Nonclassical Nucleation and Growth of Cohesive Tensile Cracks

John B. Rundle
Division 6231, Sandia National Laboratories, Albuquerque, New Mexico 87185

W. Klein
Center for Polymer Studies and Department of Physics, Boston University,
Boston, Massachusetts 02215

(Received 19 January 1989)

We analyze the nucleation and growth of cohesive tensile cracks using a field-theoretic formulation in which the free energy is written as a functional of the crack separation (offset field). Our results indicate that, for certain materials, crack nucleation and growth proceed through the formation and extension of a diffuse "halo" surrounding the classical portion of the crack. This is similar to nonclassical nucleation in magnetic systems. Theoretical considerations and numerical calculations strongly suggest that the diffuse halo can be identified with the fracture "process zone" seen in laboratory studies of advancing cracks.

PACS numbers: 64.60.Qb, 62.20.Mk

The theory of fracture began with the work of Griffith[1] who approached nucleation and growth of tensile cracks in a manner similar to the way that Gibbs treated the growth of bubbles in first-order phase transitions.[2] Under the application of a uniform tensile stress of magnitude p a crack of semilength l induces a free-energy change $\Delta F = -B^2 p^2 l^2 + 2\gamma l$, where 2γ is the energy needed to separate a unit of material at the crack tip and B depends on the elastic constants and the geometry of the solid body.[1,3,4] Crack growth occurs in the classical model when the force generated by the applied stress overcomes the resistance at the crack boundary, i.e., when $d\Delta F/dl = 0$.

The classical theory is reasonably successful in explaining fracture in brittle materials such as glass; however, crack growth in many other materials such as metals is not explained by the Griffith theory. In such materials nonclassical behavior arises from cohesion in the solid and is often manifested by the appearance of a fracture "process zone."[3,5,6] The process zone is a region of partial separation in advance of the classical crack tip and can be of considerable length compared to the classical portion of the crack.[6]

In this Letter we present a theory of fracture based on the analogy with nucleation.[7] This formulation provides a general framework that encompasses nonclassical as well as classical fracture mechanisms. Our primary result is that for certain classes of materials the crack consists of a classical part surrounded by a diffuse "halo" similar to nucleation in deeply quenched thermal systems.[8,9]

Our starting point is the observation that Griffith theory, usually thought of as describing the result of applying a variable stress p to a pre-existing crack of fixed semilength l, could equally well be a description of the growth of cracks of varying l in an applied stress field of fixed strength p. In this view, the Griffith theory is essentially a nucleation[2] theory which can be obtained from a "free-energy" functional.[10] The functional we propose[7] is of the form

$$F(\zeta) = \int d\mathbf{x} \left[-p\zeta(\mathbf{x}) + \tfrac{1}{2} \int d\mathbf{x}' \, T(\mathbf{x}-\mathbf{x}')\zeta(\mathbf{x})\zeta(\mathbf{x}') + 2\gamma' \{1 - \exp[-\zeta^2(\mathbf{x})/a^2]\} \right]. \quad (1)$$

In constructing $F(\zeta)$ we have assumed the following: (1) F is for a single lattice plane in the solid with lattice constant a. (2) The lattice plane is oriented along the x-z plane, while the tensile opening field $\zeta(\mathbf{x})$ (crack separation) and the applied stress p are normal to the lattice plane, i.e., along the y axis. Equation (1) will only describe the early, quasistatic, crack growth[10] since inertia, and hence phonon radiation, is neglected. As in nucleation in thermal systems we are assuming that the "nucleated" crack is growing so slowly that the surrounding material can be considered to be in thermal equilibrium. This is material dependent; however, one can say, in general, that the initial growth rate is proportional[8] to the inverse of the square of the radius of the nucleating droplet. For the systems we are considering this radius will be large.

