

## Phase Field Modeling of Fast Crack Propagation

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We present a continuum theory which predicts the steady state propagation of cracks. The theory overcomes the usual problem of a finite time cusp singularity of the Grinfeld instability by the inclusion of elastodynamic effects which restore selection of the steady state tip radius and velocity. We developed a phase-field model for elastically induced phase transitions; in the limit of small or vanishing elastic coefficients in the new phase, fracture can be studied. The simulations confirm analytical predictions for fast crack propagation.

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Understanding the day-to-day phenomenon of fracture is a major challenge for solid state physics and materials science. Starting with the early idea of Griffith [1], who realized that crack growth is a competition between a release of elastic energy and an increase of surface energy, various approaches have been developed to describe the striking features of cracks [2]. Usually, the motion of cracks is understood on the level of breaking bonds at sharp tips, and obviously theoretical predictions depend sensitively on the underlying empirical models of the atomic properties (see, for example, Ref. [3]). Plastic effects, however, lead to extended crack tips (finite tip radius  $r_0$ ), and it is conceivable that, for example, fracture in gels can be described macroscopically. Then a full modeling of fracture should not only determine the crack speed but also the crack shape self-consistently.

Recent phase-field models go beyond the microscopic limit of discrete models with broken translational and rotational symmetry, and encompass much of the expected behavior of cracks [4,5]; these models are close in spirit though different in details with respect to earlier approaches [6]. However, the scale of the appearing patterns is always dictated by the phase-field interface width, and thus these models have problems in the sharp interface limit. Other descriptions are based on macroscopic equations of motion but suffer from inherent finite time singularities which do not allow steady state crack growth unless the tip radius is limited by the phase-field interface width [7]. Numerical approaches which are not based on a phase field provide a selection mechanism by the introduction of complicated nonlinear terms in the elastic energy for high strains in the tip region [8], requiring additional parameters.

It is therefore highly desirable to look for minimal models of fracture which are free from microscopic details and which are based on well established thermodynamical concepts. This is also motivated by experimental results showing that many features of crack growth are rather

generic [9]; among them is the saturation of the steady state velocity appreciably below the Rayleigh speed and a tip splitting for high applied tension.

Already in our previous publication [10] we emphasized a connection between fracture mechanics and elastically induced surface diffusion processes: the Asaro-Tiller-Grinfeld (ATG) instability [11] appears to be a good starting point for the quest for a “macroscopic” theory of fracture, stating that the energy of a uniaxially stressed solid can be reduced by developing morphological perturbations of a solid surface, finally leading to fast propagating notches looking similar to cracks. In our previous model [10] we used this effect to describe fracture by surface diffusion of the solid material along the crack surfaces.

Here we propose a similar approach which describes crack growth in brittle materials by a phase transition model. In fact, it produces a nontrivial dynamical selection of the radius of the crack tip. Instead of cracks filled with vacuum, we consider for the moment a soft condensed phase inside the crack which is growing at the expense of a brittle material [7].

The difference in the chemical potentials between two phases at an interface is [12]

$$\Delta\mu = \Omega\left(\frac{1}{2}\sigma_{jk}\epsilon_{jk} - \gamma\kappa\right), \quad (1)$$

provided that the soft phase is stress-free because of negligible elastic moduli. Then the surface of the crack is free of normal and shear stresses. We assume for simplicity the mass density  $\rho$  to be equal in both phases and the elastic displacements to be continuous at the interface, which means that the two phases are coherent. Also, we assume a two-dimensional geometry. The interfacial energy per unit area is  $\gamma$ , and the interface curvature  $\kappa$  is positive if the crack shape is convex.  $\Omega$  is the atomic volume,  $\sigma_{jk}$  and  $\epsilon_{ik}$  stress and strain tensor, respectively. Stress and strain are connected by Hooke’s law for isotropic elasticity,

$\sigma_{kj} = 2\mu\epsilon_{kj} + \lambda\epsilon_{ll}\delta_{kj}$ , with the Lamé coefficient  $\lambda$  and the shear modulus  $\mu$ . Alternatively, we use Young's modulus  $E = \mu(3\lambda + 2\mu)/(\lambda + \mu)$  and the Poisson ratio  $\nu = \lambda/2(\lambda + \mu)$  as elastic constants.

