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Atomistic modeling of the interaction between self-interstitial dislocation loops and He in bcc Fe

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Abstract

The effect of a helium atom on the migration of self-interstitial dislocation loops with a Burgers vector $1/2\langle 1\,1\,1\rangle$ in bcc Fe has been investigated using molecular statics and molecular dynamics simulations. It is found that an interstitial He atom hinders the migration and coalescence behavior of dislocation loops by strongly binding to the loop on the edge sites. An unstable interstitial He atom on the loop plane easily moves to the stable edge sites by interstitial diffusion. A substitutional He atom does not significantly disturb the migration of dislocation loops, showing weak binding.

1. Introduction

Ferritic/martensitic steels are candidates for first-wall and breeding-blanket structural materials in future fusion reactor systems [1]. These materials are exposed to high-energy neutron irradiation, which produces displacement defects such as vacancies and self-interstitial atoms (SIAs). SIAs diffuse very fast three dimensionally due to their low activation barrier for diffusion and easily form self-interstitial dislocation loops by their coalescence, in addition to the SIA clusters directly formed in displacement cascades. The formed self-interstitial dislocation loops tend to migrate (usually) one dimensionally and grow as they coalesce after their continual collisions. These dislocation loops are observed with Burgers vectors, $\boldsymbol{b} = 1/2\langle 1\,1\,1\rangle$ and $\boldsymbol{b} = \langle 1\,0\,0\rangle$ in bcc Fe. $\langle 1\,0\,0\rangle$ loops have been recently proposed to form from the direct coalescence of $1/2\langle 1\,1\,1\rangle$ loops produced immediately after displacement cascades and grow by the biased absorption of $1/2\langle 1\,1\,1\rangle$ loops [2].

In addition to self-interstitial dislocation loops, helium is also generated due to (n,α) nuclear transmutation reactions and directly implanted in steels in nuclear fusion environments [1]. Since its solubility in metals is extremely low, He tends to precipitate into clusters or bubbles, enhancing void swelling and producing surface roughening and blistering as well as high-temperature intergranular embrittlement. At low temperatures, helium may also affect irradiation hardening and fatigue life by acting as an obstacle to the movement of dislocations, as do self-interstitial dislocation loops.

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Although the interactions between self-interstitial dislocation loops and He atoms play an important role in determining microstructural evolution in steels exposed to nuclear fusion environments, they have not been well understood compared to the He–vacancy interactions that have been recently studied in the frameworks of ab initio calculation [3], molecular dynamics (MD) [4,5] and kinetic Monte Carlo modeling [6,7]. The objective of this study is to understand the interactions between self-interstitial dislocation loops and both interstitial and substitutional helium atoms in bcc Fe at an atomic scale by employing both MD and molecular statics (MS) techniques. In particular, this study will focus on the effect of a helium atom on the migration and coalescence of dislocation loops.

2. Interatomic potentials and modeling methods

Both MD and MS simulations have been performed with the code MDCASK [8] and make use of the empirical interatomic potentials to describe Fe–Fe and Fe–He interactions. For Fe–Fe, we used the Finnis–Sinclair potential by Ackland et al. [9]. For Fe–He, we used the potential recently fit by Morishita et al. [4] to the ab initio calculations by Wilson and Johnson [10]. The empirical potentials used in this study predict that octahedral sites are the most stable He interstitial sites, which is not in agreement with recent ab initio calculations [3] predicting that tetrahedral sites are the most stable. However, the energy difference between octahedral and tetrahedral sites is calculated to be quite low [3]. Moreover, the activation energy of interstitial He diffusion calculated by the empirical potentials (0.08 eV) is in good agreement with the result of the ab initio calculations (0.06 eV) [3]. It is expected that substitutional He atoms diffuse dominantly by the vacancy mechanism rather than the dissociation mechanism, because the energy difference between substitutional and interstitial He atoms and indeed the dissociation energy of substitutional He is quite high; although again recent ab initio calculations [3] reveal a smaller dissociation energy of ~2.4 versus ~3.9 eV [4].

