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Simulation of the interaction between an edge dislocation and a ⟨100⟩ interstitial dislocation loop in α-iron

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Abstract

Atomic-level simulations are used to investigate the interaction of an edge dislocation with ⟨100⟩ interstitial dislocation loops in α-iron at 300 K. Dislocation reactions are studied systematically for different loop positions and Burgers vector orientations, and results are compared for two different interatomic potentials. Reactions are wide-ranging and complex, but can be described in terms of conventional dislocation reactions in which Burgers vector is conserved. The fraction of interstitials left behind after dislocation breakaway varies from 25 to 100%. The nature of the reactions requiring high applied stress for breakaway is identified. The obstacle strengths of ⟨100⟩ loops, 1/2⟨111⟩ loops and voids containing the same number (169) of point defects are compared. ⟨100⟩ loops with Burgers vector parallel to the dislocation glide plane are slightly stronger than ⟨100⟩ and 1/2⟨111⟩ loops with inclined Burgers vector: voids are about 30% weaker than the stronger loops. However, small voids are stronger than small 1/2⟨111⟩ loops. The complexity of some reactions and the variety of obstacle strengths poses a challenge for the development of continuum models of dislocation behaviour in irradiated iron.

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

1. Introduction

Ferritic steels are major structural materials of current nuclear power plants and ferritic and/or ferritic/martensitic steels are prime candidates for structural components in designs for future systems [1]. Exposure of structural components to fast neutron irradiation creates radiation damage in the form of vacancies and self-interstitial atoms (SIAs) and clusters of these defects. The present work is part of an ongoing programme to investigate the effect of damage on dislocation glide, for its presence can impede dislocation motion, thereby causing irradiation hardening and loss of ductility. Thus, an understanding of the atomic-scale mechanisms involved when dislocations gliding under applied stress encounter obstacles can provide important input for multiscale models being developed for assessment of lifetime and operational safety of materials exposed to neutron irradiation. In this approach, atomic-scale computer simulation using molecular dynamics (MD) informs continuum-level modelling of the behaviour of many dislocations, known as dislocation dynamics (DD).

In the important case of α-iron, MD has been used to investigate the interaction of a gliding edge dislocation with a variety of microstructure obstacles, including dislocation loops formed by SIAs, copper precipitates and voids (e.g. [2–7]). In ferritic and ferritic/martensitic steels that are either in current use or candidate materials for future designs, point defect clusters visible by transmission electron microscopy (TEM) have the form of small dislocation loops, and they are the subject of this paper. Their presence in irradiated iron depends on radiation dose level and temperature. The results of low-dose ion-irradiation experiments [8] and modelling [9] indicate that they do not occur easily in individual, isolated displacement cascades.

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This is supported by reports that no visible damage is found in iron irradiated by neutrons at low temperature (<100 °C) to dose levels comparable with the ion irradiations [10]. At higher neutron doses, visible defects are mostly of interstitial-type with Burgers vector, $\boldsymbol{b}$, equal to either $1/2\langle 1\,1\,1\rangle$ or $\langle 1\,0\,0\rangle$ (see Refs. [10,11] and references cited therein). The fraction of $\langle 1\,0\,0\rangle$ loops is higher after irradiation at high temperature (>250 °C) [11]. Small (≤1 nm size) cavities formed by vacancies are also present with high density [10].

Previous atomic-scale modelling of dislocation–loop interactions in iron has treated only $1/2\langle 1\,1\,1\rangle$ SIA loops [4–7]. Earlier simulations showed that these glissile loops are highly mobile and consist of arrays of closely packed, parallel $\langle 1\,1\,1\rangle$ crowdions (e.g. [12]). The studies in Refs. [4–6] used an interatomic potential for iron due to Ackland et al. [13], whereas that in Ref. [7] was based on the more recent potential due to Ackland et al. [14]. (For conciseness, these potentials, published in 1997 and 2004, respectively, are referred to as A97 and A04 in this paper.) The newer potential provides an improved description of the properties of SIAs [15] and screw dislocations [16,17], in particular. However, the results in Refs. [6,7], where comparison can be made, were broadly consistent with each other, as follows.