For phase transitions, the motion of the interface is locally expressed by the normal velocity

$$v_n = \frac{D}{\gamma\Omega} \Delta\mu \quad (2)$$

with a kinetic coefficient  $D$  with dimension  $[D] = \text{m}^2 \text{s}^{-1}$ .

It is known that nonhydrostatic stresses  $P$  at a nominally flat interface lead to the ATG instability: Long-wave perturbations of a flat interface diminish the total energy of the system, whereas short-wave perturbations are hampered by surface energy. The characteristic length scale of this instability,  $L_G \sim E\gamma/P^2(1 - \nu^2)$ , is identical to the Griffith length of a crack, up to a numerical prefactor. This instability leads to an unphysical finite time cusp singularity in the framework of the static theory of elasticity [13]: The tip radius decreases to zero and simultaneously the tip velocity grows indefinitely. In this sense, the advancing notches can be interpreted as cracks [7,10].

The elastic problem of a semi-infinite mathematical cut in an infinite (two-dimensional) solid is exactly solved by a square root singularity of stresses,  $\sigma_{ij} = Kf_{0,ij}(\theta)/(2\pi r)^{1/2}$ , using polar coordinates as depicted in Fig. 1. Here  $K$  is the stress intensity factor (static or dynamic),  $f_{0,ij}$  the universal angular distribution depending only on the mode of loading (for brevity, we suppress the velocity dependence  $v/v_R$ ;  $v_R$  is the Rayleigh speed); we concentrate on cracks of “mode I” type here. For an extended crack in an infinite environment, the square root singularity is only the slowest decaying mode; other powers can be present, and the total field can be interpreted as an expansion in the set of eigenfunctions of a straight crack:

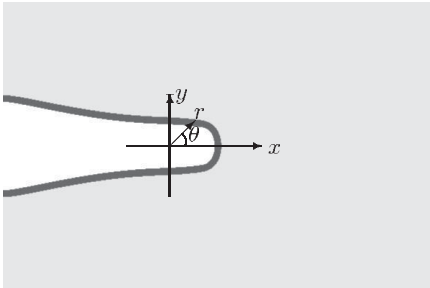


FIG. 1. Steady state growth of a crack in a strip, as obtained from phase-field simulations. A constant displacement is prescribed at the upper and lower boundary of the system. The parameters used here are  $\Delta = 2.03$  and  $D/\xi v_R = 6.18$ ; the system size is  $600 \times 400$ . The resulting velocity is  $v/v_R = 0.71$  and the radius  $r_0 = 0.69D/v_R = 4.26\xi$  are dynamically selected.

$$\sigma_{ij}(r, \theta) = \frac{K}{(2\pi r)^{1/2}} \sum_{n=0}^{\infty} \frac{A_n f_{n,ij}(\theta)}{r^n}. \quad (3)$$

Far field conditions imply  $A_0 = 1$ , whereas the other coefficients  $A_n$  are determined by the boundary conditions of vanishing shear and normal stress on the crack; modes with ascending powers of  $r$  are forbidden by boundary conditions, and even a homogeneous stress  $P$  cannot be present in an infinite system (divergent strip width  $L$ ), because this would lead to a diverging stress intensity factor  $K \sim PL^{1/2}$ . All higher order corrections in Eq. (3) scale as  $A_n \sim r_0^n$  and vanish in the sharp tip limit. From this equation follows readily that the stresses on the crack surface scale as  $\sigma \sim r_0^{-1/2}$ .

