Nodal Effects in Dislocation Mobility

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We show that, contrary to the prevailing perception, dislocations can become more mobile by zipping together to form junctions. In a series of direct atomistic simulations, the critical stress to move a junction network in a {110} plane of bcc molybdenum is found to be always smaller ($\sim 50\%$) than that required to move isolated dislocations. Our data support a previously proposed hypothesis about the nature of anomalous slip in bcc transition metals, yet offer a different atomistic mechanism for conservative motion of screw dislocation networks. The same data suggest a hierarchy of motion mechanisms in which lower-dimensional crystal imperfections control the rate of sliding along the low-angle twist boundaries.

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Dislocations are ubiquitous line defects responsible for many properties of crystalline materials. In particular, dislocation's ability to nucleate and move under stress allows materials to be worked into desired shapes and often defines a material's strength by preventing brittle cracking [1]. Understanding the mechanisms and parameters of dislocation motion is key for designing materials with improved properties. However, despite a massive body of literature [2], there remains much unknown about the subject [3]. Principally, the effect of junctions on dislocation mobility remains controversial.

In this Letter we present the first data on dislocation mobility obtained by direct atomistic simulation in which the junction effects stand out clear and unmasked. Our results decidedly show that, by forming junctions, dislocations can substantially reduce the effective lattice resistance to their motion, compared to the unconnected, stand-alone dislocations. We trace such cooperative effects to the details of atomic motion in and around junction nodes, i.e., singular zero-dimensional objects in which two dislocations join to form a junction. Our observations support an earlier conjecture that enhanced mobility of a dislocation network can contribute to anomalous slip behavior in bcc transition metals [4,5]; however, the observed atomistic mechanisms differ significantly from the earlier hypothesis. Furthermore, our data reveal a hierarchy of low dimensional crystal imperfections whose collective motion provides a mechanism for sliding along the low-angle grain boundaries in bcc materials.

Each dislocation line carries a topological charge quantified by its Burgers vector equal to one of the smallest repeat distances of crystal lattice. Unless the line tangent vector and the Burgers vector happen to be parallel (*screw* orientation), the line segment is constrained to glide in a plane defined by these two vectors, the *glide plane.* Dislocation junctions form frequently as a natural result of collisions between dislocation lines moving under stress. Depending on the incidence angle between colliding dislocations, the 4-node formed at the intersection can become unstable and reduces its energy by splitting into two 3-nodes connected by a product (junction) dislocation (Fig. 1) [6].

It has long been realized that junctions have a strong effect on dislocation mobility. A classical example is the key role junctions play in the strain-hardening behavior of fcc metals and alloys [7]. Basically, junctions are thought to limit the mobility of two parent dislocations by zipping them together and thus providing additional glide constraints to further motion. The nature of glide constraints is purely geometric: each dislocation sharing a 3-node restricts this node to move in this dislocation's glide plane. Depending on the mutual orientation of the three glide planes, the node may be restricted to move in a plane, or along a line, or its motion can be blocked entirely. There is only one case in which nodal glide is totally unconstrained: it is when all three dislocations are in pure screw orientations so that none of them provides any glide constraints. Such a situation is ideal for posing an interesting question: leaving aside the glide constraints, what is intrinsic contribution of the node to the mobility of associated dislocations? In other words, does the node itself provide extra resistance or does it facilitate dislocation motion? So far, this issue has not been explored.

In this work we quantify the effect of triple nodes on dislocation mobility in a series of direct atomistic calculations of Peierls stress, i.e., the minimal stress required for a dislocation to move at zero temperature. Peierls stress is a simple measure of dislocation-lattice coupling and, as such, allows meaningful comparisons between different

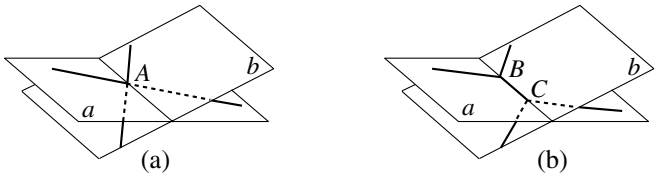

FIG. 1. (a) Two dislocation lines gliding on planes *a* and *b* collide at point *A*. (b) The 4-node *A* is unstable against zipping, resulting in a junction segment bounded by two 3-nodes *B* and *C*.

dislocations and different materials. In this work we examine the effects of junctions on dislocation motion in terms of the Peierls stress. The junction configuration considered below provides an ideal test case for our examination.

