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Study of loop–loop and loop–edge dislocation interactions in bcc iron

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Abstract

Recent theoretical calculations and atomistic computer simulations have shown that one-dimensional glissile clusters of self-interstitial atoms (SIAs) play an important role in the evolution of microstructure in metals and alloys under cascade damage conditions. Recently, it has been proposed that the evolution of heterogeneities such as dislocation decoration and rafts has serious impacts on the mechanical properties on neutron-irradiated metals. In the present work, atomic-scale computer modelling (ASCM) has been applied to study the mechanisms for the formation of such microstructure in bcc iron. It is shown that glissile clusters with parallel Burgers vectors interact strongly and can form extended immobile complexes, i.e., rafts. Similar attractive interaction exists between dislocation loops and an edge dislocation. These two mechanisms may be responsible for the formation of extended complexes of dislocation loops below the extra half-plane of edge dislocations. The interaction energies between loops and between an edge dislocation and loops has been calculated as a function of distance using ASCM and the results for long-range interactions are in good agreement with the results of isotropic elasticity calculations.

1. Introduction

In recent years, results of atomic-scale computer modelling (ASCM) of displacement cascades in metals (see [1–4] for reviews) and the theoretical treatment known as the production bias model [5–8] have emphasised the significance of intracascade clustering of self-interstitial atoms (SIAs) and the 1D diffusional transport of SIA clusters. One of the consequences of the formation of glissile SIA clusters is the creation of vacancy supersaturation, which leads to void swelling. Another important consequence of the 1D glide of SIA clusters is the creation of specific microstructural features in neutron-irradiated metals, such as decoration of dislocations by SIA loops [9,10] and formation of rafts of dislocation loops [10–13]. According to the cascade-induced source hardening (CISH) model [14], the increase in the upper yield stress during neutron irradiation occurs because most grown-in dislocations are locked due to decoration by small SIA clusters and dislocation loops. It has been shown that the 1D gliding SIA clusters produced in the cascades are responsible for the dislocation decoration and raft formation [15,16]. Dislocation–loop interactions and their effect on dislocation dynamics have been treated in terms of elasticity theory [17,18].

However, it is not known with complete confidence whether or not dislocation–loop and loop–loop interactions, especially at close distance, can be calculated accurately enough within the framework of elasticity theory. Clearly, atomic-scale simulations are necessary to eliminate this uncertainty. Even though in recent years a large number of atomic simulations have been carried out to determine the properties of SIA clusters [19–25], only a few studies have considered interactions between mobile clusters. Interactions between mobile interstitial clusters having from 19 to 127 SIAs in bcc iron (Fe) and fcc copper (Cu) have been studied in [26]. It was found that in Fe clusters/loops with $\boldsymbol{b} = 1/2\langle 1\,1\,1\rangle$

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attract each other for both parallel and non-parallel Burgers vectors. A few clusters with parallel $\boldsymbol{b}$ create a mobile complex whereas the result of interaction between clusters/loops with non-parallel $\boldsymbol{b}$ depends on their size. If one of the clusters is small (<20 SIAs) it can reorient its $\boldsymbol{b}$ and join the other one, then creating a single mobile cluster/loop with the same $\boldsymbol{b}$. In contrast, large clusters (>30 SIAs) keep their $\boldsymbol{b}$ and form immobile complexes. The situation in Cu was found to be qualitatively similar with the only difference that complexes of few clusters/loops with parallel $\boldsymbol{b}$ were found to be immobile. Interactions between a cluster of four SIAs and a straight, dissociated $1/2\langle 1\,1\,0\rangle$ dislocation in Ni were studied in [27]. For the case of non-parallel directions of the axis of the SIAs and $\boldsymbol{b}$ of the dislocation line, it was found that the cluster is absorbed by the Shockley partials in both static and gliding dislocations. The absorbed cluster creates a pinning effect and can be reoriented to the same orientation as that of $\boldsymbol{b}$ as a result of further interaction with the gliding dislocation. Investigations such as these provide atomic-level detail of some aspects of interactions involving glissile clusters, but development of a description of these interactions in elasticity theory still remains undone. The present paper addresses this problem directly by comparing the results of atomistic simulations of such interactions in bcc iron with those obtained by analytical calculations using isotropic elasticity theory. In the present work, we have studied the following problems: (a) interaction between SIA clusters and between SIA clusters and an edge dislocation at zero temperature with the aim of understanding *decoration of a dislocation by small loops*, and (b) interaction between SIA clusters at non-zero temperature and the formation of immobile complexes of mobile SIA clusters with the aim of understanding *rafts of dislocation loops*.

