Ab initio continuum model for the influence of local stress on cross-slip of screw dislocations in fcc metals

Benjamín R. Ramírez,[1,*] Nasr Ghoniem,[2] and Giacomo Po[2]

[1]*Department of Nuclear Engineering, University of Tennessee, Knoxville, Tennessee 37996, USA*

[2]*Department of Mechanical and Aerospace Engineering, University of California, Los Angeles, California 90095, USA*

(Received 14 May 2012; published 26 September 2012)

We develop a model of cross-slip in face-centered cubic (fcc) metals based on an extension of the Peierls-Nabarro representation of the dislocation core. The dissociated core is described by a group of parametric fractional Volterra dislocations, subject to their mutual elastic interaction and a lattice-restoring force. The elastic interaction between them is computed from a nonsingular expression, while the lattice force is derived from the γ surface obtained directly from *ab initio* calculations. Using a network-based formulation of dislocation dynamics, the dislocation core structure is not restricted to be planar, and the activation energy is determined for a path where the core has three-dimensional equilibrium configurations. We show that the activation energy for cross-slip in Cu is 1.9 eV when the core is represented by only two Shockley partials, while this value converges to 1.43 eV when the core is distributed over a bundle of 20 Volterra partial fractional dislocations. The results of the model compare favorably with the experimental value of 1.15 ± 0.37 eV [J. Bonneville and B. Escaig, Acta Metall. **27**, 1477 (1979)]. We also show that the cross-slip activation energy decreases significantly when the core is in a particular local stress field. Results are given for a representative uniform "Escaig" stress and for the nonuniform stress field at the head of a dislocation pileup. A local homogeneous stress field is found to result in a significant reduction of the cross-slip energy. Additionally, for a nonhomogeneous stress field at the head of a five-dislocation pileup compressed against a Lomer-Cottrell junction, the cross-slip energy is found to decrease to 0.62 eV. The relatively low values of the activation energy in local stress fields predicted by the proposed model suggest that cross-slip events are energetically more favorable in strained fcc crystals.

DOI: 10.1103/PhysRevB.86.094115 PACS number(s): 61.72.Ff, 61.72.Hh, 61.72.Lk, 61.72.−y

I. INTRODUCTION

Cross-slip is the process by which a screw dislocation crosses from its primary glide plane to a conjugate plane. It is recognized as one of the most significant mechanisms controlling the evolution of the dislocation microstructure. The process is thus critical to fundamental macroscopic plastic deformation phenomena, such as work hardening, fatigue, and creep.[1] For example, cross-slip is known to be responsible for controlling the rate of dynamic recovery during stage-III plastic deformation in fcc metals.[2,3]

Cross-slip is a thermally activated process, and its rate is influenced by the local stress field. Nevertheless, determination of the activation energy as a function of the stress state is still an open subject in dislocation mechanics. In fcc metals, the situation is complicated by the dissociated character of dislocations, which raises the question of whether and how Shockley partials recombine into an energetically unfavorable "constricted" configuration before they disassociate again on the conjugate plane. Because of its primary importance in plasticity, cross-slip has been the subject of several modeling approaches. In particular, attempts to quantify the activation energy of cross-slip in fcc metals have proceeded along two distinct paths. The first is based on the continuum elasticity theory of dislocations,[4–6] while the second focuses on atomistics, and relies on molecular statics (MS) or molecular dynamics (MD) simulations.[7–9]

Among the early continuum models of cross-slip in fcc metals, two different mechanisms were proposed by Fleischer[10] and Friedel-Escaig,[4] respectively. According to Fleischer's mechanism, cross-slip can take place without the requirement that the stacking-fault (SF) ribbon develops in a constricted configuration. Fleischer assumed that the SF ribbon could simply fold over the intersection line between primary and conjugate planes. Although this mechanism is based on a simple energetic analysis, a more detailed version (in the anisotropic framework[11]) showed that the creation of a stair-rod dislocation, which is a by-product of the process, was far more energetically expensive than the recombination of the two partials. On the other hand, the Friedel-Escaig model (developed by Escaig[4] following Friedel's idea of cross-slip[12] and expanding on the work of Stroh[13]) involves the constriction of the Shockley partials on the original glide plane, followed by redissociation on the cross-slip plane (cf. Fig. 1). In this model, the interaction among dislocations is approximated by line tension theory, and the dislocation geometry is described by circular segments, the radius of curvature of which is assumed to be very large compared to the separation between partials. Although this model results in a convenient analytical expression for the cross-slip activation energy in the limits of low and high stresses, its approximated nature introduces uncertainties in the calculation of the activation energy.

Subsequent elasticity-based models attempted to address the approximations of the original Friedel-Escaig model. The model of Duesbery[5] introduced a three-dimensional (3D) description of dislocations which improved the accuracy in the calculation of stress field and elastic energy. However, the model presents uncertainties associated not only with the size of the dislocation core (a cutoff radius was used in all calculations), but also with the recombination distance of the partials, especially for materials with narrow stacking-fault ribbon, such as Cu. Additionally, the cross-slip energy for Cu at zero stress predicted by the model is too large (3.7 eV) compared with the measured value of 1.15 ± 0.37 eV.[14,15]

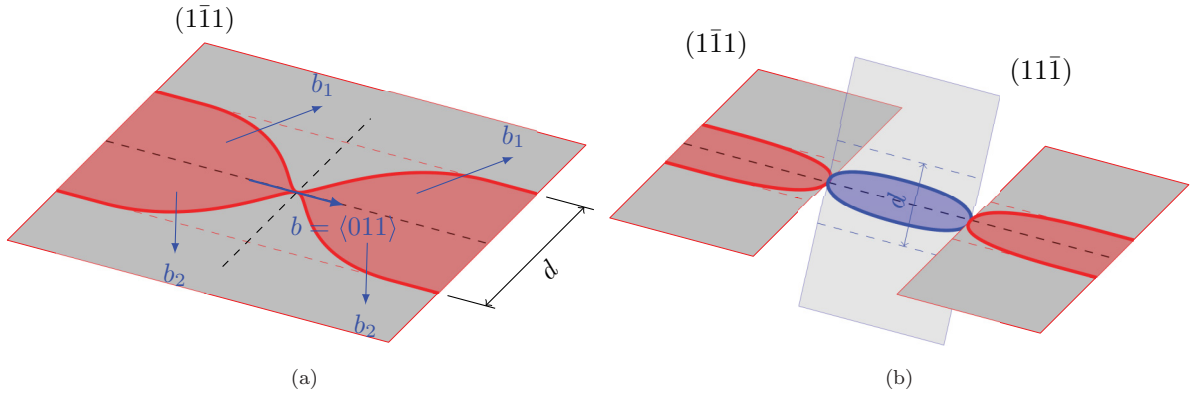


FIG. 1. (Color online) The cross-slip mechanism according to the Friedel-Escaig mode. (a) The configuration stacking-fault (SF) ribbon in the $(1\bar{1}1)$ primary plane (red area) is pinched to a point from its original equilibrium width d. (b) Cross-slip configuration with the stacking fault expanding in the $(11\bar{1})$ conjugate plane (blue area).

Other methods have tried to address the issue of the recombination energy by coupling the elasticity framework with atomistic parameters. The Püschel model[16,17] explicitly includes the dislocation core energy in the sense that the cutoff radius and the recombination distance are obtained from a one-dimensional (1D) Peierls-Nabarro model. Even though this model gives more accurate results for the cross-slip energy (1.43 for Cu), it still has uncertainties due to the geometric discontinuity (straight dislocation segments), and the geometric limitation of linear segments to represent simple core configurations.

