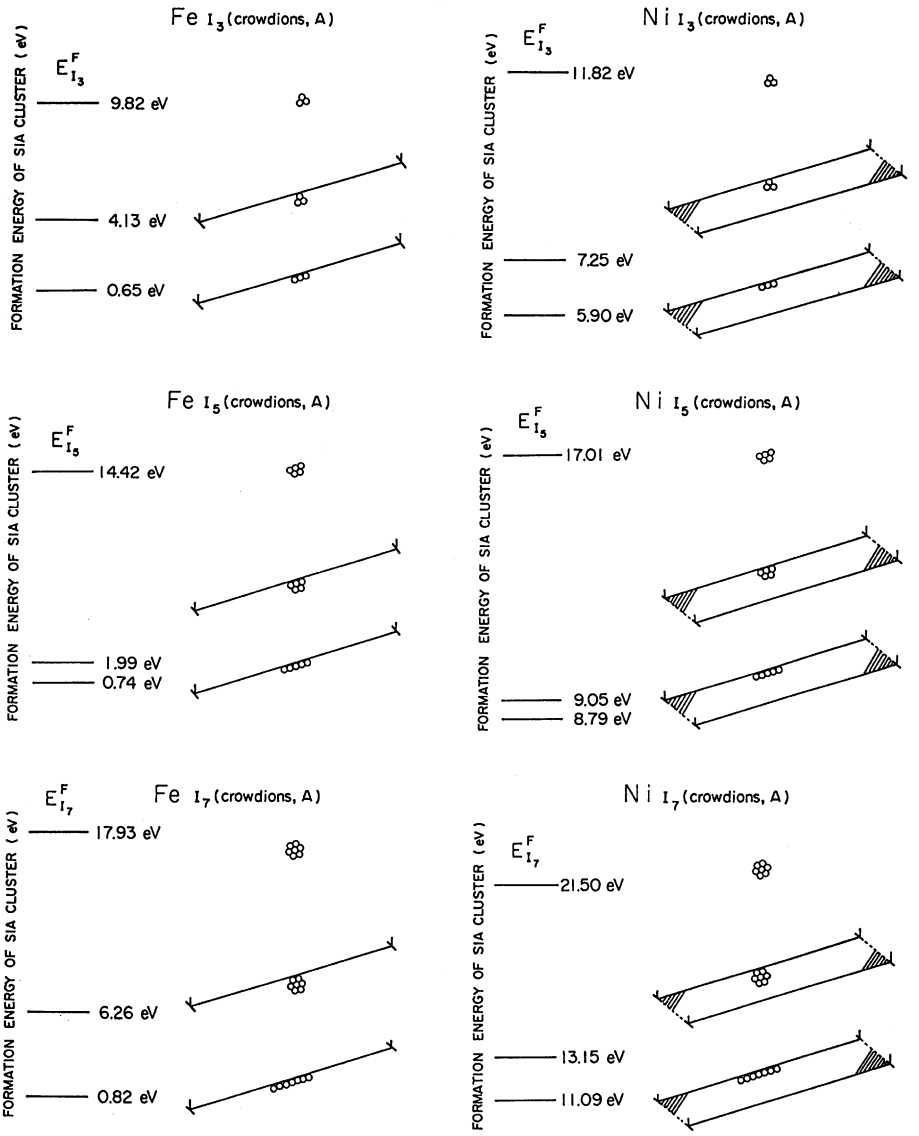

Fig. 6. Calculated results for the decrease of the formation energy for I_n ($n = 3, 5, 7$) during the absorption process into an edge dislocation core both in Fe and Ni.

Results obtained above provide a basis for the production bias mechanism, but further information on the stability of small interstitial clusters at the edge dislocation core is needed. This is the subject for future work.

4. Summary

From the viewpoint of the production bias for Fe and Ni, capture zones for interstitial clusters I_n (bundles of n crowdions, $n = 1, 2, 3, 5$) to an edge dislocation line have been calculated. The definition of the capture zone is the region where the binding energy is larger than $kT = 0.067$ eV ($T = 500$ °C). This shows increasing capture areas on the expansion side of the edge dislocation line with increasing interstitial cluster size both in Fe and Ni. The energy change from the as-trapped state of the interstitial cluster to the absorbed state into the edge dislocation core, i.e., the jogged state, was also calculated. This showed that the final stable configuration is a jogged state in Fe. This is also correct in Ni but only when the size of the interstitial cluster is larger than a certain value. These results provide a basis for the production bias mechanism.

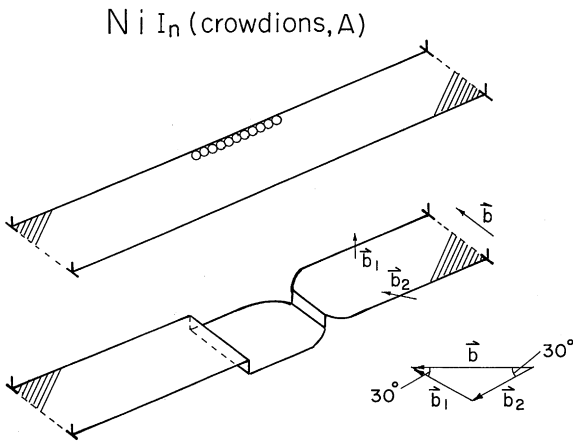

Fig. 7. Final configuration of the absorption of an interstitial cluster into an extended edge dislocation core in Ni, where both partial dislocation lines make climb motion, forming an extended jog.

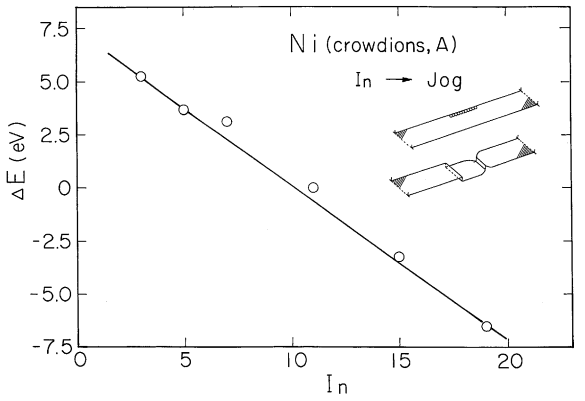

Fig. 8. Calculated energy change from the as-trapped state of an interstitial cluster to the absorbed state, that is, the fully extended jog in Ni.

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