Understanding of Irradiation Softening in α -Iron from the Viewpoint of the Direct Interaction between a Screw Dislocation and Self Interstitial Atoms under Stress

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Computer simulation of the interaction between a screw dislocation and self-interstitial atoms (SIA) under applied stress has been performed using a N -body potential (Finnis and Sinclair, 1984) for an α -iron model lattice in order to understand the irradiation softening observed at low temperatures. It was found that through the absorption of a SIA into a core of a moving screw dislocation a three-kink configuration is formed on a dislocation line, resulting in the enhancement of motion of a whole dislocation line through propagation of these kinks along the dislocation line under applied stress. This plays an important role in the irradiation-induced softening phenomenon. In this process a SIA was converted from $[\bar{1}10]$ dumbbell to $[111]$ crowdion in the dislocation core and disappeared through dissociation of an extended $[111]$ crowdion along the dislocation line. Disappearance of softening at 4.2 K can be caused by hindering propagation of these kinks through the interaction with other moving kinks. These results have possibility to explain the temperature dependence of the irradiation softening observed in α -iron.

(Received February 10, 1989)

Keywords: computer simulation, screw dislocation, self-interstitial atom, irradiation softening, iron

I. Introduction

In bcc metals, it is considered that the effect of radiation on mechanical properties at low temperatures arise mainly from an interaction between screw dislocations and radiation-induced defects, especially SIAs. Therefore, the detailed study for this interaction is required. Since in a dislocation core the strain is too large to be analysed by the theory of linear elasticity, computer simulation must be performed in model lattices. Many computer simulations for the motion of a dislocation in bcc lattices have been performed using, for example, the pairwise Johnson-Wilson potential⁽¹⁾ in order to explain the various experimental results. However, since actual transition

bcc metals have non-central character in the interatomic force, it is difficult to describe the behaviour well by pair potentials. Hence, computer simulations using Finnis-Sinclair potential⁽²⁾ will be performed in this paper. Since the more exact multi-body potential derived from tight-binding theory for a d-electron band (Masuda *et al.*⁽³⁾ Sato and Masuda⁽⁴⁾) is too complex to be used (because of insufficiency of CPU time and memory capacity of present computers) Finnis-Sinclair formulae which also include the character of d-electrons and N body effect were chosen at the present time. The size of the model crystal must be large enough to observe the whole interaction between a screw dislocation and a SIA under an applied shear stress.

Tensile tests of high-purity iron single crystals at low temperatures made after 2.5 MeV electron irradiation at 77 K (Aono *et al.*⁽⁵⁾⁽⁶⁾) showed that radiation-induced softening is observed not only at the yield point but also in the deformation stage after that, but the amount of softening decreases with increas-

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ing strain at 77 K. At 4.2 K, neither irradiation softening nor hardening were observed clearly. On the other hand, it is known that softening produced by interstitial alloying elements (for example, nitrogen, see Kitajima *et al.*⁽⁷⁾) is independent of the magnitude of deformation. This difference can be considered to come from the fact that during staining SIAs are absorbed to dislocation cores and disappear, but interstitial alloying elements are not. Therefore, computer simulation must make these facts clear, namely, absorption of SIAs into a screw dislocation core and disappearance of softening at 4.2 K. Besides this short range (core) interaction between a screw dislocation and a SIA long range interaction (Sato and Meshii⁽⁸⁾) must be taken into account to fully understand the irradiation softening effect, but in this paper only the former will be investigated.

II. Methods of Calculation

The used model α -iron lattice has a tetragonal shape of a size of about $40b \times 40b \times 99b$ (b : the strength of Burgers vector) as shown in Fig. 1. A screw dislocation was introduced at the centre of the model crystal along the longest side and a SIA was around the central position. A shear stress was applied to make the screw dislocation glide upwards. Relaxation was performed using the Newton-Raphson method under the applied stress. As shown in Fig. 1 the model crystal was divided into three zones, where zone C is a fixed zone, zone B is a relaxed zone, and zone A is a fully

relaxed zone (ten times more than zone B). In the following the iteration number N_{it} is counted in unit of one full path of relaxation in zone A, i.e., from one end to the other end of the model crystal along the direction of the dislocation line.

