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MODELING CRACK PROPAGATION: A PHASE FIELD APPROACH

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ABSTRACT

We present a continuum phase field model for crack propagation. It includes a phase field that is proportional to the mass density and a displacement field that is governed by linear elastic theory.

The phase field smoothes the sharp interface, enabling us to use equations of motion for the material rather than for the interface and thus avoiding front tracking. The interface dynamics thus emerges naturally, without making phenomenological assumptions about the crack dynamics. Our model is physically motivated, yet it avoids being specific; it does not focus on a particular material, which makes it easier to identify the basic principles of crack behavior.

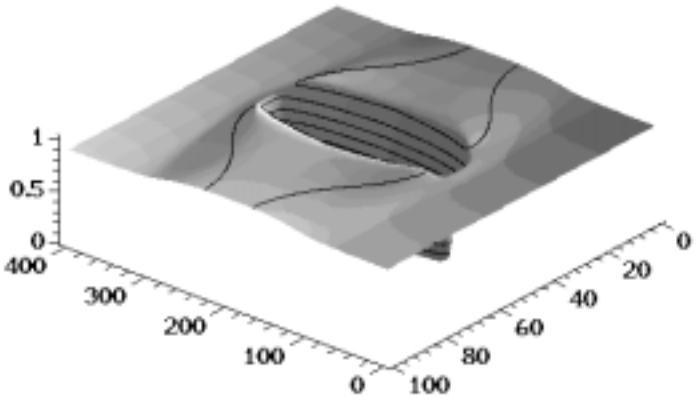

Figure 1: *A surface plot of a phase field with a growing double-ended crack.*

KEYWORDS

Fracture, phase field, multiscale, finite difference.

INTRODUCTION

The study of fracture is usually approached using mathematical descriptions and numerical simulations based on empirical observations. Finite element methods are commonly used to investigate the behavior of fractured materials on a large scale. Though these methods work well in most cases, the equations are mainly based on experimental observations.

We present a continuum description starting from basic theoretical assumptions. We introduce a phase field model, originally used to describe thermodynamic phase transitions and widely used to model solidification[1], and combine it with a displacement field. The phase field serves two main purposes. First, it smears out any sharp interfaces, averaging out microscopic detail and leaving only the necessary macroscopic variables. Second, the model gives equations of motion for the material rather than the boundaries, thus front-tracking is avoided. One of our main goals is to find macroscopic fracture laws.

The next section gives an outline of the theoretical model, presenting the main equations. This is followed by a discussion of the numerical implementation. We then describe our procedures for measuring the Griffith's threshold, before giving some concluding remarks.

THE FRACTURE MODEL

The model consists of a phase field ϕ and a displacement field $\mathbf{u}$. The former is interpreted as the normalized mass density, and typically has values between zero and one. The latter, through its derivatives, represents strain in the material. The model is based on a free energy $\mathcal{F}$ that is constructed so that the equations of motion (2–3) minimize the energy $\mathcal{F}$ with respect to time (that is, $d\mathcal{F}/dt < 0$). The free energy is given by

$$\mathcal{F} = \int_V \left(\frac{w^2}{2} |\nabla \phi|^2 + \frac{h^2}{4} \phi^2 (1 - \phi - \nabla \cdot \mathbf{u})^2 + \phi^2 \mathcal{E}(\epsilon) \right) dV \,, \tag{1}$$

where V is the volume of the system. The first term in the integrand is a gradient term discouraging spatial fluctuations in the phase field. The parameter w is proportional to the interface width. The second term is a Ginzburg-Landau double well potential, favoring values of ϕ at zero and $1 - \nabla \cdot \mathbf{u}$, representing the two phases vacuum and solid, respectively. If the material is completely unstrained, then $\nabla \cdot \mathbf{u} \equiv 0$ and the upper value is one, otherwise this value is either somewhat higher (for a compressed material) or lower (for a stretched material). The factor $1 - \phi - \nabla \cdot \mathbf{u}$ can be thought of as a density of vacancies or interstitials. The parameter h controls the height of the barrier between the vacuum and solid phases. The last term is the elastic strain energy density $\mathcal{E}(\epsilon) = (1/2) C_{ijkl} \epsilon_{kl} \epsilon_{ij}$. For a homogeneous, isotropic material, the tensor C_{ijkl} can be described by the two Lamé constants μ (the shear modulus) and λ by $C_{ijkl} \epsilon_{kl} \epsilon_{ij} = (\lambda \epsilon_{mm} \delta_{ij} + 2\mu \epsilon_{ij}) \epsilon_{ij}$. Since the elastic energy is only defined in the material (that is, $\phi \neq 0$), $\mathcal{E}(\epsilon)$ is multiplied by a factor of ϕ^2; thus the strain energy will go to zero in the vacuum. The strain is related to the displacement field by $\epsilon_{ij} = (\partial_j u_i + \partial_i u_j)/2$. This means that the divergence of the displacement field is just the trace of the strain, $\nabla \cdot \mathbf{u} = \epsilon_{mm}$.

The equations of motion for the phase field ϕ and displacement field $\mathbf{u}$ are

$$\frac{\partial \mathbf{u}}{\partial t} = -\frac{1}{\eta} \left(\frac{\delta \mathcal{F}}{\delta \mathbf{u}} + \phi \nabla \frac{\delta \mathcal{F}}{\delta \phi} \right) \tag{2}$$

$$\frac{\partial \phi}{\partial t} = -\nabla \cdot \mathbf{J} \qquad \mathbf{J} = -D \nabla \frac{\delta \mathcal{F}}{\delta \phi} + \phi \frac{\partial \mathbf{u}}{\partial t} \tag{3}$$

where η and D are the viscosity and the diffusion constant, respectively. Note that Equation (3) is the continuity equation. This means that total ϕ, or mass, is conserved. The first term in $\mathbf{J}$ is a diffusion

term, while the second term makes sure that the mass follows the motion of the displacement field. The evolution of the fields are constructed to be over-damped and downhill in the free energy.