To evaluate the binding energies of a He atom to a self-interstitial dislocation loop in bcc Fe, MS simulations have been performed. As shown in Fig. 1 a 37-SIA hexagonal loop with $\boldsymbol{b} = 1/2[1\,1\,1]$ and a habit plane of (1 1 0) is placed at the center of a $50a \times 50a \times 50a$ computational cell (250 000 atoms), where a is lattice constant of bcc Fe. Varying the location of a He atom for both interstitial and substitutional sites, the total energy was calculated through MS simulations. For an interstitial He site, an octahedral site in the bcc structure was selected. On the whole, there are two types of He atom location. One is in the directions laid on the loop plane (type I), for example, [0 0 1], $[\bar{1}\,1\,1]$, $[\bar{1}\,1\,\bar{1}]$ and $[\bar{1}\,1\,0]$, and the other is in the Burgers vector direction over the loop plane (type II) as described in Fig. 1.

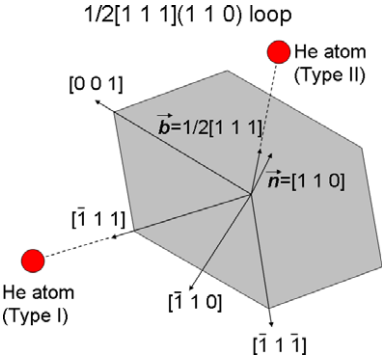

Fig. 1. Schematic illustration of a 1/2[1 1 1](1 1 0) loop with a He atom.

MD simulations have been performed with two 37-SIA hexagonal dislocation loops in a $60a \times 60a \times 60a$ computational cell (432 000 atoms) of bcc Fe at 600 and 1000 K. One 1/2[$\bar{1}\,\bar{1}$ 1](1 1 0) loop (loop A) is placed at the center of the cell and the

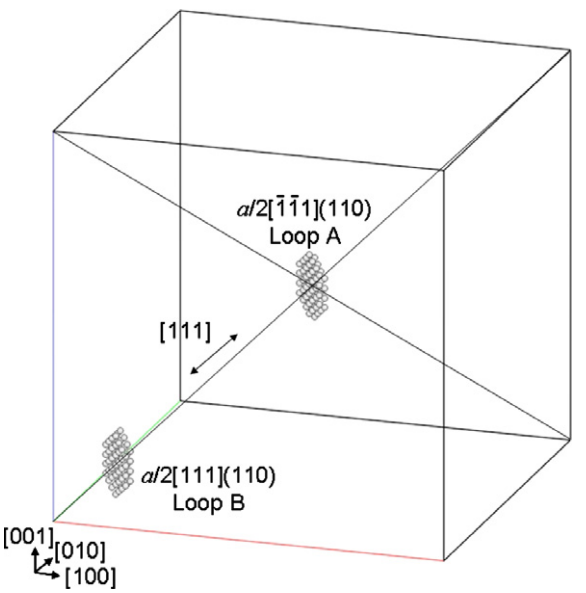

Fig. 2. Computational cell containing two 37-SIA dislocation loops (loops A and B) for MD simulations.

other 1/2[1 1 1](1 1 0) loop (loop B) is apart from the center in [1 1 1] direction as illustrated in Fig. 2. A helium atom is placed either on the edge of loop B (type I) or between the two loops in [1 1 1] direction (type II).

3. Results and discussion

The total energy relative to the well-separated He atom is plotted against He distance from the loop in Fig. 3. As the interstitial He distance decreases in $[\bar{1}\,1\,0]$ direction (type I), the total energy starts to decrease slightly from about 2.5 nm (Fig. 3(a)). However, it drastically decreases to about −1.4 eV at about 1 nm, namely, immediately on the loop edge (Fig. 3(a)). Therefore, it is expected that the interstitial He atom will quite strongly bind self-interstitial dislocation loops on the loop edge with a binding energy of about 1.4 eV. This binding energy is consistent with the value obtained by Ventelon et al. [11] who calculated the binding energy between a 20-SIA cluster and an interstitial He atom using the same potentials. Although we also calculated the binding energy on the loop edge in other directions laid on the loop plane such as $[\bar{1}\,1\,1]$, $[\bar{1}\,1\,2]$ and [0 0 1], the binding energy in $[\bar{1}\,1\,0]$ direction was the highest. For the interstitial He atom placed in the [1 1 1] Burgers vector direction (type II), the total energy decreases drastically at about 0.7 nm and then rises up to 1.2 eV at about 0.2 nm (Fig. 3(a)), indicating that an interstitial He atom will be very unstable immediately on the loop plane. The positive binding energy on the loop edge and negative binding energy immediately on the loop plane can be explained by the strain field of self-interstitial dislocation loops. While the dislocation loops induce compressive strain field on the loop plane, they induce tensile strain field near the loop edge, as Marian and coworkers [12] described. Therefore, the interstitial He atom with an approximately symmetric compressive strain field will naturally prefer to stay on the loop edge. The substitutional He atom slightly binds the loop with a lower binding energy of about 0.3 eV, as shown in Fig. 3(b), without being significantly influenced by its location, compared to the interstitial He atom.

