

COMPUTER SIMULATION OF THE INTERACTION BETWEEN AN EDGE DISLOCATION AND A
SELF-INTERSTITIAL ATOM RELATED TO A BIAS FACTOR IN VOID SWELLING

EIICHI KURAMOTO AND TETSUO TSUTSUMI

Research Institute for Applied Mechanics, Kyushu University,

6 - 1 Kasuga-koen, Kasuga-shi, Fukuoka 816 Japan

ABSTRACT

Computer simulation on the interaction between an edge dislocation and a self-interstitial atom (SIA), which plays an important role in a so-called bias effect, has been performed in model lattices of both fcc and bcc metals. The interaction between a partial dislocation and a SIA was taken into account in a fcc lattice (Au), because dislocations are extended. Not only the interaction between a straight dislocation line and a SIA, but also that between a jogged line and a SIA has been calculated. The obtained dependence of the interaction energy upon the distance from the dislocation line showed that it exists rather in a very short range, and is not so much different between the fcc and the bcc case. In the case of a jogged dislocation the lowest energy at the core site is deeper than that in the case of a straight dislocation. This suggests that the observed big difference in swelling between fcc and bcc metals could not directly come from the difference of dislocation bias.

1. INTRODUCTION

Void swelling is one of the most severe problems for the materials used in the environments of high temperature heavy irradiation. One of the important features of this phenomenon is a dislocation bias between vacancy flux and SIA flux arriving at the void surface, which enables the void nucleation and growth through the preferential absorption of excess vacancies during the irradiation. This bias effect is mainly caused by the preferential absorption of self-interstitial atoms (SIA) by an edge dislocation to vacancies. However, the interaction between an edge dislocation and a SIA has not been investigated in detail from the atomistic

viewpoint yet. Especially, in fcc lattices dislocations are dissociated and this interaction is not so simple. Not only a straight dislocation but also a jogged dislocation must be taken into account in the study of this interaction, because in the actual case SIAs are likely to be absorbed at jogged segments on a dislocation line. To clarify the basic feature of this interaction between a SIA and a dislocation line or a jogged segment on the line, computer simulation in a model lattice is definitely necessary. In the present report the result of this simulation will be presented.

2. COMPUTATIONAL METHOD

Model fcc and bcc lattices were constructed by using Finnis-Sinclair type potential (for fcc, Ackland et al (1987) (1), for bcc, Finnis and Sinclair (1984) (2)). Size of the model lattice was about $80b \times 80b \times 40b$ (b : strength of Burgers vector) for fcc (Au), and about $40b \times 40b \times 100b$ for bcc (Fe). As shown in Fig. 1 an edge dislocation was introduced into the central part of the model lattices by using an elastic solution (isotropic) as the initial configuration. The slip plane is parallel to the top or bottom surface of the model lattice. Not only a straight dislocation but also a jogged dislocation was introduced as shown in the same figure. A SIA was inserted into the site which was close to the center of the dislocation line as shown in the figure. Calculations were made for cases of different distances of a SIA from the dislocation line. Full relaxation of the model lattice was performed by a static method under the fixed boundary condition and then total energy of the whole lattice was calculated as a function of the distance between a SIA and a dislocation.

3. RESULTS AND DISCUSSION

3.1 Straight dislocation and SIA

In a fcc model lattice (Au) an extended edge dislocation was obtained after full relaxation. The distance between two partial dislocations was about $20b$ which is reasonable judging from the stacking fault energy of Au, i.e., about 35 mJ/m^2 . Two types of SIA, i.e., 100 dumbbell and 110

crowdion were introduced. A SIA was inserted below one of the partial dislocations, on the line which is perpendicular to the slip plane as shown in Fig. 1. When a SIA was very close to the dislocation core or on the core, some structural change of the SIA was observed after full relaxation, namely, from 100 dumbbell to 110 crowdion. Fig. 2 shows the obtained formation energy of a SIA against the distance between a SIA and a dislocation line. The rapid decrease of the energy is observed for both 100 dumbbell and 110 crowdion in the region which is very close to the dislocation line, which suggests that the interaction is very short range compared with that expected from the elasticity theory. The binding energy of a SIA and a dislocation line is estimated about 2 eV from this figure.

In a model bcc lattice (Fe) an edge dislocation was introduced and was relaxed, which is a perfect dislocation, not an extended one. Two types of SIA were taken into account, namely 110 dumbbell and 111 crowdion. A SIA was inserted below the dislocation line, on the line which is perpendicular to the slip plane. In Fig. 3 is shown the formation energy of a SIA against the distance between a SIA and a dislocation line. As in the fcc case the rapid decrease of the formation energy is observed in the region close to the dislocation line. The binding energy of a SIA and a dislocation is estimated about 2 eV. There is no big difference in this value between fcc (Au) and bcc (Fe) model crystal. This suggests that no big difference in a bias factor can be expected between fcc and bcc metals.