The Lamé constants are connected through Poisson's ratio ν by $\lambda = 2\mu\nu/(1-2\nu)$ [2]. In the case of plane strain, the $\nabla \cdot \mathbf{u}$ term in the double well potential turns out to be crucial to preserve this relation.

NUMERICS

We have implemented Equations (2) and (3) for a plane strain system. Thus we can perform our simulations on a two-dimensional regular finite difference grid with periodic boundary conditions in both directions. We have investigated both single-ended and double-ended cracks under mode I loading, see Figure 2.

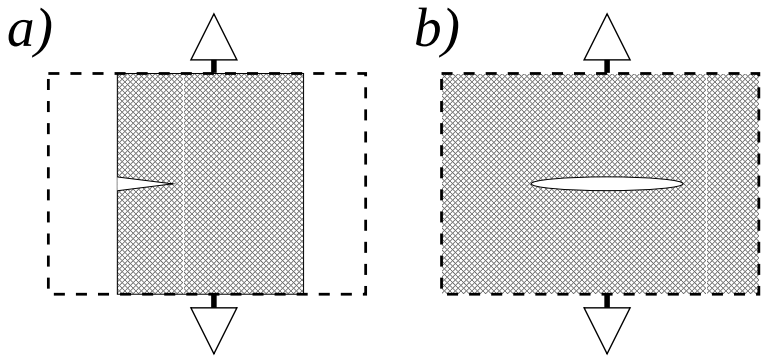

Figure 2: *A strained material with a (a) single-ended or a (b) double-ended crack. The arrows indicate the loading direction, the dashed lines the periodic boundaries.*

The system is initially strained in the y-direction with a uniform constant strain s. The strain is represented through the spatial derivatives of the displacement field $\mathbf{u}$, which means that there is an inherent discontinuity in the strain field at the y-boundary. This problem has been resolved using "skew-periodic" boundary conditions. In essence, we identify $\mathbf{u}$ on the bottom with $\mathbf{u} + \Delta\mathbf{u}$ on the top where $\Delta\mathbf{u}$ parameterizes the applied strain. Thus the strain remains continuous across the boundary. In addition to inserting a constant-slope displacement field in the y-direction, the phase field is altered from 1 to $1 - \nabla \cdot \mathbf{u}$. This is to account for the change in mass density if a material is stretched or compressed.

After straining the sample in the y-direction, a double ended crack, or slit, is inserted by removing mass (that is, setting the phase field to zero) in an elongated rectangular area in the center. The crack will grow if the strain is above some threshold value as given by the Griffith's criterion. One of our first tasks was to find this threshold value (see below).

The model described above has two different mechanisms for moving mass. One is a very slow process, which we identify as diffusion. The other is more rapid, where the phase field moves with the displacement field.

The periodic boundary conditions of the finite-difference grid allows the use of Fourier methods. To increase stability, we implemented a semi-implicit scheme[3]. The implicit parts can be solved analytically in Fourier space, which increases efficiency considerably.

MEASURING GRIFFITH'S CRITERION

One way of finding the Griffith's threshold is to measure the energy density (per unit length) of a cracked, relaxed system (that is, find the surface energy), and compare it to the energy density of a strained unfractured material. A small concern is that the measured surface energy can vary significantly if the crack is too narrow or the energy is measured too soon after the crack tip has passed. The energy of the unfractured material is just a special case of Equation (1) with $\partial_y u_y = s = \text{constant}$, $\partial_x u_x = -\nu s$ and $\phi = 1 - \nabla \cdot \mathbf{u}$; using $\lambda = 2\mu\nu/(1-2\nu)$, we get the relation

$$\mathcal{F} \approx \mu(1+\nu)s^2\,, \qquad \text{for } s \ll 1\,. \tag{4}$$

Taking the difference between the energy density in front of and behind the crack gives the energy released as a strained material is fractured and relaxed. The Griffith's criterion is reached when the strain is so low that the energy on both sides of the crack tip are the same. In our model, this happens at around 4% strain with our current choice of parameters.

Another way of finding the Griffith's criterion is by comparing the crack velocity to the energy release rate $\mathcal{G}$. This can be done using the J-integral[4]. The J-integral must be positive for the crack to grow. If the crack is parallel to the x-axis, the energy release rate $\mathcal{G}$ is equivalent to the x-component of the J-integral, J_x. Instead of performing the contour line-integral, it is common to convert it to an area-integral for increased accuracy when doing the integral numerically. The area integral is defined as

$$J_x = -\int_A \Omega(x,y)\,dx\,dy \tag{5}$$

where $\Omega(x,y) = W\partial_x q - \sigma_{ij}\partial_x u_i \partial_{x_j} q$ and $W = \phi^2 \mathcal{E}(\epsilon)$. Here q is a function that is unity around the crack tip and zero outside. Notice that if q is constant in a region, $\Omega(x,y) \equiv 0$, so in effect the line integral is replaced by a "thick line" contour integral, where the "thick line" exists everywhere q has a gradient.

CONCLUSION

We have presented a continuum phase field model of fracture, where the free energy and equations of motion are based on basic descriptions of thermodynamics. The fracture interfaces emerge and evolve naturally, avoiding the need for front tracking and phenomenological assumptions of crack growth laws. One of our main goals is to find macroscopic fracture laws.

Future work may include general three dimensional simulations, and spatial and temporal noise to represent inhomogeneities and plasticity.

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