The "interaction potential" $T(\mathbf{x}-\mathbf{x}')$ is a Euclidean tensor[7] of rank four. It describes the effect a separation at $\mathbf{x}$ has on a separation at $\mathbf{x}'$. In general, $T(\mathbf{x}-\mathbf{x}')$ is a complicated function of the material structure affected by, e.g., domain walls and defects. It does not, however, contain the effect of the local cohesive forces which are described by the exponential term in Eq. (1). The integral of $T(\mathbf{x}-\mathbf{x}')$ in a perfect infinite crystal is zero.

Attempts have been made[11,12] to calculate $T(\mathbf{x}-\mathbf{x}')$ from microscopic considerations; however, we take a different approach.[7] Since we are not interested here in calculating specific numerical quantities, but in providing a conceptual framework that encompasses nonclassical fracture mechanisms, the precise form of $T(\mathbf{x}-\mathbf{x}')$ is not important. Clearly, we require a specific form of $T(\mathbf{x}-\mathbf{x}')$ for our numerical calculations but for the discussion of the nucleation mechanism we will merely require that $T(\mathbf{x}-\mathbf{x}')$ is a function of $\mathbf{x}-\mathbf{x}'$. Therefore, the integral with respect to **x** or **x**′ is a constant, but otherwise arbitrary. Since we are considering metals and hence, systems with long-range order, we also expect that the second moment of $T(\mathbf{x}-\mathbf{x}')$ is large. This implies that saddle-point techniques[8,10,13] can be used to evaluate the nucleation process and that mean-field effects will be prominent.[8,14] It is also important to note that we assume $T(\mathbf{x}-\mathbf{x}')$ to be independent of time throughout the fracture process which also limits this approach to early time.

The term $2\gamma'\{1-\exp[-\zeta^2(\mathbf{x})/a^2]\}$ is the effective binding (free) energy due to the cohesive force of the intermolecular bonds. The quantity γ' is the binding-energy density. The derivative of the binding energy, the cohesive force, has a maximum at $\zeta(\mathbf{x})=a/\sqrt{2}$. If $T(\mathbf{x}-\mathbf{x}')$ were zero then separations greater than $a/\sqrt{2}$ would result in catastrophic crack growth. For nonzero $T(\mathbf{x}-\mathbf{x}')$ there is an additional contribution to the effective force which shifts the maximum beyond which catastrophic growth occurs. This maximum or limit of stability appears to play a role similar to that of the spinodal in thermal phase transitions. We will return to this point below.

To summarize, we consider materials with a definite but unknown past history which determines $T(\mathbf{x}-\mathbf{x}')$. The material is subjected to a constant external stress p which is assumed to have no effect on $T(\mathbf{x}-\mathbf{x}')$. Cracks appear in the material with a probability given by $\exp[-\beta F\{\zeta(\mathbf{x})\}]$, where $F\{\zeta(\mathbf{x})\}$ is given in Eq. (1). Because of the low probability of large cracks as well as the long-range nature of $T(\mathbf{x}-\mathbf{x}')$, the appearance of subcritical cracks should also have no effect on $T(\mathbf{x}-\mathbf{x}')$. We then equate the "critical crack" with the critical or nucleating droplet. Therefore, we search for saddle points[10] of the free-energy functional in Eq. (1).

The Euler-Lagrange equation is obtained by functional differentiation of Eq. (1):

$$-p+\int d\mathbf{x}'\,T(\mathbf{x}-\mathbf{x}')\zeta(\mathbf{x}') + \frac{4\gamma'}{a^2}\zeta(\mathbf{x})\exp\left[\frac{-\zeta^2(\mathbf{x})}{a^2}\right]=0\,. \tag{2}$$