In molybdenum, semiregular networks of long straight segments of $\frac{1}{2}\langle 111\rangle$ screw dislocations are often observed after moderate plastic straining [Fig. 2(a)]. These networks are geometrically equivalent to low-angle pure twist boundaries [8]. In the network, the dislocations are often seen to form junctions, as in

$$\tfrac{1}{2}[111] + \tfrac{1}{2}[\overline{1}\overline{1}1] = [001]. \quad (1)$$

In this reaction, both parents and the junction dislocations are in pure screw orientations. The predisposition to formation of $\langle 001\rangle$ junctions is a function of elastic constants and, in particular, of elastic anisotropy [9]. Using both the elasticity theory and direct atomistic simulations, we verified that the above reaction is indeed favored for the Finnis-Sinclair model [10] of Mo used in our simulations.

To eliminate unwanted surface effects and to preserve translation invariance we employ periodic boundary conditions (PBC) in combination with a special method developed in [11] for subtracting the periodic image stress. The simplest dislocation configuration compatible with PBC is a dislocation dipole. A pair of dislocations is introduced in the supercell so that their line direction is parallel to one of the supercell vectors. Subsequent relaxation of the interatomic forces using a conjugate gradient algorithm produces a well-defined dislocation dipole. Using the Parrinello-Rahman version of PBC [12], stress is then applied to drive dislocation motion in the $(\overline{1}10)$ plane. In a series of calculations with different stress magnitudes, the lowest stress at which dislocation motion takes place is taken as an approximate value of the Peierls stress, 2.40 ± 0.05 GPa, in agreement with the earlier reported values [13,14]. This rather high value of the Peierls resistance is a useful reference point for the subsequent analysis.

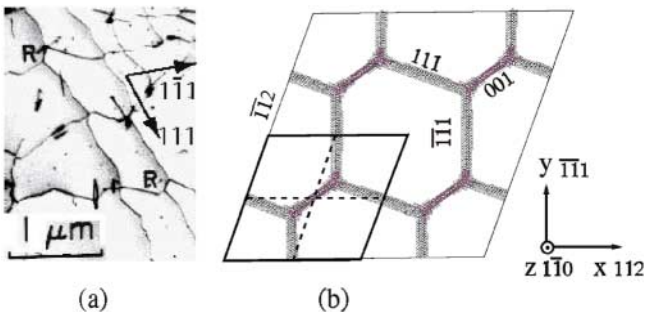

FIG. 2 (color online). (a) TEM picture showing a network of $\frac{1}{2}\langle 111\rangle$ screw dislocations forming $\langle 001\rangle$ screw junctions (marked R) at their intersections [5]. (b) A similar junction network is introduced in the atomistic model by juxtaposition of two nonparallel parent dislocations (dashed lines) in the periodic supercell (shown in the left-bottom corner). Only the atoms whose energy exceeds the bcc cohesive energy by 0.1 eV are shown.

A dipole of junctions is produced by juxtaposition of two (mixed) dislocation dipoles introduced along $[112]$ and $[\overline{1}\overline{1}2]$ directions with Burgers vectors $\frac{1}{2}[111]$ and $\frac{1}{2}[\overline{1}\overline{1}1]$ respectively, in a monoclinic supercell defined by its repeat vectors, $16[112] \times 16[11\overline{2}] \times 19[\overline{1}10]$. One such junction, or rather a fragment of the periodic junction network obtained after a conjugate gradient relaxation, is seen in Fig. 2(b). Taking advantage of the geometric equivalence of the low-angle twist boundaries and the networks of screw dislocations [8], a junction network virtually identical to the one shown in Fig. 2(b) was also created by rotating two halves of the supercell around the $[\overline{1}10]$ axis by an appropriate twist angle.

As seen in Fig. 2(b), the junction is featureless consisting of three perfectly straight screw dislocations joining at two 3-nodes. That the lines are straight is an indication of a high Peierls potential that restricts the dislocations to lie along certain crystallographic directions. We have already reported a high Peierls stress for the two $\frac{1}{2}\langle 111\rangle$ screws. Using the same computational procedure, we find that Peierls stress of a stand-alone $\langle 001\rangle$ junction dislocation is even higher, at 3.2 ± 0.2 GPa. This is the second reference value that we use below to quantify the effect of junction nodes on dislocation mobility.

A simple case that we examine here is motion in a $\{110\}$ plane that contains all three dislocations forming the junction network. In this plane alone, the network can move in two independent directions. Only two components of stress contribute to the Peach-Koehler (PK) force [15] that drives dislocation motion in this plane, i.e., σ_{xz} and σ_{yz} in the coordinate frame shown in Fig. 2(b). Below we examine network motion for a few selected directions of applied stress in the XY plane and show that both network mobility and its underlying atomistic mechanisms can be different, depending on the stress direction.

