FORMAL CONSIDERATIONS ABOUT FRACTURE: NUCLEATION AND GROWTH

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ABSTRACT

In this paper, we will answer several abstract, formal questions about the nature of crack growth and nucleation. Bringing a field theory point of view to fracture illuminates things in what I hope will be an entertaining way.

Formally, what is the crack nucleation rate? Fracture is an instability of elastic theory under tension. For thermally nucleated cracks, there is an analogy with supercooled liquids. Here the crack nucleation rate can be thought of as an imaginary part of the free energy - giving the decay rate of the metastable, stretched material. As an amusing consequence, we can formally calculate the asymptotic form for the high-order nonlinear elastic coefficients, and explicitly show that elastic theory has zero radius of convergence.

Formally, can we derive the the crack growth laws from symmetry? We can describe mixed-mode three-dimensional fracture as a moving curve in space, decorated with a description of the local crack plane, and driven by the stress intensity factors along the crack. Imposing the symmetries gives us the form of the crack growth laws in two dimensions, explaining the (well-known) fact that cracks under shear (mode II) abruptly turn until the stress becomes purely extensional (mode I). The form of the crack growth law in three dimensions will be derived, and linear stability analysis for mixed-mode fracture will be briefly summarized, with connection to factory-roof morphologies.

KEYWORDS

fracture, crack, nucleation, growth, thermal, evolution, factory roof

INTRODUCTION

In this paper, I will summarize formal work done in collaboration with Jennifer Hodgdon[1] and Alex Buchel[2, 3] on nucleation and growth of cracks in brittle, isotropic, homogeneous materials. This work is formal in the sense that bring to the problem the perspectives and approaches of theoretical physics: we'll be asking fundamental questions that most of the participants in this conference wouldn't think to ask. Sometimes answering very basic questions can be illuminating; in any case I hope it will be entertaining.

CRACK NUCLEATION

What is the crack nucleation rate? In a practical context, one may ask what the failure rate is of a component in a machine: the number of breakages per unit time. This definition depends on the size and shape of the object and the external loading. More generally, for a given material under a given load, there will be a rate of crack formation per unit volume per unit time.

the material (grain boundaries, surface heterogeneities, pre-existing microcracks, dislocation tangles). These heterogeneities usually evolve in time (fatigue, work hardening, electromigration, void formation). This makes the failure rate history dependent, and too complicated a problem to start with. So, we'll focus on brittle fracture, where we perhaps can assume that the material far from the crack tip does not irreversibly transform.

With this approximation, we have two cases. (1) The important case is when the failure is due to the inhomogeneities: distributions of microcracks[4], distributions of bond strengths[5], or other randomness[6]. In all of these cases, the rate is number of failures for a given increment of strain, not per unit time. Either the stress is large enough to trigger failure or not: a given sample, if it survives the initial loading, will survive forever. This leads to some elegant theories and simulations, but isn't what I'm focusing on today. (2) The case we study is when the material is homogeneous, and the failure is triggered by a thermal fluctuation. This basically never happens, but it's an interesting theoretical problem.

So, fundamentally, what is the fracture nucleation rate for our brittle, homogeneous material? This is actually a deep theoretical physics question. The basic problem is defining what is meant at finite temperature by a material under tension. The lowest energy state (free energy, to be pedantic) for a large cube of brittle material under external strain can easily be seen to be broken in two. The elastic energy released is proportional to the volume; the surface energy cost is proportional to the cross-sectional area; for fixed external strain there will be a length at which breaking wins. One should note that this breaking strain in real materials isn't very large: a cubic meter of iron will prefer to break in two when stretched by 10μm ($140\ \mu$m if one includes the energy lost due to plastic deformation during fracture).

Crack nucleation is precisely the mechanism by which a material goes from the metastable stretched state to the state which is broken in two. There is a close analogy to the nucleation of crystals in supercooled liquids. In supercooled liquids[7] the liquid is a metastable state with a decay rate given by the thermal probability of generating a critical nucleus. For fracture, the stretched state is a metastable state with a decay rate given by the thermal probability of generating a crack of the size given by the Griffiths threshold.