The critical droplet, or crack, for a fixed p is a spatially localized solution of Eq. (2). However, substantial information can be obtained from the spatially uniform solutions which we will consider first. For constant $\zeta(\mathbf{x})=\zeta$, Eq. (2) becomes

$$p-T\zeta=\frac{4\gamma'}{a^2}\zeta\exp\left[\frac{-\zeta^2}{a^2}\right], \tag{3}$$

where $T=\int d\mathbf{x}'\,T(\mathbf{x}-\mathbf{x}')$. The right-hand side of Eq. (3) is plotted as the solid line in Fig. 1. The dashed line in Fig. 1 is the left-hand side of Eq. (3) with an arbitrary p and positive, but otherwise arbitrary, T. For this choice of p and T there are three solutions to Eq. (3). Points labeled A and C are minima of the free energy in Eq. (1) and the point labeled B is a maximum. Although point C, which is an absolute minimum, represents a stable solution to Eq. (2), it is physically uninteresting since the separation ζ is much larger than the lattice constant a. This state is unstable to external forces such as shear which are not included in our treatment. The maximum at point B is unstable. As p is increased a critical value $p_s(T)$ is reached where points A and B coalesce. This is the so-called spinodal line which has all the properties of a line of critical points.[15] Specifically, the quantity analogous to the surface tension in thermal problems vanishes at $p_s(T)$. In analogy to nucleation, the vanishing of the "surface tension" implies that the classical droplet is no longer the dominant form of fracture.[8,9] For T negative (dotted line in Fig. 1) the same considerations apply. These spinodals can only be reached by the application of fairly large stress if T is small or, for small applied stress, in systems with considerable defects.

There is another type of spinodal that may be important for fracture. There exists an instability in materials described by Eq. (1) to fluctuations with a nonzero wave vector. Returning to Eq. (2) we assume that ζ_0 is a constant solution. Writing $\zeta=\zeta_0+\phi(\mathbf{x})$, where $\phi(\mathbf{x})$ is assumed to be small, we linearize in $\phi(\mathbf{x})$, Fourier transform, and obtain

$$-\hat{T}(\mathbf{k})\hat{\phi}(\mathbf{k})=\frac{4\gamma'}{a^2}\exp\left[\frac{-\zeta_0^2}{a^2}\right]\left[1-\frac{2\zeta_0^2}{a^2}\right]\hat{\phi}(\mathbf{k})\,, \tag{4}$$

where $\hat{T}(\mathbf{k})$ and $\hat{\phi}(\mathbf{k})$ are the Fourier transforms of $T(\mathbf{x}-\mathbf{x}')$ and $\phi(\mathbf{x})$.

Nontrivial solutions to Eq. (4) imply that there can exist unstable modes in the system[14] when $\hat{T}(0)$ is small or even zero. This spinodal is similar to the one found in crystallization of fluids.[14,16]

Returning to Eq. (2) we consider localized or droplet solutions to the Euler-Lagrange equation. We estimate the solution to Eq. (2) near the spinodal generated by a positive value for T, i.e., the instability to $|\mathbf{k}|=0$ fluc-

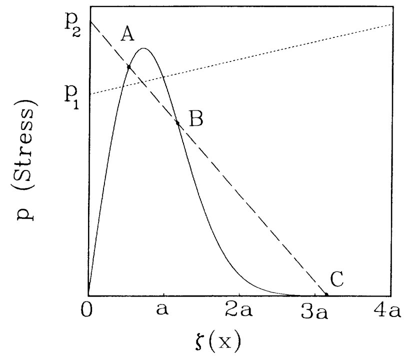

FIG. 1. The solid line is a schematic plot of the right-hand side of Eq. (3) as a function of ζ. The dashed and dotted lines are plots of the left-hand side of Eq. (3) for T positive and negative, respectively, and for different values of p.

tuations. This will be done analytically for a broad class of $T(\mathbf{x}-\mathbf{x}')$, and numerically for a particular choice.

Since we are considering the system near the spinodal we expect the critical fracture solution to Eq. (2) to be similar to a spinodal fluctuation in that it will be a large spatial extent low-amplitude droplet as seen in nucleation.[8,9] In addition, its Fourier transform should be strongly peaked about $|\mathbf{k}|=0$. This will be seen to be self-consistent.

