Bias Mechanism and Its Effects for Fundamental Process of Irradiation Damage

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In order to obtain the better understanding for bias effects under irradiation computer simulation was made and the basic view for the dislocation bias was presented from the formation energy of radiation induced defects. It was shown that the difference of the formation energy between a selfInterstitial atom and a vacancy is the most basic origin for the dislocation bias. On the other hand, for the production bias the detailed information on interstitial clusters is required and it was found in Fe model lattice that the edge dislocation line has a special character, i.e., a periodicity of b/3, but in the case of dislocation loops these stable positions distributed with a periodicity b/3 diffuse out with decreasing loop size and tend to have a periodicity of nearly b in the smaller limit of loop size. This behavior suggests that Peierls potentials which dislocation loops must overcome depend upon the loop size, and smaller Peierls stress can be expected for larger loops and an edge dislocation line probably because of finer periodicity b/3. But at finite temperatures small clusters of crowdions easily tend to have a rather loose coupling structure of composing crowdions, and slip motion as a whole cluster is not well defined, and the diffusion process as a whole might be better to represent the motion of small clusters at high temperatures.

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Keywords: bias effect in iron, dislocation bias, production bias, bundle of crowdions, dislocation loop, core structure of a loop segment

1. Introduction

In materials under irradiation various phenomena such as cascade formation, one dimensional motion of small interstitial clusters, interaction between a dislocation and interstitial clusters, three dimensional motion of radiation induced defects, dislocation bias, production bias occur and finally complicated damage structures are formed, resulting in the degradation of materials.¹⁻⁷) The first step of the total understanding of the radiation effect of materials is to obtain the information on a cascade, that is, that of vacancies and self interstitial atoms (SIAs) in a cascade. Many computer simulations have so far been made for the cascade formation⁸⁻¹⁰) and the schematic drawing of a cascade structure is shown in Fig. 1, where vacancies are mainly located inner side of a cascade and SIAs are mainly located outer side of a cascade. To obtain the information on vacancies in a cascade and SIAs in a cascade, positron annihilation lifetime measurement will be desired, especially dynamic behavior of the bundle of crowdions. In order to obtain the better understanding for bias effects under irradiation computer simulation was made and the basic view for the dislocation bias was presented from the formation energy of radiation induced defects. It was shown that the difference of the formation energy between a self-Interstitial atom and a vacancy is the most basic origin for the dislocation bias. On the other hand, for the production bias the detailed information on interstitial clusters is required and it was found in Fe model lattice that the edge dislocation line has a special character, i.e., a periodicity of b/3, but in the case of dislocation loops these stable positions distributed with a periodicity b/3 diffuse out with decreasing loop size and tend to have a periodicity of nearly b in the smaller limit of loop size. This behavior suggests that Peierls potentials which dislocation loops must overcome depend upon the loop size, and smaller Peierls stress can be expected for larger loops and an edge dislocation line probably because of finer periodicity b/3. But at finite temperatures small clusters of crowdions easily tend to have a rather loose coupling structure of composing crowdions, and slip motion as a whole cluster is not well defined, and the diffusion process as a whole might be better to represent the motion of small clusters at high temperatures.

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2. Vacancies in a Cascade

In order to investigate the state of vacancies in a cascade the positron annihilation lifetime measurement is very useful, because a positron is trapped at a vacancy site and the lifetime is determined from the surrounding electron density which is much lower at a vacancy site than that in a matrix. High purity Fe specimens refined through zone refining in hydrogen gas to high RRR (residual resistivity ratio) values above 3000 were irradiated with neutrons at very low temperature, 20 K by KUR-LTL (Kyoto University Reactor-Low Temperature Loop) to a dose of $1 \times 10^{17} \text{n/cm}^2$. The positron lifetime measurements were made for the irradiated specimens at 100 K after each isochronal annealing process. The result is shown in Fig. 3 with the same result by the electron irradiation (28 MeV electron by KURRI-LINAC, 77 K) with much less cascade effect. At 100 K both results show the almost the same positron lifetimes of about 175-180 ps, which suggests that vacancies in a cascade is almost isolated state.\textsuperscript{11,12} In Fig. 3 also the calculated result of a positron wave function trapped at a vacancy site in Fe is shown, giving the positron lifetime of 176 ps which is in good agreement with that obtained in the experiment.

3. Calculations

Model Fe lattice was constructed by using Finnis-Sinclair potential\textsuperscript{13} and into a model lattice a straight edge dislocation or bundle of crowdions of $a/2(111)$ Burgers vector was introduced. The size of the model lattice must be large enough to contain the defects with a long range strain field, such as a dislocation, and a size of simulation box is about $80b$ ($b$: magnitude of Burgers vector) cubic was used for the static calculation, but for the molecular dynamic calculation (MD calculation) usually smaller boxes were used. Relaxed structures were obtained by the static calculation or the MD calculation.\textsuperscript{15} The fixed boundary condition or the periodic boundary condition was applied depending on the defects in the model lattice, that is, the former for the bundle of crowdions and the latter for a straight edge dislocation along the dislocation line.

