

A Model for Crack-Induced Nucleation of Dislocations, Complex Stacking Faults, and Twins

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Abstract. This paper addresses a class of deformation mechanisms involving the coordinated shear of multiple, parallel slip planes. Relevant phenomena include complex stacking faults, deformation twins, and dislocation nucleation ahead of cracks in metals. As part of the theory, we revisit the notion of a multi-plane slip potential, we develop a criterion for the emergence of microtwins, and we discern the conditions that favor microtwin versus dislocation nucleation. The model is constructed using concepts from the continuum-based Peierls-Nabarro framework for extended dislocation cores.

Introduction

The deformation of metals has long been an area of intensive study. In particular, body centered cubic (BCC) metals have garnered close scrutiny due to the common use of steels for structural applications. There are several notable features that can develop during plastic deformation of BCC metals, such as dislocation nucleation and motion, stacking fault formation, crack propagation, and deformation twinning. Though BCC metals are almost always used in polycrystalline form, this paper addresses plastic deformation at the level of a single crystal.

In general, plastic deformation occurs by the motion of dislocations (see Fig 1a). Macroscopic deformations are the result of slip, which is due to the movement of full dislocations in response to an applied shear stress. Twinning is a deformation process similar to slip, involving shearing of parallel atomic planes past one another, and is associated with the motion of partial dislocations on these planes (see Fig. 1b). Twinning differs from slip on a macroscopic level in that the twinned region inherits a different crystallographic orientation than the rest of the crystal. Since BCC crystals do not have a close-packed plane on which slip is especially easy, the Peierls stress to move a perfect dislocation can be high, while the shear stress to activate the twinning process may be significantly lower. Twinning does not result in large portions of bulk plastic deformation, and twinning and slip are not “either-or” processes. While single-layer stacking faults, the type of crystalline slip that leads to twinning when it happens on successive planes, have been observed in FCC crystals, they have not been observed to occur in BCC metals. Calculations by Vitek [1] in 1970 revealed that no local fault energy minima exist for BCC crystals, and thus, single-layer stacking faults are considered to be unstable. Vitek found the first stable multi-layer stacking faults to occur on $\{112\}$ planes for n -layer faults where $n \geq 3$. When n reaches a sufficiently large number, the multi-layer stacking faults are identical to twins.

In this paper, we develop a multi-plane continuum model that for an isotropic, non-linear elastic continuum to describe deformation processes that occur on one or more slip planes ahead of a crack tip. The crack tip is assumed to be a nucleation point for slip processes. Within the framework of the multi-plane model, an empirical constitutive law is developed to describe the relationship between shear stress and displacement on the participating atomic planes. The constitutive law is defined by a parameter set which controls the deformation outcome as either (i) full dislocation formation or (ii) formation of an extrinsic stacking fault. The model is similar in

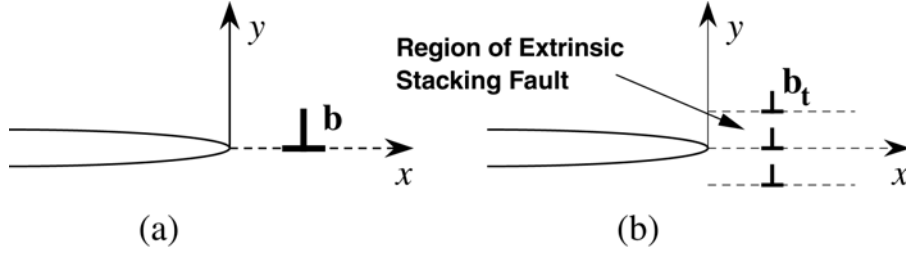


Figure 1. A crack loaded in mode II, if it doesn't propagate, either (a) emits a full dislocation or (b) emits a microtwin as a front of vertically-arrayed twinning dislocations. In BCC crystals, the full dislocation Burgers vector $\mathbf{b}$ is given by $\sqrt{3}a/2\mathbf{i}$, where a is the lattice constant. The twinning dislocation Burgers vector $\mathbf{b}_t$ is given by $\mathbf{b}/3$. The y -axis corresponds to the $[1\bar{1}2]$ crystallographic direction, and the x -axis corresponds to the $[\bar{1}11]$ crystallographic direction.