Atomistic simulations carried out in order to calculate the cross-slip activation energy were based on either finding the cross-slip energy path (Rasmussen[8]), or on parametrizing the movement of the partials (Rao[7]). Rasmussen's model, which used the nudged elastic band (NEB) method to determine the cross-slip path, discovered several characteristics of the cross-slip process. In particular, it was shown that no instantaneous redissociation on the conjugate plane takes place after a segment of the stacking-fault ribbon is constricted in the primary plane. The model also pointed out the configurational asymmetry between the edgelike and the screwlike constrictions that delimit the cross-slipped portion of a dislocation. Nevertheless, the cross-slip energy predicted by this model (2.7 eV for Cu) is significantly higher than elasticity-based models and experimental measurements. Rao and co-workers[18] recently reexamined these results, and proposed a mechanism by which cross-slip rates are enhanced. In the mechanism proposed by Rao *et al*., a screw dislocation was found to spontaneously attain a low-energy cross-slipped configuration upon intersecting a forest dislocation. The activation energy calculated with MD simulations indicated that the activation energy is a factor of 2–5 lower than that for cross-slip in isolation via the Escaig process. The MS simulations of Rao *et al*. (Rao[7]) showed that constrictions take place over 4–6 lattice planes, and that in the center of the critical configuration, the constriction is nearly equally spread over both the primary and conjugate glide planes. The results given by this model for Cu (1.07–1.28 eV) and Ni (2.35 eV) are in reasonable agreement with the values obtained from experimental measurements.[14]

Although both continuum and atomistic approaches proved effective in revealing many significant features of cross-slip, each one suffers from intrinsic limitations. The continuum approach has been plagued by the somehow arbitrary quantification of the dislocation core energy, which is a direct consequence of the singular field associated with the displacement discontinuity in classical dislocation theory.[19] Moreover, the 3D geometry of curved dislocations has been described approximately by a series of straight segments, which results in additional uncertainties related to the accuracy of the stress field at the connections between straight segments.[20] On the other hand, atomistic simulations of cross-slip have a limited scope as a result of the empirical nature of the interatomic potential, the difficulty of generating complex 3D configurations, and the restricted size of the system imposed by computational constraints. In this fashion, the influence of chemistry (impurities or solute atoms) can not be reliably studied with MS or MD. Moreover, interactions between the dislocation core during cross-slip and nearby microstructures (e.g., pileups, precipitates, grain boundaries, etc.) is not possible with atomistic simulations at the present time.

The objective of this work is to study the energetics of cross-slip of screw dislocations in fcc metals in a general local stress environment, such as the environment at the head of a dislocation pileup. The goal is to enable simulations of screw dislocation cross-slip in an evolving and complex dislocation microstructure. To meet this objective, we further develop here the planar dislocation core model of Banerjee, Ghoniem, Lu, and Kioussis (BGLK).[21] This method is essentially a two-dimensional (2D) parametrization of the original Peierls-Nabarro (PN) model, where the dislocation core is represented by a group of Volterra fractional dislocations. In this study, we consider the full 3D configuration of the dislocation core that develops during cross-slip in fcc metals. To this end, we utilize a fundamental reformulation of the parametric dislocation dynamics method, where we describe dislocation networks on the basis of abstract graph theory.[22] Moreover, for each of the fractional dislocations composing the spread core, we further improve the accuracy of energy calculations by utilizing the nonsingular continuum formulation developed by Cai *et al*.[23]

This application removes the uncertainty associated with the size of the dislocation core of fractional dislocations. The lattice-restoring force exerted on the fractional dislocations is determined from directional derivatives of the γ surface,[24] which is computed directly from *ab initio* methods.

In Sec. II, we first describe an extension of the BGLK model to nonplanar dislocation cores, the nonsingular fields of fractional dislocations composing the core, and the equilibrium configurations of fractional dislocations with the network dislocation dynamics method. This is followed in Sec. III by a presentation of results of the model for cross-slip energy and dislocation configurations in copper that show good agreement with experimental measurements. We also show an application of the model to calculations of cross-slip at the head of a dislocation pileup, with the implication that the cross-slip energy is significantly reduced for the head dislocation in a pileup. Finally, conclusions and possible future directions are discussed in Sec. IV.

II. MODEL FORMULATION

Current elasticity models for determination of the cross-slip energy are deficient in a number of ways: (a) they suffer from arbitrariness in the representation of the dislocation core, often using an *ad hoc* cutoff radius to avoid singularities, (b) they fail to accurately describe the lattice-restoring force affecting both elastic and stacking-fault energy, (c) they neglect the long-range contribution to the self-energy (e.g., using the line tension approximation), and crudely approximate dislocation interactions by discretizing dislocations with piecewise linear segments. The model presented here removes these limitations: (1) we apply a nonsingular PN framework for the elastic field of fractional dislocations, (2) we use a lattice-restoring force computed directly from *ab initio* methods, and (3) we take advantage of a network-based implementation of dislocation dynamics that guarantees continuity of the tangent vector of dislocation lines, even in the presence of topologically complex configurations. These concepts are now described in detail.

A. Extension of the PN framework to nonplanar dislocation cores

Following the BGLK model, the core of the original screw dislocation is discretized in a set of parametric fractional dislocations (PFDs). Thus, the displacement discontinuity across the original dislocation core is replaced with a stepwise distribution, the configuration of which will be determined from equilibrium. In fcc metals, the original $a/2\langle 011\rangle$ screw dislocation on the $(1\bar{1}1)$ is dissociated in Shockley partials with Burgers vector $\boldsymbol{b}_1 = a/6\langle 121\rangle$ and $\boldsymbol{b}_2 = a/6\langle \bar{1}12\rangle$, respectively. Therefore, letting $2n$ be the total number of PFDs, n of them are assigned a slip vector $\boldsymbol{b}_1/n$, while the remaining n have slip vector $\boldsymbol{b}_2/n$. As $n \to \infty$, a continuously distributed core is achieved. However, in the present numerical implementation, each fractional dislocation has a small displacement discontinuity that becomes infinitesimally small as $n \to \infty$.

The overall configuration of PFDs is illustrated in Fig. 2, where each line for a fractional dislocation can be regarded as a contour line of equal displacement vector, in increments of $\boldsymbol{b}_1/n$ for n PFDs, and $\boldsymbol{b}_2/n$ for the other half. In the initial relaxed configuration, the density ρ of PFDs per unit length normal to their line direction exhibits a double-peaked shape, with each peak centered around the location of a what is known as a Shockley partial. Conceptually, Shockley partials can be regarded as a two-delta function approximation to the original dislocation density (displacement gradient) within the core of a screw dislocation. Our representation spreads the two original Shockley delta functions to a "bundle" of PFDs that can be regarded as an equivalent n-delta function representation of the distributed core. As $n \to \infty$, the n-delta function representation yields the smoothly distributed core.

In our model of cross-slip, we imagine that the inner pair of the PFD bundle is allowed to recombine, and separate again on the conjugate $(11\bar{1})$ slip plane with their respective Burgers vectors $a/6\langle 112\rangle$ and $a/6\langle \bar{1}21\rangle$. This event locally relaxes the bundle on the primary plane and promotes cross-slip of subsequent pairs of PFDs until the bundle completely migrates to the conjugate plane. In the process, the original inner PFD pair becomes the outer pair delimiting the stacking-fault region

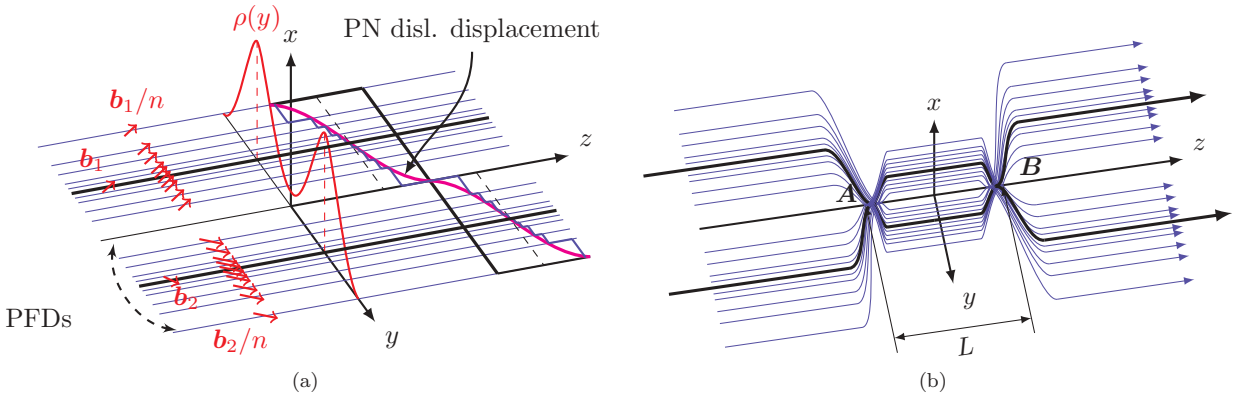


FIG. 2. (Color online) The PN model of cross-slip in fcc metals. (a) Equilibrium distribution of the bundle of parametric fractional dislocations (PFDs) composing the core of the screw dislocation, where each Shockley partial is divided in n PFDs. The density $\rho(y)$ of PFDs is a double-peaked distribution. The discretized displacement profile across the core is compared to the PN profile and to the Volterrra profile. (b) PFD configuration during cross-slip. Corresponding pairs of PDFs recombine on the cross-slip line and dissociate again in the conjugate plane. The outermost constriction points are A and B and the distance between them is L.

in the conjugate plane. We note that in this process, a series of constriction points are formed on the cross-slip line, the outermost of which are labeled A and B in Fig. 2(b). Despite the apparent overall symmetry, A and B are in locally different configurations. PFDs on the primary plane converging at A have edgelike character, while those departing from it on the conjugate plane have screwlike character. The opposite situation is encountered at B. This asymmetry, which is captured by atomistic simulations[7,8] and not by elasticity models based on the line tension approximation,[4] is present in our results.