3.1 Dislocation bias

The simulation on the interaction between a straight edge dislocation and a SIA or a vacancy placed at various surrounding positions of the dislocation was already made and much higher interaction for a SIA than a vacancy was obtained, finally giving rise to excess vacancies in a matrix which contribute to void formation, that is, dislocation bias.
effect. In the present work another fundamental view for a dislocation bias is given on the standpoint of the energy decrease of a whole crystal during the clustering of point defects. The generation of defects in the crystal by irradiation makes the crystal unstable, and the best way to recover this situation is the recombination of SIAs and vacancies, but not all of them disappear through this process, giving rise to the cluster formation of each defect, i.e., SIA clusters and vacancy clusters. Since the crystal has a periodic structure, formation and growth of planar defect clusters from isolated point defects usually recover the crystal periodicity. This is the best way to decrease the total energy of the irradiated crystal without recombination between SIAs and vacancies. Since SIAs have large strain around them, that is, large relaxation volume, the planar cluster is the only cluster morphology which actually appears in the crystal, but vacancies have both three dimensional and planar defect structure. It is obvious that the periphery of the planar shaped defect can be recognized as a dislocation line. Hence the growth of the planar defect cluster through arriving of new point defects to the peripheral region is just an absorbing such defects by the dislocation line, thus resulting in the dislocation bias when more SIAs are absorbed than vacancies into the dislocation core. This is the conventional view for the dislocation bias mechanism. But it is more fundamental to recognize that the driving force for the planar cluster formation from isolated state of point defects is the magnitude of the formation energy of a point defect, because by forming a planar defect the total formation energy significantly decreases as shown in Fig. 4 for the case of SIAs (crowdions) in Fe, where formation energy decreases to almost one tenth of the isolated state of SIAs at larger cluster of crowdions. This result suggests that the formation of a planar defect cluster is almost equal to coming back process to the perfect lattice from the defected lattice and the true origin of the bias mechanism is the difference of the formation energy between a SIA and a vacancy. In Table 1 calculated values of formation energy are shown for various metals in the case of both SIA and vacancy. To make this idea clearer the schematic drawings of planar defects of SIAs and vacancies are given in Fig. 5. In the conventional understanding of the dislocation bias the fact that the preferential absorption of SIAs than vacancies to a dislocation line gives a confirmed basis of bias mechanism due to the stronger interaction of SIAs with a dislocation line than vacancies probably based on the larger relaxation volume of a SIA than that of a vacancy. Of course this is correct, but another simple way of understanding is obtained from Fig. 5 after slight change of the viewpoint. This is based on the viewpoint that if an interstitial loop can be seen from the opposite side it is regarded as a perfect region surrounded by the vacancy planar defect existing in the outer region extending to the infinity. According to the conventional viewpoint, both SIAs and vacancies arrive at a dislocation line, e.g., the interstitial loop at the left in the figure, but from the other viewpoint this can be seen in a different way, i.e., SIAs arrive at the interstitial loop, but vacancies arrive at the outer planar defect of vacancies. This new viewpoint gives the much easier understanding for the dislocation bias, because the essential feature is just a competition between the left process (SIA clustering) and the right process (vacancy clustering) in Fig. 5, clearly showing the higher clustering tendency of SIAs than vacancies due to the higher formation energy of a SIA, which results in the dislocation bias. From this formation energy consideration, if formation energies of a SIA and a vacancy are almost equal, bias effect must be very small and void formation might be significantly suppressed. This possibility is not realized in ordinary metals, but in semiconductors, such as, Si the condition might be approximately fulfilled. Actually remarkable void formation has not been obtained in the irradiation experiments of Si.

3.2 Interstitial clusters
It has been known that the interstitial clusters which can make one dimensional motion and arrive at sinks such as

![Table 1](image-url)
dislocations significantly contribute to the production bias, resulting in the formation of voids in materials under irradiation. The interstitial cluster which can make one dimensional motion is a bundle of crowdions, i.e., dislocation loop of Burgers vector \((a/2)(111)\) in bcc crystals and \((a/2)(110)\) in fcc crystals. Bundle of crowdions \(I_n\) \((n = 7, 19, 37, 61, 91 \ldots)\) are of a hexagonal shape consisting of six edge dislocation segments all of which lie on \{110\} slip planes and make slip motion under the shear stress applied symmetrically on each slip plane as shown in Fig. 6 in the case of Fe. For this configuration important objects, such as, the detailed structure of the dislocation segment, the mobility under shear stress and the behavior of small clusters at finite temperatures must be studied, giving rise to the precious information useful for the understanding of the production bias.