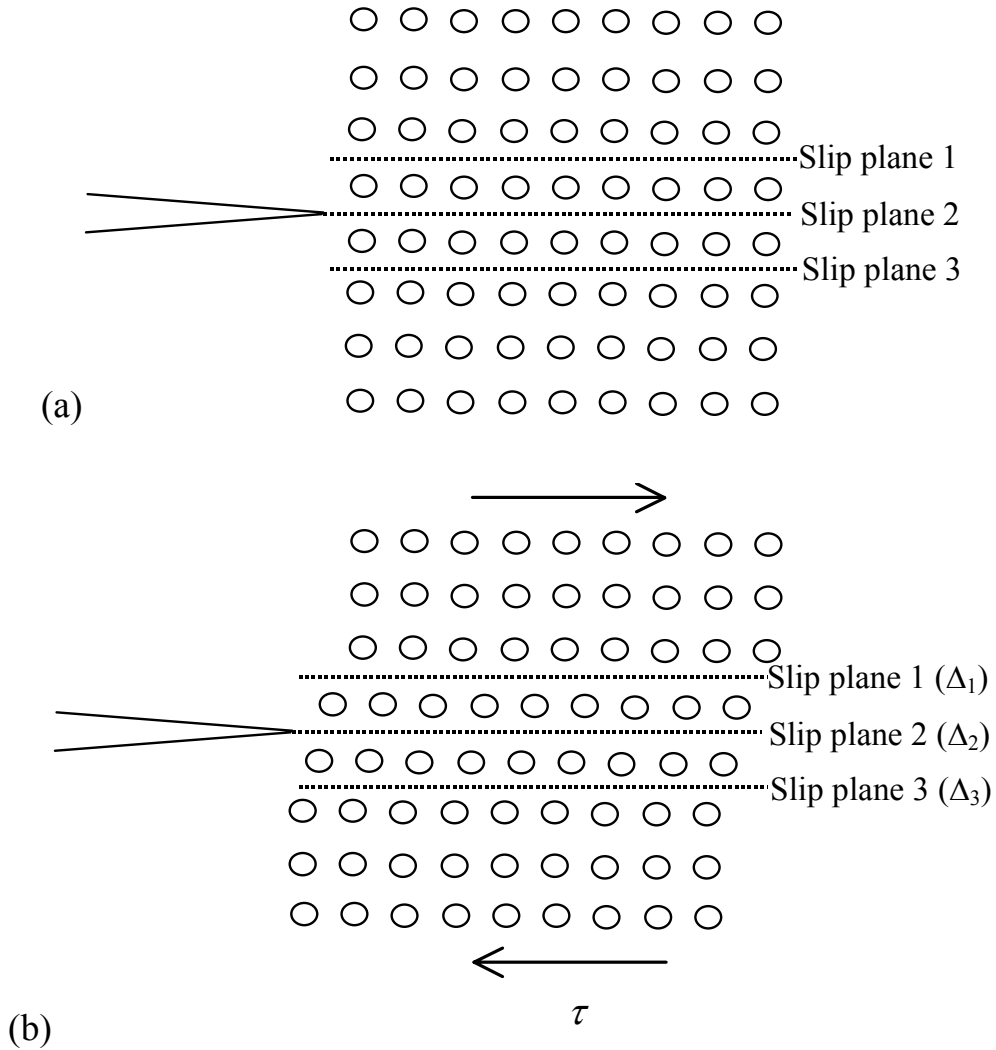


Figure 2. Multi-plane model for slip in the Peierls-Nabarro framework; (a) depicts the undeformed state while (b) depicts a mode II loading. The relative atomic displacement Δ_i refers to the horizontal shift of atoms across slip plane i , with $\Delta_i = 0$ in the undeformed state. Three parallel slip planes (one coplanar with the crack and two adjacent) slip according to the generalized interplanar potential given by Eq. 4 and shown in Fig. 3. Material external to the slip planes is modeled as a linear, elastic continuum. Within this framework, a large amount of slip concentrated on slip plane #2, with relatively small slip on planes #1 and #3 is characteristic of dislocation emission; while significant slip on all three planes is characteristic of twin formation.

spirit to recent work by Tadmor *et al.* [2] in that it exploits the Peierls concept to describe the slip of adjacent, parallel planes ahead of a crack tip. The Tadmor model has been rigorously developed for twinning in FCC crystals, a phenomenon which has been observed experimentally [3]. The current framework is somewhat more amenable to slip processes in BCC crystals.