(The analogy even extends to the practicality of the thermal nucleation mechanisms. Homogeneous nucleation of crystals in supercooled liquids almost never happens: the crystal almost always nucleates on a dust particle, or on the surface...)

Let's do this calculation explicitly, for a two-dimensional straight crack of length ℓ, in a medium under external hydrostatic tension (a pressure $P < 0$). One can solve the elastic equations to find the energy of this crack. Let α be the surface energy (energy per unit length, in two dimensions, of the crack surface), Y be the Youngs modulus, and σ be Poisson's ratio. If we define a critical crack length ℓ_c (the Griffiths[8] threshold) by

$$\ell_c = 4Y\alpha/\pi P^2(1 - \sigma^2) \tag{1}$$

then the energy of the crack is

$$E = 2\alpha\ell - \alpha\ell^2/\ell_c. \tag{2}$$

It follows that cracks with $\ell > \ell_c$ will grow to lower their energy, and that cracks with $\ell < \ell_c$ will heal (at least in our model). The energy at the top of the barrier is $E(\ell_c) = \alpha\ell_c = 4Y\alpha^2/(\pi P^2(1 - \sigma^2))$, and the probability for this critical crack to form by a thermal fluctuation is suppressed by the Boltzmann factor $\exp(-E(\ell_c)/k_BT)$. The fracture nucleation rate $\Gamma_{failure}$ per unit volume per unit time will be given by some prefactor times this Boltzmann factor:

$$\Gamma_{failure} = \Gamma_0 \exp(-E(\ell_c)/k_BT). \tag{3}$$

(Calculating this prefactor Γ_0 is quite a subtle problem[3].)

This calculation is precisely analogous to the corresponding one for a critical nucleus of solid forming in a supercooled liquid[7]. Indeed, the crack as it nucleates will be filled by a gas of vapor atoms (think of fracture in a piece of dry ice, where the vapor pressure isn't vanishingly small). The spontaneous fracture rate is precisely the nucleation rate of a gas forming in a super-stretched crystal.

Remember, though, that we claimed from a fundamental point of view the difficulty is defining the stretched material. A stretched piece of material is fundamentally a transient: how do we use equilibrium statistical mechanics to study what is only a metastable equilibrium? The precise definition of the stretched, metastable state is as an analytical continuation from the compressed state[7, 2]. In particular, suppose we study the

include the effects of thermal fluctuations producing small cracks, and then analytically continue $E(P)$ to negative pressure, one can show that it becomes complex! The decay rate (3) is proportional to the imaginary part of the energy:

$$\mathrm{Im}E(P) = C\Gamma_{failure}(P) = E_0 \exp\left(-4Y\alpha^2/\pi P^2(1-\sigma^2)k_BT\right). \tag{4}$$

Metastable states in statistical mechanics are defined by an analytic continuation of the (free) energy. The nucleation rate is defined as a particular dynamical constant prefactor Γ_0/E_0 times the imaginary part of this complex energy.

What can we derive from this formal imaginary part to the energy? The real part of the energy is related to the bulk modulus? Let's define the pressure-dependent bulk modulus $K(P)$ by

$$\frac{1}{K(P)} = -\frac{1}{V}\left(\frac{\partial V}{\partial P}\right)_T = -\frac{1}{PA}\left(\frac{\partial \mathrm{Re}(E)}{\partial P}\right)_T = c_0 + c_1 P + c_2 P^2 \cdots + c_n P^n + \cdots \tag{5}$$

where the elastic material has cross-sectional area A. c_0 is the inverse of the normal bulk modulus, and the higher order terms c_n represent nonlinear elastic coefficients. These are normally ignored, because by the time they become important plastic deformation or fracture has set in, but in principle a careful experiment could measure them. Now, if $E(P)$ is an analytic function, then it obeys Cauchy's theorem,