III. Results of Computer Simulation

1. The configuration of a SIA in a dislocation core

The stable configuration of a SIA in a screw dislocation core obtained by computer simulation is shown in Fig. 2(a), and for comparison

Fig. 2(a) The configuration of an interstitial atom in the dislocation core under the applied stress in Finnis-Sinclair potential. (A screw dislocation is introduced one atomic distance below this plane as an initial condition).

Fig. 2(b) The configuration of an interstitial atom in the dislocation core under the applied stress in Johnson-Wilson potential (A screw dislocation is introduced one atomic distance below this plane as an initial condition).

Fig. 1 A model α -iron crystal with a screw dislocation and point defects (divided into three regions A, B and C according to the extent of iteration).

is the same result obtained by using Johnson-Wilson potential shown in Fig. 2(b). In this and subsequent figures, indices I, J, K represent atom coordinates referred to orthogonal directions $[\bar{1}10]$, $[\bar{1}\bar{1}2]$ and $[111]$. To obtain the configuration of a SIA in a screw dislocation core a SIA ($[\bar{1}10]$ dumbbell) was first placed at the one atomic distance upper site from the screw dislocation core and the model crystal was stressed to move the dislocation upwards. Then, the screw dislocation encountered the SIA, which gave the final configuration of a SIA in the core. For both potentials the final configuration of a SIA in the core was $[111]$ crowdion. The conversion processes from $[\bar{1}10]$ dumbbell to $[111]$ crowdion are seen in left hand figures in Figs. 2, and the final configurations are in right hand ones. These figures are obtained by viewing the $(\bar{1}\bar{1}2)$ plane where a SIA exists from the upper side. Numbers in parentheses besides the applied stress are iteration numbers N_{it} . From the above result it is clear that $[111]$ crowdion is more stable than $[\bar{1}10]$ dumbbell in a screw dislocation core. As for the $\langle 110 \rangle$ dumbbells of different orientations, the same conversion from $\langle 110 \rangle$ dumbbell to $[111]$ crowdion was also observed, which suggests that this conversion frequently occurs on the encounter of a dislocation and a SIA in real specimens.

2. The motion of a screw dislocation under applied stress

In Fig. 3 the relaxation process of the total energy of the model crystal, u_{tot} (per atom), during iteration is shown for two cases, namely, case (i) (white marks): only a screw dislocation exists in the model crystal, case (ii) (black marks): $[111]$ crowdion exists in the dislocation core, (type A, see below). For each case three stress levels were chosen. Under the lower stress saturation is easily obtained, but under the higher stress a dislocation starts to glide and saturation does not seem to appear easily. That the top curve is at the higher level is due to a smaller volume over which the energy summation was made.

In Fig. 4 three core structures of a screw dislocation in a model α -iron lattice are shown by Vitek's differential displacement representa-

Fig. 3 Change of total crystal energy per atom u_{tot} during iteration in two cases, case (i) a screw dislocation only, case (ii) a screw dislocation and a SIA (type A).

tion (Vitek *et al.*⁽⁹⁾), where black dots are the $[111]$ atomic rows and the arrows indicate the change of the relative displacement (along the $[111]$ direction) of two adjacent atomic rows from that in a perfect crystal. The full length of an arrow (starting at one atomic row and ending the neighbouring atomic row) corresponds to $b/3$, where b is the magnitude of Burgers vector.