Multi-Plane Slip Model

In our framework, the formation of a multi-layer, or extrinsic, stacking fault is treated as a precursor to growth of a twin. This so-called “microtwin” is not yet a fully developed twin. It has been seen experimentally that deformation of BCC crystals can lead to the concomitant formation of twin dislocations and partial dislocations [4]. These partial dislocations are also known to form in as few as two or three slip planes. Thus, we limit our consideration to only those three critical atomic planes, directly ahead of the crack tip (see Figs. 1b and 2). This allows the model to remain tractable as an analytical model, while incorporating the necessary feature of multiple, coupled slip planes. The incipient microtwin is bounded on its flanks by twin planes, and is bounded horizontally by the crack tip and the partial dislocation front, respectively. The remaining material (exterior to the slipping planes along the x -axis) is treated as an elastic continuum. This allows the model to be atomistically specific in a critical region, while capturing essential mechanical details of the surrounding material. This model addresses the competition between the formation of multi-layer stacking faults versus full dislocations and even partial dislocations.

This model characterizes the behavior of BCC metals under applied shear stress by directly using an integral equation method developed by Beltz and Rice [5], built on the Peierls-Nabarro concept [6] of dislocation formation. The model assumes a *periodic* relationship between the shear stress and sliding displacement on planes just ahead of the crack tip. In order to more accurately portray a vertical stack of twin dislocations that form a twin front, or an incipient twin front, we represent them as a *vertical stack of slip distributions*. In turn, these slip distributions are discretized into a series of infinitesimal dislocations of Burgers vector of b' spaced apart by a distance dx , where b' is defined as $-(\partial\Delta/\partial x)dx$. The distribution of the infinitesimal dislocations can be made consistent with a state of stress-balance everywhere along the slip plane, and the problem of stress singularities and the associated need for a core cut-off radius are eliminated.

Fig. 2 shows a schematic of the multi-plane system before and after deformation. In considering the case of three slip planes at the crack tip, a set of coupled, nonlinear integral equations may be written to enforce stress equilibrium:

$$\begin{aligned}\tau_1[\Delta_1, \Delta_2, \Delta_3] &= \frac{K_{II}f(x, +h)}{\sqrt{2\pi x}} - \left[\int_0^\infty g_{11} \frac{d\Delta_1(s)}{ds} ds + \int_0^\infty g_{12} \frac{d\Delta_2(s)}{ds} ds + \int_0^\infty g_{13} \frac{d\Delta_3(s)}{ds} ds \right] \\ \tau_2[\Delta_1, \Delta_2, \Delta_3] &= \frac{K_{II}}{\sqrt{2\pi x}} - \left[\int_0^\infty g_{21} \frac{d\Delta_1(s)}{ds} ds + \int_0^\infty g_{22} \frac{d\Delta_2(s)}{ds} ds + \int_0^\infty g_{23} \frac{d\Delta_3(s)}{ds} ds \right] \\ \tau_3[\Delta_1, \Delta_2, \Delta_3] &= \frac{K_{II}f(x, -h)}{\sqrt{2\pi x}} - \left[\int_0^\infty g_{31} \frac{d\Delta_1(s)}{ds} ds + \int_0^\infty g_{32} \frac{d\Delta_2(s)}{ds} ds + \int_0^\infty g_{33} \frac{d\Delta_3(s)}{ds} ds \right]\end{aligned}\quad (1)$$

where Δ_1 , Δ_2 , and Δ_3 are the displacements along the three slip planes of interest, g_{ij} are the Green's functions for shear stress on plane i due to a dislocation located on plane j , and h is the interplanar spacing. Expanding upon the integral solution method utilized by Gumbsch and Beltz [7], who studied mixed-mode loading of a single slip plane ahead of a crack, the solution of this set of equations involves the determination of the K_{II} necessary to achieve any combination of displacements, Δ_1 , Δ_2 , and Δ_3 . Eq. 1 describes the entire stress distribution along the three slip planes ahead of the crack tip. The effects of slip or any displacement on a slip plane is no longer limited to just that slip plane. The interactions between the three slip planes are taken into consideration, i.e. the presence of a dislocation on any given slip plane incurs a stress on all three slip planes. Any slip that occurs along a slip plane generates stresses that are felt on all three slip

planes. Additionally, displacement can occur on all three slip planes, and the displacement is not required to be uniform across all three planes.