$$E(-P) = 1/2\pi i \oint_\gamma E(T)/T + PdT = 1/2\pi i \oint_\gamma E(T)/T \sum_{n=0}^\infty (P/T)^n dT. \tag{6}$$

with γ circling $-P$ in the complex plane. Because it divides by i, it can be used to write the real part of the free energy $E(P)$ in terms of the imaginary part. Exchanging the sum and the integral, choosing contours and checking asymptotics, we can calculate the n-th nonlinear elastic constant in equation 5 asymptotically for large n:

$$c_n \to (-1)^n(n+2)/\pi A \int_0^B \mathrm{Im}E(T)/T^{n+1}dT \tag{7}$$

So because the (complex) energy is an analytic function, the high-order nonlinear elastic constants are related to the fracture rate.

We used this to answer an extremely formal question. What is the radius of convergence of nonlinear elastic theory? We can use the ratio test: the radius of convergence equals the ratio c_n/c_{n+1} as $n \to \infty$. Using (7) and (4) and doing the integrals, we find

$$c_n/c_{n+1} \to -n^{-1/2}\left(8\beta Y\alpha^2/\pi(1-\sigma^2)\right)^{1/2} \quad \text{as n} \to \infty. \tag{8}$$

(Doing the prefactor carefully[3] with various continuum limits leaves this expression unchanged, except that the surface tension α becomes the temperature-dependent surface free energy.) The ratio goes as $n^{-1/2}$, and the radius of convergence is zero.

Should we be concerned? Hooke's law is the first term of a series that doesn't converge? First, the physical origin of this is that our brittle material is in principle unstable as soon as the pressure P becomes negative. If you're not concerned about the fact that your bridges in theory will eventually fall down because of thermal crack nucleation, perhaps the associated non-convergence of Hooke's law shouldn't distress you. Indeed, thermal fluctuations are probably too weak to make observable effects in any measurement of the nonlinear elastic constants. Second, nonlinear elastic theory has lots of company: quantum electrodynamics[9] (the most quantitatively successful theory in physics) and Stirling's series for $n!$ also have zero radius of convergence.

Intellectual curiosity aside, what of practical importance can we glean from our calculation? First, perhaps the high-order nonlinear elastic constants of disordered materials might be computed by similar means, and (disorder being important to the fracture rate) might have effects large enough to measure. Second, the imaginary part of the frequency dependent elastic constants are related to viscosities: perhaps considering both external strain and frequency together might be illuminating (vibration-induced thermal fracture rates?)

and might relate to the plastic flow rate at very early stages (before work hardening sets in). The corresponding problem in two dimensions has been well studied,[10] but it seems likely that tangling of dislocations dominates in three dimensions.

CRACK GROWTH LAWS

What are the crack growth laws? On long length and time scales, most macroscopic systems obey simple laws of motion, which depend on the properties of the material only through setting constants (like density and elastic constants) or functions (like surface energies including the crystalline anisotropy). Can we deduce the laws describing the growth of a crack front, coarse-graining over all the atoms, grains, precipitates, and plastic deformation near the crack tip, to get relatively simple laws depending on only a few materials parameters or functions?

Jennifer Hodgdon and I studied this problem, inspired by conversations with Tony Ingraffea and members of his group. Ingraffea's group[11] solves the hard part of the problem: given a complicated, three-dimensional crack, they can tell us the stress intensity along the crack tip. All they wanted was the rules for advancing the crack forward in time. The simplest problem for us to study, and the one of most current interest to their group, was quasistatic fracture in an isotropic, homogeneous medium. Including crystalline anisotropy would lead us to the physics of cleavage along the crystalline planes. Including random inhomogeneities into theories of brittle fracture leads to logarithmically rough fracture surfaces[12], but not as rugged as the experiments[13]. Including the inertial dynamics of the growing front leads to interesting traveling waves along the crack front[14] that might improve the agreement with experiment. In ductile and intergranular fracture, the roughness reflects void growth and the presence of grains and inclusions.[15] Our work did not include any of these effects.

