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Physics of Fracture

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The underlying physical bases of present-day fracture theory are examined. It is proposed that the atomically sharp crack should be taken as the cornerstone for modeling propagation processes at the fundamental level. Transmission electron microscopy evidence is presented in support of this contention. Linear continuum fracture mechanics is shown to have intrinsic limitations in its capacity to describe crack-tip phenomena; a more realistic description is provided by lattice statics, incorporating the picture of a crack as a narrow slit terminated by nonlinear linkage bonds. This description establishes a powerful starting point for understanding and predicting the effects of important crack-tip interaction processes. Two such processes, chemically enhanced slow crack growth and process-zone toughening, are discussed in this light. Finally, the nature of strength-controlling flaws in brittle ceramics is considered, with particular reference to the validity of the widely adopted hypothesis that such flaws may be regarded as true microcracks.

I. Introduction

ALONG with our ever-expanding modern-day technology has come an increasing demand for high-performance materials. Thus it is that ceramics, hitherto rejected because of their brittleness, have begun to emerge as attractive candidates for certain engineering applications. Ceramics have qualities, such as high melting points, chemical durability, and intrinsic hardness, which lend themselves to component survival at the extremes of service operating conditions. With this class of materials the chief problem in design is accordingly the containment of potential fracture processes; what properties need to be optimized to guard against the catastrophic formation and growth of cracks?

It is in response to this last question that we have witnessed the evolution of that branch of engineering science known as "fracture mechanics." The formalism of fracture mechanics stems from the basic hypotheses laid down by Griffith in his pioneering paper of 1920[1]: (i) equilibrium extension of well-developed cracks is governed by a balance between mechanical energy released and fracture surface energy gained; (ii) such cracks start from "flaws" in the stressed material. The strength of any given material is determined by both these factors; high "toughness" (resistance to crack extension) and small flaw size are prime requisites for optimal load-bearing capacity. The difficulty with ceramics is that their toughness is inherently so low that they cannot survive operational stress levels if they contain flaws of characteristic dimension 1 to 100 μm. Indeed, with optical fibers, where the operational conditions are unusually stringent, the appropriate flaw dimension may be as low as a few nanometers. What fracture mechanics does is to provide us with a mathematical formalism, based on the picture of a slitlike crack embedded in a linear elastic continuum, for handling the first of the Griffith hypotheses in a general way. Then, given all necessary information on the geometry of the critical flaw in relation to the applied stress field, one has, in principle, the means for evaluating the mechanical response of a component to failure.

For those who concern themselves primarily with the question of *when* fracture occurs, as engineers do, the methodology of fracture mechanics appears to be totally adequate as a predictive tool. However, if we ask ourselves *why* fracture occurs, things start to go wrong. For the critical processes of crack separation must occur at the very tip, and here the linear elastic continuum solutions show singularities. Thus, in inquiring how stresses remotely applied at the outer boundaries of a specimen transmit to the crack tip, there is a limit as to how far we may go with conventional fracture mechanics. The way engineers circumvent this difficulty is to write down empirical crack "laws" for extension in terms of some parameter which characterizes the *intensity* of the locally concentrated stress field, the *distribution* of stresses within the field being taken as invariant. A similar disregard for geometrical details is adopted in the description of flaws for strength analysis; the most common approach is to regard flaws simply as "microcracks," scaled-down versions of true, well-defined cracks, whose characteristic dimensions may be predetermined by empirical testing procedures. In short, engineering fracture analysts concern themselves with the *mechanics,* as distinct from the *mechanisms,* of crack growth.

Clearly, if we wish to understand fracture processes at a fundamental level our attention must turn to the latter aspect. There are two major problems which immediately become apparent.[2] The first of these concerns the assumption of linear elasticity; for a truly Hookean solid the proportionality between stress and strain has no upper limit, implying an infinite strength. Thus the mechanism of material separation at the crack tip is essentially *nonlinear.* The second problem arises in connection with the continuum approximation; the dimensions of the region in which these critical nonlinear processes operate in ceramics are calculated to be small, <1 nm. Hence, the description of separation processes strictly needs to consider the *discrete* nature of matter. What we are effectively saying here is that crack growth is ultimately governed by the complex forces which hold neighboring atoms together in the solid. It is in this context that the title theme of the present paper has its conception.