The solution consists of finding functions $\Delta_i(r)$ which satisfy Eq. 1, and to determine the maximum load for which these functions are stable. If a solution can be found for the integral equation, K_{II} is incremented and the solution procedure repeated until the solutions, $\Delta_i(r)$ converge. More details pertaining to the numerical solution procedure may be found in Refs. [5], [7], and [8]. The K_{II} at that point is considered to be the critical stress intensity factor corresponding to the load necessary for some instability to occur; *e.g.* multi-plane slip, or dislocation nucleation.

Constitutive Law

To complete the integral equation introduced in the previous section, it is necessary to develop a constitutive law for the shear response along the sliding slip planes to describe the interatomic interactions. The shear stress, $\tau[\Delta_1, \Delta_2, \Delta_3]$, is related to the actual slip that occurs along the three parallel slip planes during the deformation process. We begin by revisiting Frenkel's sinusoidal model [9] for the excess energy of a system undergoing slip on a single plane:

$$E = A\gamma_{ref} \sin^2\left(\frac{\pi\Delta}{b}\right) \quad (2)$$

where A is a dimensionless fitting parameter and γ_{ref} is an energy scale defined below. Differentiating the energy with respect to Δ gives the local shear stress:

$$\tau(\Delta) = \frac{\partial E}{\partial \Delta} = \frac{A\pi\gamma_{ref}}{b} \sin\left(\frac{2\pi\Delta}{b}\right) \quad (3)$$

and thus τ and Δ are work conjugate to each other. To generalize the Frenkel concept – that is, develop an energy appropriate for the multi-plane slip, interactions between the *multiple, parallel* slip planes must be considered. Relative displacement on one slip plane necessarily disrupts the equilibrium of atoms on neighboring planes. An empirical, yet analytic form of the energy potential is proposed as:

$$E = \gamma_{ref} \left[\begin{aligned} & A \left[\sin^2\left(\frac{\pi\Delta_1}{b}\right) + \sin^2\left(\frac{\pi\Delta_2}{b}\right) + \sin^2\left(\frac{\pi\Delta_3}{b}\right) \right] \\ & + B \left[\sin^2\left(\frac{\pi(\Delta_1 + \Delta_2)}{b}\right) + \sin^2\left(\frac{\pi(\Delta_2 + \Delta_3)}{b}\right) \right] + B \left[\sin^2\left(\frac{\pi\Delta_1}{b}\right) + \sin^2\left(\frac{\pi\Delta_3}{b}\right) \right] \\ & + C \left[\sin^2\left(\frac{\pi(\Delta_1 - \Delta_2)}{b}\right) + \sin^2\left(\frac{\pi(\Delta_2 - \Delta_3)}{b}\right) \right] + C \left[\sin^2\left(\frac{\pi\Delta_1}{b}\right) + \sin^2\left(\frac{\pi\Delta_3}{b}\right) \right] \end{aligned} \right] \quad (4)$$

The terms having coefficient A in Eq. 4 correlate to the slip of *nearest neighbor* layers of atoms – as a sum of the energies of three adjacent slip planes undergoing deformation. This contribution is just an extension, in an additive sense, of Eq. 2. The terms involving coefficient B represent *secondary* interactions generated from second-nearest-neighbor layers of atoms, and the C terms account for rotational contributions. The additional terms on the second and third lines of Eq. 4 are an attempt to include the interaction of layers within the active slip region with atomic layers above and below the active slip plane region.

For the case of *single-plane* slip, *e.g.*, $\Delta_1 \ll \Delta_3 \approx 0$, Eq. 4 reduces to $E = \gamma_{ref}(A + 2B + 2C)\sin^2(\pi\Delta_2/b)$; hence, we identify the grouping of parameters $\gamma_{ref}(A + 2B + 2C)$ as the unstable stacking energy γ_{us} . The parameter C represents an energy penalty for slip confined to one plane; *i.e.*, materials that

have a tendency to twin might be expected to have a large, positive value of C . Collectively, the parameters A , B , and C are empirical constants which should be related to material properties, and are to be determined by fitting to various existing atomistic potentials. Such procedures are described in detail by Chang and coworkers [8,10].

