Kink Asymmetry and Multiplicity in Dislocation Cores

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(Received 2 September 1997)

We propose a hierarchical classification of kink species in dislocation cores which considers three sources of broken symmetry, host lattice structure, character of the dislocation, and core reconstruction effects. Kink multiplicity in bcc and diamond cubic lattices is examined and verified directly by atomistic calculations using appropriate interatomic potential models for Mo and Si. Much of the complexity of dislocation kink mechanisms can be rationalized in terms of the identified underlying causes of symmetry breaking. [S0031-9007(97)04931-4]

PACS numbers: 61.72.Lk, 61.72.Bb, 61.72.Nn, 62.20.Fe

Understanding how crystalline materials deform noncatastrophically under an imposed load requires consideration of mobility of extended defects such as dislocations and grain boundaries. In the context of single crystal plasticity, a long-standing challenge is to describe the stress-strain response of a specimen in terms of motions and interactions of dislocation lines. While significant advances have been made recently in analyzing the behavior of interacting dislocations by direct simulation [1], atomic-level information about core mechanisms of dislocation mobility remains a bottleneck. In particular, in materials with high lattice resistance to dislocation motion it is conventional to relate dislocation mobility under stress to kink formation and migration energies through a rate equation [2]. Recent atomistic simulations revealed a more complicated picture of dislocation motion via formation, motion, and reactions of multiple species of kinks [3–5]. Despite the obvious importance of the observed *kink multiplicity,* its origin is not clearly understood.

In this Letter we show that the existence of the multiple kink species is a consequence of symmetry breaking with respect to two fundamental space operations, (a) mirror inversion relative to a plane normal to the dislocation line, and (b) 180° rotation about an axis parallel to the dislocation line. We find that symmetry breaking can occur under at least three different conditions: (1) insufficient symmetry of the crystal lattice itself, (2) mixed character of the dislocation displacement field, and (3) atomic core reconstruction. While each can result in a doubling of the number of distinct kink species, these broken symmetries, when taken together, give rise to a variety of secondary core defects. The principal implication of the present results is that for each particular dislocation the set of possible core defects and their mutual transformations are uniquely related to the hierarchy of broken symmetries.

Dislocation is a line defect of concentrated atomic disregistry given by its Burgers vector. Burgers vector is equal to one of the shortest lattice periods so that the crystal outside of a narrow core region around the line remains nearly perfect. Dislocation lines or loops move in response to applied stress and propagate through the lattice, resulting in shearing of atomic planes relative to each other. The ability of a crystalline material to respond to applied stress plastically is then directly related to the mobility properties of individual dislocations. Despite their small dimensions (dislocation core radius is typically of the order of several atomic dimensions), these crystal defects are not elementary. In materials with strong dislocation-lattice coupling, dislocations are known to move by forming double kinks and having them extend (spread) laterally along the line. Net dislocation velocity is then given, within the kink diffusion model [2], by the following rate equation:

$$v_d = \frac{\nu_D \sigma a b^3}{kT} e^{-(U_{\mathrm{DK}}/2+U_m)/k_B T}, \qquad (1)$$

where v_d is the dislocation velocity, T is the temperature, σ is the applied stress, U_{DK} is the free energy of double-kink formation, U_m is the kink migration barrier, ν_D is the Debye frequency, b is the Burgers vector, and a is the kink height. Despite its common use for the analysis of dislocation mobility, the picture of a single kink mechanism leading to this equation is not consistent with atomistic simulations [3–5]. In particular, multiple core mechanisms are observed to operate simultaneously, whereby several distinct kink species can form, move, annihilate, enter in various complex defect reactions, resulting in a rather complex picture of dislocation motion. In the following we describe a set of simple rules by which much of the observed complexity of the kink mechanisms can be rationalized *a priori,* by considering symmetry properties of the host lattice and that of the ideal straight dislocations.

We consider a double-kink structure in an otherwise straight dislocation, shown in Fig. 1, and ask what symmetry operation can transform the left and right kinks, LK and RK, into each other. For pure edge and screw dislocation segments, with Burgers vector perpendicular and parallel to the dislocation line, this operation is seen to be, respectively, a mirror inversion through the plane normal to the dislocation line [Fig. 1(a)], and a 180° rotation about an axis parallel to the dislocation line [Fig. 1(b)]. These two basic space operations, which we will call edge and screw