Equilibrium configurations of the system can be considered for different values of the distance L between the constriction points A and B. In each of these equilibrium configurations, PFDs interact through their mutual elastic field, and are subject to a lattice-restoring stress arising from the presence of the stacking fault. The elastic energy of the dislocation system is determined by calculating the mutual interaction energy between all PFDs. Including the interaction of each line with itself, this procedure naturally includes the self-energy without any local approximations (i.e., the line tension approximation). Ideally, the interaction energy between two dislocations can be calculated as a double line integral using Blin's formula.[25] However, the determination of the dislocation self-energy using Blin's formula is known to diverge as a result of idealizing the dislocation as a line with a displacement jump condition. The issue of the singularity in the elastic solution of the stress field and energy of the Volterra dislocation is avoided by considering a "finite cross section" for the dislocation line.[26] Applying this concept to each PFD, and utilizing the analytical expression derived by Cai *et al.*,[23] the nonsingular elastic energy of the system becomes

$$\begin{aligned} E_I^{ns} = -\frac{\mu}{4\pi}\oint_C\oint_{C'}\Bigg\{&\frac{(\boldsymbol{b}'\cdot d\boldsymbol{l}')(\boldsymbol{b}\cdot d\boldsymbol{l})}{R_a}\left(1+\frac{1}{2}\left(\frac{a}{R_a}\right)^2\right)\\ &+\frac{2}{m-1}\left(1+\frac{1}{2}\left(\frac{a}{R_a}\right)^2\right)\frac{(\boldsymbol{b}\cdot d\boldsymbol{l}')(\boldsymbol{b}'\cdot d\boldsymbol{l})}{R_a}\\ &-\frac{m}{m-1}\left[\boldsymbol{b}\cdot\boldsymbol{b}'\left(1+\left(\frac{a}{R_a}\right)^2\right)\right.\\ &\left.+\frac{(\boldsymbol{R}\cdot\boldsymbol{b})(\boldsymbol{R}\cdot\boldsymbol{b}')}{R_a^2}\right]\frac{d\boldsymbol{l}d\boldsymbol{l}'}{R_a}\Bigg\}, \end{aligned} \tag{1}$$

where $\boldsymbol{R}=\boldsymbol{x}-\boldsymbol{x}'$, $R=|\boldsymbol{R}|$, and, for an isotropic distribution of the core, $R_a^2=R^2+a^2$. The choice of the core spreading parameter a is particularly important when a small number of PFDs are used, and this aspect will be discussed further in Sec. II B.

B. Nonsingular description of Volterra fractional core dislocations

The treatment of the dislocation elastic energy and stress field according to the nonsingular framework requires the value of the dislocation core a, which can not be derived from continuum theory. De Wit[26] suggested using the Peierl's model to determine the distribution of infinitesimal dislocations. An attempt to obtain a from atomic considerations was developed by Schoeck,[27] who proposed obtaining a by comparing the nonsingular dislocation energy with one obtained from an atomistic treatment. The original Peierls-Nabarro[28] model is a convenient way to describe the dislocation core structure due to the planar character of the atomic misfit in crystalline solids.

Following Schoeck's model, the energy of a dislocation E^P is the sum of the elastic energy E_{el} (of the two half-spaces) and the misfit energy E_A (interplanar misfit). Furthermore, the equilibrium arrangement of the dislocation core can be obtained by minimizing the total energy ($E^P=E_{el}^P+E_A$) with respect to a suitable adjustable geometrical parameter which describes the configuration. It has been shown by Schoeck[29] that in equilibrium when the two half-spaces are assumed to be linear elastic, the atomic misfit energy E_A is equal to the prelogarithmic elastic line energy factor. So, using this result, the line energy of a single straight dislocation of orientation φ (i.e., with screw and edge components $p=b\cos\varphi$ and $q=b\sin\varphi$, respectively) for an isotropic material at equilibrium, is found to be[27]

$$\begin{aligned} E^P &= \hat{E}_L(\varphi)\left(\ln\left[\frac{R}{2\bar{w}(\varphi)}\right]+1\right),\\ \hat{E}_L(\varphi) &= \frac{\mu}{4\pi}b^2\left(\frac{1}{1-\nu}(\sin\varphi)^2+(\cos\varphi)^2\right), \end{aligned} \tag{2}$$

where E_L is the prelogarithmic elastic line energy factor, $\bar{w}$ is the average between the edge and screw components for the width. An estimate of the dislocation core width can be obtained when a 1D γ surface is constructed by parametrizing it with the shear modulus μ and the unstable stacking fault (γ_u). So, the width w of a single dislocation in an isotropic medium would then be

$$\frac{w(\varphi)}{b}=\frac{\cos^2\varphi+\sin^2\varphi/(1-\nu)}{b/c+2\pi^2\gamma_u/(\mu b)}, \tag{3}$$

where c is the interplanar spacing between glide planes. Thus, a unique value for the core width (a_S and a_E) can be obtained by requesting that the energy from the continuum model [Eq. (1)] to agree with E^P at equilibrium. Then, by comparing these results, the following values for the dislocation core width are obtained:

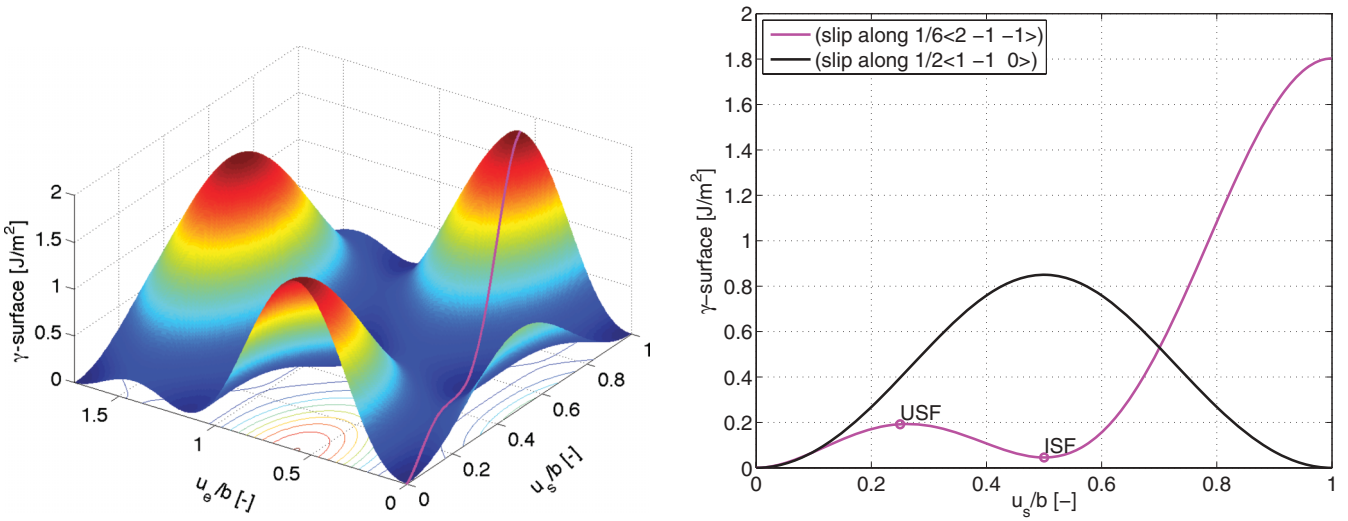
$$\begin{aligned} a_S &= \frac{2}{\sqrt{e}}\left(\frac{b}{b/c+2\pi^2\gamma_u/(\mu b)}\right),\\ a_E &= \frac{2}{e}\left(\frac{b/(1-\nu)}{b/c+2\pi^2\gamma_u/(\mu b)}\right), \end{aligned} \tag{4}$$

where e is the base of the natural logarithms. An averaged value for a can be approximated as

$$a\approx\frac{2}{e}\left(\frac{b}{b/c+2\pi^2\gamma_u/(\mu b)}\right). \tag{5}$$

