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Tension–shear coupling in slip and decohesion of iron crystals

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Abstract

Results from atomistic simulations are used to parameterize constitutive relations involving the Frenkel sinusoidal dependence of shear stress on sliding displacement and a Rose–Ferrante–Smith universal binding form for dependence of tensile stress on opening displacement, for cases where the crystal symmetry dictates that a polarity in slip displacement exists.

1. Introduction

In the past decade, the intrinsic mechanical response of crystals has been understood by building upon the concept of a periodic relation between shear stress and sliding displacement along a slip plane embedded in an elastic continuum. Using such framework, Rice [1] derived an exact solution for the nucleation of a dislocation when the slip plane and crack plane coincide. His analysis considered shear only, ignoring the coupling between the sliding displacements and tensile stress across the slip plane. This analysis revealed a new solid state parameter γ_{us}, termed the unstable stacking energy, which is defined as the energy per unit area of slip plane when one side of the lattice is shifted in shear relative to the other to the equilibrium position at, or close to, a sliding displacement of $b/2$, where b is the Burgers vector to form a complete dislocation.

Rice's solution for the critical mode II stress intensity factor K_{II} for nucleation of a dislocation edge character relative to the crack tip when the slip plane and crack plane coincide is $(1-\nu)K_{II}^2/2\mu = \gamma_{us}$, where μ is the elastic shear modulus and ν is Poisson's ratio. The left-hand side of the above equation corresponds to the energy release rate for pure mode II conditions. But since Rice's solution neglects tension–shear coupling along the slip plane, this solution is insensitive to the tensile stress distribution acting perpendicular to the slip plane, such as could be modulated through an applied mode I stress intensity factor.

Motivated by atomic models of crack behavior in crystals that revealed the importance of tension–shear coupling in easing the nucleation process (see, for example, the work by Cheung et al. [2]), various descendants of the continuum model discussed above addressed the tension/shear coupling issue by assuming a mathematical form for the

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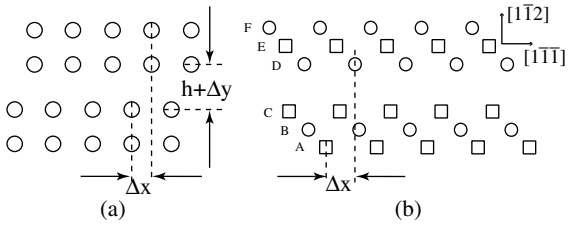

Fig. 1. Block-like lattice sliding and opening displacement of atomic layers along a slip plane. The interplanar spacing is h, and the spacing in the slip direction is b. (a) represents an idealized rectangular array; (b) depicts the sliding of {1 1 2} slip planes in a bcc structure. The atomic positions represented by squares lie $a_0/\sqrt{2}$ above and below the plane of the image, where a_0 is the lattice constant. The spacing in the horizontal direction is $\sqrt{3}a_0/2$, and the ABCDEF labelling refers to the six absolute configurations of {1 1 2} planes. Shear in the anti-twinning sense (Δx positive) is shown.

"constitutive" behavior of the slip plane [3,4]. The variables in such a relation include relative atomic displacements *along* and *perpendicular* to the slip plane, as well as the local shear stress and normal stress. These models typically assume a certain crystal symmetry. For example, a cubic, or even an orthorhombic crystal, with the slip plane aligned with the principal axes of the crystal would not undergo shear if a relative atomic separation *normal* to the slip plane were imposed. Many crystals, however, do not possess this symmetry about their active slip plane(s). For example, Fig. 1b shows a side view of the (1 1 2) plane in the bcc lattice. As will be elaborated upon later, the tension–shear coupling modes in such a crystal are more complex than what has been treated in the literature to date. The objective of this paper is to study the tension/shear coupling modes in a representative bcc metal (in this case, α-iron) and to propose an analytical representation of the slip plane constitutive response that can be used in fracture and dislocation nucleation models.

2. Combined tension–shear constitutive relations

For a uniform slip process in a crystal lattice, we imagine that a plane splits the crystal into two blocks. The upper block translates by a displacement (Δx, Δy) relative to the lower block (Fig. 1). Here Δx is the horizontal shift of the crystalline structure on one side of the slip plane, resulting in an in-plane shear. The Δy mode results in the two crystalline blocks being pulled apart (no periodicity in this direction). This paper only focuses on in-plane motions, leaving out any behavior associated with the z-direction consistent with two dimensional (plane strain) deformation.

