Role of Crack Blunting in Ductile Versus Brittle Response of Crystalline Materials

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Continuum concepts are used to evaluate the competition between crack advance and dislocation nucleation at the tip of a crack having a finite tip curvature. The analysis reveals that the favorability of crack propagation versus dislocation emission depends upon the bluntness of the crack tip. One implication is that a crack may initially emit dislocations only to reinitiate cleavage upon reaching a sufficiently blunted tip geometry. The present framework is used to classify crystals as intrinsically ductile or brittle in terms of the unstable stacking energy, the surface energy, and the peak cohesive stresses achieved during opening and shear of the atomic planes. [S0031-9007(99)09235-2]

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Ductile versus brittle behavior of crystalline materials is among the least understood of the fundamental mechanical phenomena in materials science. The conventional procedure for applying continuum-based theories to predict mechanical response of cracked bodies is to assume that the crack is atomically sharp, then to analyze how the body responds to an applied load. Rice and Thomson [1] instituted this approach by comparing the load required to propagate a given crack with the load necessary to emit a dislocation on a slip plane inclined to the crack plane and intersecting the crack front (see Fig. 1). If dislocation emission occurs at a lower load than that required for crack propagation, then the material is said to be "intrinsically ductile"; otherwise, it is said to be "intrinsically brittle." This type of physical modeling has evolved considerably over the years to account for factors such as nonlinear defect core structures, realistic slip systems, and three-dimensional dislocation configurations [2]; however, the role of crack blunting when dislocation emission initially occurs has received only limited attention [3–7]. Weertman, for example, described a mechanism by which a crack blunting by emitting dislocations may reach a limit in its ability to continue emitting [4]. Atomistic studies [5,6] agree on one major point: the favorability of crack advance versus dislocation emission can change as the crack tip blunts. In this Letter, we show that a crystal should not be classified as intrinsically ductile or brittle based on the emission of the first dislocation, but rather on the *ongoing* competition between crack propagation and subsequent dislocation nucleation as the crack-tip curvature evolves toward steady state. The present analysis identifies the critical material parameters that predict the outcome of this competition.

We first consider crack propagation. According to the Griffith theory [8], a sharp crack will advance when the applied energy release rate, $\mathcal{G}$, attains the value $2\gamma_s$, that is, the energy per unit area required to create two free surfaces. Formally, $\mathcal{G}$ is the rate of decrease of stored elastic energy in the system per unit area of crack advance; it scales directly with the intensity of loads applied to the body, and is related to the stress intensity factor, K, from fracture mechanics by the Irwin relation [9]

$$\mathcal{G} = \frac{(1 - \nu^2)K^2}{E}, \tag{1}$$

where E is Young's modulus and ν is Poisson's ratio. For illustration, we consider pure mode I loading, wherein the symmetry of the applied load is such that the crack faces tend to open rather than shear against one another (the formalism can be readily extended to mixed-mode loading). The material parameter $2\gamma_s$ is graphically depicted in Fig. 2, and represents the area under the stress versus separation curve for the atomic planes undergoing separation during the fracture process. In the Griffith theory, the critical load for fracture does *not* depend on σ_p, the maximum of the stress versus separation curve, but only on the

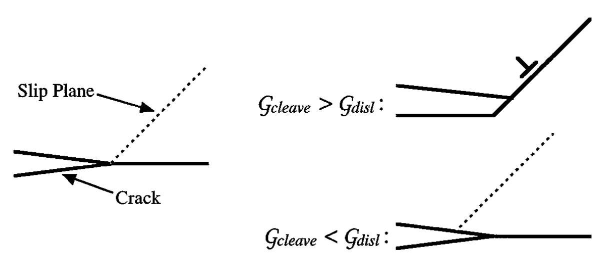

FIG. 1. A sharp crack with intersecting slip plane (left), showing the competition between dislocation emission (upper right) and cleavage decohesion (lower right). A blunt crack with an angular profile is shown, similar to that studied by Schiøtz *et al.* [5].

