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Atomistic simulation of the $a_0\langle 100\rangle$ binary junction formation and its unzipping in body-centered cubic iron

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Abstract

Molecular dynamics simulation is used to study the formation of the $a_0\langle 100\rangle$ binary dislocation junction in body-centered cubic Fe. Results show that under an applied strain two intersecting ½ $a_0\langle 111\rangle$ dislocations, one mobile edge and one immobile screw, form an $a_0\langle 100\rangle$ binary junction of mixed character in the glide plane of the mobile edge dislocation. It appears, however, that the binary junction does not necessarily lay in one of the three possible $\{110\}$ glide planes of the screw dislocation. The binary junction starts to unzip as the impinging edge dislocation bows around and moves away, which results in the formation of a screw dipole along its Burgers vector. The dipole eventually annihilates, completing the unzipping process of the junction, which liberates the edge dislocation. The effects of temperature and strain rate on the unzipping of the junction are quantified by the critical release stress needed to detach the edge dislocation from the screw one. The critical stress decreases when the temperature increases from 10 to 300 K, whereas it increases with increasing applied strain rate, or dislocation speed. The interaction mechanism and strength of the $a_0\langle 100\rangle$ binary junction as an obstacle to the edge dislocation are compared to that of other types of defect, namely nanosized voids, Cu and Cr precipitates, and dislocation loops in Fe. It appears that the binary junction strength is in the lowest range, comparable to that of a coherent Cr precipitate.
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1. Introduction

In the dislocation-assisted plastic deformation of crystalline materials, strain hardening derives from the multiplication of mobile dislocations and their interaction with other dislocations [1–4] or microstructure defects such as nanosized voids [5–9], secondary phase precipitates [8–15], dislocation loops [16–21] and grain boundaries [22–27]. Among these mechanisms dislocation–dislocation interactions play a substantial role in the strain hardening of metallic materials. The existing theory relates strain hardening to the pairwise interaction of dislocations whereby two intersecting dislocations form a junction that ties the dislocations together [1–3]. This type of junction is believed to lay at the intersection of the two dislocation slip planes [28–31]. It is usually not mobile and, therefore, represents a strong barrier to further dislocation motion, until the local stress reaches a critical value at which the junction is destroyed and the two dislocations can pass each other [32]. During plastic deformation, the dislocation density increases and, as a result, the number of such events continuously increases, thus leading to strain hardening through forest hardening [32,33].

The dislocation junctions are formed when n gliding dislocations reduce their total energy by interacting with each other and forming an $(n+1)$th dislocation segment. The Burgers vector b_j of the resulting junction depends on the Burgers vector b_i of the interacting dislocations, as $b_j = \Sigma b_i$. Given that the energy of a dislocation is proportional to the square of its Burgers vector, one can estimate the

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possibility of a junction to be created using the Frank energy criterion [34]. It implies that n dislocations may react to form an $(n+1)$th dislocation provided $b_j^2 < \sum b_i^2$. In addition to the energy criterion, the dislocations reaction depends on topological constraints of the dislocations, such as the length and relative geometry of the interacting dislocations [28–30], as well as the Peach–Koehler force [35] they experience.

Studies done by using discrete dislocation dynamics (DDD) simulations indicate that binary junctions contribute substantially to the strengthening of cubic crystalline materials [22,23,33,36], where they can provide nucleation sites for energetically stable ternary junctions in body-centered cubic (bcc) materials [32,37]. Forest hardening through the $a_0\langle 100\rangle$ binary junction in bcc materials and particularly in bcc Fe in a wide range of temperatures has been the subject of various DDD simulations [29,31–33,38,39] and transmission electron microscopy (TEM) studies [40–43]. Naamane et al. [38] have studied the role of binary junctions in the strain hardening of bcc Fe at temperatures from 50 to 250 K using DDD simulations. This study has shown that although, at low temperatures, e.g. 50 K, screw dislocations play a main role in the strengthening of bcc Fe, the number of binary junctions is significant. With increasing temperature, up to 250 K, the contribution of junctions to strengthening increases as the number of junctions rises. This is due to the evolution seen in the microstructure from mainly straight screw dislocations at 50 K to rather mixed or edge dislocations at 250 K. It should be noted that the $a_0\langle 100\rangle$ binary junctions at low temperatures may form due to the interaction of two ½ $a_0\langle 111\rangle$ screw or near screw dislocations, which was observed by Louchet and Kubin [40] using TEM in bcc Nb at 50 K. The hardening induced by the $a_0\langle 100\rangle$ junction has also been reported in the interaction of a ½ $a_0\langle 111\rangle$ gliding dislocation with nanometric dislocation loops with Burgers vectors ½ $a_0\langle 111\rangle$ or $a_0\langle 100\rangle$, using molecular dynamics (MD) simulations [19,44,45]. It is noted that the resistance given by this junction to the gliding dislocation is controlled by its mobility and unzipping towards its parent dislocations.