Fig. 4 presents MD snapshots of the interaction between two 37-SIA dislocation loops at 1000 K without the presence of the He atom. Initially, loop A was 7.4 nm away from loop B in [1 1 1] direction. As soon as the MD simulation begins, loop A is driven toward loop B in the [1 1 1] direction as a result

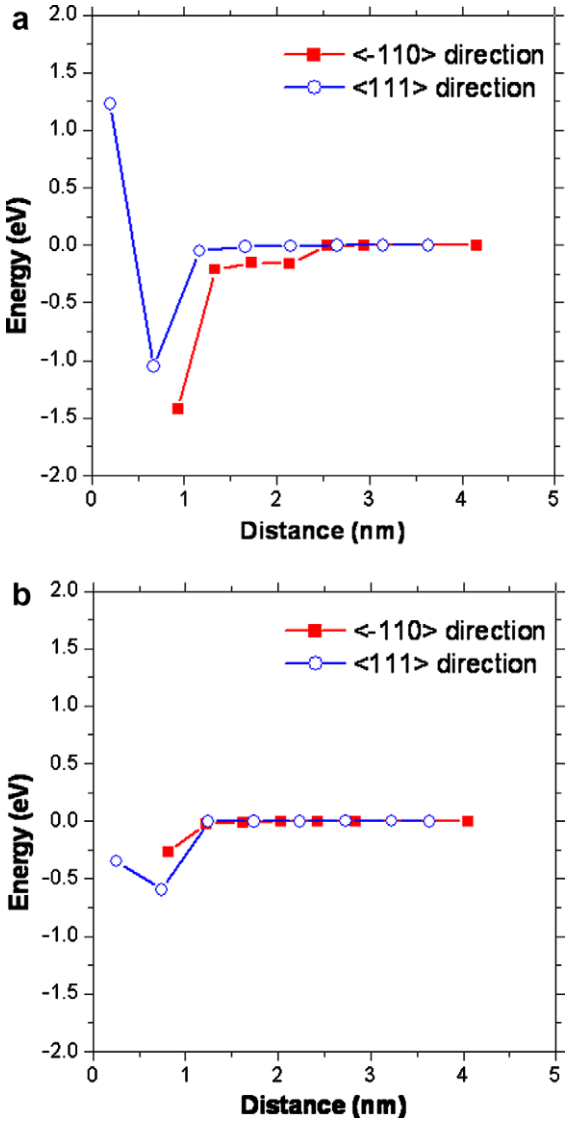

Fig. 3. Total energy variation, relative to the well-separated He atom, with (a) interstitial and (b) substitutional He distance from the loop center.

of the long-range elastic interaction (Fig. 4(a)). At about 18 ps, the two dislocation loops collide near the center of the cell. As shown in Fig. 4(b), immediately after the collision, several segments with $\boldsymbol{b} = [0\,0\,1]$ form according to the following reaction:

$$1/2[1\,1\,1] + 1/2[\bar{1}\,\bar{1}\,1] \rightarrow [0\,0\,1]. \quad (1)$$

Although these [0 0 1] segments repeat the appearance and disappearance in our short-time simulation, Marian et al. [2] demonstrated the propagation of the $\langle 1\,0\,0\rangle$ segments through a kinetic process in their

