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Competing processes in reactions between an edge dislocation and dislocation loops in a body-centred cubic metal

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Molecular dynamics simulation was used to investigate reactions of a $\frac{1}{2}\langle 1\,1\,1\rangle\{1\,1\,0\}$ edge dislocation with interstitial dislocation loops of $\frac{1}{2}\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ type in a model of iron. Whether loops are strong or weak obstacles depends not only on loop size and type, but also on temperature and dislocation velocity. These parameters determine whether a loop is absorbed on the dislocation or left behind as it glides away. Absorption requires glide of a reaction segment over the loop surface and cross-slip of dipole dislocation arms attached to the ends of the segment: these mechanisms depend on temperature and strain rate, as discussed here.

Keywords: Edge dislocation; Dislocation loop; Molecular dynamics; Iron

The microstructure of neutron-irradiated ferritic alloys, which are important structural materials for nuclear reactors, typically contains dislocation loops, nanovoids and second-phase particles. At sufficiently high doses (a few dpa), defects detectable by transmission electron microscopy (TEM) in body-centred cubic (bcc) Fe and Fe-based alloys are mainly self-interstitial atom (SIA) dislocation loops with Burgers vector, $\boldsymbol{b}_L$, equal to either $\frac{1}{2}\langle 1\,1\,1\rangle$ or $\langle 1\,0\,0\rangle$ (see Refs. [1,2] and references cited therein). Loops present in the matrix can pin dislocations and thereby obstruct their motion by either contact or elastic interaction, which leads to an increase in the yield stress and a reduction in ductility, the phenomenon known as "matrix hardening" (e.g. [3,4]). Rationalization of the dislocation–loop interaction mechanism requires detailed atomic-level information, which is why this problem is primarily addressed using molecular dynamics (MD) techniques.

A series of MD studies of the interaction of a $\frac{1}{2}\langle 1\,1\,1\rangle\{1\,1\,0\}$ edge dislocation with a periodic row of loops in Fe with $\boldsymbol{b}_L$ equal to either $\frac{1}{2}\langle 1\,1\,1\rangle$ or $\langle 1\,0\,0\rangle$ [5–9] has already been reported. For $\frac{1}{2}\langle 1\,1\,1\rangle$ loops it was revealed that those with $\boldsymbol{b}_L$ parallel to the dislocation glide plane do not offer significant resistance to the glide of an edge dislocation and can be easily absorbed or dragged by it: we do not consider them further here. Loops with $\boldsymbol{b}_L$ inclined to the glide plane are attracted by an edge dislocation and react with it [7]. Small loops (e.g. containing up to 37 SIAs) are easily absorbed as superjogs on the dislocation line (an effect which is equally true for both edge and screw dislocations) [7,10]. Larger ones (>100 SIAs) react with the dislocation to form a segment with $\boldsymbol{b}$ of $\langle 1\,0\,0\rangle$ type, which is sessile in the dislocation glide plane and thus pins the dislocation [5,7,8]. The reaction mechanism and the critical stress, τ_C, required to unpin the dislocation depends on temperature and loop size [5–8]. The results obtained so far suggest that even relatively large $\frac{1}{2}\langle 1\,1\,1\rangle$ loops (331 SIAs) can be completely absorbed at sufficiently high temperature ($\geqslant$300 K).

Dislocation reaction with a $\langle 1\,0\,0\rangle$ loop forms a segment with Burgers vector $\frac{1}{2}\langle 1\,1\,1\rangle$, which, in contrast with the $\langle 1\,0\,0\rangle$ segment on a $\frac{1}{2}\langle 1\,1\,1\rangle$ loop, results in a wider variety of outcomes, ranging from total loop absorption by the edge dislocation to none [9]. However, $\langle 1\,0\,0\rangle$ loops with $\boldsymbol{b}_L$ lying in the dislocation slip plane are strong barriers to dislocation glide, whereas others are weak.

In this paper, $\frac{1}{2}\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ loops that offer strong resistance to edge dislocation glide are considered specifically, since they have the greatest potential to affect the plastic response to load. We therefore study

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reactions of the $\frac{1}{2}[1\,1\,1](1\,\bar{1}\,0)$ edge dislocation with loops with $\boldsymbol{b}_L = \frac{1}{2}[1\bar{1}1]$ or $[0\,0\,1]$ and size up to 8.6 nm under both static (temperature $T = 0$ K) and dynamic ($T < 600$ K) conditions. The conditions of temperature, applied strain rate and loop size that affect whether a loop is a strong obstacle for an edge dislocation are assessed. We show that the mechanism of loop absorption by the dislocation is important in this regard, and that glide of a reaction segment and cross-slip of dipole side arms are necessary steps in the process.

The $\frac{1}{2}[1\,1\,1](1\,\bar{1}\,0)$ edge dislocation was constructed using the model developed in Ref. [11]. Periodic boundary conditions were imposed in the directions of $\boldsymbol{b}$ and the initially straight dislocation line. Dislocation glide was induced by applying a $[1\,1\,1](1\,\bar{1}\,0)$ shear strain to rigid boundary atoms in the $[1\,\bar{1}\,0]$ direction at a constant rate, $\dot{\gamma}$, in the range 10^6 to 5×10^7 s^{-1}. The corresponding shear stress–strain (τ–γ) relationship for the dislocation reacting with a periodic row of identical loops was obtained by estimating the stress acting on the outer rigid parts of the crystallite that were subject to the shear displacement. Earlier work [11] has shown that the effect of periodicity along [1 1 1], which creates a periodic array of parallel dislocations, is insignificant, even for strong obstacles, if the model dimension along [1 1 1] is large enough, as here (see below).