C. *Ab initio* determination of the crystal lattice slip-resistance force

In the presence of partial dislocations, the total energy of the system includes a contribution due to the existence of the stacking-fault ribbon bounded by pairs of partial dislocations. The variation in stacking-fault energy associated with a change of width of the ribbon, on either primary or conjugate plane, gives rise to a configurational force on partial dislocations on that plane. The stacking-fault energy and the corresponding lattice force can not be determined from continuum elasticity



(a) (b)

FIG. 3. (Color online) (a) The generalized stacking-fault energy (GSFE), or γ surface on the $(1\bar{1}1)$ plane of Cu, plotted vs displacement components $u_e^* = u_e/b$ and $u_s^* = u_s/b$, in the edge direction $\langle 21\bar{1}\rangle$ and screw direction $\langle 011\rangle$, respectively. The magenta line represents the energy profile along the direction of the Shockley partial $1/6\langle 121\rangle$. (b) Comparison of the GSFE profile of a screw dislocation and a Shockley partial dislocation when projected on the $u_e^* = 0$ plane. The unstable stacking-fault (USF) energy and intrinsic stacking-fault (ISF) energy are marked.

considerations. In our model, they are computed using the concept of generalized stacking-fault energy (GSFE), or γ surface.[24] A process to construct the γ surface has been developed by Schoeck[30] and more recently by Xiao-Zhi *et al.*[31] First, the lattice parameter a of the material is calculated by minimizing the energy of its unit cell. Then, the γ surface is determined as a function of the relative coordinates $u_e^* = u_e/b$ and $u_s^* = u_s/b$, representing components of displacement imposed to a unit cell, in the edge direction $\langle 21\bar{1}\rangle$ and screw direction $\langle 011\rangle$, respectively. The γ surface has translational periodicity equal to $\sqrt{3}$ in the u_e^* coordinate, and equal to 1 in the u_s^* coordinate. Taking advantage this periodicity, the γ surface can be parametrized as

$$\begin{aligned}\frac{\gamma(u_s^*,u_e^*)}{c_{111}b} = {} & c_0 + c_1\cos(4\pi u_s) + c_2\left[\cos\left(\frac{2\pi u_e^*}{\sqrt{3}} + 2\pi u_s^*\right)\right. \\ & \left. + \cos\left(\frac{2\pi u_e^*}{\sqrt{3}} - 2\pi u_s^*\right)\right] + c_3\cos\left(\frac{4\pi u_e^*}{\sqrt{3}}\right) \\ & + c_4\cos\left(\frac{8\pi u_e^*}{\sqrt{3}}\right) + a_1\left[\sin\left(\frac{2\pi u_e^*}{\sqrt{3}} + 2\pi u_s^*\right)\right. \\ & \left. + \sin\left(\frac{2\pi u_e^*}{\sqrt{3}} - 2\pi u_s^*\right)\right] + a_2\sin\left(\frac{4\pi u_e^*}{\sqrt{3}}\right),\end{aligned} \tag{6}$$

where the coefficients c_0, c_1, c_2, c_3, c_4, a_1, and a_2 are found by fitting Eq. (6) with data obtained from *ab initio* calculations. Of particular interest during the fitting process are the values γ_u of the unstable stacking-fault (USF) energy and the value γ_i of the intrinsic stacking-fault (ISF) energy. These two values correspond to the local maximum and local minimum encountered along the direction of the Shockley partial $1/6\langle 2\bar{1}\bar{1}\rangle$ at $\boldsymbol{u}^* = (1/4, \sqrt{3}/12)$ and $\boldsymbol{u}^* = (1/2, \sqrt{3}/6)$, respectively. In this work, the γ surfaces for Cu and Ni were constructed using the VASP code.[32–35] The characteristic values γ_u and γ_i, were found to be 182 and 42 mJ/m^2 for Cu, while these values for Ni were determined to be 270.5 and 138.3 mJ/m^2, respectively. The γ surface for Cu is plotted in Fig. 3(a), where the energy curve corresponding to the direction of the Shockley partial is highlighted. In Fig. 3(b), this curve is projected on the plane $u_e^* = 0$ for comparison of the energy profile of a pure screw dislocation.

Once the γ surface is determined, the lattice-restoring force on a dislocation can be obtained from derivative of γ along the direction of the slip vector of that dislocation. In particular, if a Shockley partial having slip vector $\boldsymbol{s}$ ($|\boldsymbol{s}| = b/\sqrt{3}$) is discretized by n PFDs, the lattice force per unit line on the ith PFD becomes

$$f_i^L = -\frac{1}{b}\left.\frac{\partial\gamma}{\partial\boldsymbol{u}^*}\right|_{\frac{is}{nb}} \cdot \frac{\boldsymbol{s}}{n}. \tag{7}$$

We remark that this force acts in the glide plane of the dislocation line and normal to the dislocation tangent vector.

D. Determination of equilibrium states by network dislocation dynamics

We study the total energy of the dislocation system (elastic plus stacking fault) for different values of the cross-slip length L. For each value of L, the energy is computed in the *equilibrium* configuration, i.e., when dislocations stop moving and the system becomes stationary. Dislocation dynamics (DD) is used to study dislocation motion and reach equilibrium configurations. The configuration of the dislocation core during cross-slip, illustrated in Fig. 2(b), suggests that the concept of planar dislocation lines with constant Burgers vector should be abandoned when formulating the DD framework. On the cross-slip line, for example, not only

PFDs give rise to a 3D configuration by changing their glide plane, but also their Burgers vector changes (yet in a way that their sum is constant). In order to represent this complex geometric and topological structure, we adopt a network-based implementation of dislocation dynamics. The present model is based on a recent formulation of constrained network parametric dislocation dynamics (CN-PDD).[22] In this framework, a dislocation network $\mathcal{N}$ is represented by a collection of vertices (dislocation nodes) $\{\alpha_i\}$, connected by a set of directional edges (dislocation line segments) $\{(\alpha_i,\alpha_j)\}$, each carrying a vectorial flow quantity (Burgers vector).

Based on thermodynamic considerations, it can be shown that the equation of motion of an arbitrary dislocation network can be cast in the following weak form:

$$\sum_{(\alpha_i,\alpha_j)\in\mathcal{N}} \int_{\alpha_i}^{\alpha_j} (\boldsymbol{B}\boldsymbol{v} - \boldsymbol{f})\cdot\delta\boldsymbol{v}\, dl = 0, \tag{8}$$

where $\boldsymbol{B}$ is a positive-definite tensor of dislocation mobility, $\boldsymbol{v}$ is the velocity vector along the dislocation line, and $\boldsymbol{f}$ is the force per unit line of dislocation. When lattice friction is taken into account, the total force per unit line of dislocation can be expressed as $\boldsymbol{f} = \boldsymbol{f}^E + \boldsymbol{f}^L$, where $\boldsymbol{f}^E$ is the Peach-Koehler force induced by the total elastic stress field, and $\boldsymbol{f}^L$ is the lattice-restoring force. If the position of each dislocation edge is prescribed in parametric form as $\boldsymbol{r}(u,t) = \boldsymbol{H}(u)\boldsymbol{q}(t)$, with $\boldsymbol{H}(u)$ being a matrix of shape functions and $\boldsymbol{q}_i(t)$ a vector of nodal degrees of freedom, the velocity vector on each dislocation lines becomes $\boldsymbol{v} = \boldsymbol{H}(u)\dot{\boldsymbol{q}}(t)$ and standard assembling techniques allow us to rewrite Eq. (8) in global form as

$$\boldsymbol{K}\,\dot{\boldsymbol{Q}} = \boldsymbol{F}, \tag{9}$$

where $\boldsymbol{K}$ is the stiffness matrix of the network, $\dot{\boldsymbol{Q}}$ is the global vector of vertex generalized velocities, and $\boldsymbol{F}$ is the global vector of vertex forces. Numerical solution of Eq. (9) yields the nodal generalized velocities, which are used to update the dislocation network configuration at each time step of simulation.