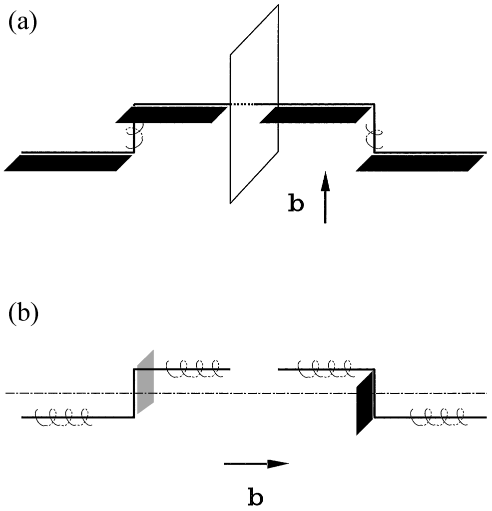

FIG. 1. Displacement field of dislocation kinks viewed from above the glide plane. Right and left helices indicate the sense of Burgers displacement in the screw segments, while the extra half-planes inserted from above (dark) and from below (light) the glide plane show the sense of Burgers displacement in the edge segments. Mirror plane and rotation axis are shown in (a) and (b), respectively.

transformations, provide the basis for determining whether LK and RK should be considered as identical. In what follows we will establish that kink asymmetry can arise from a hierarchy of causes—asymmetry of the underlying lattice, mixed character of a dislocation, and atomic core reconstruction—each one is sufficient to make LK and RK distinct from each other. Moreover, the combination of reconstruction defect with either lattice asymmetry or mixed dislocation character leads to kink-defect complexes which further enrich the multiplicity of kink species. For verification, specific examples of dislocation kinks in the bcc and diamond cubic lattices are examined, and their relaxed atomic configurations are determined by simulations of the type described in [4] using many-body potentials for Mo [6] and Si [7].

The most basic underlying cause of kink asymmetry arises when the host lattice is not symmetric with respect to the two space operations just described. Figure 2 shows a double kink in the $\frac{a}{2}[111]$ screw dislocation in Mo where, as a consequence of broken symmetry in the 180° rotation, LK and RK are different. First recognized in [8], this kink asymmetry is a generic property in bcc materials. A corresponding example involving broken mirror symmetry is the case of $\frac{a}{2}[110]$ edge dislocation lying along a $[1\bar{1}2]$ direction in diamond cubic Si.

Next in the hierarchy of sources of asymmetry is the dislocation character. When dislocation has both edge and screw components, there exists no space operation which transforms LK and RK into each other. One can therefore conclude that in mixed dislocations LK and RK must be different. Two prominent examples in Si are the 60° full and 30° partial dislocations lying along the $[1\bar{1}0]$ direction in the glide plane. In Fig. 3(a) the different structures of LK and RK can be seen in the bonding topology in the kink cores, a behavior which can be traced to the mixed dislocation character since the host lattice is symmetric with respect to both edge and screw transformations. A comprehensive analysis of the different kink forms in this dislocation has been given in [4].

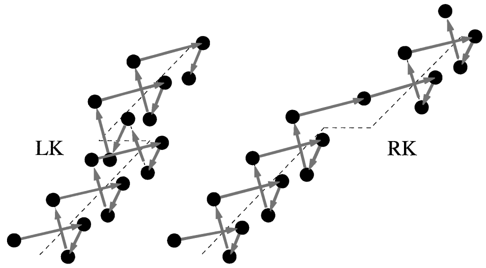

FIG. 2. LK and RK in $\frac{a}{2}[111]$ screw dislocation in bcc Mo. Only the atoms nearest to the geometric center of the dislocation are shown, connected by arrows representing relative atomic displacements in the direction of **b** with breaks (kinks) in the helical sequence. Helix period is equal to Burgers vector b and the arrows are scaled by their maximum length of $b/3$. LK appears as a step with W-shaped pattern of arrows, with two extra atoms in the helical sequence, whereas in RK, only one extra atom appears.

The third cause of kink asymmetry, that of core reconstruction, differs from the first two in that it is specifically dependent on the details of interatomic interaction. Consider the 90° partial dislocation in the same $(\bar{1}11)$ glide system in Si as Fig. 3(a). Because mirror symmetry is preserved in both the lattice and kink displacement fields, one might expect no difference between left and right kinks. Indeed Fig. 4(a) shows LK and RK are mirror twins in the unreconstructed core. However, when the core reconstructs, Fig. 4(b) shows this symmetry no longer holds. The screw dislocation $\frac{a}{2}[110]$ in Si is another example where symmetry, in this case the 180° rotation, is broken by core reconstruction. Given that reconstruction depends on interatomic interaction, it has been argued that such a process may be suppressed in III-V and II-VI diamond cubic compounds due to repulsion between the anions or cations in the dislocation core [9].