Sun et al. [3] suggested an analytic form for the combined slip and opening displacements between two atomic planes with an initial separation h. It is expressed in terms of a potential corresponding to the energy per unit area Φ_0, given by:

$$\Phi_0 = 2\gamma_s\left[1 - \left(1 + \frac{\Delta y}{L}\right)e^{-\frac{\Delta y}{L}} + \sin^2\left(\frac{\pi\Delta x}{b}\right)\left\{q + \left(\frac{q-p}{1-p}\right)\frac{\Delta y}{L}\right\}e^{-\frac{\Delta y}{L}}\right], \tag{1}$$

where γ_s is the surface energy for one of the decohered surfaces, b is the Burgers vector, L is the characteristic length of the decohesion process (i.e., tensile stress undergoes a maximum at $\Delta y = L$ in the absence of any shear deformation), and p and q are dimensionless material constants that quantify the degree of tension–shear coupling. Specifically, q is defined as the ratio $\gamma_{us}/2\gamma_s$ (here, γ_{us} refers to an unrelaxed shear process, as elaborated upon by Sun et al. [3]), and p is related to the dilatation undergone by the crystal when it shears to its unstable stacking position at zero normal stress. The potential above is related to stress through its derivatives

$$\tau = \frac{\partial\Phi}{\partial\Delta x}; \quad \sigma = \frac{\partial\Phi}{\partial\Delta y}. \tag{2}$$

This constitutive relation is designed to reduce to the Frenkel sinusoidal form [5] in a shear mode (sliding by Δx) when $\Delta y = 0$ and the Rose–Ferrante–Smith [6] universal binding relation for tensile deformation (opening by Δy) when $\Delta x = 0$. It has also been used in a micromechanics framework for understanding the decohesion of elastic/plastic adherends in the special case where $p = q$ [7]. Eq. (1) does not account for the fact that in real crystals, when the crystal halves are separated in

the y-direction, shear stresses develop due to asymmetry of atomic positions with respect to the vertical axis. In order to make the constitutive relation more applicable to asymmetric crystal deformation, an additional contribution to the deformation potential is proposed, which takes the form

$$\Phi = \Phi_0 + 2\gamma_s \frac{\pi \Delta x \Delta y a e^{-\Delta y/L}}{bL}. \quad (3)$$

Thus, an additional fitting parameter a, which represents the strength of a coupling mode that allows shear stress to accumulate when crystal halves are pulled apart ($\Delta x = 0$ and $\Delta y \neq 0$), must be determined in order to best match data obtained from simulations, or optimistically, experimental measurements. One weakness of the new term is that it ceases to be periodic in Δx for $\Delta y \neq 0$. The impact of this is minimal, as (i) the loss of periodicity only applies to the normal stress σ when Eq. (2) is imposed, and (ii) the continuum models that make use of such constitutive relations typically do not apply them beyond approximately $\Delta x \approx b/2$, i.e., well within the first period of oscillation.

3. Atomistic simulations

The molecular dynamic simulations described in this section use an N-body potential of the Finnis–Sinclair type [8,9], applied to an iron crystal at 0 K under plane strain. The potential is consistent with the elastic constants $C_{11} = 2.433$, $C_{12} = 1.45$, and $C_{44} = 1.16 \times 10^{11}$ Pa. The simulated crystal consists of 198 atomic planes in the $[\bar{1}\,1\,0]$ direction, 200 planes in the $[0\,0\,1]$ direction, and three planes in the $[1\,1\,0]$ direction, where periodic boundary conditions are utilized. Traction-free boundary conditions are applied in the other directions, similar to those used in Ref. [8]. The small thickness in the latter direction is sufficient to include the whole range of interactions in the bcc lattice for this potential under plane strain conditions. The crystal is divided into two parts, divided by the $[\bar{1}\,1\,1]$ diagonal. The upper part is fixed, and the lower part is gradually displaced (step by step) in the $[\bar{1}\,1\,1]$ direction, using a step $0.01b$ where $b = a_0/2\langle 1\,1\,1\rangle$ is the Burgers vector in a bcc crystal (a_0 is the lattice constant, equal to 2.8665 Å). During this rigid sliding along a $(1\,\bar{1}\,2)$ plane (which contains the $[\bar{1}\,1\,1]$ slip direction), the total potential energy in the system is calculated as

$$\Phi = \frac{E_{\mathrm{POT}}(\Delta x, \Delta y) - E_{\mathrm{POT}}(0,0)}{NA_{112}}, \quad (4)$$