Hermite shape functions and degrees of freedom are typically used in dislocation dynamics. When linear Hermite shape functions are used, the network is discretized in piecewise straight segments and the continuity of tangent vector, Peach-Koehler force, and lattice force at the intersection of segments is violated (as in Ref. 5). The lack of an accurate description of the dislocation core geometry at various stages of cross-slip is improved by describing dislocations with cubic Hermite splines. With this choice, the generalized degrees of freedom of a dislocation segment (α_i,α_j) are

$$\boldsymbol{q} = [\boldsymbol{p}_i\ \boldsymbol{t}_i\ \boldsymbol{p}_j\ \boldsymbol{t}_j]^T, \tag{10}$$

where, in general, $\boldsymbol{p}_k$ and $\boldsymbol{t}_k$ are the position and parametric tangent of the kth vertex in the network, respectively. In order to further reduce the total number of degrees of freedom in the network, the nodal tangents can be enslaved to nodal positions by prescribing a linear relationship between them. In defining this relationship, we take advantage of the network structure and used

$$\boldsymbol{t}_i = \sum_{\alpha_j\in\mathcal{O}_i} \frac{\boldsymbol{p}_j - \boldsymbol{p}_i}{c_{ij}} + \sum_{\alpha_j\in\mathcal{I}_i} \frac{\boldsymbol{p}_i - \boldsymbol{p}_j}{c_{ij}}, \tag{11}$$

where $\mathcal{O}_i$ is the set out-neighborhood of the vertex i (i.e., the set of vertices connected to vertex i by links departing from i), $\mathcal{I}_i$ is the set in-neighborhood of the vertex i (with analogous definition), $c_{ij} = |\boldsymbol{p}_i - \boldsymbol{p}_j|^\alpha$, and α is an appropriate tension parameter. This rule can be seen as a generalization of Catmull-Rom curves, which, for $\alpha = 0.5$, enjoy useful properties such as smoothness and non-self-intersection.[36] During the assembly process, relationship (11) is included in the stiffness matrix of the network, therefore the method presented here allows the description of long curved dislocation segments with a minimal number of degrees of freedom. Moreover, since both position and tangent continuity are guaranteed at each dislocation node, even in the presence of 3D configurations and complex topological connections, dislocation elastic fields can be computed with a high level of accuracy.[20]

III. RESULTS FOR THE INFLUENCE OF DISTRIBUTED DISLOCATION CORES AND THE LOCAL STRESS

We now present results of calculations of the activation energy of cross-slip using the extended Peierls-Nabarro model described above. The formation energy of the system can be expressed as the difference between the total elastic energy and the total stacking-fault energy:

$$E = E^{el} - E^{\mathrm{SF}}. \tag{12}$$

The total stacking-fault energy can be computed approximating the area integral of the γ surface. In particular, splitting the contributions from the primary and conjugate planes, we write

$$E^{\mathrm{SF}} = \int \gamma\, dA \approx \sum_{k=1}^{n} \gamma(\boldsymbol{u}_k^*)\big(A_k^p + A_k^c\big) \tag{13}$$

with n being the number of PFDs composing a Shockley partial, $\boldsymbol{u}_k^* = k\boldsymbol{s}/(nb)$ the coordinate of the slip vector at the kth PFD, and A_k^p and A_k^c the area enclosed between the kth and $(k-1)$th pair of partials in the primary and conjugate planes, respectively. The change in formation energy during the cross-slip process is calculated with respect to the final configuration, illustrated in Fig. 2(b), and the reference configuration of Fig. 2(a). Different final configurations are obtained as equilibrium states of the system for different values of the cross-slip length $L = \overline{AB}$ [Fig. 2(b)]. The change in energy therefore becomes

$$\begin{aligned}\Delta E(L) &= \Delta E^{el} - \Delta E^{\mathrm{SF}} = \Delta E^{el} - \sum_{k=1}^{n} \gamma(\boldsymbol{u}_k^*)\big(\Delta A_k^p + \Delta A_k^c\big)\\ &= \Delta E^{el} + \sum_{k=1}^{n} \gamma(\boldsymbol{u}_k^*)\big(S_k^p - S_k^c\big).\end{aligned} \tag{14}$$

In Eq. (14) we introduced the areas $S_k^p = -\Delta A_k^p$ swept by PFDs on the primary plane and the corresponding areas $S_k^c = \Delta A_k^p$ swept on the conjugate plane. We note that when only two Shockley partials are used, Eq. (14) simplifies to the expression found in Ref. 37:

$$\Delta E = \Delta E^{el} + \gamma_i(S^p - S^c), \tag{15}$$

where γ_i is the intrinsic stacking-fault energy of the material.

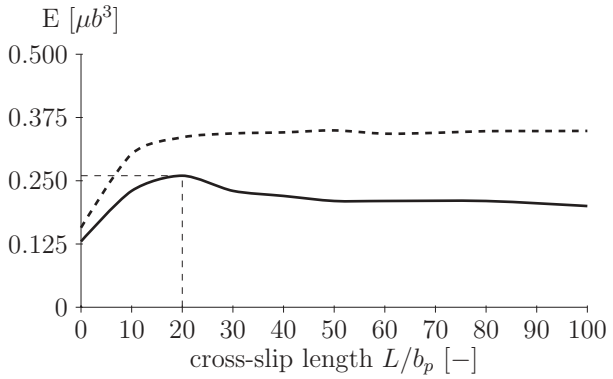


FIG. 4. Comparison of the energy of the unstressed configuration as a function of the relative cross-slip length L/b_p, where $b_p = b/\sqrt{3}$: the dashed line represents the result obtained with only two partials ($n = 1$), while the solid line represents the result for the PN model with 20 fractional dislocations.

Figure 4 shows the energy ΔE as a function of the parameter L for two limiting cases of the model: (a) a simplified case including only two Shockley partials ($n = 1$), corresponding to the compact cross-slip mechanism,[4] and (b) a generalization of the model with 20 PFDs ($n = 10$) participating in the cross-slip process. In either case, the value $\Delta E(0)$ represents the energy of the 2D constricted configuration in the primary plane. As L increases, the energy experiences a rapid increase, which finds its physical origin in the extra energy required to separate the two constriction points and expand the PFDs in the cross-slip plane. However, the mutual interaction between the two constricted regions decays rapidly with L, therefore leading to the plateau observed in the energy curve for sufficiently large L. This dependence of the cross-slip energy on the separation between the two constrictions on the cross-slip plane is well documented and has been observed in other elasticity[4,5] and atomistic models as well[8,9] and Ref. 16. The plateau is reached at $L \approx 45b_p$ and the corresponding energy is $\Delta E = 0.34[\mu b^3] \approx 1.9$ eV. This value, which corresponds to the activation energy computed by the proposed model for $n = 1$, is significantly lower than a value of ≈3.7 eV estimated by Duesbery,[5] 2.7 eV determined by Rasmussen, and close to the range of values calculated by Püschl and Schoeck[16] (see Ref. 17 for a critical review). However, this result is higher than the experimental measurement obtained by Bonneville and Escaig: $\Delta E = 1.15 \pm 0.37$ eV. We also observe that the energy value at the plateau is approximately twice the constriction energy $\Delta E(0)$, therefore suggesting that each of the two 3D constrictions is energetically equivalent to the 2D constriction at $L = 0$.

The improvement in the accuracy of the cross-slip energy of the present model is attributed to two factors: (1) a very accurate representation of the cross-slip configuration with smoothly curved lines, and (2) the utilization of atomistically informed nonsingular elastic fields with less ambiguity on the contribution of Shockley partial cores. However, the value determined here (1.9 eV) is outside the range of experimental observations of Bonneville and Escaig, and indicates that the rate of cross-slip through thermal fluctuations alone will be insignificant.