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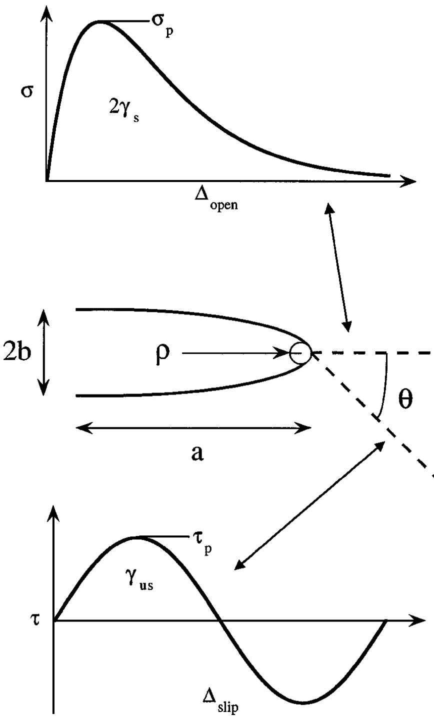

FIG. 2. A finite crack is represented as a slender elliptical slit with major axis a and minor axis b, which in turn prescribe the radius of curvature at the tip, $\rho = b^2/a$. Along the slip plane (inclined by angle θ with respect to the crack plane), the slip displacement adheres to the Peierls-like τ vs Δ_{slip} relationship. Along the crack front, the opening displacement adheres to a σ vs Δ_{open} relationship. The parameters τ_p and σ_p characterize the critical stress required for slip or decohesion, respectively.

area beneath it. This lack of dependence on σ_p is borne out by cohesive zone models [10–12] which do not make use of Griffith's theory at all.

We envision a crack that is continuously blunting on the atomic scale due to crack-tip dislocation emission on slip planes intersecting the crack front. We propose the use of a slender elliptical slit to approximate a blunting crack (Fig. 2) and to make our calculations tractable while introducing a length scale, ρ (radius of curvature of the tip), into the analysis. The elliptical crack-tip profile represents a drastic departure from the sharp corner (and its associated stress singularity) that would result, from a continuum viewpoint, when dislocations emit along a single slip plane (see Fig. 1). The angled crack tip (which does retain a sharp corner) has received some attention in the literature, notably from Schiøtz *et al.* [5], but other atomistic simulations [6,13] suggest that, at the atomic scale, it makes little sense to exploit a shape that contains a stress singularity in the continuum sense.

Consider an infinite solid containing an elliptical cutout with long semiaxis a and short semiaxis b. A remote stress of magnitude σ_∞ is applied perpendicular to the major axis of the ellipse. The radius of curvature at the tip, ρ, is given by b^2/a. The elasticity solution for this problem, given by Inglis [14] and Muskhelishvili [15], predicts the stress at the crack tip is

$$\sigma_{\text{tip}} = \sigma_\infty\left(1 + \frac{2a}{b}\right) = \sigma_\infty\left(1 + 2\sqrt{\frac{a}{\rho}}\right). \quad (2)$$

Assuming the crack is not sharp, thereby departing from the Griffith theory, we impose the condition that the crack propagates in a brittle fashion when the local stress given by Eq. (2) achieves the cohesive strength of the solid, σ_p. To a remote observer who sees the cutout simply as a finite-length crack, conventional fracture mechanics [16] gives the stress intensity factor as $K_I = \sigma_\infty\sqrt{\pi a}$. Combining Eqs. (1) and (2) and solving for the critical energy release rate gives

$$\mathcal{G}_{\text{cleave}} = \frac{\pi\sigma_p^2}{E'(\frac{1}{\sqrt{a}} + \frac{2}{\sqrt{\rho}})^2} \approx \frac{\pi\sigma_p^2\rho}{4E'}, \quad (3)$$