where E_{POT} denotes potential energy in the system, N is the number of atoms along the diagonal, and A_{112} is the area per atom in the $(1\,\bar{1}\,2)$ plane ($A_{112} = 2d_{110}b$, where d_{110} is the interplanar distance between neighboring $\{1\,1\,0\}$ planes). The simulations are repeated for prescribed increments in Δx and Δy (with no other relaxation allowed), and the specific results for $\Phi(\Delta x, \Delta y)$ are discussed in the next section. Earlier work by Machová et al. [8] has revealed that the effects of crystal size are negligible for the assemblage considered here. Additional details concerning the geometry and the method of solution, as well as the determination of local stresses, may be found in earlier work by Machová et al. [8]. We note that in this work, the block-like shear is applied in the *anti-twinning* direction, that is, in a sense that leads to dislocation formation rather than twinning.

4. Results and discussion

The primary results from the atomistic modeling are summarized in Figs. 2–4. In Fig. 2, we show Φ as a function of Δx for various levels of crystal separation Δy. As expected, the energy levels return to values similar to where they started ($\Delta x = 0$ vs. $\Delta x = b$), reflecting the inherent periodicity in the lattice. When the crystal is separated, we note that the minimum of $\Phi(\Delta x)$ shifts away from $\Delta x = 0$, indicative of a tendency for the lattice to shear as it is separated (i.e., there is a tendency for actual slip or the necessity for shear stress τ to develop to prevent a slip-like deformation). As emphasized earlier in this paper, this phenomena would not be expected in a crystal of cubic or orthorhombic symmetry with principal axes aligned with the slip and opening directions. The curve for $\Delta y = 0$ remains essentially symmetric about the midpoint $\Delta x = b/2$, not completely

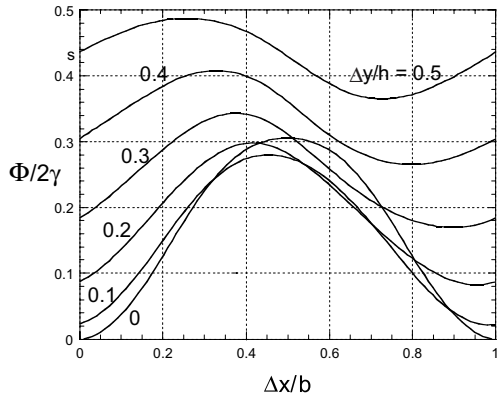

Fig. 2. The atomistically derived potential energy $\Phi(\Delta x, \Delta y)$ as a function of the sliding displacement Δx for α-iron. The interplanar spacing h is given by $h = a_0/\sqrt{6} = 2b/3\sqrt{2}$.

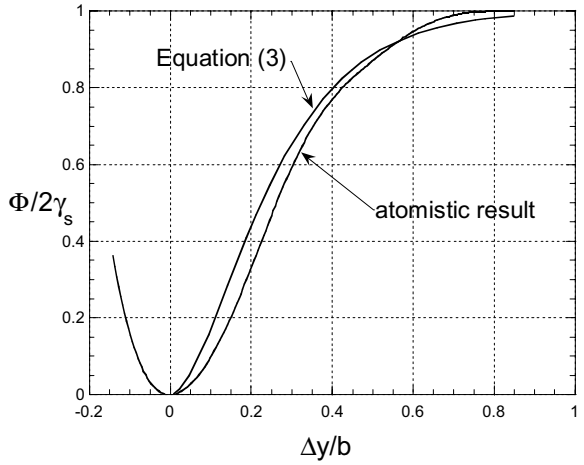

Fig. 3. The potential energy $\Phi(\Delta x, \Delta y)$ as a function of the opening displacement Δy for $\Delta x = 0$. The results from atomistic calculations and modeling based on the analytical formula, Eq. (3), are shown.

expected due to the crystal symmetry, but in surprisingly good agreement with the form proposed by Frenkel [5]. The peak energy in this case is identified as the unrelaxed unstable stacking energy [3]. At further levels of separation, the peak in potential energy shifts, not unexpectedly due to the crystal symmetry. Fig. 3 shows the potential energy as a function of normal separation Δy, not only from the atomistic model, but also from the analytic fit discussed in Section 2 (more details to