To address this discrepancy, we investigate here a mechanism in which cross-slip does not take place through the constriction of two Shockley partials on the primary slip plane to an infinitesimally small screw segment, followed by its dissociation into two equivalent Shockley partials on the conjugate plane. An energetically more favorable mechanism is proposed such that cross-slip is a gradual process by which small parts of the dislocation core are sequentially transferred and assembled on the cross-slip plane. A study of this mechanism requires that the dislocation core should have a distributed displacement field on both primary and conjugate planes. To represent such distributed cores, we use bundles of PFDs, as described earlier. Calculations of the dislocation core structure are complex because of the truly 3D nature of PFDs during the cross-slip process. Numerical tests indicated that convergence in core configuration and calculated activation energy are obtained with $n \geqslant 10$ (i.e., 20 PFDs). The energy values obtained from our simulations (cf. Fig. 4) show a constriction energy of $E_0 = 0.125[\mu b^3] = 0.7$ eV, which is lower than what is obtained for $n = 1$, and that the activation energy is slightly more than twice the initial constriction energy. Moreover, it can be observed in Fig. 5 that the dislocation configuration near the two constriction regions is asymmetric, due to an asymmetric rotation of the dislocation lines in order to minimize the energy by lengthening the screw component and shortening the edge component. This aspect was previously observed by Rasmussen[8] using atomistic simulations. In the mechanism described here, the innermost PFD constricts first, then the constricted fractional screw segment dissociates into two partials and those expand on the conjugate slip plane as the outermost PFDs there. The process continues, where the second to the innermost PFD cross-slips to the second outermost on the conjugate plane. This gradual process continues until all PFDs are transferred to the conjugate plane. The energy cost of this gradual process is lower than the traditional two-Shockley partial model because PFDs can quickly separate apart, leading to a corresponding reduction in the overall energy. Thus, cross-slip of a distributed core is energetically more favorable than that of the two-Shockley core with concentrated displacement jumps across the Shockley partial dislocation lines. The

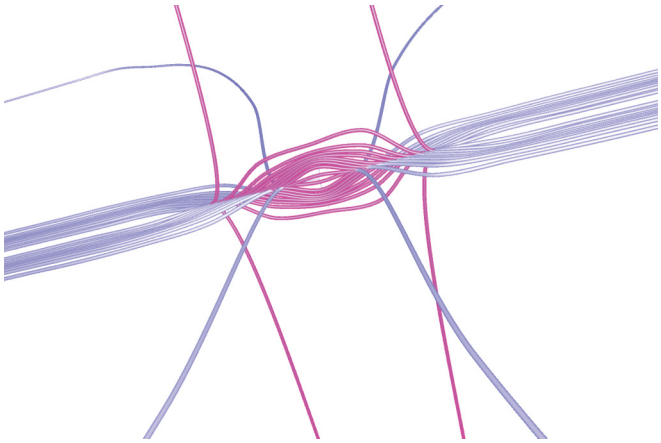


FIG. 5. (Color online) Cross-slip configuration with 20 PFDs corresponding to $L = 5b_p$.

cross-slip activation energy in this case is calculated to be $E_{cs} = 0.256[\mu b^3] = 1.43$ eV for Cu, corresponding to a critical length of 11.5[b]. This value for the activation energy falls between Rasmussen's result (2.7 eV) and Rao's (1.07–1.28 eV) for the unstressed configuration and within the range of experimental measurements obtained by Bonneville and Escaig[14] ($\Delta E = 1.15 \pm 0.37$ eV).

To understand the general discrepancy between cross-slip models and experimental observations, which show a greater ease by which cross-slip takes place, locally favorable stress states have been proposed.[4,7,38,39] Earlier proposals by Seeger[38] invoked unrealistically large dislocation pileups, while a more recent investigation by Rao *et al.*[7] used atomistic simulations to show that cross-slip close to dislocation junctions in Cu requires an activation energy of only 1.28 eV. More recently, Rao *et al.*[18,40] evaluated the cross-slip activation barrier for a screw dislocation when intersecting a forest dislocation in both Ni and Cu. The calculated activation energies for Ni and Cu from the fully cross-slip plane state to the partially cross-slipped state forming a Lomer-Cottrel (LC) junction are found to be 0.68 and 0.67 eV, respectively. The activation energies for cross-slip were found to be a factor of 2–6 lower than the activation energy for cross-slip in Cu estimated by Friedel-Escaig analysis. Escaig *et al.*[14] indicated that the heterogeneity of the cross-slip nucleation process (i.e., it occurs at favorable sites in the crystal) might result in a lower cross-slip energy. This observation is consistent with the idea of introducing jogs (preexisting constriction points) along the dislocation line to lower the energy.[41] In the recent work of Bonneville *et al.*, even lower activation energy was measured.[42] These overall conclusions are also consistent with the work of Rao *et al.*,[7] in which further assistance from a nearby dislocation junction reduces the energy of an activated state.

In order to determine the effects of an applied stress on cross-slip, we recall that Shockley partials have Burgers vector with the same screw components and opposite edge components. It follows that any uniform applied stress acting on the screw components causes the stacking-fault ribbon to translate rigidly, while a stress acting on the edge components compresses or expands the ribbon. Therefore, only τ_e, the resolved shear stress on the dipolar component of the partials (or Escaig stress[4,39]), affects the activation energy of cross-slip. The effect of Escaig stress is equivalent to a contribution $\gamma_e = -b\tau_e u_e^*$ to the γ surface and, according to Eq. (7), results in an additional force $f_e = \pm b\tau_e/(2n\sqrt{3})$ on each pair of PFDs. The case that most favors cross-slip is achieved when the applied load increases the width of the ribbon in the cross-slip plane while decreasing it on the original plane. For the active slip system $(1\bar{1}1)[011]$, this can be obtained by applying a uniaxial stress state $\boldsymbol{\sigma} = \sigma_0 \hat{\boldsymbol{m}} \otimes \hat{\boldsymbol{m}}$ with direction of stress $\hat{\boldsymbol{m}}$ falling in region B in Fig. 6(a), and for an appropriate sign of σ_0. Letting $\hat{\boldsymbol{n}}'$ be the plane normal and $\hat{\boldsymbol{e}}'$ and the dipolar direction on the primary plane, and $\hat{\boldsymbol{n}}''$ and $\hat{\boldsymbol{e}}''$ the corresponding quantities on the conjugate plane, Escaig stresses on these planes are $\tau_e' = \sigma_0(\hat{\boldsymbol{m}} \cdot \hat{\boldsymbol{n}}')(\hat{\boldsymbol{m}} \cdot \hat{\boldsymbol{s}}')$ and $\tau_e'' = \sigma_0(\hat{\boldsymbol{m}} \cdot \hat{\boldsymbol{n}}'')(\hat{\boldsymbol{m}} \cdot \hat{\boldsymbol{s}}'')$, respectively. Choosing $\hat{\boldsymbol{m}}$ in region B as shown in Fig. 6(a), σ_0 was varied such that an Escaig stress τ_e'' in the range $0.0001[\mu] \leqslant \tau_e'' \leqslant 0.004[\mu]$ was produced in the cross-slipped plane (for $\hat{\boldsymbol{m}} = [225]$), which is the direction shown in-between [112] and [113] in Fig. 6(a), this becomes $\tau_e' = -0.7143\tau_e''$. The dependence of the activation energy