Circular $\frac{1}{2}\langle 1\,1\,1\rangle$ SIA loops were created below the dislocation slip plane, while square $\langle 1\,0\,0\rangle$ loops with sides oriented along $\langle 1\,1\,0\rangle$ directions were placed so that the dislocation could intersect them. The number of SIAs in the loops was varied from 37 to 1225, corresponding to loop diameter, D, in the range 0.5–9 nm. Simulation of reactions with the largest loops was performed in crystals containing up to 6×10^6 atoms, whereas reactions involving smaller loops were modelled in crystals containing $\sim 1 \times 10^6$ atoms. The length, L, of the dislocation line along the periodic direction was varied from 20.5 to 61.5 nm and the crystal size along [1 1 1] was varied from $100b$ up to $200b$ depending on the loop size and simulation temperature. The size of the crystal along the $[1\,\bar{1}\,0]$ direction normal to the slip plane was 20 nm. Thus, the dislocation density was in the range $1–2 \times 10^{15}$ m^{-2}, resulting in a free-flight dislocation velocity ranging from 2 to 200 m s^{-1} for the strain-rate range specified above. Simulations were performed within the NVE ensemble without additional temperature control, varying the MD integration time step from 2 to 5 fs. All simulations used the many-body interatomic potential for Fe from Ref. [12].

An edge dislocation can fully absorb small loops of up to ~61 SIAs under all the conditions considered, and larger loops are also absorbed under certain conditions, as discussed later. The absorption mechanism is briefly the following. First, the geometry must allow for intersection of the dislocation line and a loop edge. For this, $\frac{1}{2}[1\,\bar{1}\,1]$ loops, which have a glide prism inclined to the $(1\,\bar{1}\,0)$ plane, can be positioned below the dislocation glide plane of a positive edge dislocation and glide under attraction so that the two cores meet. Loops with $\boldsymbol{b}_L = \langle 1\,0\,0\rangle$ have lower mobility and have to be positioned more precisely so that they intersect the glide plane. Second, the compete absorption of a loop with $\boldsymbol{b}_L = \frac{1}{2}[1\,\bar{1}\,1]$ reported in Refs. [5,7,8] involves the formation of a $[0\,1\,0]$ reaction segment that pins the dislocation, which bows out under increasing stress until a screw dipole is formed. The $[0\,1\,0]$ segment then glides across the loop surface and converts $\boldsymbol{b}_L$ to $\frac{1}{2}[1\,1\,1]$, after which the loop is absorbed as a double superjog on the $\frac{1}{2}[1\,1\,1]$ dislocation. For the $\langle 1\,0\,0\rangle$ loops, several mechanisms occur [9], depending on their orientation and structure. Here we consider the case when $\boldsymbol{b}_L = [0\,0\,1]$, the loop sides have $\langle 1\,1\,0\rangle$ directions and the uppermost loop segment lies in the dislocation glide plane. An absorption reaction proceeds as follows. The dislocation, being attracted to the loop, moves towards it and undergoes an energetically favourable reaction with the upper side of the loop to form a $\frac{1}{2}[1\,1\,\bar{1}]$ segment. The latter propagates across the loop surface, converting $\boldsymbol{b}_L$ to $\frac{1}{2}[1\,1\,1]$, after which the loop is incorporated in the dislocation line as two superjogs. The superjogs rearrange into a U-shape with segments aligned along $\langle 1\,1\,2\rangle$ directions and the dislocation continues to glide.

However, as we now explain, whether or not these mechanisms of complete absorption of a loop by an edge dislocation actually occur depends on the simulation conditions. Furthermore, the critical stress at which the dislocation is released varies significantly with loop size, ambient temperature and/or strain rate. Consider first the effect of temperature on τ_C. Plots of τ_C vs. T for $\frac{1}{2}[1\,\bar{1}\,1]$ and $[0\,0\,1]$ loops containing 169 SIAs (i.e. $D \sim 3$ nm) are shown in Figure 1a. At low temperature no absorption occurs and the dislocation is unpinned via

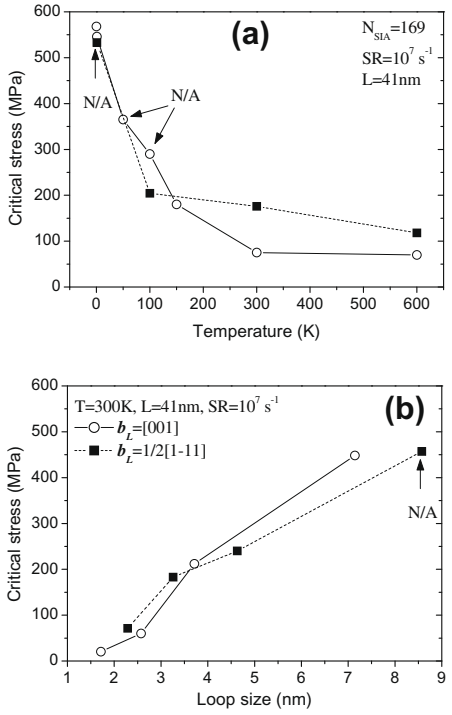

Figure 1. τ_C for the edge dislocation to pass a periodic row ($L = 41$ nm) of loops with $\boldsymbol{b}_L = [0\,0\,1]$ or $\frac{1}{2}[1\,\bar{1}\,1]$ at $\dot{\gamma} = 10^7$ s^{-1}. (a) τ_C vs. T for loops containing 169 SIAs. (b) τ_C vs. D at $T = 300$ K. Label N/A denote reactions where the pre-existing loop was not absorbed.