Continuum Theory of Fracture

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September 28, 2006

Abstract

We present a continuum theory of fracture which describes the fast 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 the selection of the steady state tip radius and velocity. Two different numerical approaches are presented to solve this problem. A sharp interface approach allows to study the steady state regime by the means of a series expansion technique. Also, 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, and the results of both numerical approaches are in excellent agreement with each other.

Keywords: Fracture Mechanics, Pattern Formation, Sharp Interface Modeling, Phase Field Methods

1 Introduction

Even though fracture and material failure are frequently encountered in many scientific and industrial fields, their description still remains a major challenge for solid state physics and materials science. It was Griffith's [1] idea to describe crack growth as a competition of two different effects: the release of the elastic energy in the material and the increase of surface energy due to crack growth. This idea proved to be very fruitful and since then, numerous approaches have been developed to describe the various features of cracks [2].

The most conventional approach is to understand cracks on the level of breaking bonds between atoms. This approach assumes sharp crack tips and requires detailed information, either theoretical or empirical, about the atomic properties and interactions. This in turn makes any quantitative description depend heavily on the chosen model and its parameters.

On the other hand, it is known that due to plastic effects, real crack tips are often not sharp, but rounded with a finite tip radius r_0. If one also looks at fracture in gels, a macroscopic approach seems feasible. Other experimental results also indicate that certain features of crack growth are generic [3]. For example, it has been observed that the steady state velocity of the crack tip saturates well below the Rayleigh speed, which is the theoretical upper limit [2]. When high tensions are applied, tip splitting occurs.

Our aim is to find minimal models for fracture in such a way that not only the crack speed, but also the crack shape can be determined self-consistently. Those minimal models should be free of microscopic details and be based on well established thermodynamical concepts. One technique that is suited for the above sketched path is phase field modeling, where one does not deal with a sharp boundary that has to be tracked explicitly, but rather with a diffuse interface. That way, a set of differential equations can be derived which are valid in the whole bulk and can be solved numerically.

Recent phase field models, though close in spirit but different in details compared to earlier approaches [4], comprise much of the expected crack behavior [5, 6] and go beyond the microscopic limit of discrete models with broken translational and rotational symmetry. The used phase field models should produce the correct behavior in the sharp interface limit, which is not always the case when the appearing patterns are of the order of the interface width. 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.

In order to find a minimal macroscopic model of fracture, the Asaro-Tiller-Grinfeld (ATG) instability [9] provides a good starting point. It states 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. We already emphasized that connection between fracture mechanics and elastically induced surface diffusion processes in a previous publication [10], where we used the ATG instability to describe fracture by surface diffusion of material along the crack surfaces.

It is important to point out that this model for fast crack propagation in brittle materials is substantially different from conventional fracture mechanics. The crack has a finite tip radius, and therefore propagation requires a mass transport process. In the spirit of a lubrication approximation, plasticity in a thin region around the tip can effectively be described by surface diffusion processes along the crack contour, and is therefore contained in our descriptions [10]. Thus, it contains an effective full modeling of a thin process zone.

As another consequence, fracture mechanics can now be understood in the framework of interfacial pattern formation processes. This means that for all surface points of the extended crack the interface motion has to be expressed through the local driving forces. Simultaneously, the difficulty arises that the elastic fields have to be determined in domains that continuously change their shape in the course of time and are not known in advance. The profit, however, is that no guesses for the equations of motion, especially at an otherwise singular tip, have to be made, but instead the propagation is based on thermodynamically well established concepts. In particular, the splitting of cracks is automatically contained in the description. The conventional fracture mechanics with sharp crack tips is contained in the sense of an integral energy balance.

Here we propose a different approach to describe the fast growth of cracks driven by phase transition kinetics and present two different numerical methods that are used to explore it numerically. The first method is based on a sharp interface approach and is designed in particular for steady state growth. In contrast to other methods, the limit of fully separated length scales is performed analytically, leading to a very efficient numerical scheme. The method is based on a series expansion technique, and the satisfaction of the elastic boundary conditions on the crack contour reduces to a linear matrix problem, whereas the bulk equations of dynamical elasticity are automatically satisfied. Nevertheless, finding the correct crack shape and speed remains a difficult nonlinear and nonlocal problem.