Differentiating Eq. 4 results in expressions for local, interplanar shear stress to be used in conjunction with Eq. 1; i.e.,

$$\tau_i(\Delta_1, \Delta_2, \Delta_3) \equiv \frac{\partial E}{\partial \Delta_i} \quad (5)$$

While the model is developed on the atomic level, and the underlying atomic structure gives rise to the functional forms developed here, the formulation of the constitutive law is inherently a continuum one. For the purpose of visualizing the energy profile of the constitutive law, the case of multi-plane slip will be presented in this paper with the constraint that $\Delta_1 = \Delta_3$, with Δ_1 and Δ_2 plotted against energy. This special case is chosen since Δ_1 and Δ_3 are expected to be identical in value – i.e., they lie equidistant from the central slip plane – and the geometry and loading considered here are symmetric about the x -axis.

The surface profile of the potential energy can assume several different shapes, with features depending to some extent on the nature of the critical point at $(\Delta_1, \Delta_2) = (b/2, b/2)$: there may exist a peak (that is, a relative maximum), a trough (that is, a relative minimum), or a saddle point. The parameters A , B , and C dictate which one of these classes the energy surface falls into. The type of profile can be determined by considering the second partial derivatives of Eq. 4 with respect to Δ_1 and Δ_2 (again, with Δ_3 identified with Δ_1) at the critical point, along with the determinant of the Hessian operator (the so-called “second derivative test”) [11].

Dislocation Formation

Fig. 3a shows the energy contour for the case of $A = 1.0$, $B = 0.5$, and $C = 0.1$. For this parameter set, the energy surface shows no relative minima, except for cases where the lattice has undergone one full lattice translation vector (that is, at the corners of the plot). In this situation *full* dislocation formation is favored. Additionally, the lowest energy path from $(0,0)$ to the next point of zero excess energy is along the “ Δ_2 edge,” indicating that slip-like displacement will be concentrated on the 2nd (middle) slip plane, consistent with the formation of a single, or planar, dislocation. Moreover, the 2nd derivative test is consistent with a saddle point at the critical point $(b/2, b/2)$. Thus, it would be unlikely for the atomic planes to displace, even locally, into a metastable state in the range $0 < \Delta_i < b$.

Fig. 4a shows the displacement results from the multi-plane model for the three main combinations of slip plane motion, plotting the displacement along each slip plane, along the y -axis, against the distance from the crack tip in units of Burgers vectors, along the x -axis. As expected, most of the displacement occurs on the middle slip plane (#2). Minimal slip does occur on slip planes 1 and 3 as well, since the slip planes are not artificially held stationary and are allowed to react to activity occurring on neighboring planes. Additionally the maximum amount of slip, which occurs right at the crack tip, is about $b/2$, and quickly decreases away from the crack tip, which is in agreement with the Rice/Beltz model [5] for dislocation nucleation. The displacements shown are the amounts of slip on each slip plane just prior to dislocation emission.

In addition to predicting the deformation mechanism that occurs when the lattice is under applied shear stress, the multi-plane model isolates the threshold for instability in terms of $\mathcal{G}/\gamma_{us}$, where $\mathcal{G}$ is the energy release rate [given by $(1 - \nu)K_{II}^2 / 2\mu$] and γ_{us} is the unstable stacking energy