Naturally, Ingraffea's group already had a working solution. For mode I fracture, the material is described by a crack growth velocity $v(K_I)$. For mode II fracture, the crack turns abruptly until it is mode I (the principle of local symmetry[16]). There were two other rules in the literature for picking the crack growth direction: one maximizing the energy release[17], and one moving into the direction of minimum strain energy density[18]. All three rules seemed to predict crack paths which agreed well with one another[19]. At that time (around 1990) they were just moving into 3D fracture, and were quite interested in more crack growth laws for more general geometries.

Jennifer Hodgdon and I decided to try to write the most general crack growth law allowed by symmetry. Let us describe the local crack front with an orthonormal triad of vectors: $\hat{\mathbf{b}}$ perpendicular to the local crack face, $\hat{\mathbf{t}}$ tangent to the crack front, and $\hat{\mathbf{n}}$ pointing in the direction along which the crack was last growing. Our theory is valid on long length and time scales: in particular, we assume that the curvatures of the the radii of curvatures for the crack surface and crack front are large, so to zeroth order the crack is straight and flat (we'll expand in the curvatures). There are then three symmetries of the crack: the reflection R_{plane} in the $\hat{\mathbf{n}} - \hat{\mathbf{t}}$ plane of the crack, the reflection R_{cross} in the $\hat{\mathbf{n}} - \hat{\mathbf{b}}$ plane perpendicular to the crack front $\hat{\mathbf{t}}$, and the 180° rotation about $\hat{\mathbf{n}}$ (which is the product of the two other symmetries).

The first convenient thing to fall out of the symmetry analysis is the decomposition of the strain field into modes. The linear elastic solution near the crack tip can be decomposed into a superposition of solutions with definite symmetries under R_{plane} and R_{cross}. Mode I is symmetric under both transformations, mode II is antisymmetric under reflections in the plane but symmetric to reflections perpendicular to the front, and mode III is antisymmetric under both. Jennifer found that there was yet another mode (mode IV?) which is symmetric under R_{plane} and antisymmetric under R_{cross}. Presumably Hodgdon's mode IV is usually ignored because it does not introduce a crack opening.

We then assume that the body being cracked and the radii of curvature of the local crack front and crack surface are all large compared to the inhomogeneities in the material and the nonlinear zone around the crack tip. This is what is needed to ensure that there is a region around the crack tip where the elastic displacement fields scale with the square root of the distance r to the crack tip. (In general[1, 20] the displacement field for each mode can be expanded in a series of all half-integer powers of r. The less singular terms are important only far from the crack, and are determined by the boundary conditions and the crack shape; the more singular

for example, we describe ductile fracture only if the body is much larger than the plastic zone. We write the growth laws of the crack in terms of the three stress-intensity factors K_I, K_{II}, and K_{III} in this (so-called K-dominant) region, their gradients along the crack front, and the curvatures of the crack front and crack surface. We impose the symmetries of the problem described above, plus a gauge symmetry[21, 1] associated with reparameterization of the crack front, to find the most general law of motion allowed by symmetry.

In two dimensions, we found that the most general crack growth law was of the form

$$\partial \mathbf{x}/\partial t = v(K_I, K_{II}^2, K_{III}^2)\hat{\mathbf{n}}, \qquad\qquad \partial\hat{\mathbf{n}}/\partial t = -f(K_I, K_{II}^2, K_{III}^2)K_{II}\hat{\mathbf{b}}, \qquad (9)$$

where $\mathbf{x}$ is the location of the crack tip, v is the velocity of the crack, and f represents the tendency for a crack to turn under the external load (hence changing the direction $\hat{\mathbf{n}}$ pointing along the crack).