The other method is a phase field description which also allows to study e.g. the tip splitting of cracks and is not limited to steady state growth. However, it requires enormous computational efforts, and therefore it is much more difficult to obtain quantitative results of the same quality as the series expansion technique.

The paper is organized as follows: First, we introduce the minimum model for fast crack propagation processes. Then, in section 3 we present the series expansion technique to solve the arising pattern selection problem for the crack shape and velocity self-consistently. In section 4 the phase field approach is outlined. Finally, the results from both techniques are presented and discussed.

2 Model Description

Imagine that the crack is filled with a soft condensed phase instead of vacuum, and the growth is then interpreted as a first order phase transformation of the hard solid matrix to this soft phase [7, 10, 11]. The inner phase becomes stress free if its elastic constants vanish. For simplicity, we assume the mass density ρ of both phases to be equal; together with the premise of coherency at the interface this implies that the solid matrix is free of normal and shear stresses at the crack contour, i.e. $\sigma_{nn} = \sigma_{n\tau} = 0$, which serves as boundary conditions. In the bulk, the elastic displacements u_i have to fulfill Newton's equation of motion,

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i. \tag{1}$$

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

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

provided that the soft phase is stress free because of negligible elastic moduli. For simplicity, we assume a two-dimensional geometry. The interfacial energy per unit area is γ, and the interface curvature κ is positive if the crack shape is convex. Ω denotes the atomic volume, σ_{jk} and ϵ_{ik} are stress and strain tensor respectively. Stress and strain are connected via Hooke's law for isotropic elasticity, $\sigma_{kj} = 2\mu\epsilon_{kj} + \lambda\epsilon_{ll}\delta_{kj}$, with the Lamé coefficient λ and the shear modulus μ. 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

$$v_n = \frac{D}{\gamma\Omega} \Delta\mu \tag{3}$$

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

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

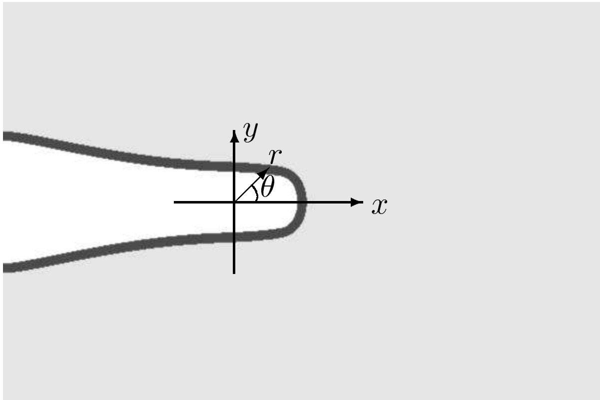

Figure 1: Steady state growth of a crack in a strip with mode I loading, as obtained from phase-field simulations.

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, $\sigma_{ij} = K f_{ij}^{(0)}(\theta)/(2\pi r)^{1/2}$, using polar coordinates as depicted in Fig. 1. Here K is the stress intensity factor (static or dynamic), $f_{ij}^{(0)}$ 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 also concentrate on cracks of "mode I"-type here. However, for a crack with finite tip radius, the elastic situation is substantially modified, and we will present suitable methods for solution of this problem in the subsequent sections.

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 co-moving 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 Eq. (2) scale as $\mu \sim 1/r_0$ and thus by virtue of the equation of motion (3), $v \sim 1/r_0$. 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 vr_0/D remains as dimensionless parameter. All other parameters combine to $\Delta = K^2(1-\nu^2)/2E\gamma$, which is the dimensionless driving force; $\Delta = 1$ 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. (2) and (3), the shape equation reads

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

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.

In the tail region, however, the elastic stresses have decayed, and the shape equation therefore becomes simply $-vy' = Dy''$. Its general solution, $y(x) = h/2 + B\exp(-vx/D)$, with h being the opening of the crack far behind the tip, 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 diffusion process [10], a finite opening h 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, the velocity enters into the equation of motion not only as vr_0/D but also as v/v_R. Now a rescaling is impossible, and both, the propagation velocity v and the tip radius r_0, are dynamically selected.