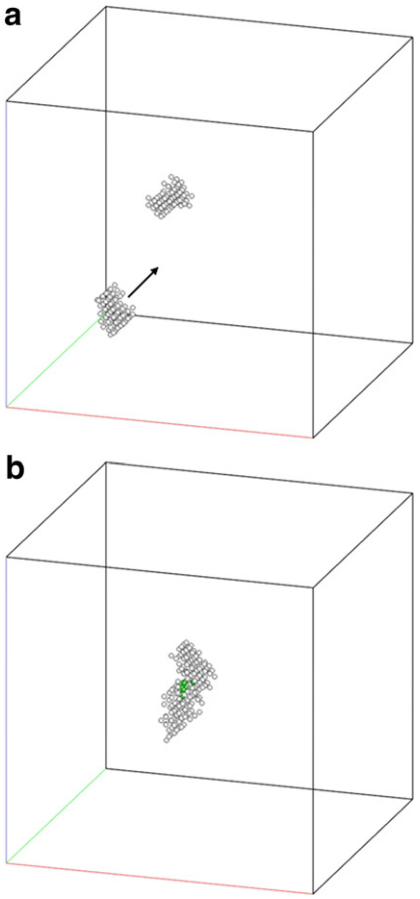

Fig. 4. MD snapshots showing the interaction between loops A and B, which are 7.4 nm apart, at (a) 13.4 and (b) 18.2 ps at 1000 K. The green atoms represent [0 0 1] segments. The arrow indicates the migration direction of loop B. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

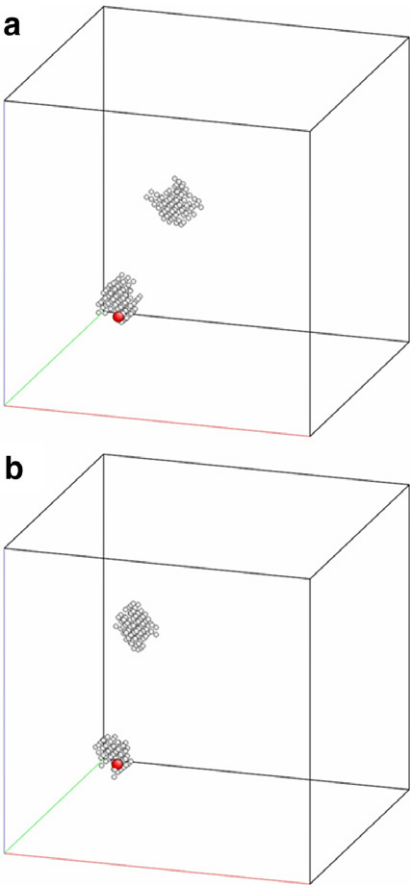

Fig. 5. MD snapshots showing the interaction of an interstitial He atom on the edge of loop B in $[1\,\bar{1}\,0]$ direction with loops A and B, which are 5.0 nm apart, at (a) 10 and (b) 100 ps at 1000 K. The red atom represents the He atom. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

prolonged MD simulation, which might be responsible for the formation of $\langle 1\,0\,0\rangle$ loops.

Snapshots showing the interaction of the interstitial He atom on the edge of loop B in $[1\,\bar{1}\,0]$ direction (type I) with the two dislocation loops 5.0 nm apart from each other at 1000 K are given in Fig. 5. Although the distance between loops A and B is closer than the case in Fig. 4, loop B does not easily migrate toward loop A being strongly bound by the interstitial He atom, as expected from a binding energy of about 1.4 eV. Even in the prolonged simulation up to 100 ps, the He atom still binds loop B, thus keeping loop B from migrating toward loop A (Fig. 5(b)). When we reduced the distance between the two loops below 5 nm, loop B succeeded in escaping from the He atom at about 18 ps, finally leading to the coalescence of the two loops. Hence, the elastic interaction energy between the two loops within 5 nm seems to be enough to overcome the binding between loop B and the interstitial He atom.

