Micromechanics of Fracture: Connecting Physics to Engineering

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Introduction

Humpty Dumpty sat on a wall
Humpty Dumpty had a great fall
All the king's horses and all the king's men
*Couldn't put Humpty together again.**

This nursery rhyme is one of the oldest, most familiar, and shortest treatises on fracture mechanics in the literature. Nevertheless, it makes several important points: (1) fracture occurs in response to some driving force (for Humpty, a "great fall"), (2) fracture involves material separation, and (3) fracture is irreversible.

Of these, the driving force for fracture is probably the best-understood aspect. Fracture generally occurs because of the propagation of crack-like defects under the influence of a surrounding stress field. If the surrounding material behaves like a linear elastic solid (i.e., it follows Hooke's law), the stress state near the crack tip is described by

$$\sigma_{ij} = \frac{K}{\sqrt{2\pi r}} f_{ij}, \qquad (1)$$

where r is the distance from the crack tip, f_{ij} is a function of the angular position relative to the crack tip (which depends on the material's elastic constants), and K is the stress-intensity factor that depends on the mode of crack loading. Three modes are possible: Mode I involves opening of the crack; Mode II involves sliding of the crack faces perpendicular to the crack front; Mode III is also a sliding mode, but with the direction of sliding parallel to the crack front. The opening mode, Mode I, is of the greatest significance in practical applications and has received the most attention in the engineering and materials science fields. However, the sliding modes are what cause earthquakes, and so they are of great interest to geophysicists. In addition, in heterogeneous solids, such as composites and multilayers, the mismatch in mechanical properties leads to mixed-mode behavior (i.e., opening and sliding) in the vicinity of the crack tip, even if the remote loading is purely Mode I. The function f_{ij} depends on the mode of loading, but is otherwise independent of the forces that act to cause crack growth. All of the details about the geometry and the forces only affect the value of K. The physical significance of Equation 1 is that the energy available to drive crack growth, the energy-release rate $\mathcal{G}$, is proportional to K^2.

Whether or not the driving force (for Humpty, the height of the fall) is sufficient to cause fracture depends upon the presumed presence of unavoidable flaws or small cracks (in fracture, as in many other subjects, growth is much better understood than nucleation). Given a solid body with an initial crack subject to some external forces, will the crack grow, or will it remain stationary? To decide this, a fracture criterion is needed. Such a criterion has to connect the physics of the actual material-separation process to the driving force. Fracture mechanics dates from Griffith's work, where he postulated that a crack will grow when the energy-release rate reaches the value needed to make new crack surface; that is, when the energy-release rate is 2γ, where γ is the surface energy (extending the crack makes two surfaces). This holds for brittle solids. For an ideal brittle solid, only the breaking of bonds on the crack plane is involved. Real materials are different: the linear elastic response that is assumed in Equation 1 ceases to hold in regions sufficiently close to the crack tip. Not only does the response become nonlinear, but irreversible deformation processes occur (which is what makes putting Humpty together again so difficult). This has two far-reaching consequences: (1) the local stress state deviates strongly from that in Equation 1, and (2) crack growth requires more energy than just that needed for creating new surface. It was Irwin's[1] great insight that the Griffith scenario still holds if one interprets γ as the surface energy plus the plastic dissipation in the advancing crack-tip region. This interpretation is valid provided that the region over which dissipative and nonlinear effects predominate is small compared with the region over which Equation 1 holds (small-scale yielding). To illustrate that the additional term can be large, the surface energy of many materials with very different fracture resistances is of the order of 1 J/m^2; the energy-release rate of structural metals (e.g., aluminum and steel alloys) is typically one to two orders of magnitude greater.

The success of engineering fracture mechanics has been to relate measurements of the effective γ from tests on small laboratory specimens to the initiation of crack growth in structures and components. The approach is a purely phenomenological one: the fracture energy is not related to the underlying physical processes. The focus of this article is on the interaction between the dominant dissipative mechanism in crystalline metals, dislocation plasticity, and material separation. First, however, we point out some other challenging unresolved issues in fracture.