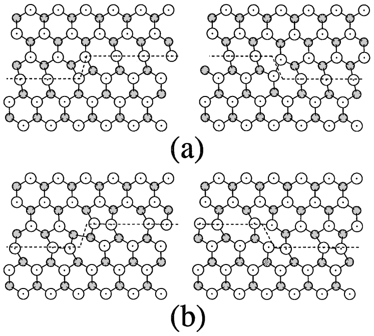

FIG. 3. Kinks in a 30° partial in Si with atoms above and below the glide plane shown as open circles and closed circles, respectively. (a) LK and RK in unreconstructed core. (b) Alternative kinks LK$'$ and RK$'$ in reconstructed core.

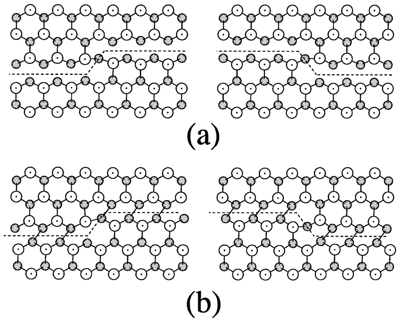

FIG. 4. Same as in Fig. 3 but for 90° partial, (a) identical LK and RK in unreconstructed core, (b) LK and RK after reconstruction which breaks the mirror symmetry.

Another characteristic distinction of the core reconstruction relates to the double degeneracy of the reconstructed ground state structure, giving rise to the existence of reconstruction defects, or solitons [10]. Solitons appear as faults that separate two core segments reconstructed in the opposite sense. The direction of symmetry breaking in the entire dislocation can be reversed by a soliton passing along the dislocation line from one end to the other. In particular, as the soliton traverses along the line all kinks of LK variety will be converted to RK, and vice versa. This is in contrast to the other two sources of multiplicity discussed above, in which the sense of left-right kink asymmetry is permanently fixed for a given dislocation, once its character and Burgers vector are defined.

Besides changing the sense of left-right kink asymmetry, solitons can produce new kink species by binding to kinks and forming kink-soliton complexes (KSC) [4]. Such KSC are kinks and solitons at the same time and, depending on interatomic interaction, they may be either stable or completely unstable with respect to spontaneous dissociation into the parent defects—regular kinks and solitons. Thus, symmetry breaking reconstruction will not necessarily result in multiple kinks, but rather introduces a *possibility* for the existence of additional kink species, each with its own distinct topological characteristics related in a unique way to the sense of core reconstruction. The set of possible core defects, kinks, and solitons alike, as well as their degeneracies, can be deduced from the particular sense of the symmetry breaking with respect to an appropriate space operation. For example, in the above case of 90° partial in Si, two kinds of solitons can exist [11] as well as four different kinks [5], including two KSC defects. The solitons are nondegenerate while the four kinks are doubly degenerate, each having two mirror-twin forms. The case of screw dislocation in Si is similar, yet different. Again, using the screw transformation as a test we find that only one doubly degenerate soliton, one fourfold degenerate kink, and two doubly degenerate kinks can exist in this case.

The simple hierarchy of broken symmetries is useful for classifying kink mechanisms in various dislocations. We now examine three cases in which one of the sources of kink asymmetry is combined with a secondary core reconstruction, resulting in a rather complex set of kinks and solitons. The first case is the same $\frac{a}{2}[111]$ screw dislocation in bcc transition metals. Depending on the subtle details of interatomic interaction, these dislocations experience a particular core reconstruction in the form of a nonplanar core splitting, this time breaking another symmetry—[110] diad symmetry [12]. This nonplanar core structure is doubly degenerate so that two kinds of defects are present, termed p and n solitons in [3]. As was discussed above, lattice asymmetry makes LK and RK different (Fig. 2). In the reconstructed core these two kinks can bind with either of the two solitons, making up to four additional kink species (KSC) and bringing the total number of kinks to six. In this case kink multiplicity arises from the left-right asymmetry of the lattice combined with the secondary nonplanar core reconstruction.

As discussed earlier, the mixed character of the 30° partial dislocation in Si is responsible for LK and RK being different [Fig. 3(a)]. Additional core reconstruction breaks another symmetry, this time translational, doubling the structural period along the core from b to $2b$. Because the reconstructed structure is doubly degenerate, solitons are present in the core. Similar to the case of full screw dislocation in Si, only one kind of soliton is possible. The latter can bind to the two kinks and form two additional KSC, bringing the number of possible kink species to four. Each of these kinks can have alternative configurations, related to the normal kinks by a specific bond-switching transformation in which the kink center translates by half a period, as shown in Fig. 3(b). It was found [4] that kinks move along the core in a series of such transformations, as in $RK \rightarrow RK' \rightarrow RK \rightarrow \ldots$. In [13] such low energy bond-switching path was not considered, leading to an overestimation of RK migration barrier in 30° partial. Additional kink multiplicity in this dislocation results from a combination of left-right kink asymmetry due to a mixed dislocation character with additional core reconstruction.