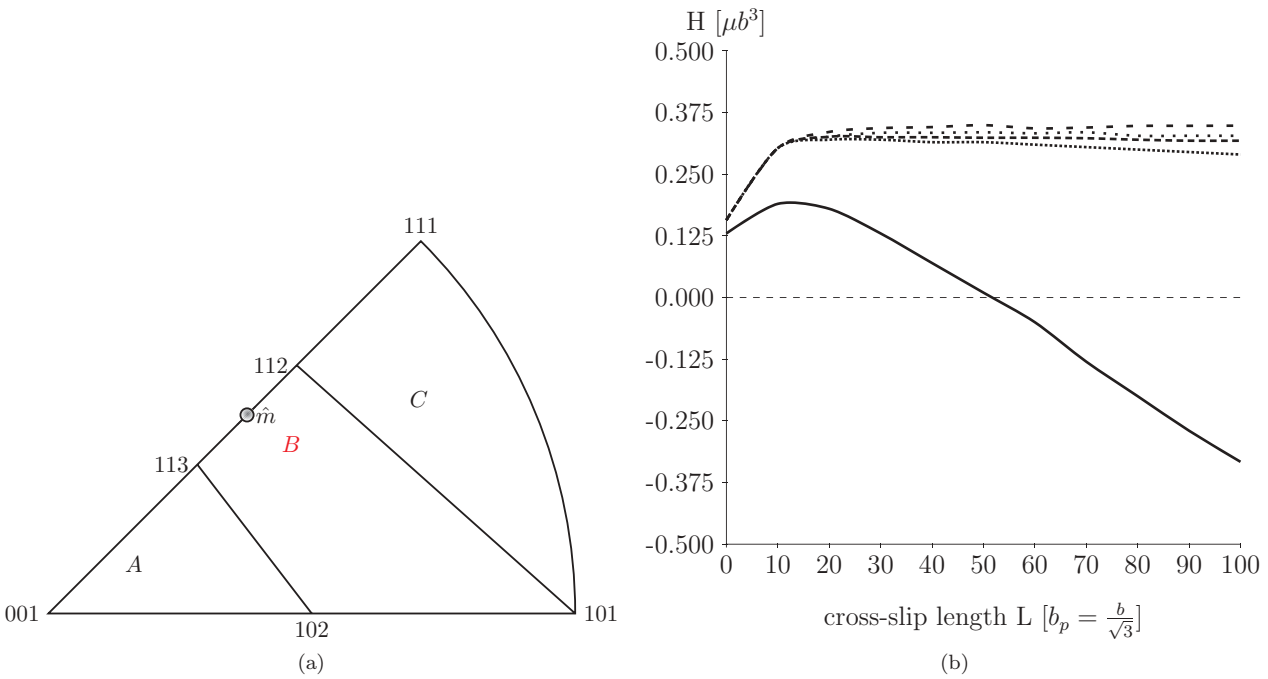
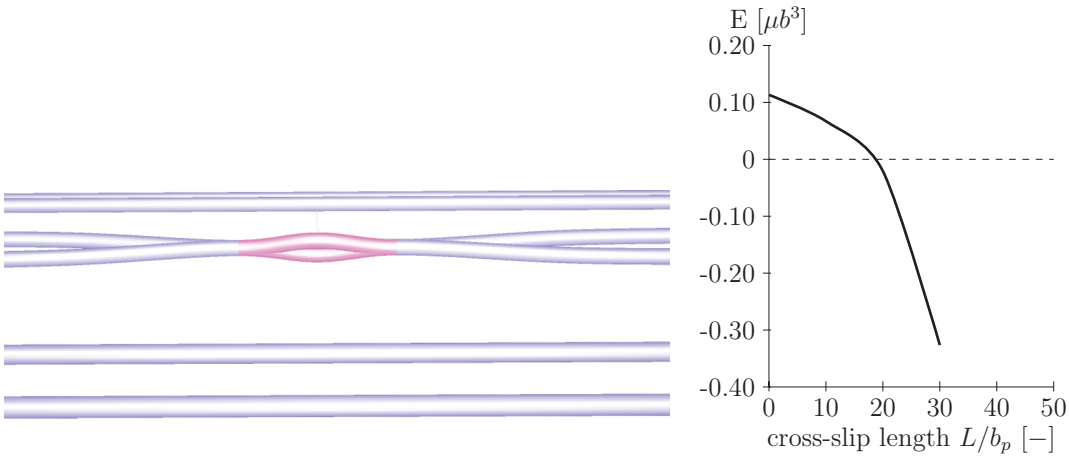


FIG. 6. (Color online) Effects of applied stress on activation energy. (a) Stereographic projection of the $(1\bar{1}1)[011]$ slip system showing the regions where the Escaig stresses on primary and conjugate planes change sign. (b) Parametric plot of ΔE vs L for different values of Escaig stress (τ_e): $\tau_e/10^{-4} = 40\ \mu$ (solid line), $\tau_e/10^{-4} = 3\ \mu$ (close dotted line), $\tau_e/10^{-4} = 2\ \mu$ (close dashed line), $\tau_e/10^{-4} = 1\ \mu$ (sparse dotted line), and $\tau_e/10^{-4} = 0\ \mu$ (sparse dashed line).



(a)Cross-slip detail (b)Cross-slip activation energy

FIG. 7. (Color online) Effects of dislocation pileups on cross-slip activation energy in Cu. (a) A simulation detail showing the head of a configuration with five pairs of Shockley partials piled up against a Lomer-Cottrell dislocation. (b) Corresponding energy curve $\Delta E(L)$.

on the reaction coordinate L, $\Delta E(L)$, was determined for different values of τ_e'', and the results are shown in Fig. 6(b). The results indicate that increasing the applied stress on the complex reduces not only the activation energy, but also the activation length required for the process. For $\tau = 0.004[\mu]$, we obtained an activation energy of $E_{cs} = 0.17\mu b^3 = 0.95\,\text{eV}$ and an activation length of $12b$ when two partials were used. In this case, it is also shown that ΔE becomes negative at $L \approx 52b$, indicating that when the partials are separated by this value on the cross-slip plane, the dislocation core will expand spontaneously at this value of the Escaig stress.

As stated earlier by Seeger,[38] pileups may provide a mechanism that enhances the rate of the cross-slip by reducing the width of the stacking-fault ribbon on the primary glide plane. Although the idea of requiring a large number of pileup dislocations to increase cross-slip rates (Seeger suggested about 100 dislocations) has been challenged by experimental data (Mughrabi[43]), it may not be necessary to require such large pileups.

The influence of an applied stress on cross-slip has been studied by Lu, Bulatov, and Kioussis using an *ab initio* method. Their results indicate that the critical stress for cross-slip to be 1.68 and 0.32 GPa Ag and Al, respectively.[44] To determine the effects of an inhomogeneous stress state on cross-slip, we assume that a representative pileup is composed of five pairs of Shockley partials, and is piled up against an obstacle. It is noteworthy that dislocation pileups containing as large as 20 dislocations have been experimentally observed.[43] We also use a modest applied shear stress of 0.0001μ ($\approx$5 MPa) to investigate the feasibility of cross-slip under this scenario. A series of relaxed configurations describing the cross-slip process were determined, and their energy calculated. An equilibrium configuration of the two leading dislocations in the Shockley partial pileup, and the LC lock is displayed in Fig. 7(a). The first dislocation at the top of the figure is a LC dislocation, which is sessile and has a Burgers vector of $\langle 110 \rangle$. The dislocation at the head of the pileup (second from top) is a screw dislocation, dissociated into two Shockley partials. The stress acting on this head dislocation is a result of the applied stress, the stress generated by the trailing four dislocations in the pileup, and the LC dislocation. It is thus a spatially varying stress field (inhomogeneous), which causes the head screw dislocation to cross slip, as shown in the figure. The results of the activation energy, shown in Fig. 7(b), indicate that the constriction energy was reduced by $\approx 50\%$ compared with the unstressed case. It is interesting to note that the energy associated with the constriction configuration is the highest of all configurations. The activation energy for cross-slip is only the energy required to form the constriction configuration alone ($\approx$0.62 eV), and once this configuration is formed in the pileup stress field, the expansion of the Shockley partials on the conjugate plan is spontaneous. The implication of investigating this scenario is that cross-slip of screw dislocations is very common in fcc metals, as a result of homogeneous or inhomogeneous stress fields that are inevitable as dislocations move through an evolving microstructure.