The core structure directly obtained after relaxation from the initial elasticity solution is shown in (a), which seems isotropic and is close to the elasticity solution. This is called unpolarized type core structure. The polarized type core also exists in this model lattice as shown in (b), which was obtained by giving small displacements along the $\langle 111 \rangle$ direction to the central three atomic rows constituting a screw dislocation core, or stressing the unpolarized core to the next stable position. The well relaxed energy for these two core structures are very close each other (slightly lower in the polarized type core). Besides these two core structures a split type core structure is also observed as shown in (c) which was obtained by introducing a screw dislocation at the mid-

Fig. 4 Various core structures of a screw dislocation.

dle point between two stable positions. This configuration is a metastable configuration between the two stable positions. (Refer to Takeuchi⁽¹⁰⁾ for naming of these core structures)

Figure 5 shows the motion of a screw dislocation (here only the unpolarized type is taken into account) in a model crystal under applied shear stress, where successive behaviour of a dislocation line viewed from an inclined upper angle are drawn. In the top left part of this figure the $\langle 111 \rangle$ view of this model crystal is shown, where next central position of a dislocation is also denoted by a dotted triangular. It is seen from the main figure that under shear stress 0.015μ ($\mu = (C_{11} - C_{12} + C_{44})/3 = \text{shear modulus for the } \langle 111 \rangle \text{ direction in the } \{110\} \text{ plane}$) the left hand part of a dislocation line already glided to the next stable position. Under the higher stress the whole dislocation line moved to the next stable position. This means that Peierls stress for a screw dislocation in this model α -iron lattice is about 0.015μ . The forward motion of a screw dislocation line was followed by the side motion of a kink

Fig. 5 Motion of a screw dislocation under applied shear stress.

which is denoted by hatching in the figure. The shape of the kink is not 'abrupt'.

3. Interaction between a screw dislocation and a SIA under stress

Before going into a detailed investigation of the interaction between a screw dislocation and a SIA it is useful to study qualitatively behaviour of the dislocation core when it absorbs a SIA (the [111] crowdion which is the stable configuration in the core as mentioned in III.1). The unpolarized type core (Fig. 4(a)) is taken here. In Fig. 6 is shown the shift of a screw dislocation centre (denoted by the circle) to a neighbouring stable position by giving certain $\langle 111 \rangle$ displacement to one of the three atomic rows (centre in each figure) in the core. For example, in the top right figure the dislocation centre is completely shifted to the upper stable site by the displacement $-b/3$ ($-$ is the downward direction of the paper plane). The displacement $2b/3$ (the upper direction of the paper plane) gives the same result. In the bottom centre figure the dislocation centre is shifted to the right hand stable position by the displacement $b/3$. From these two figures it is simply predicted that the absorption of [111] crowdion into a screw dislocation core causes a shift of the dislocation core to two different neighbouring sites depending on the side of the crowdion, because the crowdion has equal and

opposite $\langle 111 \rangle$ displacements on either side of itself. This suggests that a screw dislocation line must be kinked in a complicated way when it absorbs a SIA ([111] crowdion). The actual computer simulation in the following will show that this complex structure is suitable to be called a 'three-kink configuration'. The last one of the three kinks is a 'bridge' of the two kinks formed directly by the $\langle 111 \rangle$ strain of an absorbed crowdion.

In order to clarify how the interaction between a screw dislocation and a SIA under stress depends on the relative position between them, computer simulations for various relative positions shown in Fig. 7 were performed, where a circle indicates the original position of a screw dislocation line, and A, B, C, D, E and F are the positions where SIAs were inserted. Type A, E and F are first nearest neighbouring positions of the centre of the dislocation. Type B and type D are in the second and the third nearest zones, respectively. Positions in each group (1st to 3rd nearest neighbours) are equivalent under no applied shear stress. However, the equivalency is not kept under applied shear stress. Then simulation for all cases are required. Furthermore, in order to clarify the more complex and actual interaction between a screw dislocation and a few SIAs computer simulation was also performed for the case where one interstitial atom is in the core (position A) and the other one is outside the core (position D). Simulation for type F will not be presented because of its less importance for the enhancement of a dislocation motion. The case of type C is similar that of type D, then this will also be omitted.

Fig. 6 Formation of "three-kink configuration". (Only a central atomic row is displaced upward or downward without any relaxation).

Fig. 7 Various relative positions between a screw dislocation and a SIA.