The prementioned tip splitting for high applied tensions is possible due to a secondary ATG instability: Since we have $\sigma \sim K r_0^{-1/2}$ 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.

3 The Series Expansion Method

We will now present the first numerical method for the calculation of steady state propagation of a semi-infinite crack in an isotropic medium. As mentioned before, we restrict ourselves to the two-dimensional case and plane strain. The general setup is that of an elastic medium exposed to mode I loading and the crack is moving with a given constant velocity v along the x axis, as shown in Fig. 1. We start with the description in the laboratory frame of reference. Following Ref. [2, 14], we now introduce two real functions $\phi(x, y, t)$ and $\psi(x, y, t)$ which are related to the displacements u_i as follows,

$$u_x = \frac{\partial\phi}{\partial x} + \frac{\partial\psi}{\partial y}, \quad u_y = \frac{\partial\phi}{\partial y} - \frac{\partial\psi}{\partial x}.$$

Decomposing the displacements in the above way, we can now decouple the bulk equation (1) into two wave equations,

$$c_d^2\nabla^2\phi = \partial_{tt}^2\phi, \quad c_s^2\nabla^2\psi = \partial_{tt}^2\psi. \tag{5}$$

with the dilatational sound speed c_d and the shear sound speed c_s. The expressions for the sound speeds are $c_d = \sqrt{E(1-\nu)/\rho(1-2\nu)(1+\nu)}$ and $c_s = \sqrt{E/2\rho(1+\nu)}$, respectively.

If we now exploit the steady state situation and change into a co-moving frame of reference ($x \to x - vt$), the time derivatives in Eqs. (5) vanish. Also introducing rescaled coordinates perpendicular to the crack, $y_d = \alpha_d y$ and $y_s = \alpha_s y$, with $\alpha_d^2 = 1 - v^2/c_d^2$ and $\alpha_s^2 = 1 - v^2/c_s^2$, leaves us with Laplace equations

$$\frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y_d^2} = 0, \quad \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y_s^2} = 0 \tag{6}$$

instead of the above wave equations. These Laplace equations can be used to find all eigenmodes of a straight growing cut.

In order to solve the elastodynamic problem of a crack with finite tip radius r_0, we use a series expansion

$$\sigma_{ij} = \frac{K}{(2\pi r)^{1/2}} \left(f_{ij}^{(0)} + \sum_{n=1}^{N=\infty} \frac{A_n f_{ij,d}^{(n)} + B_n f_{ij,s}^{(n)}}{r^n} \right).$$

The functions $f_{ij,d}^{(n)}(\theta_d, v)$ and $f_{ij,s}^{(n)}(\theta_s, v)$ are the universal angular distributions for the dilatational and shear contributions which can be obtained from Eq. (6). They also depend on the propagation velocity.

For the unknown coefficients of expansion A_n and B_n, one has to solve the linear problem of fulfilling the boundary conditions $\sigma_{nn} = \sigma_{n\tau} = 0$ on the crack contour. The tangential stress $\sigma_{\tau\tau}$ is determined only through the solution of the elastic problem. As it enters into the equations of motion (2) and (3), it leads to a complicated coupled and nonlocal problem.

The idea for solving this problems has been developed originally in the context of dendritic growth [15]. The strategy is as follows: first, for a given guessed initial crack shape and velocity, we determine the unknown coefficients A_n and B_n from the boundary conditions. In a second step, the chemical potential and the normal velocity at each point of the interface is calculated. Afterwards, we obtain the new shape by advancing the crack according to the local interface velocities. This three-step procedure is repeated until the shape of the crack remains unchanged in the co-moving frame of reference, providing a natural way to solve the problem, as it follows the physical configurations to reach the steady state.