The single-crack picture implicit in the considerations just described implies that fracture splits an object into two pieces, but this is not always the case. In a sufficiently ductile material, the crack may arrest before it severs the solid into separate pieces. For brittle solids, once a crack begins to run, it runs very fast. The crack repeatedly bifurcates,[2,3] with the solid eventually shattering into many pieces. This transition from crack growth to fragmentation is a topic of current research interest and is far from completely understood. There is not yet a complete answer, for example, to the question of what constitutes the limiting crack speed in a brittle

*The real Humpty Dumpty is said to have been a powerful cannon used during the English Civil War (1642–1649). It was mounted on top of St. Mary's at the Wall Church in Colchester, defending the city against siege in the summer of 1648. The church tower was hit by the enemy and the top of the tower was blown off, sending Humpty tumbling to the ground.

solid. What is clear, both theoretically and experimentally, is that crack speeds can exceed elastic wave speeds, and such intersonic cracks are accompanied by shock waves.[4] Crack growth faster than an elastic wave speed occurs more readily under Mode II (sliding) conditions than under Mode I (opening) conditions, and differences in elastic properties (as across an interface) promote such fast crack growth. The prediction of the crack path, the total consumed energy, the fracture-surface characteristics, and so on are current topics of research. These aspects are crucial in order to address issues of design of fracture-resistant materials. In heterogeneous materials, cracks meander through the microstructure, and microscale alterations in the crack path can have a major effect on macroscale fracture resistance. Dissipative mechanisms in crystalline metals include mesoscale dislocation plasticity in the crack-tip region and larger-scale (hundreds of microns to millimeters) plasticity associated with the nucleation and coalescence of voids at second-phase particles. Chemical and electrical interactions in the crack-tip region can affect the energy required for fracture. For example, the diffusion of impurities to the crack-tip region may directly affect either dissipative processes or cohesion there. Another chemical effect of importance is the creation of an oxide layer on newly exposed free surface.

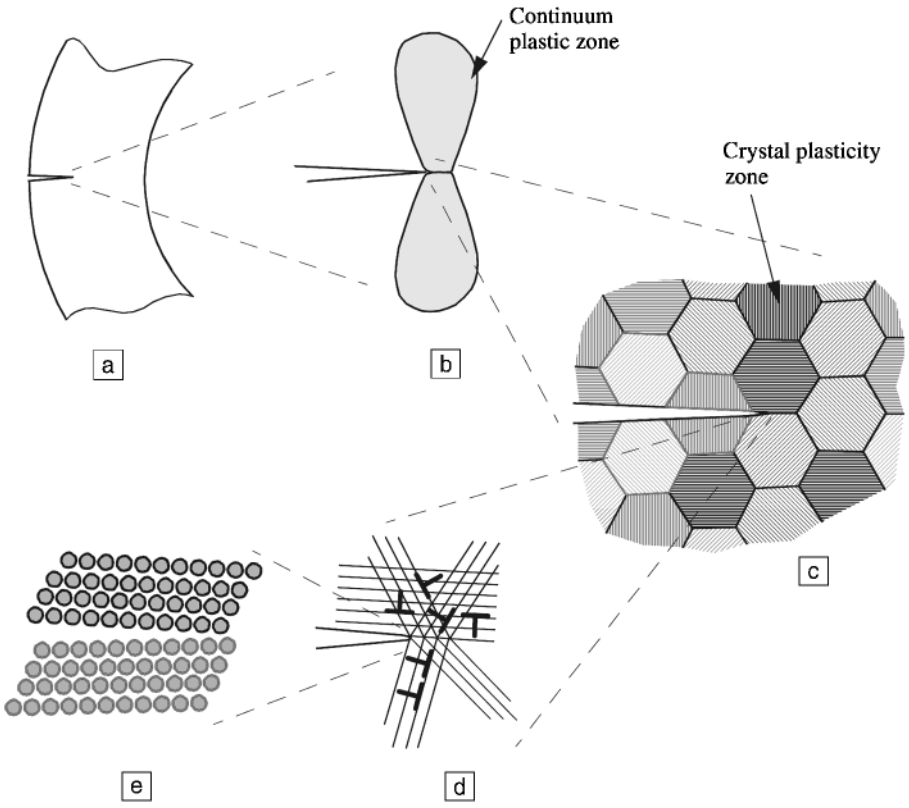

Figure 1. The various relevant scales that may determine the response of a crack in a macroscopic component (a). Zooming in to the near-tip region, we observe (b) the plastic zone governed by macroscopic continuum plastic flow, inside of which we notice that (c) the material is polycrystalline, with the plastic deformation being different in different grains. Even closer to the tip of the crack, we observe that (d) plastic deformation occurs via localized slip on particular slip planes, caused by the motion of individual dislocations. The final illustration (e) shows the atomic arrangement on either side of the crack.