### 3.2.1 Stable positions of the dislocation loops

The inherent lattice resistance to the slip motion of dislocation loops of the edge character, i.e., Peierls stress was calculated in the previous paper and the decreasing tendency with increasing loop size was obtained. In the present paper the stable positions of the dislocation loops were investigated in order to obtain the information on the Peierls potential. Stable positions of the cores of the dislocation loops were obtained for hexagonal shaped dislocation loops of various sizes, i.e., \(I_{19}, I_{217}, I_{817}, I_{1951}\), and also for a straight edge dislocation. The central position of the dislocation core was obtained by the plotting the distribution of Burgers vector, i.e., the displacement between two atomic planes just above and below the slip plane, some examples of which are shown in Fig. 7, where the displacement increases from zero to one \((b)\) from negative infinity to positive infinity and the central position is defined as the position where the displacement becomes 0.5 \(b\). Basically stable position of the dislocation core is usually distributed with a period of \(b\) (magnitude of Burgers vector) along \{111\} direction on the slip plane \{110\}, but the edge dislocation line has a special character, i.e., a periodicity of \(b/3\) as shown in the inserted figure in Fig. 8, and actually the calculated values of Peierls energy at these points distributed with a periodicity \(b/3\) are exactly equal as shown in Fig. 8. In this figure the values of stable points are calculated ones, but the potential shape is schematic because of the difficulty of the calculation of Peierls potential. On the other hand, in the case of dislocation loops these stable positions are split into two opposite directions as shown in Fig. 8 by a dotted line, that is, the value of \(x\) decreases with decreasing loop size. This decreasing behavior of \(x\) is shown in Fig. 9, suggesting that through the decrease of a loop size dislocation loops tend to have a periodicity nearly \(b\). The important point of this feature is that Peierls potentials which dislocation loops must overcome depend upon the loop size, and smaller Peierls stress can be expected for larger loops and an edge dislocation line probably because of finer periodicity \(b/3\). The calculated result of decreasing tendency of Peierls stress with the increase of a loop size was previously obtained.
3.2.2 Behavior of dislocation loops at finite temperatures

Since a straight dislocation makes a slip motion by the aid of the thermally activated kink pair formation, it is reasonably considered that the same mechanism might occur for the case of motion of dislocation loops. But in the case of smaller limit of dislocation loops some change might occur for this mechanism, because the ratio \( R = D/b \), where \( D \) is the diameter of a loop and \( b \) is the periodic distance of the motion, the magnitude of Burgers vector, might probably become an important parameter which determines the behavior of motion. By the analytic calculation for this problem by using a conventional string model [21], it can predict that in the case of the ratio \( R \) smaller than a critical value meta-stable configuration such as kink pair does not exist, suggesting that in this case of smaller dislocation loops the motion might be regarded as a whole motion of a cluster of crowdions just like a diffusion.

In order to clarify this feature the molecular dynamics calculation was made for a small dislocation loop \( I_{19} \) at 10 and 100 K. In Fig. 10 shows a snap shot of the thermally motion of this cluster, showing the dispersed motion of each crowdion composing a bundle of crowdions. This means that at finite temperatures small clusters of crowdions easily tend to have a rather loose coupling structure of composing crowdions, and slip motion as a whole cluster is not well defined, and the diffusion process as a whole might be better to represent the motion of small clusters at high temperatures. Much more detailed investigations will be required for this thermally activated motion of small interstitial clusters.

4. Summary

It is well known that in the process of damage structure evolution in materials under irradiation so-called bias effects, \( i.e., \) dislocation bias and production bias are playing important roles. For the better understanding for these bias effects computer simulation has been made and the basic view for the dislocation bias was obtained from the consideration of the formation energy of radiation induced defects. It was shown that the difference of the formation energy between a self-interstitial atom and a vacancy is the most basic origin for the dislocation bias. On the other hand, for the production bias the detailed information on the stable positions of small interstitial clusters, \( i.e., \) the stable position of the core of a dislocation segment of a bundle of crowdions in Fe was obtained from the computer simulation on the viewpoint of the inherent lattice resistance stress for the clusters which can be also called Peierls stress.

It was found that the edge dislocation line has a special character, \( i.e., \) a periodicity of \( b/3 \), but in the case of dislocation loops these stable positions distributed with a periodicity \( b/3 \) diffuse out with decreasing loop size and tend to have a periodicity of nearly \( b \) in the smaller limit of loop size. This behavior suggests that Peierls potentials which dislocation loops must overcome depend upon the loop size, and smaller Peierls stress can be expected for larger loops and an edge dislocation line probably because of finer periodicity \( b/3 \).

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