Recently, a complex reconstruction was found for the 90° partial dislocation in Si [14] where, in addition to breaking the mirror symmetry, as was shown in Fig. 4(b), a period doubling takes place similar to the above case of 30° partial. The new double-period (DP) structure was predicted to have lower energy than the commonly accepted single-period (SP) one, resulting in a wide variety of possible kinks and solitons. The latter can be counted as follows. The ground state structure is fourfold degenerate and can host up to five topologically distinct solitons which we term "translation soliton" T, "mirror solitons" M_1 and M_2, and "translation-mirror solitons" TM_1 and TM_2, after the broken symmetries that cause their existence. T soliton is fourfold degenerate while the other four solitons are each doubly degenerate. Binding of these solitons to kinks LK and RK makes up to six more KSCs, bringing the total number of topologically distinct kinks to eight. Similar to the case of 30° partial, each of these eight kink families contains at least two members, related to each other by a bond-switching rearrangement of core atoms corresponding to kink translation along the core. Still more low energy core defects in the 90° partial can be expected due to the nearly identical energies of the DP and SP structural states; depending on the method used, the predicted difference ranged from several meV to several tens of meV per Å of dislocation line [14]. Since the latter value is of the order of kT (at 900 K), the core is likely to contain a number of short SP segments shifted by one-half lattice spacing from a normal DP position. Half-kinks at the boundary between DP and SP segments can exist in various forms, depending on the sense of core reconstruction in the adjacent DP and SP segments. We expect these half-kinks to play an important role in dislocation mobility, since their energies might be close to or lower than the energies of the full kinks discussed in [14]. This is because elastic contribution to the kink energy is proportional to the square of kink height [2]. Based on the reported energy difference we estimate that full kinks will gain energy by splitting into two half-kinks separated by a narrow SP segment of a few lattice spacings. The motion of such extended kinks can proceed by translation of the leading and trailing half-kinks (partials), in close analogy to the motion of extended dislocations in diamond cubic and fcc crystals. It remains to be seen which of the predicted multiple kink species, full and partial, are involved in the low energy pathways for dislocation motion.

As a thought experiment for observing kink asymmetry, one may imagine a mixed dislocation, say $\frac{a}{2}[110]$ 60° dislocation in Si, pinned between two strong obstacles at a small (vicinal) angle with respect to the ideal line direction. Depending on the sign of the vicinal angle, there will be a certain number of *geometrically necessary* kinks of one kind, either left or right. By applying an appropriate stress, it should be possible to force the kinks to move toward one pinning point, giving rise to a bow out of the pinned segment. If the mobilities of LK and RK are sufficiently different, then the rates of stress-induced bowing out also will be different for two dislocation segments pinned at equal but opposite vicinal angles. Another possibility involves misfit dislocations in strain-mismatched heteroepitaxial thin films [15]. *In situ* TEM experiments have shown that mobilities of two seemingly equivalent threading dislocations can differ by a factor of 2 or more [15,16]. Since the measurements do not resolve the exact sense of the Burgers vector, it is tempting to relate the observed anomalous mobilities to possible unresolved kink asymmetry.

In summary, we have examined three different sources of multiple kinks in two different materials with high lattice resistance to dislocation motion, diamond cubic Si and bcc Mo. We showed that the observed richness of the secondary core excitations, including solitons and kinks, can be rationalized in terms of the underlying asymmetries of the host lattice, displacement fields of mixed dislocations, and symmetry-breaking core reconstructions. Asymmetries of the host lattice and those of the mixed dislocations are geometric by nature and are permanently associated with a given dislocation. On the other hand, kink asymmetries caused by core reconstructions are not permanent and may or may not be realized, depending on the interatomic interaction. The usefulness of the proposed approach is that for any given dislocation the entire set of core defects and their transformations contributing to dislocation motion can be gleaned just by considering the symmetries of the host lattice and that of the straight *defectless* dislocation. The present analysis of secondary core defects underscores the effectiveness of symmetry considerations for characterization of excitations in solids. It appears that our simple intuitive approach can be incorporated into a more formal and systematic analysis of topological characteristics of crystal defects developed earlier by Pond [17] in connection with surface and interfacial behavior.

This work was supported by the MIT MRSEC Program of the National Science Foundation under Award No. DMR 94-00334. V. V. B., W. C., and S. Y. acknowledge support from LLNL under Agreement No. B332671.

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