where $E' \equiv E/(1 - \nu^2)$ for plane strain. We have used the approximation in Eq. (3) that $\rho \ll a$; i.e., the crack is of some macroscopic, "laboratory" dimension, while ρ is of atomic dimension. Although Eq. (3) is linear in ρ, it is expected to break down as ρ approaches zero. In order to maintain a finite toughness in the ideally sharp limit, the Griffith theory must prevail as ρ becomes vanishingly small. This is indicated schematically in Fig. 3: as ρ approaches zero, the applied energy release rate for crack advance approaches $2\gamma_s$. For larger ρ, it should asymptote to the straight line given by Eq. (3). The transition zone between the two limits has been assumed to be smooth in the schematic of Fig. 3. Detailed mechanical analyses of the exact form of $\mathcal{G}_{\text{cleave}}(\rho)$, assuming a specific form of the stress versus separation curve in Fig. 2, are in progress, but initial results confirm the basic behavior indicated in Fig. 3.

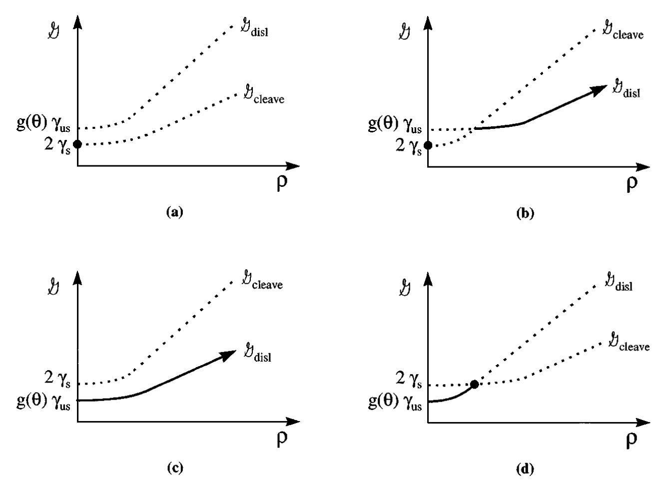

FIG. 3. (a) Represents an intrinsically brittle material where $2\gamma_s < g(\theta)\gamma_{\text{us}}$ and $\sigma_p < \tau_p/\cos\theta\sin\theta$; (b) represents an intrinsically brittle material where $2\gamma_s < g(\theta)\gamma_{\text{us}}$ and $\sigma_p > \tau_p/\cos\theta\sin\theta$; (c) represents an intrinsically ductile material where $2\gamma_s > g(\theta)\gamma_{\text{us}}$ and $\sigma_p > \tau_p/\cos\theta\sin\theta$; (d) represents a material that initially blunts but later reinitiates cleavage where $2\gamma_s > g(\theta)\gamma_{\text{us}}$ and $\sigma_p < \tau_p/\cos\theta\sin\theta$.

The crossover value for ρ, below which blunting effects are not significant and Griffith fracture prevails, is $8\gamma_s E'/\pi\sigma_p^2$ (on the order of three to four Burgers vectors for α-Fe, using data extracted from Shastry *et al.* [17]). This crossover seems consistent with atomistic results given by Schiøtz *et al.* [5] and Gumbsch [6], where only moderate increases in crack initiation load above the Griffith limit are noted for slight excursions from an ideally sharp crack tip. In the latter study, more significant increases in the failure thresholds were noted for blunter cracks.

Dislocation nucleation follows an analogous treatment. Recently, Rice and co-workers [18,19] provided an analysis of the threshold load for dislocation nucleation at a crack tip. They considered a slip plane intersecting a sharp crack. The slip plane was taken to obey an interplanar potential associated with rigid block sliding in a homogeneous lattice (see Fig. 2). The principal result is that the critical applied $\mathcal{G}$ (the prevailing energy release rate *if* the crack were to move as a classical singular crack, without a shear or decohesion zone at its tip) associated with dislocation nucleation is given by

$$\mathcal{G}_{\rm disl} = \frac{8\gamma_{\rm us}}{(1 + \cos\theta)\sin^2\theta} \equiv g(\theta)\gamma_{\rm us}\,, \qquad (4)$$