We consider a crack as it might have developed in the late stage of the ATG instability, as depicted in Fig. 1. The macroscopic length of the crack is not considered here, and instead the stress intensity factor  $K$  is given. At first, we demonstrate that steady state growth using only the static theory of elasticity is impossible; in fact, this is the reason for the mentioned cusp singularity.

Assume that  $y(x)$  in Cartesian or  $r(\theta)$  in polar coordinates describes the steady state shape of a crack in the comoving frame of reference, corresponding to a specific tip radius  $r_0$  and velocity  $v$ . According to the results above, both contributions to the chemical potential equation (1) scale as  $\mu \sim 1/r_0$  and thus by virtue of the equation of motion (2),  $v \sim 1/r_0$ . Hence a rescaling of the steady state equation is possible. In other words, the explicit length scale  $r_0$  drops out of the equations, and only the phase transformation rate  $v r_0/D$  remains as dimensionless parameter. All other parameters combine to the dimensionless driving force  $\Delta = K^2(1 - \nu^2)/2E\gamma$ ;  $\Delta = 1$  corresponds to the Griffith point. Notice that this rescaling is only possible in the framework of the static theory of elasticity; otherwise, the stress field itself becomes velocity dependent, introducing the ratio  $v/v_R$  as an additional parameter in the system.

Using the steady state condition  $\dot{y} = -vy'$  together with Eqs. (1) and (2), the shape equation reads

$$\kappa = \frac{\sigma_{ik}\epsilon_{ik}}{2\gamma} + \frac{vy'}{D(1 + y'^2)^{1/2}}, \quad (4)$$

which is a nonlocal equation due to the long range elastic interactions. The boundary conditions at the tip are given by the arbitrary choice of the origin,  $r(0) = r_0$  and  $r'(0) = 0$ , since we are interested in symmetrical shapes,  $r(\theta) = r(-\theta)$ . Thus the entire shape is a function depending only on the parameter  $v$ .

On the other hand, in the tail region, the elastic stresses have decayed, and the shape equation therefore becomes simply  $-vy' = Dy''$ . Its general solution,  $y(x) = A + B \exp(-vx/D)$ , contains a growing exponential which is inconsistent with the boundary conditions of the straight crack. Therefore the solution must be arranged such that  $B = 0$ . Notice that in contrast to the surface

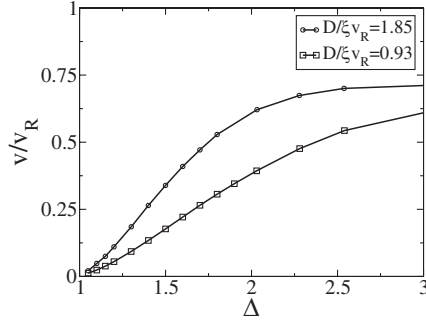


FIG. 2. Steady state velocity versus dimensionless driving force  $\Delta$ ;  $\Delta = 1$  is the Griffith point.

diffusion process [10] a finite opening  $A$  cannot be excluded since we do not have to obey mass conservation here. At a first glance, suppression of the exponential seems to lead to a selection of the steady state velocity  $v$  as the only available parameter. However, from the rescaling behavior explored above it follows immediately that  $B \sim 1/v$  (notice that  $B$  has the dimension of a length), and therefore a finite velocity cannot be selected. Consequently, a steady state solution for a growing crack in the framework of the static theory of elasticity does not exist.

The situation is different for the dynamical theory of elasticity: Here velocity enters into the equation of motion not only as  $vr_0/D$  but also as  $v/v_R$ . Since now a rescaling is impossible, both the propagation velocity  $v$  and the tip radius  $r_0$  are selected.

A tip splitting is possible for high applied tensions due to a secondary ATG instability: Since  $\sigma \sim Kr_0^{-1/2}$  in the tip region and the local ATG length is  $L_G \sim E\gamma/\sigma^2$ , an instability can occur, provided that the tip radius becomes of the order of the ATG length. In dimensionless units, this leads to the prediction  $\Delta_{\text{split}} \sim \mathcal{O}(1)$ .