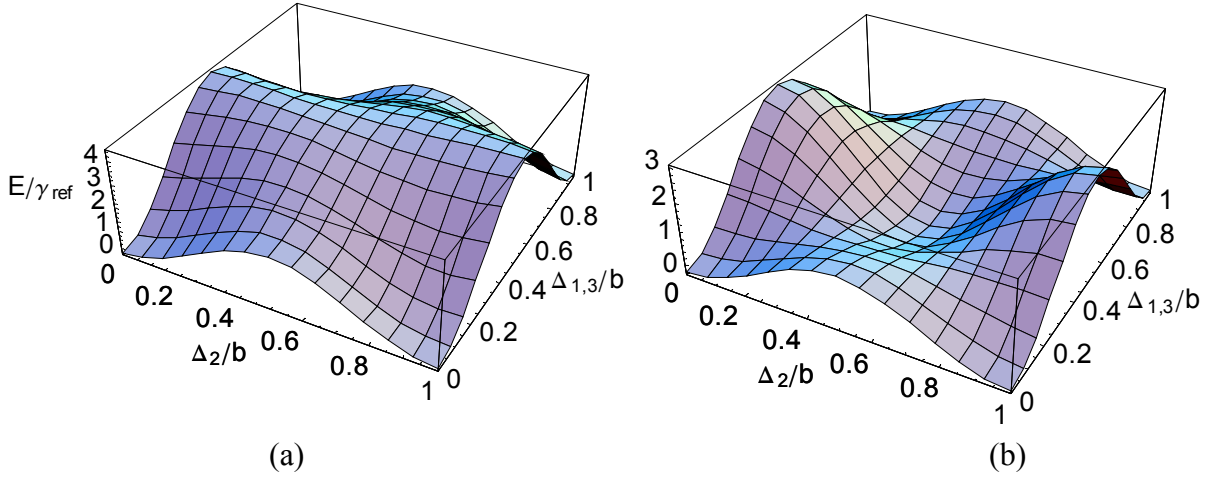


Figure 3. Multi-plane interplanar potentials characteristic of (a) full dislocation formation ($A=1.0$, $B=0.5$, $C=0.1$) and (b) twinning ($A=-0.7$, $B=0.5$, $C=0.6$). The curves represent the local excess energy due to slipping one, two, or three parallel slip planes in any combination with the constraint that the slip on planes #1 and #3 are identical (consistent with the symmetry considered in this paper). Here, b denotes the magnitude of a *full* Burgers vector, $\sqrt{3}a/2$, where a is the lattice constant.

discussed earlier. The model starts with an initial G/γ_{us} , finds a solution to the integral equations, then increases G/γ_{us} and repeats the solution procedure. Here, the system becomes unstable at $(G/\gamma_{us})_{max} \approx 1.05$, which may be thought of as the *effective* unstable stacking energy of single dislocation formation for the multi-plane slip model. As expected, this is very close to the expected result $G = \gamma_{us}$ for dislocation nucleation in the single-plane version of the model as developed by Rice and Beltz [5].

Microtwin Formation

Multi-plane slip is favored when an unstable minimum exists in the potential energy surface of the constitutive law. To illustrate this, we consider the parameter set $A = -0.7$, $B = 0.5$, and $C = 0.6$. A stacking fault forms when the slips on the three adjacent slip planes settle into a state of metastable equilibrium associated with the minimum depicted in Fig. 3b, with *partial* Burgers vectors.

In contrast with the case of dislocation formation presented in the previous section, here C has increased, from $C = 0.1$ to $C = 0.6$; B remains the same, and A is decreased significantly. Comparing Figs. 3a with 3b, it can be seen that multi-plane slip is associated with a lesser energy barrier than single plane slip. The displacement profile results for this case are shown in Fig. 4b, indicating the formation of a stacking fault. Slip plane 2 (midplane) still experiences the most slip, since it is located in line with the crack. However, the adjacent slip planes 1 and 3 also experience significant slip. As with the previous case, the displacement decays quickly, and within a few Burgers vector lengths from the crack tip, the material is essentially unaffected by the presence of the newly formed stacking fault.

As seen from the energy profile, the displacements of the three-slip plane prior to instability are less than the value $b/2$ that was seen for the single dislocation case, further indicating the formation of a stacking fault. The potential well sits directly in the center of the energy profile of Fig. 3b. Though the true displacement profile does not take place along either of these idealized paths, but rather some combination of multi-plane slip, they are good guides for visualizing the deformation, and the point of instability should occur near these points. Indeed, the results show the maximum displacement of slip plane 2 to be around $0.32b$, which correlates to the point of