4 Phase Field Modeling

As alternative method to solve the equations of motion for growing cracks with finite tip radius, we developed a phase field code that contains elastodynamics. 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 ϕ denote the phase field with values $\phi = 0$ for the soft and $\phi = 1$ for the hard phase. The energy density contributions are

$$f_{el} = \mu(\phi)\epsilon_{ij}^2 + \lambda(\phi)(\epsilon_{ii})^2/2$$

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 ξ. Finally,

$$f_{dw} = 6\gamma\phi^2(1-\phi)^2/\xi$$

is the well-known double well potential. Thus the total potential energy is

$$U = \int dV \left(f_{el} + f_s + f_{dw}\right). \tag{7}$$

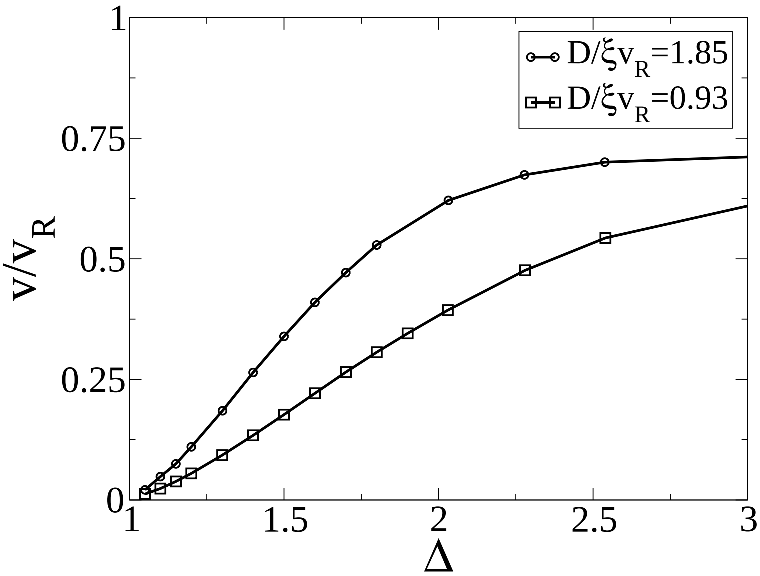

Figure 2: Steady state velocity as a function of the dimensionless driving force Δ.

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

$$\rho \ddot{u}_i = -\frac{\delta U}{\delta u_i}, \tag{8}$$

and the dissipative phase fields dynamics follows from

$$\frac{\partial \phi}{\partial t} = -\frac{D}{3\gamma\xi}\frac{\delta U}{\delta \phi}. \tag{9}$$

These equations lead in the limit $\xi \to 0$ to the correct sharp interface limit above, as described by Eqs. (2) and (3). This was carefully proven in [7] for the case of static elasticity.

For the numerical realization, we employ explicit representations of both the elastodynamic equations and the phase field dynamics, where the elastic displacements are defined on a staggered grid [16]. The derivation of the elastodynamic equations of motion from a discretized action integral obeying invariance against time inversion guarantees long time stability. We then choose a rectangular strip with fixed displacements at its upper and lower boundary to study crack growth. The grid can be shifted horizontally in order to always keep the crack tip in the center of the system. Thus, crack growth can be studied over long times in relatively small systems. Typical dimensions used here are 1000×500 grid points, the phase field interface width is $\xi = 5\,\Delta x$ (Δx is the lattice unit) and the Poisson ratio is $\nu = 1/3$. In the soft phase, we typically set the elastic constants to one percent 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 Δ and the kinetic coefficient D; in the numerical realization, also the phase field width ξ and the strip width L appear.