2. Calculational method

Molecular statics was used to study the energy of cluster–cluster and cluster–dislocation interactions at zero temperature. The crystallite used was oriented along $[1\,\bar{1}\,0]$, $[1\,1\,\bar{2}]$ and $[1\,1\,1]$ directions with size approximately 21 nm × 8.3 nm × 14 nm and contained about 220 000 mobile atoms. The usual boundary conditions for static dislocation studies were applied, i.e., periodic along the dislocation line direction $[1\,1\,\bar{2}]$ and rigid along other two directions. Atoms in the rigid boundaries were displaced according to the elastic solution for the dislocation. One of the clusters (usually the larger one) or an edge dislocation with $\boldsymbol{b} = 1/2[1\,1\,1]$ along line direction $[1\,1\,\bar{2}]$ was created initially and then relaxed. A cluster with the same Burgers vector was then created in the $(1\,1\,1)$ plane at a desired distance $\boldsymbol{r}_{\langle 1\,1\,0\rangle}$ along the $[1\,\bar{1}\,0]$ axis, below the extra half-plane, and the crystallite was relaxed again. Interactions between clusters containing 19–127 SIAs were studied. Interaction energy was calculated as the difference between the energy of a crystallite containing a particular defect configuration and the (calculated) energy when the defects (clusters or cluster and dislocation) are infinitely separated.

Theoretical estimation of loop–loop interaction energy in an isotropic elastic medium was obtained in [28] and for co-planar loops with the same Burgers vector $\boldsymbol{b}$ the interaction energy is given by

$$E_{\mathrm{INT}} = -\frac{\mu b^2 S_1 S_2}{4\pi(1-\nu)}\frac{1}{r^3}, \tag{1}$$

where μ is the shear modulus, ν the Poisson ratio, S_1 and S_2 the areas of the two loops and r is the distance between their centres. Loop–dislocation interaction energy has been obtained in [29] and for the case studied can be written as

$$E_{\mathrm{INT}} = -\frac{\mu b^2 S}{2\pi(1-\nu)}\frac{1}{r}, \tag{2}$$

where S is the loop area. In addition to the assumption of isotropic elastic behaviour, Eqs. (1) and (2) are based on the infinitesimal loop approximation, i.e., $r^2 \gg S$, so that loop size and geometry are ignored. In the following, the values obtained by these expressions are compared with the results of atomistic simulations.

Molecular dynamics (MD) was used to investigate cluster–cluster interaction at non-zero temperature. Complexes containing two–five clusters of self-interstitial atoms, each having 19–91 SIAs, were studied in the temperature range 250–800 K. The SIA platelets were taken to be hexagonal in shape, and to lie in a $(1\,1\,1)$ habit plane with Burgers vector $\boldsymbol{b} = 1/2[1\,1\,1]$. Simulations were carried out for crystallites with up to 85 000 mobile atoms for time up to 2.5 ns. The analysed parameters include the jump frequency and correlation factor of the centre of mass (CM) of each cluster and of the whole complex, and the mean square displacement of atoms in the simulated crystallite. In both statics and dynamics simulations, we used a many-body potential obtained for α-Fe in [30].