where θ is the inclination of the slip plane with respect to the crack plane. Equation (4) assumes the Burgers vector lies completely within the plane of Fig. 2 (i.e., has no component parallel to the crack front). It also overestimates $\mathcal{G}_{\rm disl}$ for $\theta > 0$ because it ignores shear-tension coupling (i.e., the effects of tension normal to the slip plane) and uses an approximate stress solution on inclined slip planes [18–20]. The crack-tip shear stress, $\sigma_{r\theta}$, along the inclined slip plane is given approximately by

$$\tau_{\rm tip} \approx \sigma_\infty\left(1 + 2\sqrt{\frac{a}{\rho}}\right)\cos\theta\sin\theta\,, \qquad (5)$$

which is essentially Eq. (2) scaled by the appropriate Schmidt factor. Equation (5) is valid for slip plane inclination angles up to about 70°, beyond which the equation breaks down because the maximum shear stress does not occur directly at the crack tip. Equating (5) with the peak shear stress, τ_p, and solving for the critical applied energy release rate for dislocation nucleation gives

$$\mathcal{G}_{\rm disl} \approx \frac{\pi\tau_p^2\rho}{4E'\cos^2\theta\sin^2\theta}\,. \qquad (6)$$

Again, $\mathcal{G}_{\rm disl}$ scales linearly with ρ and must not be interpreted physically for ρ approaching zero, whereupon $\mathcal{G}_{\rm disl}$ must approach the value given by Eq. (4), as shown in Fig. 3. The crossover crack-tip curvature is given approximately as $32\gamma_{\rm us}E'\cos^2\theta/\pi\tau_p^2(1 + \cos\theta)$, which corresponds to 10–20 b for α-Fe [17].

Based upon the threshold criteria motivated above, we can now differentiate between an intrinsically ductile and an intrinsically brittle crystal. Imagine a material with an initially sharp crack. Knowledge of the parameters γ_s, $\gamma_{\rm us}$, σ_p, and τ_p (and elastic moduli) enables the construction of plots of $\mathcal{G}_{\rm disl}$ and $\mathcal{G}_{\rm cleave}$ vs ρ, which can follow only one of four possibilities, as indicated in Fig. 3. For each case, we cite a particular material example. When the peak shear stress or tensile stress is not directly given in a particular reference, we have used estimates based on the universal bonding relation [12,21,22] for σ_p and the Frenkel model [2,18–20] for τ_p.

Case (i).—As depicted in Fig. 3(a), $2\gamma_s$ is less than $g(\theta)\gamma_{\rm us}$ and σ_p is less than $\tau_p/\cos\theta\sin\theta$. When the material is loaded, the crack advances by crack-tip cleavage. Because the condition for dislocation nucleation is never satisfied, no blunting occurs, and we classify this material as intrinsically brittle. Many ceramics below their ductile-to-brittle transition temperature and glasses below their glass transition temperature would fall into this category. Using material parameters for a specific cleavage plane in silicon reported by Sun *et al.* [19], $2\gamma_s = 3.12$ J m^{-2} which is less than $g(\theta)\gamma_{\rm us} = 12.9$ J m^{-2}, and $\sigma_p = 15.9$ GPa is less than $\tau_p/\cos\theta\sin\theta = 85.8$ GPa, thus predicting that silicon is intrinsically brittle.

Case (ii).—As depicted in Fig. 3(b), $2\gamma_s$ is less than $g(\theta)\gamma_{\rm us}$, but σ_p is greater than $\tau_p/\cos\theta\sin\theta$, giving rise to a crossover between $\mathcal{G}_{\rm disl}(\rho)$ and $\mathcal{G}_{\rm cleave}(\rho)$. Again, cleavage is favored over dislocation nucleation, and a sharp crack remains sharp. This material is intrinsically brittle; however, it is evident that a preexisting, sufficiently blunt crack could maintain ductile behavior and continue to blunt. The latter behavior is, however, metastable, as a perturbation in the local crack-tip curvature could cause it to spontaneously sharpen and proceed to extend via cleavage. Analysis of the critical parameters of α-Fe results in this predicted behavior [17]. We predict this system to be brittle for very sharp crack geometries because $2\gamma_s = 2.84$ J m^{-2} is greater than $g(\theta)\gamma_{\rm us} = 6.54$ J m^{-2}; however, dislocation nucleation becomes energetically favorable when the crack-tip curvature is greater than ~20 Å because $\sigma_p = 31.7$ GPa is greater than $\tau_p/\cos\theta\sin\theta = 21.1$ GPa.