Defining $\Delta p \equiv p_s - p$ and writing $\zeta(\mathbf{x}) = \zeta_0 + \psi(\mathbf{x})$, we expand the exponential in Eq. (2) keeping terms up to quadratic in $\psi(\mathbf{x})$. We also expand $\hat{T}(\mathbf{k})$ in powers of $|\mathbf{k}|$ and keep terms to second order. Combining these manipulations results in the equation for the crack profile $\psi(\mathbf{x})$:

$$-R^2\nabla^2\psi(\mathbf{x}) + \Delta p - a\psi^2(\mathbf{x}) = 0\,, \tag{5}$$

where $-R^2$ is the second moment of $T(\mathbf{x}-\mathbf{x}')$ which is assumed to be large and the coefficient of the ψ^2 term $(a>0)$ will not vanish at the spinodal $\Delta p = 0$.

Equation (5) is identical to the Euler-Lagrange equation obtained for nucleation near the spinodal in magnetic systems and binary fluids and alloys.[8,13] The solution to Eq. (5) is known[8] to be given in the form $\psi(\mathbf{x}) \sim (\Delta p)^{1/2}\tilde{\psi}(|\mathbf{x}|/\xi)$, where the correlation length $\xi \sim (\Delta p)^{-1/4}$. This is precisely the low-amplitude large-spatial-extent solution we expected.

Additional information about the structure of the critical cracks in this regime can be obtained from the analogy with nucleation. First, we should expect that the crack near the spinodal is a fractal and should be describable as a percolation cluster.[8,17] Second, the critical crack will become more classical or Griffith-like when the applied stress p is significantly less than p_s. From nucleation studies we know that the structure should be that of a Griffith-like classical crack surrounded by a fractal halo.[9] Third, we know that nonclassical nucleation and, by analogy, nonclassical fracture depends on the proximity of the spinodal. This in turn requires that there be some property of the system that stabilizes it against fracture for deep quenches, i.e., large p. From the nucleation studies[8] we know that stability requires that the parameter R in Eq. (5) be large. Consequently it is the second moment of the stress tensor $T(\mathbf{x}-\mathbf{x}')$ that determines the degree to which nonclassical fracture is important. This is, of course, material and history dependent.

In order to investigate the dynamic evolution of the fracture we adopt the form of $T(\mathbf{x}-\mathbf{x}')$ given in Eq. (6):

$$T(\mathbf{x}-\mathbf{x}') = -\left[\frac{2\mu}{a\pi(1-\nu)}\right]\frac{1}{(x-x')^2-1}\,, \tag{6}$$

where we have assumed symmetry in the z-coordinate direction and stress in the y direction. In Eq. (6), μ is the macroscopic shear modulus and ν is the macroscopic Poisson's ratio.[18] The form chosen for $T(\mathbf{x}-\mathbf{x}')$ is dic-