Fig. 6 shows snapshots showing the interaction of the interstitial He atom, which is 3.5 nm away from loop A and 1.5 nm from loop B in [1 1 1] direction (type II), with loops A and B 5.0 nm apart, at 1000 K. When the simulation begins, loop B starts to migrate toward the He atom and then it contacts the He atom at about 9 ps. However, immediately after they contact, the He atom soon moves from the plane of loop B to the edge (Fig. 6(a)). This is because the He atom prefers the stable edge site to the unstable plane site, as observed in our MS simulation (Fig. 3(a)). This fast movement of the interstitial He atom is enabled by the interstitial diffusion

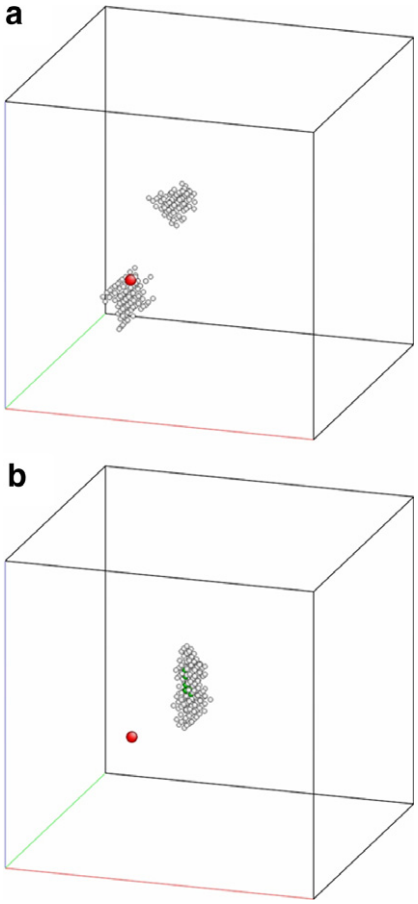

Fig. 6. MD snapshots showing the interaction of an interstitial He atom, which is 3.5 nm away from loop A and 1.5 nm from loop B in [1 1 1] direction, with loops A and B at (a) 9.6 and (b) 17.0 ps at 1000 K. The red and green atoms represents the He atom and [0 0 1] segments, respectively. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

of He in bcc Fe with a very low activation barrier, as mentioned earlier. Although the He atom that moved to the edge of loop B slightly binds loop B, loop B overcomes the binding and then finally collides with loop A (Fig. 6(b)), because the two loops are within 5 nm as in the previous paragraph.

In contrast to the interstitial He atom, the substitutional He atom on the edge of loop B does not bind loop B strongly. Loop B overcomes the binding of about 0.3 eV at 1000 K, although its migration is slightly disturbed by the binding. It reaches loop A at about 28 ps. A substitutional helium atom placed between loops A and B has little effect on the loop migration and coalescence process. Because the substitutional He atom cannot diffuse without another vacancy (and has an ~3.9 eV barrier for thermal dissociation), it does not move as loop B approaches. Loop B easily passes through the substitutional He atom at 1000 K by forming a mixed Fe–He dumbbell (crowdion). The formation of the mixed dumbbell (crowdion) is also supported by the fact that the position of the He atom after the passage shifts by ($0.5a$, $0.5a$, $0.5a$). The so-called 'kick-out' mechanism observed by Ventelon et al. [11], in which the He atom is ejected from a substitutional to an interstitial position when contacting a SIA cluster, is not observed in this case. This is presumably because the 37-SIA dislocation loop encountered the substitutional He atom in the center of the loop, rather than at the periphery where recombination and kick-out could have occurred. Notably, MD simulations by Kuramoto [13] have shown that vacancy–SIA recombination does not occur when similar size SIA dislocation loops encounter vacancies at the loop center, rather than at the periphery. MD simulations of the same configurations were also performed at 600 K, although the results are quite similar to those at 1000 K, and are thus not reported here.

4. Conclusions

Atomistic simulations have been employed to elucidate the effect of a helium atom on the migration of self-interstitial dislocation loops with $\boldsymbol{b} = 1/2\langle 1\,1\,1\rangle$ in bcc Fe. The MD simulations reveal that an interstitial He atom at the edge of a dislocation loop hinders the migration of the loop, thereby suppressing the coalescence of dislocation loops. An interstitial He atom on the plane of a dislocation loop easily moves to the stable edge sites by interstitial diffusion. It is found that the binding energy of a substitutional He atom to a 37-SIA dislocation loop is significantly lower (~0.3 eV), and does not significantly disturb loop migration. A substitutional helium atom on the loop plane is not ejected to an interstitial site and thus a dislocation loop passes through it by forming a mixed Fe–He dumbbell (crowdion).

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