IV. SUMMARY AND CONCLUSIONS

The main purpose of this investigation is to theoretically determine the influence of local stress fields on the activation energy for cross-slip in fcc metals and compare the results with experiments. Strong variations in the local stress field are common in strained crystals, where the externally applied stress is shielded and substantially modified by the internal microstructure. Models that are based on atomistic or *ab initio* simulations alone may have difficulties accessing this mesoscopic regime of physics because of computational limitations on the simulation size. Previous elasticity-based calculations of the activation energy have been limited by two essential problems: (1) uncertainty of the contribution of Shockley partial dislocation cores to the calculated energy, and (2) utilization of linear segments, which inevitably leads to numerical error associated with tangent discontinuities at connections between linear segments. On the other hand, atomistic simulations suffer from the uncertainty in quantifying the effect of the empirical potential on calculated

energies. Empirical potentials, by their nature, rely on fitting equilibrium parameters that do not include the energetics of interplanar slip, which is a key parameter that determines the dislocation core structure. Estimates of elastic models for the cross-slip activation energy are typically high, and questions on the influence of the two factors described above remain lingering. Atomistic simulations for thermal cross-slip energy (without stress) have also given values as high as 2.7 eV for Cu, implying that cross-slip rates in the range of $\frac{1}{3}T_m - \frac{1}{2}T_m$ would be negligibly small. However, strong experimental evidence suggests that cross-slip rates in copper are high, leading to dislocation network recovery in stage III of single-crystal hardening.[15] In earlier atomistic models,[8] the large difference between atomistic results and experiment may be due to unrealistic boundary conditions, where image interactions complicate interpretation of the results, and where constrictions distort the lattice when they exit the atomistic simulation box. Also, empirical potentials may have difficulties in accurately determining the resistance to slip or the γ surface, as accurately done here with *ab initio* calculations.

In a complex local stress environment, for example at the head or a dislocation pileup, in the vicinity of an external or an internal interface, or near a sessile junction, a model that can capture such strong stress variations and accurately evaluate the activation energy for cross-slip is developed. A cross-slip model within the framework of the nonsingular continuum dislocation theory has been implemented to avoid the effects of the dislocation core cutoff radius on the activation energy. Thus, the interaction energy between partial fractional dislocations is calculated without local approximations (e.g., line tension), and with a core parameter that is calibrated with the *ab initio* determined gamma surface.

Accurate description of 3D dislocation configurations has been accomplished by decomposing dislocation networks in piecewise parametric splines with position and tangent continuity at the nodes. This description allows accurate determination of relaxed dislocation configurations, and does not require an *ad hoc* decomposition of interdislocation forces into self and interaction types. Consequently, this description not only provides a unique method for calculation of interaction forces, but it also gives the capability of describing complex 3D dislocation core configurations. This feature allows the model the potential of simulating the activation energy of cross-slip in real environments that are difficult to capture with purely *ab initio*, atomistic, or elasticity calculations.

The introduction of physically realistic values for the dislocation core width a using the PN model and a 1D generalized stacking-fault energy surface was implemented for the two-Shockley partials model. When PFDs are introduced, the dislocation core parameter a was scaled with the PFD Burgers vector, thus endowing the model with atomistic (*ab initio*) level fidelity. The present model with smooth, 3D partial fractional Volterra dislocations of arbitrarily small Burgers vector overcomes several difficulties that have persisted in elasticity-based models, yet provides a description of a more gradual mechanism of cross-slip, where smaller parts of the core are transferred in a way that minimizes the core energy over and beyond what can be achieved with Shockley partials alone. *Ab initio* fidelity is maintained where needed, and that is in evaluating the interplanar shear resistance during a complex core transformation. The consistency of the model with experimental measurements, while reasonable for unstressed cross-slip events, underscores the importance of local stress states on substantially enhancing cross-slip rates in fcc crystals. The present results on the effects of local stress states, obtained within the framework of the BGLK extended PN model, are consistent with recent evaluations of Rao and co-workers[18] using MD simulations. In addition to the *ab initio* level of calculational fidelity, the present model can be directly incorporated into dislocation dynamics descriptions of microscale plasticity, where local stress states are routinely determined for complex dislocation topologies, close to precipitates, interfaces, and external crystal surfaces.

*bramire2@utk.edu

[1] J. Poirier, Rev. Phys. Appl. **11**, 731 (1976).
[2] J. Koehler, Acta Metall. **1(5)**, 508 (1953).
[3] P. Jackson, Mater. Sci. Eng. **57**, 39 (1983).
[4] B. Escaig, Le Journal De Physique **29**, 225 (1968).
[5] M. S. Duesbery, Acta Metall. Mater. **40**, 149 (1992).
[6] G. Saada, Mater. Sci. Eng. A **137**, 177 (1991).
[7] S. Rao, T. Parthasarathy, and C. Woodward, Philos. Mag. A **79**, 1167 (1999).
[8] T. Rasmussen, Phys. Rev. Lett. **79**, 3676 (1997).
[9] S. Rao, D. Dimiduk, J. El-Awady, T. Parthasarathy, M. Uchic, and C. Woodward, Philos. Mag. **89**, 3351 (2009).
[10] R. L. Fleischer, Acta Metall. **7**, 134 (1959).
[11] A. J. E. Foreman, Acta Metall. **3**, 322 (1955).
[12] J. Friedel, *Dislocations* (Addison Wesley, Reading, MA, 1964).
[13] A. Stroh, Proc. Phys. Soc., London, Sect. B **67**, 427 (1954).
[14] J. Bonneville and B. Escaig, Acta Metall. **27**, 1477 (1979).
[15] J. Bonneville and B. Escaig, Acta Metall. **36**, 1989 (1988).
[16] W. Püschl and G. Schoeck, Mater. Sci. Eng. A **164**, 286 (1993).
[17] W. Püschl, Prog. Mater. Sci. **7**, 415 (2002).
[18] S. Rao, D. Dimiduk, T. Parthasarathy, J. El-Awady, C. Woodward, and M. Uchic, Acta Mater. **59**, 7135 (2011).
[19] J. M. Burgers, Proc. Kon. Ned. Akad. Wetenschap **42**, 293 (1939).
[20] N. M. Ghoniem, S. H. Tong, and L. Z. Sun, Phys. Rev. B **61**, 913 (2000).
[21] S. Banerjee, N. Ghoniem, G. Lu, and N. Kioussis, Philos. Mag. **87**, 4131 (2007).
[22] G. Po and N. Ghoniem (unpublished).
[23] W. Cai, A. Arsenlis, C. R. Weinberger, and V. V. Bulatov, J. Mech. Phys. Solids **54**, 561 (2006).
[24] V. Vitek, Philos. Mag. **18**, 773 (1969).
[25] J. Blin, Acta Metall. Mater. **3**, 199 (1955).
[26] R. deWit, in *Solid State Physics*, edited by F. S. Turnbull and David (Academic, New York, 1960), pp. 249–292.
[27] G. Schoeck, Phys. Status Solidi B **247**, 265 (2010).
[28] F. R. N. Nabarro, Proc. Phys. Soc., London **59**, 256 (1947).
[29] G. Schoeck, Acta Metall. Mater. **43**, 3679 (1995).
[30] G. Schoeck, Philos. Mag. A **69**, 1085 (1994).
[31] X.-Z. Wu, R. Wang, S.-F. Wang, and Q.-Y. Wei, Appl. Surf. Sci. **256**, 6345 (2010).

[32]G. Kresse and J. Hafner, Phys. Rev. B **47**, 558 (1993).
[33]G. Kresse and J. Hafner, Phys. Rev. B **49**, 14251 (1994).
[34]G. Kresse and J. Furthmüller, Comput. Mater. Sci. **6**, 15 (1996).
[35]G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).
[36]C. Yuksel, S. Schaefer, and J. Keyser, Computer-Aided Design **43**, 747 (2011).
[37]D. Caillard and J. Martin, *Thermally Activated Mechanisms in Crystal Plasticity*, Chap. 5 (Pergamon, New York, 2003).
[38]A. Seeger, in *The Mechanism of Glide and Work Hardening in Face-centered Cubic and Hexagonal Closed-pack Metals*, edited by J. C. Fisher (Wiley, New York, 1957), pp. 243–332.
[39]B. Escaig, in *Cross-slipping Process in the f.c.c. Structure*, edited by A. Rosenfield, G. Hahn, A. Bement Jr., and R. Jaffee (McGraw-Hill, New York, 1968), pp. 655–677.
[40]S. Rao, D. Dimiduk, J. El-Awady, T. Parthasarathy, M. Uchic, and C. Woodward, Acta Mater. **58**, 5547 (2010).
[41]T. Vegge and K. W. Jacobsen, J. Phys.: Condens. Matter **14**, 2929 (2002).
[42]T. Rasmussen, T. Vegge, T. Leffers, O. B. Pedersen, and K. W. Jacobsen, Philos. Mag. A **80**, 1273 (2000).
[43]H. Mughrabi, Philos. Mag. **18**, 1211 (1968).
[44]G. Lu, V. Bulatov, and N. Kioussis, Phys. Rev. B **66**, 144103(5) (2002).