On the other hand, big difference in a bias factor between fcc and bcc crystals has been proposed to explain the void swelling behaviours, especially in austenitic stainless steels (fcc, large swelling) and ferritic stainless steels (bcc, small swelling) (3, 4, 5). The origin of the bias difference is considered to be the difference of the relaxation volume of a SIA in fcc crystals (about 2 atomic volume) and in bcc crystals (about 1 atomic volume), which was obtained from X-ray diffraction method. But, no discussion has been made for the fact that dislocations are extended in fcc lattices, then a SIA interacts with a partial dislocation which has a smaller strain field around it than that of a perfect dislocation. Namely, in fcc crystals a SIA of a larger relaxation volume interacts with a smaller strain field of a dislocation, and vice versa in bcc crystals. This is not contradictory to the present result of computer simulation, namely, similarity between fcc and bcc crystal mentioned above.

3.2 Jogged dislocation and SIA

Since it is considered that SIAs rather interact with jogs on dislocation lines during the irradiation, computer simulation was also made for this case. If this process is repeated by successive arriving of SIAs, it contributes to climbing of a dislocation line, which is definitely necessary to cause a dislocation bias effect, namely, preferential absorption of SIA flux to vacancy flux. As shown in Fig. 1 a SIA was inserted to sites below a jog, and the total energy of a model lattice was calculated after full relaxation. In a model fcc lattice (Au) a dislocation is extended and jogged (total two jog sites, each partial dislocation has one), and a SIA was placed below one of them. The obtained energy - distance functions for fcc (Au) and bcc (Fe) cases are shown in Figs. 4 and 5, respectively. They are again very short ranged as those in the cases of a straight dislocation, but the lowest energy at the core site is deeper and almost zero. This can be understood by considering that a SIA absorbed into the core of a dislocation at a jog site is converted to the jog itself, namely, the jog was advanced one atomic distance ahead on the dislocation line. In bcc case the dislocation is not extended and this is easily seen, but in fcc case, i.e., extended case it is not so simple to understand.

To clarify this point the actual atomic configuration around a jog is drawn in Fig. 6 obtained by seeing from the top to bottom direction of the model lattice, where black points are on an upper atomic plane and white points are on a lower atomic plane. The vertical dotted line denotes the position of one of the two partial dislocations, and the other one is in the right direction out of the figure. The horizontal dotted line shows the position of the step of stacking fault, namely, in the upper region of the dotted line in this drawing the stacking fault is between black (upper) and white (lower) atomic plane, and in the lower region of the dotted line stacking fault is on the one atomic distance upper plane. A SIA is absorbed at the crossing point of a vertical and a horizontal dotted line where the distance of two adjacent black mark atoms (left and right) is larger than others. The final configuration is that where all black marked atoms existing on a row on the right hand side of a SIA are shifted to the right direction by half an atomic distance. This corresponds to one atomic distance advance (downwards in this figure) of the stacking fault region. On the way to this final configuration some potential barrier exists and the

conversion needs some agitation of the atoms involved. In an actual case, especially in high temperature environment this transformation may occur in thermally assisted way.

References

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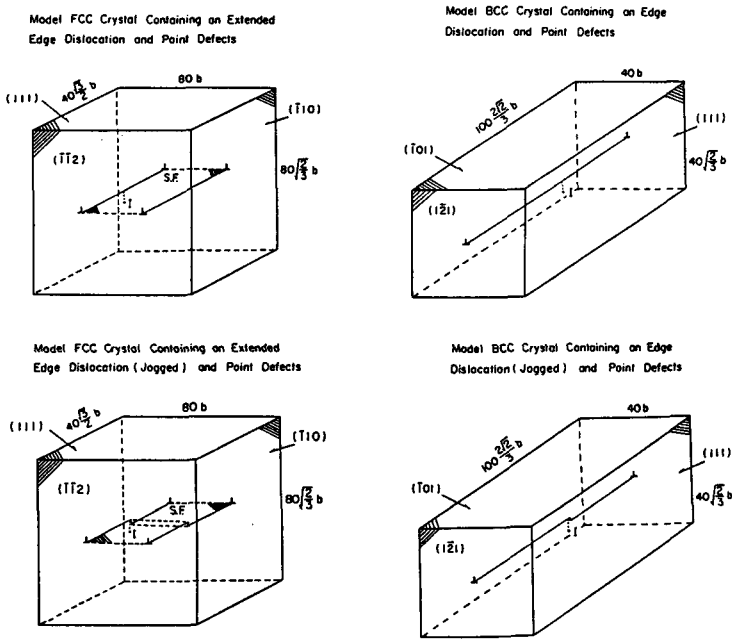


Fig. 1 FCC and BCC model lattices containing an edge dislocation and a SIA (not only a straight dislocation but also a joggled edge dislocation is drawn).