The first case is when the stress is applied along the $[110]$ direction, i.e., perpendicular to the Burgers vector of the $[001]$ junction dislocation. Regardless of the magnitude of applied stress, the junction dislocation does not move. Nevertheless, after ramping the stress up to 1.4 GPa, motion of the network is observed, strictly in the direction along the junction line. The motion takes place by unzipping the junction at its trailing node, leading to nucleation and propagation of kinks on both $\frac{1}{2}\langle 111\rangle$ dislocations joining the junction. To complete the motion cycle, the kinks pass through the periodic boundaries, converge on the leading node, and rebuild the junction, effectively translating the whole network along the junction line direction [Fig. 3(a)]. Remarkably, it would have taken much higher stress, $\sim$2.7 GPa along this stress direction, to move any of the two dislocations if they were unconnected. This is the first clear indication that the presence of junction nodes significantly affects dislocation mobility. In order to examine if and how these observations depend on the size of the

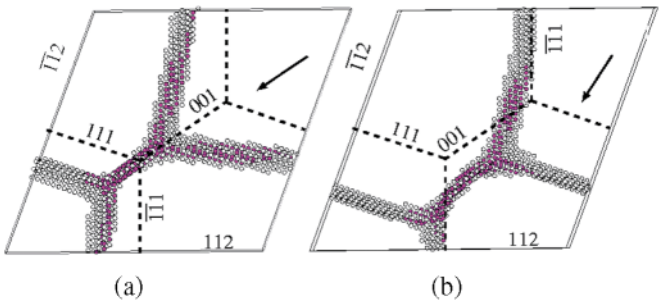

FIG. 3 (color online). The network moves under stress from its initial position shown by the dashed lines. (a) Network motion under stress applied perpendicular to the junction line. (b) Network motion under stress applied perpendicular to one of the parent screw dislocations. Arrows show approximate directions of network motion.

simulation cell, we performed similar simulations in periodic boxes ranging from 16 000 to 310 000 atoms (the standard size for most of our simulations was 74 000 atoms). Using the method reported in [11], the accuracy of our Peierls stress calculations is estimated at about 10%, determined by the size and shape of the periodic supercell. Within this accuracy, both Peierls stress and the underlying motion mechanism are found to be independent of the size of the simulation box.

Next, we examine a situation in which the more difficult motion of the junction dislocation, perpendicular to its line direction, is induced. In this case stress is applied along the $[001]$ direction. Here again the motion cycle starts as a kink appears, at random, at one of the two junction nodes. This time, however, the first kink nucleates and propagates along the $[001]$ junction dislocation followed by kink activity on the two $\frac{1}{2}\langle 111\rangle$ dislocations. As a result, the whole network moves perpendicular to the junction line preserving its overall shape. In this case, the stress required to initiate the network motion is 2.6 GPa, which is again significantly lower than the Peierls stress of a stand-alone junction dislocation (3.2 GPa), whose motion is clearly assisted by kink nucleation at the triple nodes.

The last case we discuss here is when stress is applied along the $[112]$ direction so that the PK force is zero on the $\frac{1}{2}[11\bar{1}]$ dislocation [vertical line in Fig. 2(b)]. Remarkably, all three dislocations in the network, including the unstressed one, move once the stress reaches 1.9 GPa. Motion takes place in a sequence in which several kinks nucleate and propagate on the more mobile $\frac{1}{2}[111]$ dislocation, followed by kink formation on the junction line. As the kinks propagate, the two lines move in the directions of their respective PK forces while the unstressed $\frac{1}{2}[11\bar{1}]$ dislocation still remains in its initial position. However, the $\frac{1}{2}[111]$ dislocation moves faster than the junction dislocation which leads to the accumulation of distortion at the node, manifest in bending of the unstressed $\frac{1}{2}[11\bar{1}]$ dislocation [Fig. 3(b)]. Finally, this distortion is released by kinks rushing along the unstressed line towards the other node, so that this dislocation moves to the left. From then on, this motion cycle repeats in which all three dislocations move in a cooperative fashion so that the whole network moves in response to applied stress. Consistent with the first two cases, the stress required to move the network, at 1.9 GPa, is considerably lower than Peierls stress of any of its constituent dislocations. Given the screw character of the network, it could be expected to move in the direction exactly perpendicular to stress (as it does in the first two cases). However, apparently due to the different mobilities of the participating dislocations, preservation of line connectivity at the node requires the network to drift left, i.e., perpendicular to the driving force, in addition to moving downward, i.e., along the force.