3. Results and discussion

3.1. Energy of a straight dislocation

It can be seen that the interaction energies in Eqs. (1) and (2) are determined in isotropic elasticity theory by the self-energy factor for a straight dislocation line $2A = \mu/(2\pi(1-\nu))$ [31]. For an anisotropic crystal, this factor does not have a unique value, independent of line direction and $\boldsymbol{b}$, and must be obtained either by

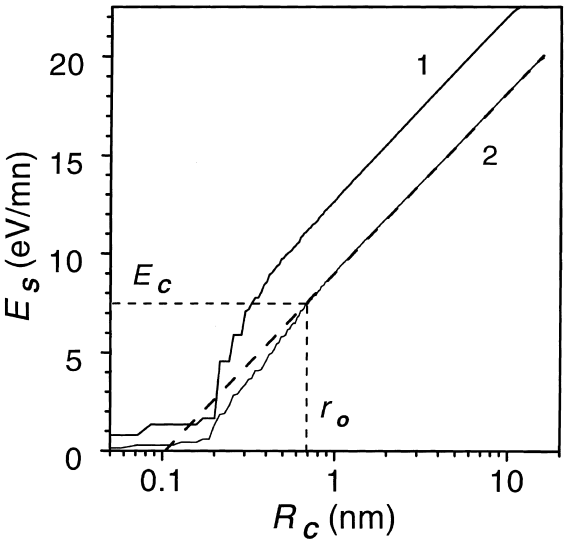

Fig. 1. Elastic energy stored in the cylinders of radius R_C containing the edge dislocation $1/2[1\,1\,1][1\,1\,\bar{2}]$: (1) before relaxation; (2) after relaxation.

anisotropic elasticity theory [32] or by atomistic simulation [33]. We have applied the latter since it gives the energetic factor for the particular interatomic potential employed and takes into account the atomic structure of the dislocation core. The method is based on the evaluation of the strain energy E_S within the cylinder containing the dislocation along its axis. This energy can be expressed (per unit length of line) as $E_S = Ab^2 \ln(R_C/r_0) + E_C$, where R_C is the radius of the cylinder, r_0 the core radius and E_C is the core energy. The slope of a plot of E_S vs $\ln(R_C)$ (in the region where it is linear) defines the factor A (see Fig. 1). Parameters estimated for the edge dislocation modelled here are: $A = 3.99$ eV/nm, $r_0 = 0.67$ nm and $E_C = 7.43$ eV/nm.

3.2. Loop–dislocation interaction

The interaction energy of a 37-SIA cluster with the edge dislocation as a function of separation $\boldsymbol{r}_{\langle 1\,1\,0\rangle}$ is presented in Fig. 2. Estimation of the same energy by Eq.(2) is shown with a full line. In Fig. 2(a), both dependencies appear to be in close agreement, whereas in Fig. 2(b), where E_{INT} is shown versus the reciprocal separation distance, a significant difference at short distance can be clearly seen. Thus, the simple isotropic elasticity theory seems to describe the long-range interactions quite well, even with the infinitesimal loop approximation. In contrast, the short-range interactions ($\boldsymbol{r}_{\langle 1\,1\,0\rangle} \leqslant 1$ nm) are not well described with such a simple approximation and it seems as if the real structure of the dislocation and cluster needs to be taken into account. An important consequence of the present results is that