What does this equation imply about the crack growth? If $K_{II} = 0$, the crack won't turn; otherwise it will turn (if $f > 0$) so as to reduce K_{II} in magnitude. Thus we agree with the principle of local symmetry, except that our cracks will turn gradually towards this direction, rather than jump abruptly to the new orientation. Over what turning radius does our crack turn? Using results of Cotterell and Rice[22], Hodgdon showed that if the angle of the crack differs from the angle that makes $K_{II} = 0$ by a small amount $\Delta\theta$, then $K_{II} = K_I\Delta\theta/2$; this implies that $\Delta\theta \ \exp(-fK_I x/2v)$, and the angle decays exponentially to pure mode I with a material-dependent decay length of $2v/fK_I$. We expect this length scale to be set by a microscopic scale characteristic of the material: the atomic size in a glass, the size of the nonlinear zone in a ductile material, etc. This means, in essence, that our analysis agrees with the traditional prescription that the crack turns abruptly. We think of writing the crack growth laws as differential equations replaces the atomistic short-distance cutoff with a smooth one.

Our analysis did not make any assumptions about microscopic mechanisms. We believe that arguing whether the crack turns to maximize the energy release or minimize the strain energy density is misguided: if you turn the crack according to the wrong rule, in the succeeding step it'll keep turning and you'll converge to the same final trajectory (making $K_{II} = 0$) with a radius of curvature given by the step size in your algorithm.

So much for reinventing what's already known. What about three dimensions? Now everything depends on where we are along the crack front. If we let s measure arclength along the crack front, then up to first order in gradients

$$
\begin{aligned}
\partial x/\partial t = &\qquad\qquad\qquad v\hat{n} + w\hat{t} \\
\partial\hat{n}/\partial t = &\ -\left[\frac{\partial v}{\partial s} + w\frac{\partial\hat{t}}{\partial s}\cdot\hat{n}\right]\hat{t} + \left[-fK_{II} + g_I K_{III}\frac{\partial K_I}{\partial s} + g_{II}K_{II}K_{III}\frac{\partial K_{II}}{\partial s} + g_{III}\frac{\partial K_{III}}{\partial s} + \right. \\
&\ \left. h_{tb}\frac{\partial\hat{t}}{\partial s}\cdot\hat{b} + h_{nt}K_{II}\frac{\partial\hat{n}}{\partial s}\cdot\hat{t} + (h_{nb}K_{II}K_{III} + w)\frac{\partial\hat{n}}{\partial s}\cdot\hat{b}\right]\hat{b},
\end{aligned}
$$
$$(10)$$

where f, g_α, and h_{ij} are functions of K_I, K_{II}^2, and K_{III}^2, and the velocity v can be a function of these and a number of gradient terms[1]. Only f among these constants, which gives the turning radius for mode II fracture, is expected to be large (as discussed above): the others should be all of the same order of magnitude.

What can we do with this expression? First, if the crack begins nearly flat and straight, we can do perturbation theory to see if the crack becomes flatter and straighter, or if it goes unstable. Jennifer Hodgdon[23] found that cracks under mode I are stable (as expected), but that cracks under mixed mode I and mode III (twisting) can be stable or unstable depending on the materials constants: in particular, if $g_I > 0$, steady-state mode III cracks are unstable to small perturbations. Experimentally, she found that cracks under mode III turned to form a helical crack surface: such turning wasn't allowed for in our perturbation theory, which assumed periodic boundary conditions. Others find, for longer cracks, that mode III fracture is unstable to the formation of a "factory roof" morphology. It wasn't possible at the time to test Hodgdon's results with realistic crack-growth simulations, and this work remains unpublished.[23]

Second, we can use it to propagate real 3D cracks in simulations, and compare to experiments and more microscopic simulations. I anticipate that our symmetry analysis will prove important and useful, but that there will be additional internal variables (perhaps crack-tip curvature[24]) that will be necessary for describing the crack, and which may induce crack branching and other effects missing in our existing theory.

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