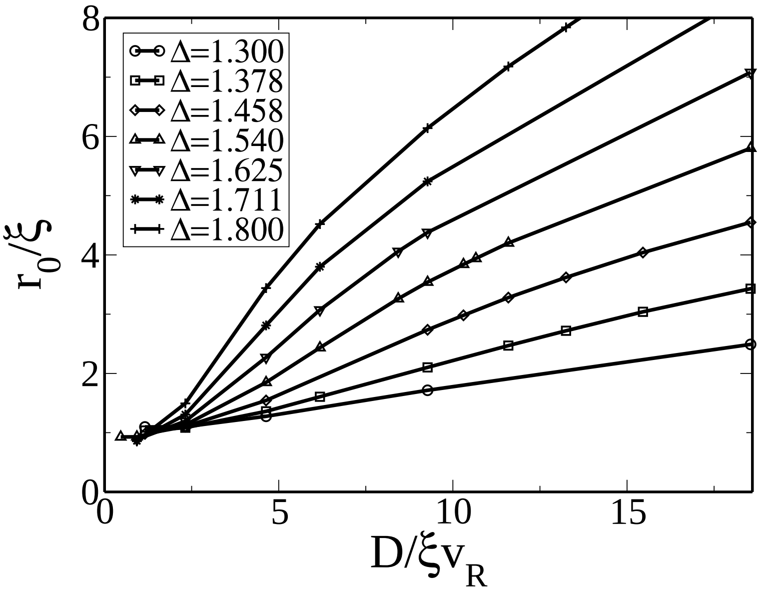

Figure 3: Tip radius r_0 as a function of the kinetic coefficient, for different driving forces Δ.

5 Results

The main goal was to substantiate that elastodynamics allows steady state growth without collapsing into the finite time cusp singularity of the ATG instability, selecting both a non-zero tip radius (see Fig. 3) and a propagation velocity below the Rayleigh speed (see Fig. 2). The simulations performed with the two methods confirm this prediction, and a typical steady state shape is shown in Fig. 4. Below the point $\Delta \approx 1.14$ dissipative solutions do not exist [17]. The tip radius is then determined by a microscopic length scale, which can be mimicked by the phase field interface width ξ. 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).

For phase field simulations, the tip radius is cut off by the interface width ξ only for very low kinetic coefficients. Otherwise it is fairly 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 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 Δ alone, we conclude that r_0 depends linearly on the kinetic coefficient. Notice that also the tail opening h is of the scale $h \sim D/v_R$.

The tip curvature becomes negative for $\Delta > 1.8$ using the series expansion method, indicating the onset of a tip-splitting instability (see also Fig. 4). Snapshots of a typical tip splitting scenario obtained from phase field simulations for relatively high driving forces are shown in Fig. 5. 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 continuum theory of fracture, based only on the linear theory of elastodynamics and phase transition kinetics has been developed. The model shows the possibility of steady state growth of cracks and a tip splitting instability. Numerical investigations of this model have been

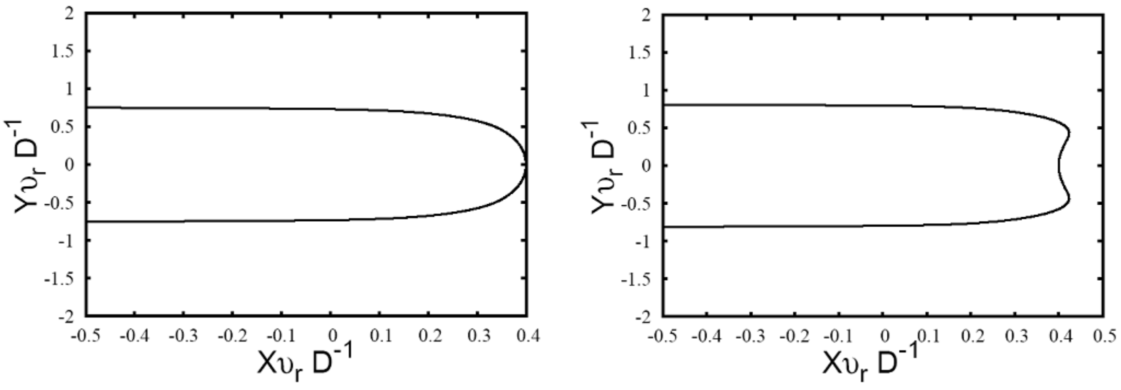

Figure 4: Crack shape obtained for $\Delta = 1.3$ and $\Delta = 2.3$, using the series expansion method. The negative tip curvature can cause tip splitting.

Figure 5: Irregular tip splitting scenario. We used $D/\xi v_R = 1.85$ and $\Delta = 3.6$; the system size is 600×400. Time is given in units D/v_R^2.

done by a series expansion method and phase field modeling. The results of these completely independent approaches are in excellent agreement with each other.

This work has been supported by the Deutsche Forschungsgemeinschaft under grant SPP 1120.

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