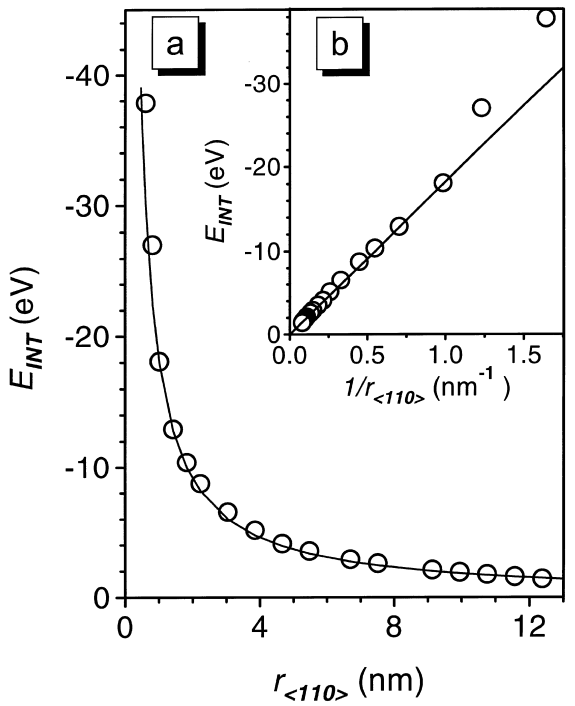

Fig. 2. Interaction energy of a 37-SIA cluster with an edge dislocation: (a) versus $r_{\langle 1\,1\,0\rangle}$ (distance between dislocation line and loop centre below the extra half-plane); (b) versus reciprocal distance $1/r_{\langle 1\,1\,0\rangle}$. Circles are simulation data, solid line is the Eq. (2) with A estimated from Fig. 1.

the interaction energy can be estimated with the simple approach at separation distances much greater than it is possible to simulate directly. For example, for the above case of a 37-SIA cluster, the estimated interaction energy of 0.1 eV corresponds to a separation of about 170 nm. This model also can be used for the estimation of interaction energy in cases when the loop plane and extra half-plane of the dislocation are different (see [28]).

The atomistic simulation also shows how the presence of an SIA cluster modifies the stress field around a dislocation. We present, in Fig. 3, the hydrostatic pressure distribution calculated at the atomic sites when the 37-SIA cluster was relaxed at a distance of 6.9 nm from the dislocation core.

3.3. Loop–loop interaction

The results for the interaction energy of a 19-SIA cluster with clusters of 19, 61 and 127 SIAs, and of a 61-SIA cluster with a 127-SIA cluster, for co-planar clusters separated along the $[1\,\bar{1}\,0]$ direction are presented in Fig. 4. The lines in Fig. 4 show the elastic description of the interaction energy according to Eq. (1) for the interaction of pairs of clusters of sizes 19–19, 19–127 and 61–127. It can be seen that in general, Eq. (1) gives a

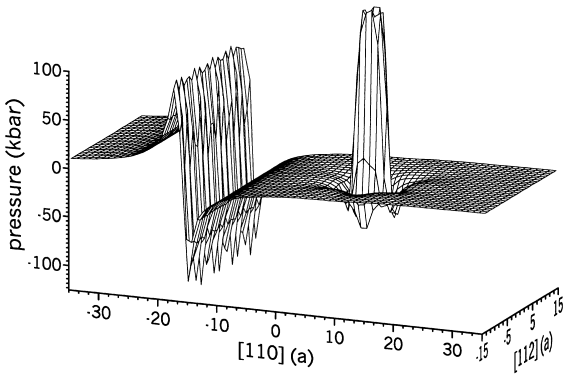

Fig. 3. Pressure distribution in the (1 1 1) plane containing the extra half-plane of the $1/2[1\,1\,1][1\,1\,\bar{2}]$ edge dislocation and the habit plane of a 37-SIA cluster ($r_{\langle 1\,1\,0\rangle} = 6.9$ nm).