When the Burgers vector, $\boldsymbol{b}_{\mathrm{L}}$, of the loop is inclined to the dislocation glide plane, e.g. $1/2[1\,\bar{1}\,1]$ inclined to $(1\,\bar{1}\,0)$, it is attracted by the moving dislocation (with $\boldsymbol{b} = 1/2[1\,1\,1]$) and reacts with it by gliding to intersect the glide plane. The defect arrangement created by the reaction and the maximum stress required for continued dislocation glide depend on temperature, applied strain rate and loop size. Loops containing either 37, 169 or 331 SIAs (which correspond to sizes of 1.6, 3.5 or 5.0 nm) in crystals deformed at strain rates from 10^6 to $10^8\ \mathrm{s}^{-1}$ and temperatures from 1 to 600 K were modelled in Refs. [6,7]. Small loops are readily transformed by the reaction so that their Burgers vector becomes the same as that of the dislocation line and they are simply absorbed on it as a set of superjogs. These impose only a small resistance to glide of the dislocation. The larger loops react so that one side forms a segment on the line with $\boldsymbol{b} = [0\,1\,0]$, which is sessile in the $(1\,\bar{1}\,0)$ plane. The loop therefore presents a strong obstacle to dislocation glide and the dislocation side arms joined to the loop are pulled into screw orientation at the critical (maximum) stress. At 1 K, the dislocation breaks away from this segment by annihilation of the dipole by screw cross-slip and leaves a loop behind. At higher temperatures, the controlling mechanism is propagation by glide of the $[0\,1\,0]$ segment over the loop surface under the applied stress, coupled with cross-slip of the screw side arms. This transforms the Burgers vector of the loop to that of the dislocation line and the loop transforms to form superjogs. The critical stress increases with increasing strain rate and decreasing temperature, the effect of the latter being more significant. Importantly, edge dislocations are seen to provide a means for removing interstitial damage via the formation of superjogs.

As noted above, loops with Burgers vector of $\langle 1\,0\,0\rangle$ type are also created in iron by radiation damage. It is therefore important to understand their interaction effects on a dislocation line of the $\langle 1\,1\,1\rangle\ \{1\,\bar{1}\,0\}$ slip system. It does not seem possible to predict their effects from the results for $1/2\langle 1\,1\,1\rangle$ clusters because the energetically favourable reaction would produce a $1/2\langle 1\,1\,1\rangle$ segment rather than a $\langle 1\,0\,0\rangle$. The occurrence of $\langle 1\,0\,0\rangle$ loops has long been considered surprising because the magnitude of $\langle 1\,0\,0\rangle$ is larger than that of $1/2\langle 1\,1\,1\rangle$ and this implies that their elastic strain energy, which is proportional to $\boldsymbol{b}_{\mathrm{L}}^2$, is larger. This paper is not concerned with the cause of their origin and growth, only with their presence, and so it is not necessary to review the various explanations in the literature, such as those in Refs. [18,19], which are not consistent with recent calculations of defect stability using either ab initio or empirical interatomic potential methods [15]. We note, however, that recent MD simulations have shown that $\langle 1\,0\,0\rangle$ interstitial loops can form by the interaction of three glissile $1/2\langle 1\,1\,1\rangle$-type loops [20]; and both vacancy and interstitial loops can occur in displacement cascades arising from primary knock-on atoms with much higher atomic mass than that of iron [9]; Furthermore, Dudarev et al. [21] have shown recently that the anisotropic elastic energy of a dislocation loop with $\boldsymbol{b} = \langle 1\,0\,0\rangle$ falls below that of a $1/2\langle 1\,1\,1\rangle$ loop because of changes in the elastic constants of iron as temperature increases towards the $\alpha - \gamma$ transition.

We have therefore applied large-scale MD simulations to study interaction between an edge dislocation and a row of $\langle 1\,0\,0\rangle$-type interstitial dislocation loops. All three orientations of $\boldsymbol{b}_{\mathrm{L}}$ have been considered and the position of the loop with respect to the dislocation glide plane has been varied. Large loops (>100 nm) that are clearly resolved by TEM in samples irradiated at high temperature with a high dose of ions or electrons lie perpendicular to $\boldsymbol{b}_{\mathrm{L}}$ and have square or rectangular geometry with sides along the $\langle 0\,0\,1\rangle$ directions [22,23]. The geometry of small SIA loops found in neutron-irradiated material is not known. It seems likely that they also have edge character and are square with $\langle 0\,0\,1\rangle$ or $\langle 0\,1\,1\rangle$ sides, since these directions are the most closely packed for a loop in a $\{1\,0\,0\}$ plane. The only SIA loop found so far in MD simulation of displacement cascades in iron was of 30 SIAs and had sides mainly along the $\langle 0\,1\,1\rangle$ directions [9]. The difference in the formation energy of the two loop types is very small with the interatomic potentials used here [24], and so we have considered both types.

In view of the large number of possible configurations and reactions, we have modelled interaction of an edge dislocation with loops containing a similar number of SIAs (162 or 169) at one temperature ($T = 300$ K) and one applied strain rate ($\dot{\varepsilon} = 10^7\ \mathrm{s}^{-1}$). Both the newer and older interatomic potentials, A04 and A97, respectively, have been used for this work in order to test the sensitivity of the results to choice of potential.

As reviewed above, the visible damage in neutron-irradiated iron consists of a mixture of $1/2\langle 1\,1\,1\rangle$ and $\langle 1\,0\,0\rangle$ loops and small cavities. The resistance that $1/2\langle 1\,1\,1\rangle$ loops and