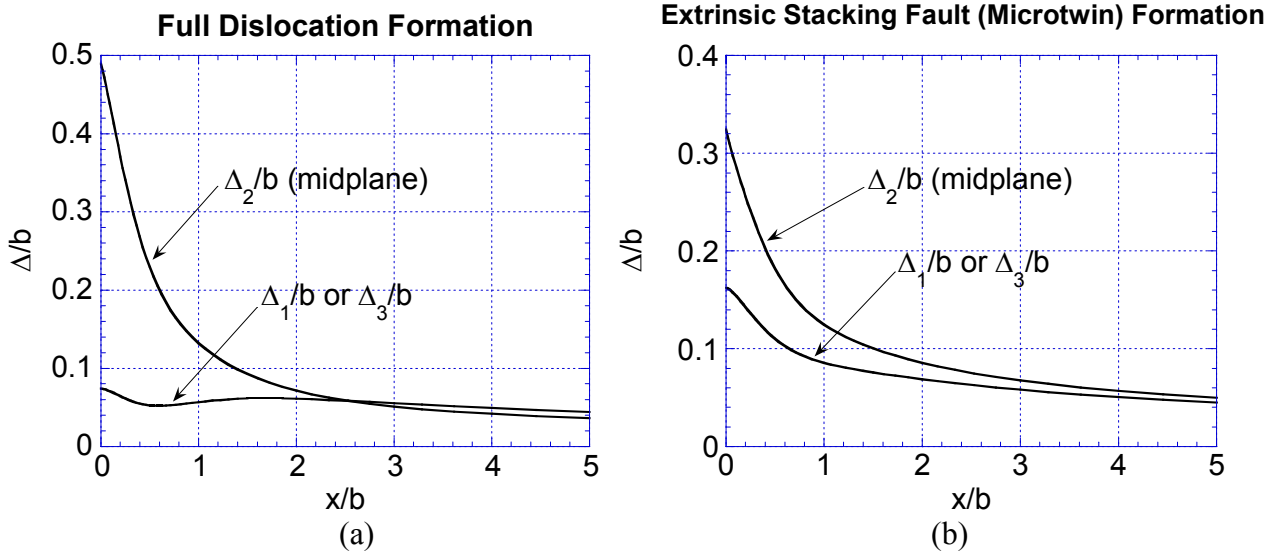


Figure 4. Profiles of relative atomic displacement on three parallel slip planes obtained from the numerical solution of Eq. 1 with the interplanar potentials given by Eq. 4. Twinning is characterized by non-negligible shear displacement accumulating on multiple, parallel planes, consistent with the system reaching an energy state in the interior of the plot given in Fig. 3b. Here, b denotes the magnitude of a *full* Burgers vector, $\sqrt{3}a/2$, where a is the lattice constant.

instability, or the top of the potential energy “hill” before the displacement falls into the potential well, thus forming a stacking fault.

The onset of instability occurs at $G/\gamma_{us} \approx 0.6$, a modestly *lower* value than for the dislocation emission considered in the previous section, consistent with the system avoiding the energy barrier associated with single plane slip.

Conclusion

The unique characteristic of the multi-plane slip model is the ability for multiple slip planes to operate, allowing for the possibility of deformation features other than the oft-modelled single dislocation emission. Given the appropriate set of parameters for the multi-plane energy potential, the lattice response of the model results in slip occurring along multiple planes, which can lead to stacking fault formation, and ultimately, twinning.

The model produces clear distinction between stacking fault formation and full dislocation formation. The case of single dislocation emission produces realistic displacement results, with displacement occurring on all three slip planes. The majority of the slip occurs on the middle, central slip plane as expected, but the other two slip planes also experience some slip, although of a magnitude less than that on the central slip plane. This is interesting to note, since it demonstrates the mobility that is allowed and always present in the system; the secondary slip planes are not “locked” and do experience some small deformation in response to the large displacement occurring on the central slip plane.

The situations in which stacking fault formation arises differ in that significant slip occurs on all three planes, and is distributed along all three planes, though it is not necessary for the slip to be equal on all three planes. The symmetry of the system requires that the slip planes above and below the crack plane experience equal but opposite amount of displacement, and this is observed in the results of the model.

This model is currently limited to an idealized case of mode II loading of a crack tip that is coplanar with the slip planes. Further expansions for the model should include a consideration of inclined slip planes, mixed mode loading effects, and perhaps most importantly, a more robust family of slip plane constitutive laws that can be fit to the behavior of real crystals.

Acknowledgements

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