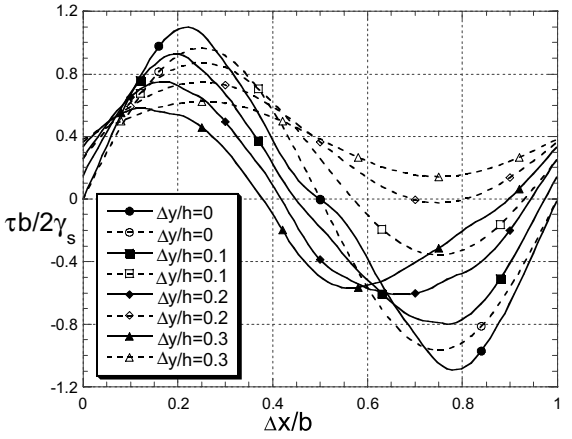

Fig. 4. The local shear stress as a function of the sliding displacement Δx for various values of Δy. The results from atomistic calculations appear as solid lines, and the analytic results appear as dashed lines.

follow). The characteristic form discussed by Rose et al. [6] is apparent. In addition, we show profiles of shear stress as a function of slip displacement in Fig. 4 for various $\Delta y \neq 0$.

A useful exercise would be to determine values of the parameters a, p, and L/b that give the most accurate representation of the energy associated with crystal deformation. The primary advantage of this parameterization is that a class of continuum models, based on the Peierls–Nabarro concept, directly utilize equations of the form $\tau(\Delta x, \Delta y)$ and $\sigma(\Delta x, \Delta y)$, and the direct use of atomistically derived data in those models is potentially cumbersome. In addition, a wide range of material classes could be studied using such continuum models simply by investigating the effects of p, q, a, and L/b. As mentioned earlier, q is already dictated by the atomistic potential, as it corresponds to the ratio $\gamma_{us}/2\gamma_s$. The strategy we use to determine the remaining parameters is to choose them such that the peak stresses τ and σ undergone by the crystal during separation ($\Delta x = 0$) agree, and that the peak shear stresses during shear for separations other than zero agree. The values of the constants are determined to be $q = 0.307$, $p = 0.360$, $L/b = 0.134$, and $a = 0.332$. In Figs. 5 and 6, respectively, we show the variation in σ and τ as the crystal is separated. While

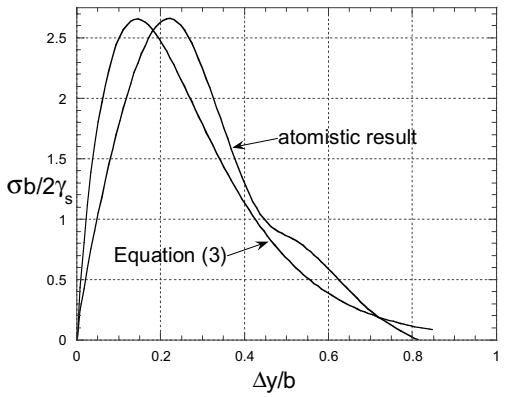

Fig. 5. Normal stress σ versus opening displacement for $\Delta x = 0$. The fitting scheme used in this paper ensures that the peak stresses, as well as the area under the curves (ideal work of separation), agree.

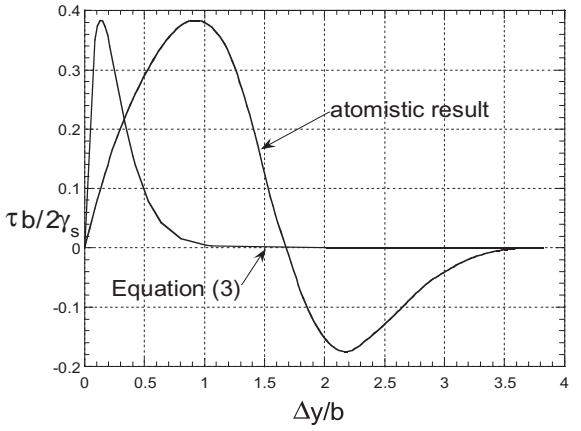

Fig. 6. Shear stress τ versus opening displacement for $\Delta x = 0$. The fitting scheme used in this paper ensures that the peak stresses agree.

the analytic form does an excellent job in reproducing the value of the peak stresses, we note that it is not robust enough to reproduce the particular values of Δx and Δy at which the maxima occur. Other modifications to Eqs. (1)–(3), such as a "skew" term introduced by Xu et al. [4], may provide the basis for further improvements to the analytic fit proposed in this paper.

5. Conclusion

The tension–shear coupling for combined slip and decohesion of the $\{2\,1\,1\}$ plane in α-iron is examined using an atomistic model based on the embedded atom method. An analytic form to characterize the development of local stresses as a function of the shear and opening displacements is proposed and is found to represent satisfactorily the atomistically derived results.

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