Overall, we have computed the network Peierls stress for four distinct directions in the XY plane, three of which are discussed above. Figure 4 quantifies the nodal effect on dislocation mobility. The hexagonal envelope corresponds to conditions when at least one of the three dislocations sees a resolved stress exactly equal to its Peierls stress reported earlier for stand-alone dislocations. The nodal effect is manifest in the fact that four simulation data points lie well inside this envelope. This means that the nodes significantly reduce the effective lattice resistance to motion of dislocations once they are incorporated in the network. Since the cases examined so far sample all distinctly different situations, we conclude that the nodes enhance network mobility for all orientations of the applied stress in the XY plane.

In addition to revealing the generic effects of junction nodes on dislocation motion, our results shed light on a long-standing controversy over the mechanisms of anomalous slip observed in bcc transition metals at low temperatures. It was suggested that enhanced dislocation activity in the anomalous slip plane (which has relatively small resolved shear stress) is due to cooperative motion of planar

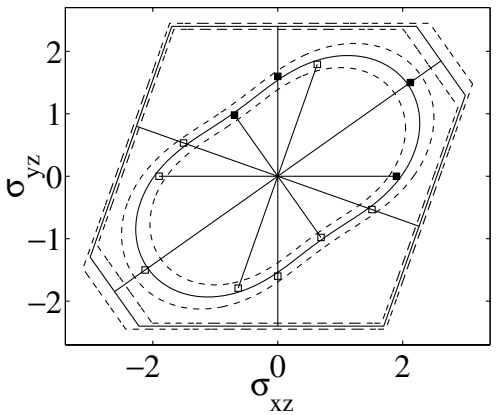

FIG. 4. Peierls stress of the dislocation network as a function of stress orientation. Filled symbols show the values of critical stress for the four directions actually tested. Open symbols are obtained by symmetry. Dashed lines indicate the range of error in the computed Peierls stress.

networks of screw dislocations [4]. Even though motion of planar networks similar to that shown in Fig. 3(a) was directly observed in *in situ* TEM [16], the issue remained controversial. In particular, it was argued that conservative motion of planar networks requires motion against applied stress and, as such, may not be possible [17]. With time, the controversy subsided but was never fully resolved, due to the lack of mechanistic understanding. In particular, the original mechanism was thought to involve kink emission at the leading node of the junction while the possibility of network motion in directions other than [001] was never considered. This is contrary to our observation that the kinks form by splitting off the trailing node of the junction [see Fig. 3(a)]. Furthermore, our simulations prove that planar networks of $\frac{1}{2}\langle 111\rangle$ dislocations can move conservatively in all directions in the (110) plane and that dislocation mobility is markedly enhanced by the presence of junction nodes.

Yet another interpretation of the results reported here has to do with the mentioned geometric equivalence of the planar dislocation networks and the low-angle grain boundaries. Indeed, the network motion discussed above is nothing but conservative sliding of a low-angle $[\bar{1}10]$ pure twist grain boundary. Therefore, all the parameters and mechanisms revealed here by atomistic simulations also describe the sliding mobility of such low-angle boundaries. Our observations suggest that mobility of 2D defects (grain boundaries) is controlled by the behavior of its constituent 1D defects (dislocations), whose motion is initiated by the emergence of kinks at 0D defects (junction nodes). Ultimately, it is the properties of the 0D defects (junction nodes and kinks) that define the resistance to intergranular sliding along the low-angle twist boundaries.

We observe that for the nodes to enhance dislocation mobility two conditions should be satisfied: Peierls stress for dislocation glide in the absence of nodes should be high, and, simultaneously, lattice resistance to kink migration along the dislocation should be low. For the FS model of Mo employed here both conditions are met: Peierls stress for kink migration is only 0.02 GPa, 2 orders of magnitude lower than 2.4 GPa for a straight screw dislocation. In contrast, we found that in another glide system Peierls stress for stand-alone dislocations is low, at 0.07 GPa, whereas after the dislocations are incorporated into a junction network their Peierls stress actually increases to 0.2 GPa [18].

In summary, contrary to the anticipated constraining effect of the junction nodes, formation of screw dislocation junctions is predicted to enhance dislocation mobility in bcc molybdenum. This effect can play a role in low temperature deformation in Mo and other bcc metals, where screw dislocations and junction networks are often observed.

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