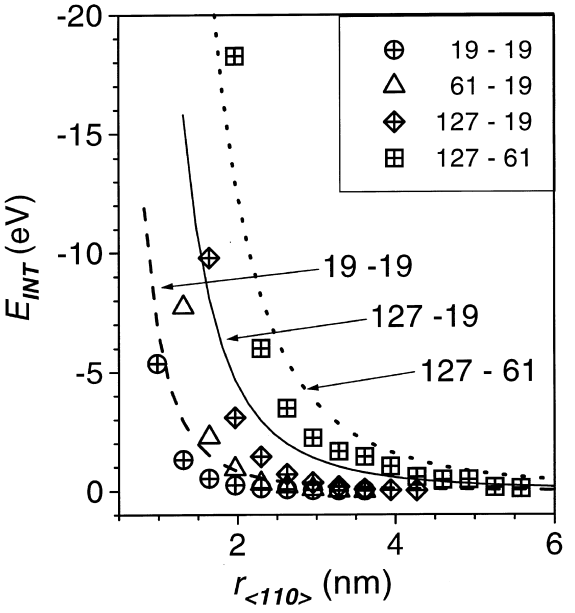

Fig. 4. Interaction energy of pairs of different $1/2[1\,1\,1](1\,1\,1)$, co-planar SIA clusters versus distance, $r_{\langle 1\,1\,0\rangle}$, between their centres along the $[1\,\bar{1}\,0]$ direction. Theoretical curves were obtained via Eq. (1) for: dashed line – interaction between two 19-SIA clusters, solid line – interaction between 127- and 19-SIA clusters and dotted line interaction between 127- and 61-SIA clusters.

poor description of loop–loop interaction at both long and short distances. The atomic-level simulation gives an energy dependence versus distance which is much stronger than $\propto r^{-3}$. For example, a simple fit yields an exponent between -5 and -6. Therefore, the interaction between small loops at short distances cannot be described by the isotropic interaction of infinitesimal loops. However, the larger the clusters, the stronger the interaction and the better the description of the long-range interactions, and in the case of 61–127 SIA interactions all data except points for the two shortest distances (i.e., r larger than the diameter) can be described by $\propto r^{-3.4}$. The finding that larger clusters obey the theoretical behaviour for long-range interactions is possibly related to a criterion for which clusters can be described as dislocation loops in the continuum elasticity treatment.

3.4. MD simulation of complexes of glissile SIA clusters

The main aim of this part of the present work is to define conditions when glissile clusters can be converted into an immobile state and remain in the system during damage evolution. As a general trend, we find that the larger the number of clusters in a complex, the lower is its mobility. Simulation shows that although each individual cluster in a complex remains mobile, the characteristics of motion are changed. In particular, the correlation factor (see [19–25]) decreases from about 3–5 to less than unity. The jump frequency of an individual cluster changes only weakly while the displacements of the CM of the complex decreases. In small complexes, individual clusters move (jump) forward and backward around their common CM,which is also mobile, whereas the CM of large complexes remains immobile. For example, the complex of a compact set of five clusters of size 19, 19, 37, 61 and 91 SIAs separated by a mean distance equal to the average cluster diameter is immobile and at $T < 500$ K does not produce displacements of atoms. The mechanism preventing mobility of large complexes of mobile clusters is related to broken correlations in jumps of individual clusters separated by different distances. A more detailed description of the behaviour of individual clusters in large complexes will be presented elsewhere. Here, we simply emphasise the main qualitative result that mobile SIA clusters can create immobile complexes, which may act as nuclei for rafts of dislocation loops. Due to the spatial spread of such complexes, their effective cross-section for interaction with other SIA clusters is much larger than that of a compact cluster (loop) of the same total number of SIAs.

4. Conclusions

1. MD simulations have demonstrated that glissile SIA clusters form stable complexes. Complexes containing more than five different clusters have low mobility and can serve as nuclei for rafts of dislocation loops.
2. The loop–loop interaction energy of clusters (loops) up to 127 SIAs cannot be described within the isotropic approximation for infinitesimal loops although the validity of such an approximation improves for larger clusters.

3. Long-range interactions between SIA clusters and an edge dislocation are well described by the isotropic approximation for infinitesimal loops.
4. The short-range nature of both cluster–cluster and cluster–dislocation interactions are unlikely to be described accurately in terms of isotropic elasticity theory: atomistic simulation is an appropriate tool for its study.

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