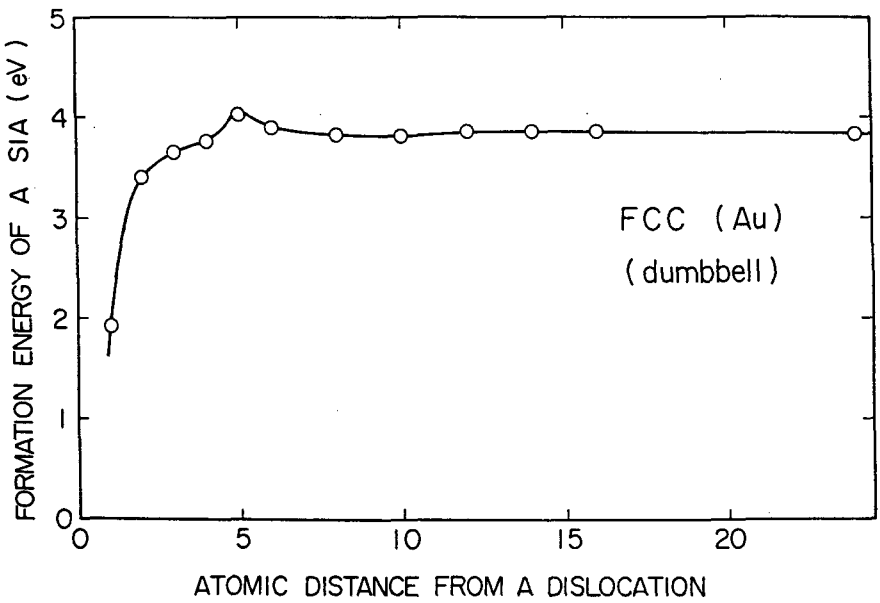


Fig. 2 Calculated formation energy of a SIA against a distance from the extended dislocation line in a fcc model lattice (Au).

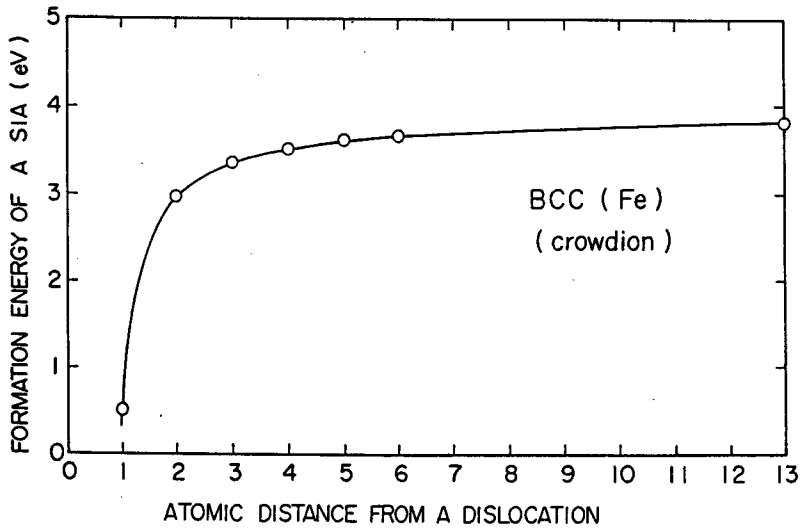


Fig. 3 Calculated formation energy of a SIA against a distance from the dislocation line in a bcc model lattice (Fe).