The Scales in Fracture

The micromechanics of fracture attempts to link the macroscopic fracture resistance to the underlying physical mechanisms of irreversible deformation and material separation. The specific physical mechanisms are material-dependent and, in general, involve a broad range of length and time scales. To make matters specific, we focus on room-temperature crack growth in crystalline metals under circumstances where dislocation glide is the dominant mechanism of plastic dissipation. However, many of the issues are generic and are pertinent in a broader range of circumstances.

Figure 1 is a highly simplified illustration of the important length scales involved for cleavage crack growth in a relatively ductile polycrystalline metal. The relevant length scales range from that of the macroscale object to the atomic scale, including the various microstructural length scales in between that are associated with, for example, particles, grains, and defect structures.

The challenge lies in the fact that all scales are connected, and all may contribute to the total fracture energy. It is worth noting that although the atomistics of the separation of surfaces may only contribute a small fraction of the total energy-release rate, it can still be controlling. This is because dissipative mechanisms can operate only if fracture is delayed sufficiently to allow them to come into play. Indeed, as pointed out in Reference 5, the surface energy can play a valve-like role because small changes in atomic-scale fracture resistance can lead to large changes in plastic dissipation.

Even though the example in Figure 1 is highly idealized, it is useful to consider the various scales and their connections in some more detail:

- When the size of the plastic zone spans sufficiently many grains (Figure 1b), one may describe the plastic deformation by means of a macroscopic, and often isotropic, continuum model. This gives rise to stress and strain fields (referred to as the HRR fields)[6,7] that differ from Equation 1, but which share several key characteristics with it: (1) the stresses are singular (the stress is infinite at $r = 0$, when the crack is modeled as being mathematically sharp), but the singularity depends on the strain-hardening characteristics of the material; (2) the stress distribution near the crack tip depends on the material properties, but is independent of the loading conditions and the geometry; and (3) there is a single parameter characterizing the amplitude of the singularity that embodies the effects of geometry and loading.
- At smaller scales, this description loses accuracy because the anisotropic nature of the individual grains becomes noticeable, which gives rise to stress and strain fluctuations with wavelengths equal to the grain size (Figure 1c). These can be described by means of crystal plasticity models, which are continuum-based but which recognize the discrete nature of the slip systems along which plastic flow occurs. If the plastic zone is in a single crystal, the near-tip fields are completely different from the HRR fields. When hardening at the crystal level can be ignored, the stress field is piecewise uniform in

various sectors around the tip,[8,9] with stresses of the order of the critical resolved shear stress for slip.

- Zooming in to the tip of the crack, the individual dislocations that mediate plastic flow become noticeable (Figure 1d). At this scale, energy dissipation is associated with the motion of large numbers of dislocations moving through the lattice. Each dislocation induces a localized stress concentration that gives rise to large local stress fluctuations. This landscape continuously changes as dislocations move or are generated from the crack tip itself or from nearby sources.
- The actual separation process takes place at the atomic scale (Figure 1e) and occurs inside the dislocation plasticity zone (for a recent perspective on atomistic analyses of fracture phenomena see the May 2000 issue of *MRS Bulletin*[10]). The stress fields from the next higher-up scale cause local bonds between atoms to be stretched and broken when the stresses at this scale reach values of the order of the bond strength. This process may be assisted by other atoms that have diffused to the crack tip from the environment.

Many details are left out in this discussion, but it emphasizes that fracture—that is, the creation of new surface—is a highly localized effect at the atomic scale that is driven by the applied load via the stress fields on smaller and smaller length scales. It is the precise communication down these scales that determines whether or not crack growth occurs and how much energy is dissipated along the way (e.g., see Reference 11). The success of predictions of macroscopic fracture properties on the basis of atomic properties relies entirely on the accuracy with which the intermediate scales can be bridged. In transferring information between models at different size scales, there are subtle issues of capturing the behavior at the smaller size scale in some appropriate average sense, particularly when defect structures are involved.

Dislocation Dynamics Near Crack Tips

We now focus on the dislocation scale illustrated in Figure 1d, because the stress concentrations at this scale play a key role in determining whether crack growth will take place in a ductile or brittle manner. At this scale, the dislocations can be modeled as line singularities in an elastic solid; that is, the elastic effect of interatomic interactions is averaged out, but the dislocations as carriers of plastic deformations are represented discretely. The long-range interactions between dislocations are accounted for through their continuum elasticity fields. Short-range dislocation interactions are incorporated by a set of constitutive rules that in principle can be derived from atomistic modeling.