Case (iii).—As depicted in Fig. 3(c), $g(\theta)\gamma_{\rm us}$ is less than $2\gamma_s$ and σ_p exceeds $\tau_p/\cos\theta\sin\theta$. Now, dislocation nucleation is the preferred response to applied load. As the crack blunts and ρ continues to increase, $\mathcal{G}_{\rm disl}$ remains less than $\mathcal{G}_{\rm cleave}$, and persistent dislocation nucleation remains the preferred mode; thus, we classify the material as intrinsically ductile. Most fcc metals at room temperature would fit this description. Aluminum is an excellent example of an intrinsically ductile material and its critical parameters predict this behavior [19]. Dislocation nucleation is always energetically favorable because $g(\theta)\gamma_{\rm us} = 0.537$ J m^{-2} is less than $2\gamma_s = 1.13$ J m^{-2} and $\tau_p/\cos\theta\sin\theta = 4.80$ GPa is less than $\sigma_p = 9.06$ GPa.

Case (iv).—As in the previous case, $g(\theta)\gamma_{\rm us}$ is less than $2\gamma_s$, and initial dislocation nucleation is preferred. However, $\sigma_p < \tau_p/\cos\theta\sin\theta$ and crossover occurs at a critical ρ, as shown in Fig. 3(d). At a finite crack-tip blunting, cleavage is the favored mode and the crack advances. This behavior is most likely to occur on metal-ceramic interfaces. We use data obtained from Hong *et al.* [21] for MgO/Ag interfaces, with a slip plane (in Ag) inclined at $\theta = 70.5°$ with respect to a (100) fracture plane. In this study, the silver atoms are positioned directly above the magnesium atoms. The value of $g(\theta)\gamma_{us} = 1.01\ \mathrm{J\,m^{-2}}$ is just slightly lower than $2\gamma_s = 1.08\ \mathrm{J\,m^{-2}}$, which allows for initial dislocation nucleation. This behavior is soon superseded by cleavage, due to the fact that $\sigma_p = 6.90$ GPa is less than $\tau_p / \cos\theta \sin\theta = 8.96$ GPa. It is to be understood that metal/ceramic interfaces represent the crudest application of our theory in its current form, since the present analysis applies to homogeneous, isotropic solids.

Several issues need to be resolved in extending the present treatment to a more general description of material fracture. The model is limited to predicting the early competition between cleavage and blunting and lacks the ability to account for the development toward a mature crack, the behavior of which is often dominated by larger-scale processes including the development of a plastic zone, the presence of grain boundaries, and heterogeneities such as second-phase particles. Furthermore, the appropriateness of using a rounded tip versus an angled one in continuum models remains an outstanding issue.

The motion of surrounding dislocations in the crystal is not accounted for in this treatment, nor are three-dimensional aspects associated with dislocation nucleation on "oblique" slip planes that intersect the crack tip at a point rather than along the entire crack front. For the cases described above where dislocations are emitted from the crack tip, the applied energy release rates should rigorously be interpreted as those based on the local, fully screened, crack-tip field, which can differ from the macroscopic field due to other dislocations or nonlinear effects in the system. The shielding effect of previously emitted dislocations can lower the stress field around the crack and therefore increase the critical applied load for dislocation nucleation and cleavage. Although emitted dislocations are assumed to be swept sufficiently far away that we may ignore these shielding effects, background dislocations and plastic dissipation have been shown to play a critical role in the actual applied loads necessary to maintain the "local" loads described in this paper [23–27], and are therefore expected to influence the ductile versus brittle competition. This notion can be exploited to predict the macroscopic fracture toughness, as well as to explain the large dependence of ductile versus brittle fracture energies on temperature, e.g., as in work by Lipkin *et al.* [27], where it was found that shielding effects can increase the applied loads by up to 3–4 orders of magnitude from the loads discussed in the present work.