(1) Simulation of the type A configuration

In Fig. 8(a) the [111] crowdion was placed on the first atomic row (position A in Fig. 7) in the dislocation core. The shear stress was applied so as to move the dislocation upwards in the figure. Even with no shear stress, a three-kink configuration appeared just in front of the dislocation line. When the applied stress increased beyond the critical shear stress ($F=0.005$ to 0.007μ), these three kinks started to propagate along a dislocation line under increasing applied stress or iteration number. Two of the three kinks propagated to the left and the other to the right in this figure. Corresponding to this behaviour, in Fig. 8(b) is shown the strain distribution along the [111] atomic row where the [111] crowdion was absorbed. Exactly speaking, deviation of the interatomic distance from b on the [111] atomic row is shown as a function of the atom position K , and negative values correspond to the compression state. In other words, this is an extended structure of the [111] crowdion in a

screw dislocation core. It is seen that the strain distribution gradually changes with increasing number of the iteration N_{it} and increasing stress. With no applied stress the strain distribution was localized, but started to propagate to either direction under higher stress than 0.005 – 0.007μ . Namely, dissociation of the extended [111] crowdion occurred, which is identical to the migration of kinks in opposite directions in Fig. 8(a), resulting in the enhancement of forward motion of a whole dislocation line. Figure 8(a) and (b) show that the critical shear stress for a screw dislocation to move was reduced through the nucleation and propagation of three kinks compared with the case of no absorption of a SIA ($F=0.015 \mu$). This must give a significant contribution to the irradiation softening. The [111] crowdion will finally disappear as diffusing away of three kinks on the dislocation line.

(2) Simulation of the type B configuration

In Fig. 9(a) the 111 crowdion was placed out-

Fig. 8(a) Motion of a screw dislocation under applied shear stress in type A configuration.

Fig. 8(b) Strain distribution (change of the interatomic distance) along the [111] atomic row where [111] crowdion exists.

side and in front of the dislocation core (position B in Fig. 7). In this case more complicated structure appeared after relaxation as shown in the figure. The centre of the screw dislocation seems to be shifted to two atomic distant neighbouring position, and this part and the original dislocation line must be connected, finally resulting in four-kink configuration as shown in the figure. To understand this situation the same trial as that in Fig. 6 was made and is shown in Fig. 9(b), where $\langle 111 \rangle$ displacements are given on the atomic row at the B position. When the displacement is $b/2$ or $-b/2$ (bottom, right figure), a new dislocation centre appears at the site (denoted by the dotted circle) which is two atomic distant from the original position of the dislocation. This is considered to be an essential feature in fig. 9(a). When the applied stress became larger than the critical shear stress ($F=0.01 \mu$), propagation of kinks started, and two of four kinks propagated to the left and the other two to the right in this figure, which indicates that also in

this case the softening occurs.

(3) Simulation of the type D configuration

In Fig. 10 $[\bar{1}10]$ dumbbell was placed outside and in front of the dislocation core and in a perpendicular direction to the slip plane (position D in Fig. 7), where $[\bar{1}10]$ dumbbell is more stable than $[111]$ crowdion. Simulation was carried out in detail only for this direction of $\langle 110 \rangle$ dumbbell, but similar results will be obtained for other orientations. Without applied shear stress there occurred no change in a dislocation line. When the applied stress became $F=0.015 \mu$ ($N_{it}=360$), a dislocation began to move forward but $[\bar{1}10]$ dumbbell was not converted into $[111]$ crowdion yet. The conversion and three-kink formation occurred at about 0.02μ and migration of kinks took place with increasing number of iteration as well as other cases (type A and B). In this case no softening was observed, because a screw dislocation line itself must glide one atomic distance before it encounters a SIA.

(4) Simulation of the type E configuration

In Fig. 11(a) the $[111]$ crowdion was placed on the back atomic row (position E in Fig. 7) in the dislocation core. Without applied shear stress the three-kink configuration appeared behind the dislocation line. However, this

Fig. 9(a) Motion of a screw dislocation under applied shear stress in type B configuration.

