Dynamic instabilities of fracture under biaxial strain using a phase field model

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We present a phase field model of the propagation of fracture under plane strain. This model, based on simple physical considerations, is able to accurately reproduce the different behavior of cracks (the principle of local symmetry, the Griffith and Irwin criteria, and mode-I branching). In addition, we test our model against recent experimental findings showing the presence of oscillating cracks under bi-axial load. Our model again reproduces well observed supercritical Hopf bifurcation, and is therefore the first simulation which does so.

In recent years, the physics community has seen a rebirth of interest in the problem of dynamic fracture. This rebirth was kindled by a series of experiments revealing that the current engineering approach to crack propagation, namely the coupling of linear elasticity to an empirical energy balance law for crack tip motion, cannot account for the richness of actual fracture phenomenology. Specifically, dynamical instabilities which drive the system away from a single crack propagating in a straight line require more sophisticated attention to the actual tip region, the so-called process zone.

Given the above, it is clear that one needs a framework which can couple local degrees of freedom involved in breaking inter-atomic bonds to global elasticity. One approach, referred to as phase-field modeling of fracture, accomplishes this task by introducing an order-parameter field (the degree of “broken-ness”) which then couples to the elastic strain in a fundamentally continuum-level formulation. The fact that the system does not need to be placed on a lattice avoids dynamical artifacts associated with the breaking of translational and rotational symmetry. One such phase-field model due to Karma, Kessler and Levine (KKL) has been shown to correctly encompass much of the expected behavior of mode III (out-of-plane) cracks.

Here, we extend the KKL model to full vector elasticity and test its genericity. Our major interest is in seeing whether a recently discovered supercritical Hopf bifurcation to oscillating cracks under biaxial loading (see Fig. 1) is in fact reproduced by KKL; we will see that in fact it is. This first-ever successful simulation of the crack oscillation has the dual benefit of demonstrating that the instability is not dependent on any special properties of the specific materials used in the experiment (rubber) and also of giving us more confidence in the phase-field methodology.

We start with the KKL phase field model. Here, a sheet of fractured elastic material is represented by the elastic displacement field $u_x$, $u_y$ and by a phase field variable $\phi$ that can be interpreted as the proportion of intact inter-atomic links. The evolution equation of $u_x$ and $u_y$ derives from a modified elastic energy:

$$E = \int \int dx \, dy \, g(\phi)(\frac{1}{2} \lambda \epsilon_{ii}^2 + \mu \epsilon_{ij}^2)$$  \hspace{1cm} (1)

where $g = (4 - 3\phi)^3$ is a function of $\phi$ chosen such that $g(0) = 0$, $g(1) = 1$, and $g'(0) = g'(1) = 0$; this specific choice is discussed in [3]. The tensor $\epsilon_{ij}$ is the strain tensor which has the following form:

$$\epsilon_{ij} = \frac{1}{2}(\partial_i u_j + \partial_j u_i)$$  \hspace{1cm} (2)

The evolution equations for $u_x$ and $u_y$ are then:

$$\rho \partial_t u_i = \frac{\delta E}{\delta u_i}$$  \hspace{1cm} (3)

The corresponding evolution equation of $\phi$ is

$$\tau \partial_t \phi = \Delta \phi - \frac{dV(\phi)}{d\phi} - \frac{dg(\phi)}{d\phi}(E_\phi - \epsilon_c)$$  \hspace{1cm} (4)

where $V(\phi) = 4(\phi(1-\phi))^2$ is a double well potential and

$$\begin{cases} E_\phi = \frac{1}{2} \lambda \epsilon_{ii}^2 + \mu \epsilon_{ij}^2 \quad \text{if } tr(\epsilon) > 0 \\ E_\phi = \frac{1}{2} \lambda \epsilon_{ii}^2 + \mu \epsilon_{ij}^2 - \alpha K_{lame} \epsilon_{ii}^2 \quad \text{if } tr(\epsilon) < 0 \end{cases}$$  \hspace{1cm} (5)

where $K_{lame} = (\lambda + \mu)/2$ is the modulus of compression for a plane strain configuration; $\alpha$ is an arbitrary coefficient chosen to be bigger than 1. This breaking of the symmetry between compression and extension is a key ingredient not present in previous phase field approaches to in-plane fracture. If a material is simply compressed, having $\alpha > 1$ will guarantee that it will not break; also, compression will increase the threshold needed for inducing a fracture through shear. The parameters values used here are: $\epsilon_c = 1$, $\tau = 5$, $\lambda = \mu = 1$ and $\alpha = 1.5$.

We proceed to study this model computationally in a box of width $W$ and length $L$. Simulations were performed using a grid spacing of $\delta x = 0.15$ and a time step of $\delta t = 0.001$ (Decreasing to $\delta x = 0.075$ and $\delta t = 0.0005$ leads to no significant difference in the results). The time...
stepping scheme was the forward Euler method while the spatial operators were computed using a discretization that conserves the discretized energy of Eq. 1 (The use of other scheme lead to long term numerical instabilities). In our simulations, we used both fixed grids of different sizes along the $x$ axis and a grid moving with the fracture tip along the $x$ axis. Boundary conditions for the fixed grid were as follows: at the $y = W$ ($y = 0$) boundary, $u_y$ was kept equal to $\Delta_y (0)$ and on both lateral edges $u_x = x\Delta_x/L$. At the $x = L$ ($x = 0$) boundary, $u_x$ was kept equal to $\Delta_x (0)$ and no flux boundaries were used for the $u_y$ field. In the case of the moving grid, the boundary conditions at $y = W$ and $y = 0$ were unchanged whereas the boundary conditions at the horizontal ends of the grid were modified. First we introduced an artificial viscosity in a thin layer at both ends (This mimics partially absorbing boundary conditions). Also, at the leftmost end the $u_x$ field was kept constant between each displacement of the grid. We checked that those modifications did not affect the behavior of the crack when compared to results obtained using a long enough fixed grid, thereby allowing us to simulate the crack propagation along an infinite strip along the $x$ axis. The initial conditions were constructed as follows: a small initial crack was created by setting $\phi = 0$ in a small region of fixed width and variable length and by letting the system evolve following a damped version (see later) of the evolution equation of elasticity (while $\phi$ was kept constant) until a stationary state was reached.