We developed a phase-field code together with elastodynamics to describe phase transformations under stress, including, for example, also martensitic transformations. In the limit of vanishing shear modulus in one of the phases, this approach can be used to study melting and solidification processes which are induced by elastic forces [7]. For a very soft secondary phase, crack propagation can be studied in the framework of a continuum theory, since then the usual boundary conditions of vanishing normal and shear stress are recovered. Let  $\phi$  denote the phase field with values  $\phi = 0$  for the soft and  $\phi = 1$  for the hard phase. The energy density contributions are  $f_{\text{el}} = \mu(\phi)\epsilon_{ij}^2 + \lambda(\phi)(\epsilon_{ii})^2/2$  for the elastic energy, with  $\mu(\phi) = h(\phi)\mu^{(1)} + [1 - h(\phi)]\mu^{(2)}$  and  $\lambda(\phi) = h(\phi)\lambda^{(1)} + [1 - h(\phi)]\lambda^{(2)}$ , where  $h(\phi) = \phi^2(3 - 2\phi)$  interpolates between the phases and the superscripts denote the bulk values. The surface energy is  $f_s(\phi) = 3\gamma\xi(\nabla\phi)^2/2$  with the interface width  $\xi$ . Finally,  $f_{dw} = 6\gamma\phi^2(1 - \phi)^2/\xi$  is the well-known double well potential. Thus the total potential energy is

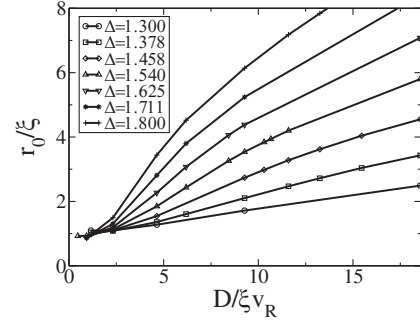


FIG. 3. Tip radius  $r_0$  as a function of the kinetic coefficient  $D$  for different driving forces  $\Delta$ . In the intermediate linear regime the length scales are well separated.

$$U = \int dV(f_{\text{el}} + f_s + f_{dw}). \quad (5)$$

The elastodynamic equations are derived from the energy by the variation with respect to the displacements  $u_i$ ,

$$\rho\ddot{u}_i = -\frac{\delta U}{\delta u_i}, \quad (6)$$

and the dissipative phase fields dynamics follows from

$$\frac{\partial \phi}{\partial t} = -\frac{D}{3\gamma\xi} \frac{\delta U}{\delta \phi}. \quad (7)$$

These equations lead in the limit  $\xi \rightarrow 0$  to the correct sharp interface limit above, as described by Eqs. (1) and (2). For the case of static elasticity, this was carefully proved in Ref. [7].

For the numerical realization, we employ explicit representations of both the elastodynamic equations and the phase-field dynamics. The elastic displacements are defined on a staggered grid [14]. The derivation of the elastodynamic equations of motion from a discretized action integral obeying invariance against time inversion guarantees long time stability.

We study crack growth in a rectangular geometry of a strip with fixed displacements at its upper and lower boundary. The grid can be shifted horizontally in order to keep the crack tip always in the center of the system. Thus, crack growth can be studied over long times in relatively small systems. Typical dimensions used here are  $600 \times 200$  grid points, the phase-field interface width is  $\xi = 5\Delta x$

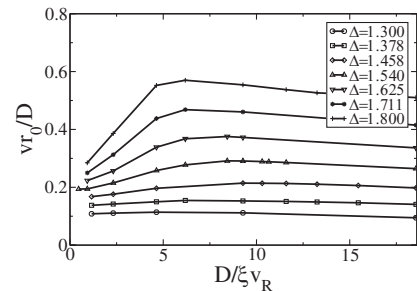


FIG. 4. The quantity  $vr_0/D$  as a function of the kinetic coefficient for different driving forces  $\Delta$ .