Much work has been done on correlating γ_{us} and $2\gamma_s$ with observed fracture processes, especially in the area of numerical simulations of fracture. The model described in this Letter highlights the relevance of the parameters σ_p and τ_p. The roles of peak tensile stresses (e.g., as determined by Rose *et al.* [22]) and peak shear stresses (e.g., as determined by Cleri *et al.* [20]) in the ductile versus brittle behavior of crystals should be assessed in future simulations and experiments on fracture.

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[1] J. R. Rice and R. Thomson, Philos. Mag. **29**, 73 (1974).
[2] G. Xu, A. S. Argon, and M. Ortiz, Philos. Mag. A **75**, 341 (1997).
[3] G. J. Dienes and A. Paskin, J. Phys. Chem. Solids **48**, 1015 (1987).
[4] J. Weertman, *High Cycle Fatigue of Structural Materials: In Honor of Professor Paul C. Paris* (TMS, Warrendale, PA, 1997), p. 41.
[5] J. Schiøtz, L. M. Canel, and A. E. Carlsson, Phys. Rev. B **55**, 6211 (1997).
[6] P. Gumbsch, J. Mater. Res. **10**, 2897 (1995).
[7] G. E. Beltz and L. L. Fischer, Philos. Mag. A (to be published).
[8] A. A. Griffith, Philos. Trans. R. Soc. London A **221**, 163 (1920).
[9] G. R. Irwin, J. Appl. Mech. **24**, 361 (1957).
[10] G. I. Barenblatt, Appl. Math. Mech. **23**, 622 (1959).
[11] G. I. Barenblatt, Adv. Appl. Mech. **7**, 55 (1962).
[12] J. R. Rice and J.-S. Wang, Mater. Sci. Eng. A **107**, 23 (1989).
[13] D. Farkas (private communication).
[14] C. E. Inglis, Trans. Inst. Naval Architects **55**, 219 (1913).
[15] N. I. Muskhelishvili, *Some Basic Problems on the Mathematical Theory of Elasticity: Fundamental Equations, Plane Theory of Elasticity, Torsion and Bending* (Noordhoff, Groningen, 1975).
[16] H. Tada, P. C. Paris, and G. R. Irwin, *The Stress Analysis of Cracks Handbook* (Del Research Corporation, St. Louis, 1985).
[17] V. Shastry and D. Farkas, Model Simul. Mater. Sci. Eng. **4**, 473 (1996).
[18] J. R. Rice, J. Mech. Phys. Solids **40**, 239 (1992).
[19] Y. Sun, G. E. Beltz, and J. R. Rice, Mater. Sci. Eng. A **170**, 67 (1993).
[20] F. Cleri, S. Yip, D. Wolf, and S. R. Phillpot, Phys. Rev. Lett. **79**, 1309 (1997).
[21] T. Hong, J. R. Smith, and D. J. Srolovitz, Acta Metall. Mater. **43**, 2721 (1995).
[22] J. H. Rose, J. R. Smith, and J. Ferrante, Phys. Rev. B **28**, 1835 (1983).
[23] J. Weertman, Acta Metall. **26**, 1731 (1978).
[24] R. Thomson, J. Mater. Sci. **13**, 128 (1978).
[25] G. E. Beltz, J. R. Rice, C. F. Shih, and L. Xia, Acta Mater. **44**, 3943 (1996).
[26] D. M. Lipkin and G. E. Beltz, Acta Mater. **44**, 1287 (1996).
[27] D. M. Lipkin, D. R. Clarke, and G. E. Beltz, Acta Mater. **44**, 4051 (1996).