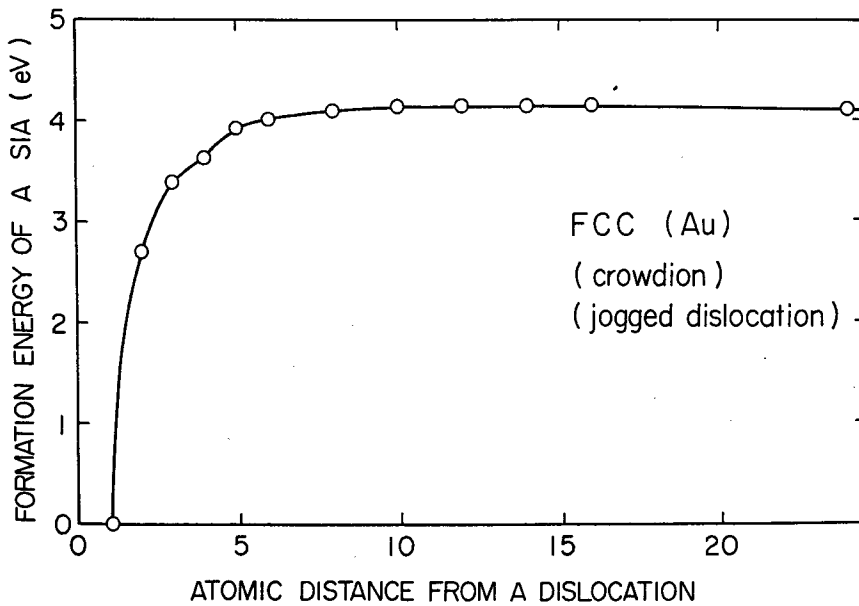


Fig. 4 Calculated formation energy of a SIA against a distance from the jogged extended dislocation line in a fcc model lattice (Au).

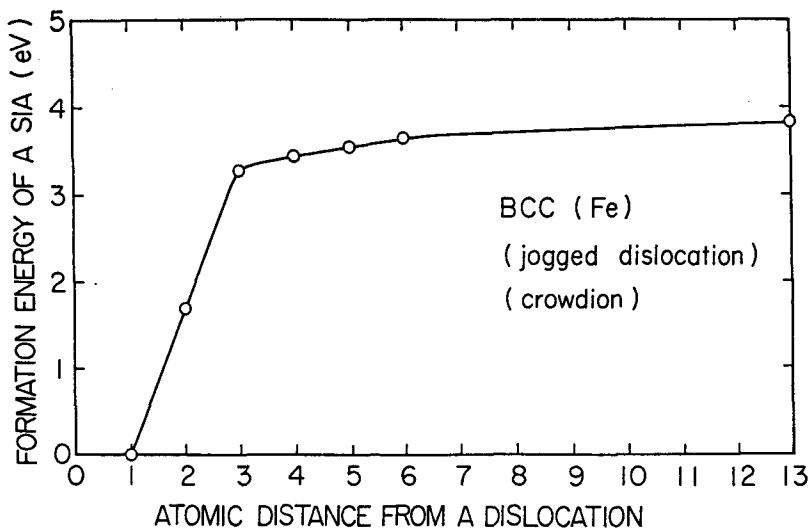


Fig. 5 Calculated formation energy of a SIA against a distance from the jogged dislocation line in a bcc model lattice (Fe).

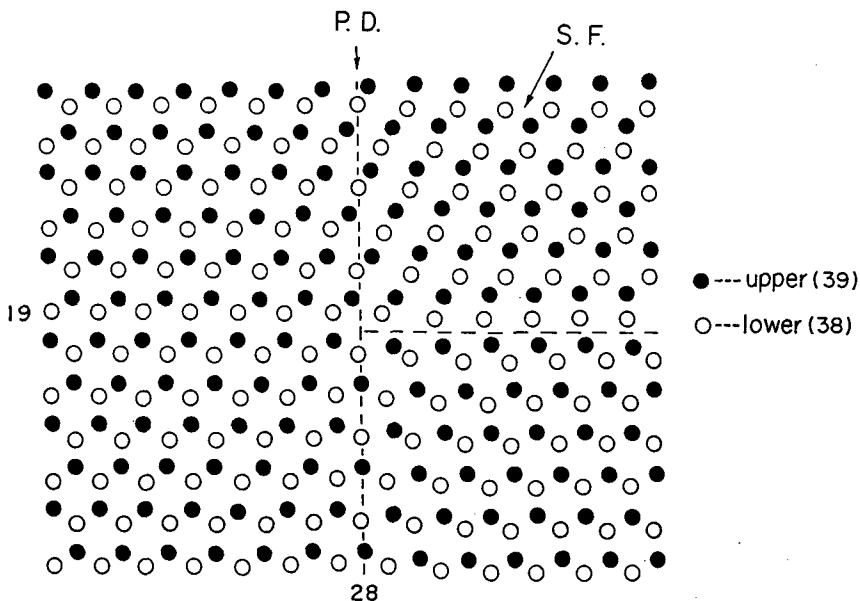


Fig. 6 Atomic configuration around a jog in a fcc model lattice (Au), (black marked atoms are on an upper plane, and white marked atoms are on the lower plane)