In bcc materials, dislocations with either of the four ½ $a_0\langle 111\rangle$ Burgers vectors associated with either of the three $\{110\}$ or three $\{112\}$ slip planes constitute the main slip systems that contribute to the plastic deformation in bcc metals [46–50]. The corresponding dyadic product of these degrees of freedom results in 24 slip systems, with a high probability of binary junction formation at the intersection of those glide planes. The resultant binary junction is a dislocation segment with a Burgers vector $a_0\langle 100\rangle$ through the following type of reaction:

$$\frac{1}{2}a_0[1\,-1\,-1]+\frac{1}{2}a_0[111]=a_0[100] \tag{1}$$

Due to the possible interacting slip systems, three types of generic junction may form. There are two types involving junctions of mixed character and one type involving a junction of edge character. Presuming that the glide of the parent dislocations is constrained to their slip plane, the line direction of the mixed character junctions is $\langle 111\rangle$, whereas in the case of the edge junction it is $\langle 010\rangle$ [28–31].

The available studies using theoretical [1–3], experimental [40–43] and DDD simulation [22,23,32,33] approaches have shown the importance of the ½ $a_0\langle 111\rangle\{110\}$ dislocations interaction and formation of the $a_0\langle 100\rangle$ binary junction in bcc structures. Although DDD simulation can predict to some extend the junction strength using continuum elasticity theory of dislocations, an explicit study of the ½ $a_0\langle 111\rangle\{110\}$ dislocations intersection at atomistic scale and evaluation of the interaction strength is needed to give further insight into the formation and unzipping process of the binary dislocation junctions in bcc materials, particularly in bcc Fe. It is important to study the effects of the thermal activation and speed of impinging dislocation on the formation mechanism of the $a_0\langle 100\rangle$ binary junction and the level of stress that is needed to unzip it. Hence, in this study, we investigate the formation and unzipping processes of the $a_0\langle 100\rangle$ junction and quantify its strength using MD simulation. For that purpose, we simulate the interaction of a ½ $a_0[-111]$ edge dislocation moving on (101) glide plane with a ½ $a_0[111]$ screw dislocation in bcc Fe. The interaction and the stress needed to release the moving edge dislocation from the screw dislocation are studied as a function of temperature and strain rate. The strengthening induced by the formation of the binary junction is then discussed in comparison to the strengthening due to different nanosized defects, namely the void, Cu and Cr precipitates, and the different dislocation loops in iron.

2. Simulation technique

The MD simulation of the interaction of the edge dislocation with the screw dislocation in bcc Fe at different temperatures and applied strain rates is made using a model that has been developed by Schäublin and Chiu [51]. This model has already been successfully used in the study of the ½ $a_0\langle 111\rangle\{110\}$ dislocation mechanisms and its interaction with various nanosized defects in bcc Fe [11,12,52,53]. The dislocations are introduced using anisotropic elasticity of the continuum with the code DISLOC [51]. Deformation of the specimen is achieved using the code MOLDY [54] using the embedded atom method with the so-called "Marinica 10" Fe empirical interatomic potential [55], the later version of the Mendelev 03 [56] potential with a modified fitting to slightly different parameters database. The dislocation core structure, particularly that of the screw dislocation in bcc Fe, has an influence on its mobility and interaction with obstacles. The potential used in this work predicts a compact core structure for the ½ $a_0\langle 111\rangle$ screw dislocation, which is consistent with the core structure predicted by ab initio calculations [55,57]. However, using the Marinica 10 potential, a local

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