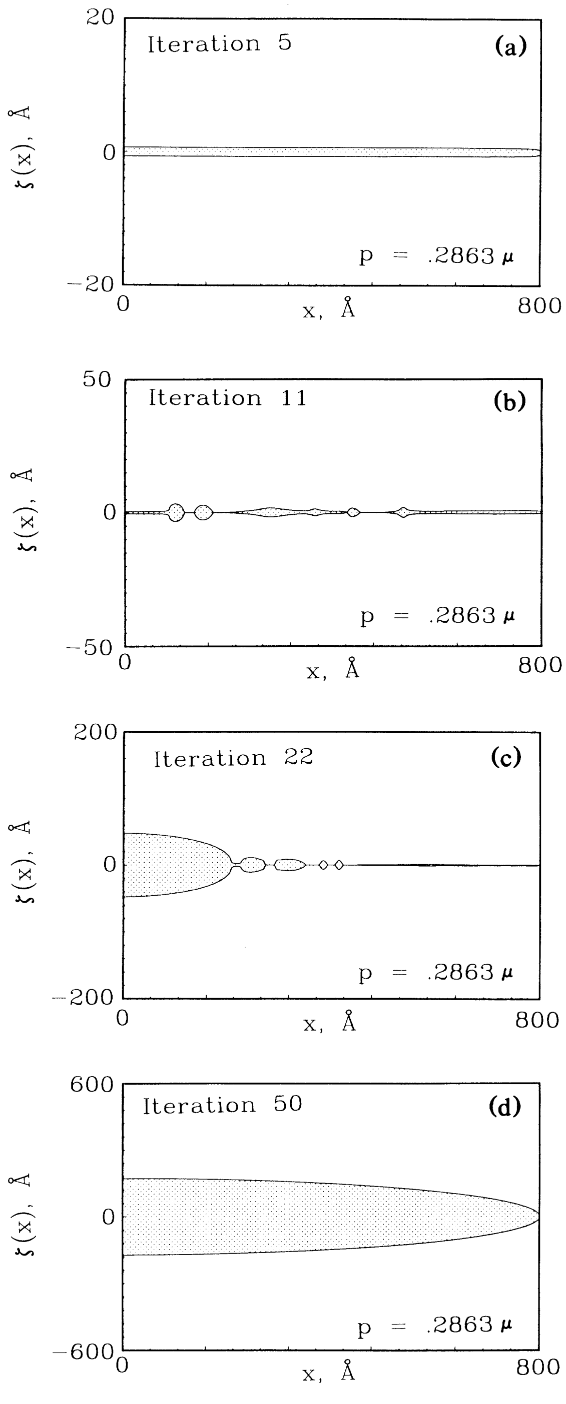

FIG. 2. Plot of the offset field $\psi(x)$ as a function of x for an applied uniform stress in the y direction. Symmetry is assumed in the z direction (out of the page). (a) After 5 iterations and before the noise is switched on; (b) after 11 iterations and the mean offset field is zero; (c) after 21 iterations (note change in vertical scale); and (d) after 50 iterations. These were generated with Langevin dynamics using the stress tensor in Eq. (6) with $\mu = 3\times10^{11}$ dyn/cm^2, $\nu = 0.25$, $\gamma' = 3\times10^{-9}\mu$, $p = 0.2863\mu$, and $a = 2$ Å.

tated by the assumption that on the coarse-grained length scales inherent in free energies of the form assumed in Eq. (1), the stress tensor can be taken as the elastic stress Green's function.[7] This is the stress tensor appropriate to a defect-free elastic solid and that $\int d\mathbf{x} \times T(\mathbf{x}-\mathbf{x}')=0$ when the solid is infinite.

Using Langevin dynamics with a Gaussian random noise we solve for the offset field ζ numerically in the region near the spinodal value of p. Specifically we coarse grain our system and iterate the equation of motion. It should be noted that the computational requirement of a finite system results in a finite positive value for T and a breaking of translation symmetry in the x direction.

The results of the computation are summarized in Fig. 2. In Fig. 2(a), the tensile offset is shown for the chosen value of p after five iterations and with no random noise. This is the value of the offset in the "metastable state." At five iterations the noise is turned on and for ten iterations the system fluctuates about the metastable state with no change in the average offset from that seen in Fig. 1(a). Figure 2(b) shows a representative lattice profile. At ~ 15 iterations the mean offset begins to grow, bubbles form and begin to more toward regions of a larger tensile force $\int d\mathbf{x}\,\zeta(\mathbf{x})T(\mathbf{x}-\mathbf{x}')$. Figure 2(c) shows a relatively late stage of this process. Finally, in Fig. 2(d) we show the crack evolved into a classical object.

Several interesting predictions as well as indications of directions of further research result from this work. First, there is considerable experimental evidence[5,19,20] in support of nonclassical crack extension by processes similar to those indicated in Fig. 2. The extension of cracks through the growth and absorption of voids in the nonclassical ramified region or process zone is generally termed "microvoid coalescence" or "dimple rupture" when it occurs in metals.[19,20] Usually this is attributed to pre-existing defects or inclusions but homogeneous fracture with microvoid coalescence also occurs.[20] In our model this process occurs as a consequence of the nucleation process contained in the free-energy functional of Eq. (1).

Second, our theory is general enough to contain both classical and nonclassical fracture. Moreover, a specific physical characteristic of the material, the second moment of $T(\mathbf{x}-\mathbf{x}')$, and the "spinodal" that goes along with large values of this moment, are seen to be necessary for nonclassical fracture.