In what follows an attempt will be made to sketch some of the more important advances in fundamental fracture theory. Inevitably, the selection of topics and the corresponding interpretations will reflect a personal viewpoint. The presentation will focus around one central assertion, that brittle cracks are atomically sharp and propagate by the sequential rupture of bonds. In the first part the justification for making this assertion, and the evidence which supports it, will be given. This will set the scene for modeling two important fracture phenomena in ceramics, slow crack growth due to chemical interactions with environmental species and toughening due to the operation of energy-dissipative pro-

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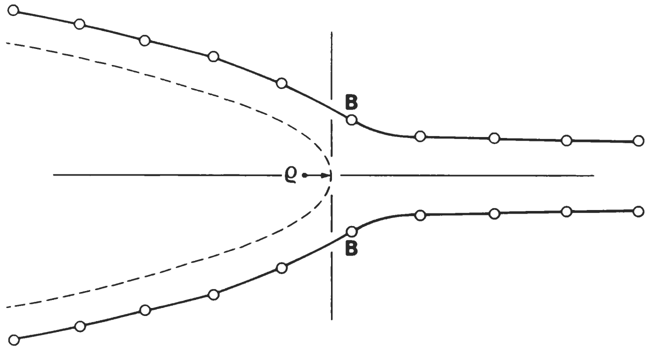

Fig. 1. Tip contours for equilibrium crack in silica glass, as computed from linear elastic fracture mechanics. Crack-tip radius is seen to be significantly smaller than intermolecular spacing.

cesses within the near field of the crack. It will be argued that, by considering events at the sharp tip in isolation from the remainder of the crack system, the potential exists, for the first time, for making *a priori* predictions of propagation laws for particular material systems. Finally, the extent to which small flaws may be regarded as true microcracks will be examined in the light of recent controlled-indentation studies.

II. The Atomically Sharp Crack as the Cornerstone of Brittle Fracture Theory

(1) *Intrinsic Limitations of Linear Elastic Continuum Models*

We begin with an outline of the now familiar picture of a slitlike crack in a linear elastic, isotropic continuum.[2,3] In accordance with appropriate boundary conditions (i. e. remotely applied tensile loads, traction-free crack walls), the solutions for the near-field stresses and displacements about a crack tip in a material with Young's modulus E and Poisson's ratio ν are of the general form

$$\sigma_{ij}=[K/(2\pi r)^{1/2}]f_{ij}(\theta) \tag{1a}$$

$$u_i=(K/E)(r/2\pi)^{1/2}g_i(\theta,\nu) \tag{1b}$$

where r,θ are polar coordinates. The distribution characteristics of the field are determined by the separable coordinate-dependent terms: of these, the radial component is particularly noteworthy, for it shows immediately how the stresses and strains become infinite at $r\rightarrow 0$; the angular quantities $f_{ij}(\theta)$ and $g_i(\theta,\nu)$ are explicit functions which are obtainable from any standard reference source on fracture mechanics (e. g. Refs. 2 and 3). The remaining quantity K uniquely determines the intensity of the field, and is appropriately termed the stress intensity factor. This factor embodies the essential boundary conditions of the crack system; it scales directly with the applied load and is a function of characteristic crack dimensions.

The stress intensity factor is a particularly appealing parameter in engineering mechanics, for, not only does it quantify the driving force on the crack, it satisfies the laws of linear superposition. Consequently, there has developed a strong tendency to formulate crack extension laws exclusively in terms of K. Such laws are of two main types. (i) *Equilibrium* laws, which specify that cracks may extend (stably or unstably) at some critical stress intensity factor, $K=K_c$, which defines the material toughness. In the event that the toughness is determined entirely by the reversible work of free surface creation, γ, it can be demonstrated[2] that $K_c=(2\gamma E)^{1/2}$. Then, coupled with the standard solution for cracks of characteristic length c subjected to uniform applied tensile stress σ, $K=Y\sigma c^{1/2}$ (where Y is a crack geometry term), we obtain an instability condition $\sigma_f=(2\gamma E/Yc_f{}^{1/2})$, which is the famous Griffith strength formula.[1] (ii) *Kinetic* laws, where, at some subcritical configuration $K<K_c$, the crack can extend at some specifiable velocity, $v=v(K)$. The most important example of kinetic crack growth is that due to chemical interactions with environmental species.