Conventional continuum plasticity theory (Figures 1b or 1c) predicts that stress levels at a blunted crack tip are limited to being of the order of a few times the flow strength (roughly 10^{-3} times Young's modulus). However, the strength of atomic bonds, as predicted (for instance) from first-principles computations, is roughly an order of magnitude larger. Thus, a key issue is how stresses that are high enough to cause atomic separation are transmitted to the crack tip. Our recent dislocation dynamics study[12] indicates that this gap may be bridged by the stress concentrations associated with discrete dislocations (see also References 13 and 14).

The calculations in Reference 12 have significant limitations: they are two-dimensional; the short-range dislocation-interaction rules are plausible choices rather than directly derived from atomistics; and to numerically resolve relevant length scales, the calculations are carried out using a cohesive strength that is lower by a factor of 3–4 than expected from atomistics. Nevertheless, the results are instructive regarding the role of dislocation structures in transmitting high stresses to the crack tip. A typical result of such simulations is shown in Figure 2. The opening stress reaches sufficiently high values ahead of the crack tip to open the cohesive surface and thus for the crack to propagate. The peak stress level, according to conventional continuum plasticity, is about a factor of 4 lower, and crack growth would not be predicted by such an analysis.

These calculations[12] indicate that dislocations play a dual role in the fracture process. On the one hand, dislocation activity gives rise to values of the crack driving force at initiation that are significantly higher than for an elastic solid with the same cohesive properties. On the other hand, it is the local stress concentration associated with discrete dislocations in the

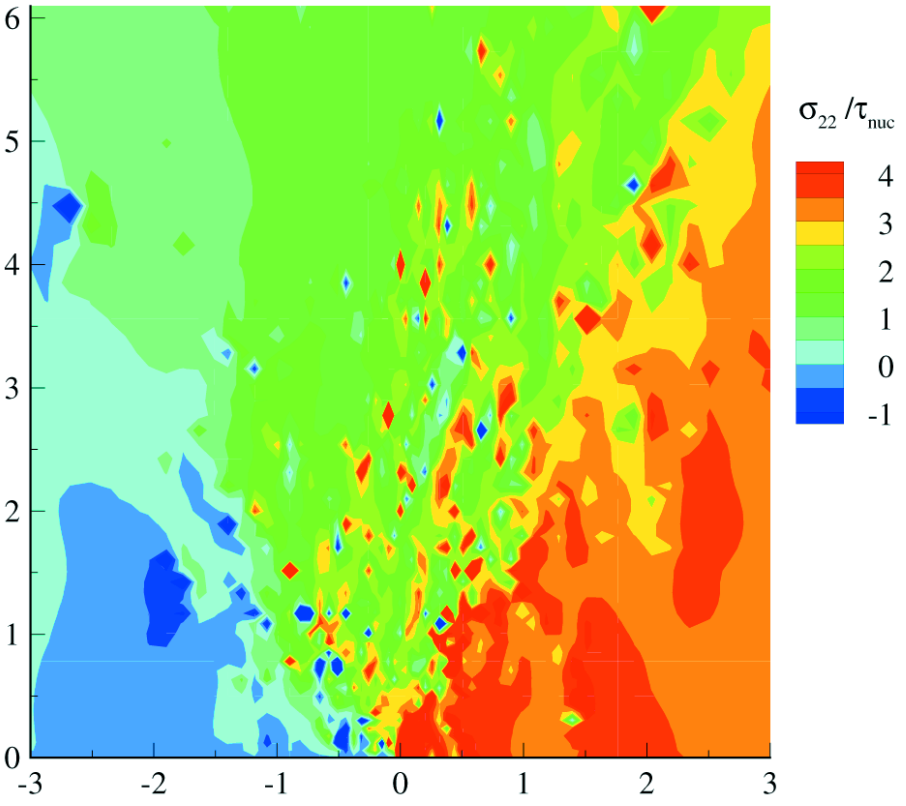

Figure 2. Distribution of the opening stress σ_{22} (i.e., in the vertical direction) near the tip of a stationary crack in a crystal with three slip systems (slip planes oriented at 0 and ±60° with respect to the horizontal crack plane; all lengths in micrometers). Beyond a distance of 0.5–1 μm, the average stress fields agree rather well with continuum slip solutions where the stress is uniform in sectors around the tip and is of the order of the flow strength. Inside the very near-tip region of 0.5–1 μm, however, the opening stress attains much higher values.

vicinity of the crack tip that leads to stress levels of the magnitude of the cohesive strength, causing the crack to propagate.