Fig. 9(b) Formation of "four-kink configuration". (Only a central atomic row is displaced upward or downward without any relaxation).

Fig. 10 Motion of a screw dislocation under applied shear stress in type D configuration.

Fig. 11(a) Motion of a screw dislocation under applied shear stress in type E configuration.

three-kink configuration did not expand but contracted under increasing applied shear stress as shown in the figure. This is also seen in Fig. 11(b), which shows the strain distribution along the $[111]$ atomic row where $[111]$ crowdion exists. This indicates that the three-kink configuration behind a dislocation behaves as an obstacle for the forward motion of a screw dislocation. This can be understood by comparing type E with type A (Fig. 8(a)). Two kinks moving to the left are sited on the left side in type A but on the right side in type E, and the other right moving one which has a maximum Schmid factor is vice versa. Therefore, three-kink configuration in type E must constrict inwards when the stress is applied so as to move the dislocation upward. Under the applied stress which was smaller than $F=0.03 \mu$ ($N_{it}=360$), the dislocation was pinned at the original position and beyond this stress the pinning point disappeared and $[111]$ crowdion was left behind the dislocation line. However,

Fig. 11(b) Strain distribution (change of the interatomic distance) along the $[111]$ atomic row where $[111]$ crowdion exists.

in Fig. 11(a) even under lower stress the remaining part of the dislocation line already started to move. The reason was not so clear, but it seems reasonable to conclude that the type E configuration contributes to hardening through the pinning mechanism.

(5) Hybrids of type A and type D: (i) type A & D, (ii) type D & A

During low temperature deformation of specimens irradiated at low temperatures, a screw dislocation must glide on a slip plane interacting SIAs successively. In rough estimate, a screw dislocation segment of length of the order of " μm " encounters a SIA at every jump over the Peierls potential in the specimen irradiated to the level of $10^{18}\text{e}/\text{cm}^2$. In the matrix of bcc metals a SIA has a $\langle 110 \rangle$ dumbbell structure. But there must be a certain probability of generation of a SIA in a screw dislocation core as $\langle 111 \rangle$ crowdion during low temperature irradiation. There the three-kink configuration is already formed, which must be a starting point of dislocation motion after irradiation. This is the reason why we consider the hybrid case of type A and type D. This pattern will occur successively because $[\bar{1}10]$ dumbbells will convert to $[111]$ crowdions on encountering with a moving screw dislocation. Two cases should be considered for the relative position between two SIAs because three-kink configuration is not symmetrical in the direction of a dislocation line as mentioned above. We distinguish these two by type A&D and type D&A, where the order of A and D corresponds to the increasing order of " K " (Z-coordinate of a lattice point). The relative distance between two SIAs was taken to be $20b$ along the $[111]$ direction.

In Fig. 12 for the type A&D $[111]$ crowdion (type A) was placed at $K=40$, and the $[\bar{1}10]$ dumbbell (type D) was placed at $K=60$. As increasing the applied shear stress and the iteration number, two things occurred, namely the kink of highest Schmid factor propagated to the right in the figure ($F=0.01\mu$) and the second one, which is more important, is that $[\bar{1}10]$ dumbbell was converted into $[111]$ crowdion, resulting in the formation of a new three-kink configuration, before propagating two kinks

Fig. 12 Motion of a screw dislocation under applied shear stress in type A & D configuration.

(from position A) arrived at this position ($F=0.02\mu$). The right going kink in this newly formed three kinks must encounter the two left going kinks from position A, which makes an obstacle point for the forward motion of a whole dislocation line just like the type E mentioned above. Then in this type A&D softening cannot be expected but hardening will occur. But, if the collision of these kinks going in opposite directions can be avoided, namely, the conversion takes place after the two left going kinks passed away, we can expect softening even in this type A&D. This depends on the kink mobility, which may increase with increasing temperature.