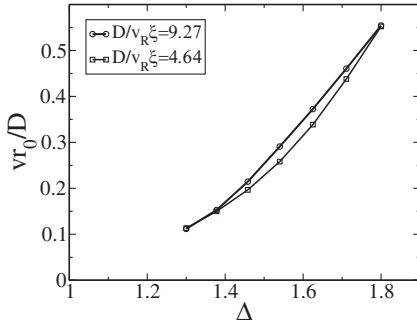


FIG. 5.  $vr_0/D$  as a function of the driving forces  $\Delta$ ; the curves for different kinetic coefficients do not differ significantly, in agreement with the theoretical prediction.

( $\Delta x$  is the lattice unit), and the Poisson ratio is  $\nu = 1/3$ . In the soft phase, we typically set the elastic constants to 1% of the values in the hard phase; however, these values are qualitatively not significant. Notice that after rescaling the equations of motion depend only on the driving force  $\Delta$  and the kinetic coefficient  $D$ ; in the numerical realization, also the phase-field width  $\xi$  and the strip width  $L$  appear.

First, we studied the growth of cracks in the vicinity of the Griffith point. Here, the tip radius is not determined by the length scale  $D/v_R$  but by the phase-field interface width  $\xi$ . In the strip geometry, the dimensionless driving force is  $\Delta = u_0^2(\lambda + 2\mu)/4L\gamma$  with the fixed vertical displacement  $u_0$  applied to the strip. As a nontrivial test, the numerical results validate the analytical prediction of the Griffith point  $\Delta = 1$  in the framework of the model, as the propagation velocity tends to zero (see Fig. 2).

The main goal was to prove that elastodynamics allows steady state growth without collapsing into the finite time cusp singularity of the ATG instability, selecting both a nonzero tip radius and a propagation velocity below the Rayleigh speed. The simulations confirm this prediction, and a typical steady state shape is shown in Fig. 1. Obviously, the tip radius is not determined by the intrinsic phase-field length scale  $\xi$ . This can also be seen in Fig. 3, where we plotted the steady state tip radius  $r_0$  as a function of the kinetic coefficient  $D$  for various driving forces  $\Delta$ . Only for very low kinetic coefficients is the tip radius cut off by the interface width  $\xi$ , otherwise it is clearly bigger; for high kinetic coefficients the saturation is induced by the system size. In between, however, the scales are well separated and the radius  $r_0$  is a linear function of  $D$ , in



FIG. 6. Irregular tip splitting scenario. We used  $D/\xi v_R = 1.85$  and  $\Delta = 3.6$ ; the system size is  $600 \times 400$ . Time is given in units  $D/v_R^2$ . Minor numerical noise breaks the symmetry of the competing sidebranches.

good agreement with the theoretical analysis: since both parameters  $v/v_R$  and  $vr_0/D$  are predicted to be universal functions of the driving force  $\Delta$  alone, we conclude that  $r_0$  should depend linearly on the kinetic coefficient. Notice that also the tail opening  $A$  is of the scale  $A \sim D/v_R$  instead of  $A \sim \xi$ . Furthermore, the phase transformation rate  $vr_0/D$  is rather independent of the kinetic coefficient (Fig. 4) and thus its universal behavior can be extracted (Fig. 5). We believe that the results can be improved by increasing the system size and by a better separation of the length scales, which will be done in the near future.

Snapshots of a typical tip splitting scenario for relatively high driving forces are shown in Fig. 6. Repeated irregular splitting of the crack tip occurs, followed by symmetrical growth of the sidebranches. After a while, one finger wins the competition, moves back to the center of the strip and can finally split again.

In summary, a phase-field model has been developed to describe crack growth, based on thermodynamically well-defined equations with a valid sharp interface limit. The model shows the possibility of steady state growth of cracks and a tip splitting instability, in agreement with analytical predictions. In contrast to other models previously discussed it provides a selection of the tip radius by the scale  $D/v_R$ .

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