Third, since nonclassical fracture is predicted to be the same as nonclassical nucleation we expect that the nonclassical fracture process starts before any increase is detected in the mean value of the offset field. This is the analog of the fractal droplet in magnetic systems which initiates the metastable state decay with no detectable magnetization change. In analogy with the nucleation problem, this implies that the nonclassical initial crack can be characterized as a particular type of percolation cluster. This has the additional benefit of severely limiting the kinds of percolation models that will give an accurate picture of fracture.[21]

Finally, the nucleation analog suggests several additional fracture mechanisms such as the instability to $|\mathbf{k}| \neq 0$ fluctuations discussed above. We can also suggest two experiments to further test our theory. If the process zone is a "spinodal effect" we would predict from our theory that the size of the process zone should increase with p for fixed large R as $[p_s(T)-p]^{-1/4}$ and should also increase linearly with R for large fixed p.

We wish to thank J. R. Rice for a helpful discussion. This research was supported by DOE Contract No. DE-AC04-76DP00789 and by Contract No. CD-11 from the NASA Crustal Dynamics Program at Sandia Laboratories and by a grant from the ONR at Boston University.

---

[1] A. A. Griffith, Philos. Trans. Roy. Soc. London A **221**, 163 (1920).

[2] See, for example, A. C. Zettlemoyer, *Nucleation* (Dekker, New York, 1969).

[3] See, for example, M. Kanninen and C. H. Popelar, *Advanced Fracture Mechanics* (Oxford, New York, 1985).

[4] G. R. Irwin, *Fracture of Metals* (American Society for Metals, Metals Park, OH, 1948).

[5] D. S. Dugdale, J. Mech. Phys. Solids **8**, 100 (1960).

[6] P. L. Swanson, in *Fracture Mechanics of Ceramics,* edited by R. C. Bradt (Plenum, New York, 1986), Vol. 8; J. F. Labuz, S. P. Shaw, and C. H. Dowding, J. Rock Mech. Min. Sci. **24**, 235 (1987).

[7] J. B. Rundle, J. Geophys. Res. (to be published).

[8] C. Unger and W. Klein, Phys. Rev. B **29**, 2698 (1984).

[9] C. Unger and W. Klein, Phys. Rev. B **31**, 6127 (1985).

[10] J. S. Langer, Ann. Phys. (N.Y.) **41**, 108 (1967).

[11] R. Thomson, V. K. Tewary, and K. Masuda-Jindo, J. Mater. Res. **2**, 619 (1987), and references therein.

[12] G. J. Dienes and A. Paskin, in *Atomistics of Fracture,* edited by R. M. Latanison and J. R. Pickens (Plenum, New York, 1983).

[13] J. W. Cahn and J. E. Hilliard, J. Chem. Phys. **28**, 258 (1958).

[14] W. Klein and F. Leyvraz, Phys. Rev. Lett. **57**, 2845 (1986).

[15] D. W. Heermann, W. Klein, and D. Stauffer, Phys. Rev. Lett. **49**, 1262 (1982).

[16] J. Yang, H. Gould, and W. Klein, Phys. Rev. Lett. **60**, 2665 (1988).

[17] L. Monette, W. Klein, M. Zuckermann, A. Khadir, and R. Harris, Phys. Rev. B **38**, 11 607 (1988).

[18] S. K. Crouch, Internat. J. Numer. Methods Engrg. **10**, 301 (1976).

[19] R. B. Bates, in *Fracture: Interactions of Microstructure, Mechanisms and Mechanics,* edited by J. M. Wells and J. D. Landes (The Metallurgical Society of the ASME, New York, 1984).

[20] C. D. Beachem, Trans. Am. Soc. Met. **56**, 318 (1963), and references therein.

[21] B. Khang, G. G. Batrouni, S. Redner, L. de Arcangelis, and H. J. Herrmann Phys. Rev. B **37**, 7625 (1988), and references therein.