In Fig. 13 for the type D&A $[111]$ crowdion (type A) was placed at $K=60$, and the $[\bar{1}10]$ dumbbell (type D) was placed at $K=40$. Under the applied shear stress $F=0.01\mu$ the kink of highest Schmid factor propagated to the right in the figure and encountered the $[\bar{1}10]$ dumbbell, resulting in the conversion of $[\bar{1}10]$ dumbbell into $[111]$ crowdion, namely the formation of a new three-kink configuration. The differ-

Fig. 13 Motion of a screw dislocation under applied shear stress in type D & A configuration.

ent point from the case of type A&D is that the conversion occurred after the right going kink from the position A passed away. This avoided the formation of an obstacle for the forward motion of a whole screw dislocation line. Hence in this case of type D&A we can expect softening.

IV. Discussion

Using the model iron lattice constructed by Finnis-Sinclair potential the relatively low Peierls stress for a screw dislocation was obtained (0.015μ , which is much lower than the value obtained in Johnson-Wilson potential 0.052μ , (see Kuramoto *et al.*⁽¹¹⁾⁽¹²⁾, Aono *et al.*⁽¹³⁾). Although this value is still higher than that obtained in 4.2 K experiments for pure iron single crystals (0.005 – 0.007μ : Aono *et al.*⁽⁵⁾⁽⁶⁾), this situation enabled the detailed study on the interaction between a screw dislocation and SIAs under applied shear stress. By relaxing the model crystal under low applied stress to a large extent, the three-kink propagation in

type A or the four-kink propagation in type B were fully observed at a very low stress level (0.005μ , almost equal to the experimental level), suggesting that the absorption of a SIA into a dislocation core is a very important factor for the irradiation softening effect. As a result of these kink propagations SIAs disappear along the screw dislocation line as the dissociation process of the extended $[111]$ crowdion on a $[111]$ atomic row in the screw dislocation core. This can explain the fact that the softening disappears with increasing amount of deformation of the irradiated specimens at low temperatures (Aono *et al.*⁽⁶⁾), namely, the exhaustion effect of SIAs.

In type E the absorption of a $[111]$ crowdion into the core acts as a pinning point and causes a hardening effect. However, these unfavourable three-kink configuration plays an important role in understanding the temperature dependence of softening observed in the experiments. The results of computer simulation are considered to correspond to the experiments at 4.2 K where almost no softening was observed (Aono *et al.*⁽⁵⁾⁽⁶⁾). At higher temperatures kinks have higher mobility, which will change the situation to a large extent, resulting in the remarked softening (observed at 77 K). This will be the same in the case of type A&D, where three-kink configurations are formed successively and the key point is timing of nucleation of the second one (before or after a coming kink arrives). The result of simulation presented here showed the case of bad timing for the softening. In the case of type D&A the example of good timing was obtained. This depends on the kink mobility (i.e., temperature and presence of impurity atoms) and the orientation of the applied shear stress.

A schematic representation of a case where successive formation of three-kink configuration is shown in Fig. 14. In real specimens irradiated at low temperatures SIAs are randomly distributed like Fig. 14(a) and in this case unfavourable type A&D must appear as shown in the figure. In Fig. 14(b) is shown the case of a rather artificial distribution of SIAs which gives only favourable type D&A. But this must be seldom observed in actual specimens. Then we must consider that Fig. 14(a) is the actual

Fig. 14 Illustrations of a slip plane where successive interactions between a gliding screw dislocation and SIAs occur. (case (a); expected at 4.2 K (solid line) and 77 K (dotted line), case (b); rather artificial configuration of SIAs which is favourable for softening).

case in specimens, which gives almost no softening at 4.2 K and remarkable softening at higher temperatures (e.g., 77 K), where kink mobility is higher. The solid and dotted lines in the figure correspond to these two cases, respectively.

This study must be extended more to cases where higher numbers of SIAs are existing on slip planes and adjacent planes, and under

more complicated stress conditions (not only shear stress but also normal stress), namely under actual tensile condition of different orientations, and so on. These will be made in the near future.

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