Let us now take a closer look at the crack field solutions at the tip itself. As an illustrative example, consider silica glass for which $E=70$ GPa, $\nu=0.2$, and $K_c=0.75$ MPa·m$^{1/2}$ (as determined from direct observations of crack growth in large-scale test pieces).[4] Figure 1 shows appropriate equilibrium crack-tip contours evaluated from Eq. 1(b). The solid contours represent displacements for planes initially separated by one Si–O–Si bond linkage distance across the crack plane, 0.32 nm; the circles along these contours correspond to this same linkage unit, and are to be taken as an indication of the average molecular density rather than of the true atomic structure. It is apparent that the strains ahead of the crack-tip origin are well beyond the Hookean range; the "bond" BB, for instance, has undergone a normal strain of 60%. The dashed contour in Fig. 1 represents the displacements for the initially contacting crack walls. From Eq. 1(b) it can be shown that this contour is parabolic with tip radius $\rho=(4/\pi)(K/E)^2$; for the equilibrium configuration shown, $\rho_c=0.14$ nm, which is less than one-half the intermolecular separation. Of course, as the crack enters the subcritical region, $K<K_c$, the radius becomes smaller still. It is clear, therefore, that the parabolic crack-tip contour is a physically meaningless concept in terms of the molecular structure; the continuum model cannot be used to describe curvature at the subatomic level. The conclusions drawn here, which can be demonstrated to apply to ceramics in general (at least at room temperatures), suggest that brittle cracks may be more realistically represented as narrow slits terminated at their ends by nonlinear connecting springs of atomic dimensions.

Before pursuing this point in detail it should be pointed out that there exist alternative viewpoints concerning the fundamental nature of crack processes in brittle materials. One of these takes note of the clear evidence for localized plastic zones at crack tips in metals and polymers, and argues that similar zones must exist in ceramics, even if on a submicroscopic scale.[5] Such plastic zones, it is claimed, are necessary to account for the fact that some ceramics have measured toughness values in excess of those expected from surface-energy considerations alone. In this view, fracture is effectively controlled by bulk deformation properties. Another modeling procedure, used extensively by those who study chemically assisted failure, involves the assumption that the crack tip is indeed rounded, and that fracture ensues as a result of some stress-enhanced "sharpening" mechanism (e. g. by preferential dissolution of the fissure walls).[6] Now it is surface chemistry which is the important factor. We should acknowledge here that neither of these two alternatives is totally inconsistent with the sharp-crack concept: for the first, *limited* plasticity (or any other energy-dissipating process) can occur within the near field without altering the essential nature of the sequential bond rupture mechanism; for the second, sharpening may well be feasible, but not beyond the limit of atomic dimensions as already discussed, in which case the model envisaged relates more properly to crack *initiation* from a starting *notch*. It is nevertheless our contention that a truly propagating brittle crack has certain properties that only a nonlinear, atomistic theory can predict, and in this sense the distinctions made above between the different approaches extend beyond the realm of mere semantics.

(2) *Direct Observations of Crack Tips and Interfaces: Transmission Electron Microscopy*

Until recently, virtually all the evidence cited in favor of one crack-tip model or another in brittle ceramics could be regarded as "circumstantial." Because of the extremely small scale on which the essential separation processes are expected to operate, direct, confirmatory observations have generally lain beyond the reach of ordinary microscopic techniques. (For a survey, see Ref. 7.) However, transmission electron microscopy (TEM), with its ultimate potential for resolving detail at the atomic level (albeit only in solids with a regular, crystalline array), has changed all that. The beautiful work of B. J. Hockey stands alone in this area,[8–10] and here we shall examine some of the findings from his observations which bear on the crack-tip question.

Hockey's studies have been carried out on four select materials, silicon, germanium, silicon carbide, and aluminum oxide, covering a broad spectrum of covalent-ionic bonding. Specimens are indented with a Vickers pyramid to produce the requisite cracks, and are then thinned into a foil, as indicated in Fig. 2(A). A typical TEM micrograph of the overall damage pattern produced is shown