The source of dislocations in the crack-tip region is material-dependent. In some materials, such as silicon, the sole source of dislocations is the crack tip itself. Then, the key question for brittle or ductile response is whether dislocation nucleation precedes decohesion or vice versa (e.g., see Reference 15). Other materials have an abundance of sources in the crack-tip region (this is the situation modeled in Reference 12). In either case, two conditions need to be met for the material to behave in a ductile manner: (1) the dislocations must be nucleated, and (2) they need to be mobile (see also Reference 14).

If very few dislocations are nucleated, the stresses near the crack tip are essentially those given by Equation 1, with local deviations caused by the presence of isolated dislocations. In such source-limited circumstances, crack growth takes place, with the energy-release rate differing only slightly from the surface energy. On the other hand, if ample dislocations nucleate and can glide, unobstructed, away from the crack-tip region, dislocation motion relaxes the stresses near the crack tip, leading to continued blunting without crack propagation. In fact, fracture in crystalline metals rarely occurs by cleavage when there is large-scale plasticity. Continued crack-tip blunting leads to large plastic strains over a large enough region to activate mechanisms of void nucleation, growth, and coalescence. This microvoid fracture mechanism, where the governing processes take place over a size scale of microns to hundreds of microns, is what gives rise to the very high energy-release rates of ductile structural metals. Intermediate between these two limits are the circumstances in Figure 2, where both plastic flow and cleavage separation take place.

Discrete dislocation considerations are of particular importance for fatigue crack growth and for crack growth at metal–ceramic interfaces. Atomistic calculations of MgO/Ag adhesion[16] give cohesive strengths of 2–10 GPa and values of the work of separation of the order of 0.1–1.0 J/m^2, with the lower values accounting for effects of small concentrations of impurities and segregants. Macroscopically measured values of the work of separation are typically 2–5 J/m^2 for segregated interfaces with sharp cracks and greater than 200 J/m^2 for clean interfaces with blunt cracks.[17] The macroscopically inferred values of the cohesive strength are several times the flow strength of the metal.[17] Thus, there is a significant discrepancy between "top-down" and "bottom-up" estimates of the fracture properties. This gap may be bridged through consideration of the dislocation structures that form near an interface crack.

Crack growth under cyclic loading conditions (fatigue-crack growth) is undoubtedly the most important mode of fracture in practical applications. The essence of fatigue is that crack growth occurs even when the driving force for crack growth is much smaller than what is needed for the same crack to grow under monotonic loading conditions. This is what makes fatigue fracture so dangerous in practice and so difficult to understand fundamentally. Although much is known about the phenomenology of fatigue, an understanding is lacking of why fracture occurs at lower values of the crack driving force under cyclic loading conditions.

For crystalline metals, the irreversibility of dislocation motion plays an essential role in fatigue-crack growth. Under cyclic loading conditions, the internal stress state generated by the discrete dislocations provides the bias for the evolution of the dislocation structure that increases the near-crack-tip opening stress and thus provides the driving force toward fracture.

Challenges and Outlook

Fracture is an archetypical multiscale problem: length scales from the electronic structure for chemical effects to the macroscopic can all come into play in determining the fracture resistance of a structure or component. Engineering fracture mechanics, which involves identifying fracture parameters and transferring results from small-scale tests to larger-scale structures, is a well-developed subject, even though a fundamental understanding of some issues is still lacking. The main promise for multiscale fracture modeling lies in applications to small-scale structures and to designing materials with improved fracture resistance.

Multiscale modeling of fracture processes can proceed in two ways: (1) by means of data compression and transmission across scales through passing effective properties from one scale to a higher scale, or (2) by the direct coupling of regions modeled at one scale to another (e.g., an inner region modeled atomistically, to an intermediate region modeled in terms of discrete dislocations, to an outer continuum region). In this latter case, a key issue that remains to be resolved is how to pass defects from one size scale to the next. It is also worth noting that as a general rule, computations on smaller size scales require smaller time steps. More often than not, time-step, rather than spatial-integration, considerations are the computationally limiting factor.

Multiscale modeling of fracture is in an early stage of development, but there is great potential for improving not only the fracture resistance under mechanical loading, but also the fracture resistance when environmental effects come into play, for example, through chemical interactions and/or the presence of electrical and magnetic fields. Traditionally, the component or structure of interest has been of a macroscopic size (centimeters to meters or larger), but the reliability of micromechanical and microelectronic structures and components is likely to be of increasing importance.

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