We first tested the model for damped dynamics obtained by replacing $\partial_t u$ by $\partial_t$. For pure mode I loading, the fracture began to propagate once the imposed elastic energy was higher than the fracture energy (see later). In addition, in this case, the stress intensity factor at the tip of a steady crack was found to be constant for various loading configuration, hence obeying the Irwin criterion 8 (data not shown). More interestingly, numerical simulations in the case of pure mode II loading showed that the model respects the local symmetry principle: the fracture propagates in the direction which nullifies the stress intensity factor for mode II (see Fig. 2b). Hence this model reproduces well the behavior of a single crack in the damped regime. Note that this result depends on our asymmetry parameter $\alpha$: allowing breakage under compression leads to a model which does not follow the local symmetry principle (Fig. 2b, inset). The results for different $\alpha$ ranging from 1 to 2 were similar.

Next, we turn briefly to results obtained in the dynamic (non-damped) case under pure mode I loading. As expected by analogy with the results of 8 for the case of mode III loading, the initiation of crack propagation appeared at the Griffith threshold with good accuracy. Indeed, according to the Griffith criterion, one would expect a crack to begin to propagate for a value of the $y$ extension $\Delta_y$ bigger than $\Delta_c$ which is solution of:

$$W \left( \frac{1}{2} \lambda + \mu \lambda^2 \right) = 2 \int_0^1 d\phi \sqrt{2(1-g(\phi)) + V(\phi)}$$

(6)

This formula was derived in 8 and follows from the asymptotic solution of the model in the region far behind the crack tip. For the parameter values used here, this threshold is at 9.5 whereas in our simulations the crack begins to propagate for $\Delta_y$ bigger than 9.7 ± 0.1; this 2% discrepancy is due to discretization and finite width effects and gives some measure of the accuracy of our com-
computations. The speed of the stable crack behaved qualitatively as expected when loading was increased. When loading was further increased, the dynamic fracture exhibits a branching instability and a secondary crack begins to propagate (see Fig. 3). This branching instability is compatible with what has been observed experimentally in a wide range of materials [10, 11]. A complete analysis of the branching phenomenon will be addressed in further work.

We now turn to our major interest here, the case of a dynamic crack propagating under biaxial stress. Experimental work by Deegan et al. [3] has shown that for a given imposed strain in the \( y \) direction (see Fig. 4), there is a threshold value of the \( x \) strain for which the crack propagation is no longer straight; instead, the crack tip position begins to oscillate. In fact, the instability appears to be supercritical and the tip trajectory is well-approximated by a sinusoidal line with finite wavelength and amplitude. Recall that in our calculations strains are applied by moving the rightmost border of the sheet by \( \Delta x \) and by moving the top border by \( \Delta y \); hence, if \( \Delta x = 0 \), the system is set to pure mode I. The experimental results translate into the prediction of a Hopf bifurcation that should occur as we cross a threshold value of \( r = W \Delta_x/L \), with \( \Delta_y \) being fixed.

The results of our numerical simulations for two sets of \( \lambda, \mu \) and different values of \( \Delta y \) faithfully reproduces the aforementioned phenomenology. Namely, the fracture tip trajectory indeed undergoes a Hopf bifurcation when the \( x \) extension is increased over a threshold value that depends on both parameter regime and the vertical extension. This bifurcation is characterized by the fact that below threshold, the tip position shows damped oscillations (see figure 3) and ends up propagating along a straight line, whereas above threshold those oscillations are amplified and the restabilized state corresponds to the situation where the fracture tip oscillates at a finite wavelength with a finite amplitude (see figure 3). We checked that this instability was not due to waves reflecting at the boundaries that can create periodic markings called Wallner lines [12]. Indeed, the expected wavelength of such markings would be \( \lambda = W \sqrt{v/c \sqrt{1 - \nu^2/c^2}} \), that is about 10 s.u. while the wavelength observed here is about 300 s.u. This is confirmed by the fact that switching to quasi-absorbing boundary conditions at the \( y = W \) and \( y = 0 \) lines does not affect the oscillations.

When the restabilized state is reached, the trajectory of the tip is almost indistinguishable from a sinusoidal line, as in Fig. 3. One can also note that the horizontal tip speed oscillates with a frequency equal to two times the frequency of the vertical position, so that the maximum of the horizontal tip speed are reached when the instantaneous tip velocity is directed along the \( x \) axis. In addition, the tip speed tangent to its trajectory is kept almost constant (up to numerical errors) and for different values of \( r \) (r varying between 7 and 8), we did not find significant changes in the tip speed (less than a few %). A picture of this state is presented in Fig. 4.

We now describe the changes in the oscillating restabilized state when the strain along the \( x \) axis is increased. As seen in figure 5, the amplitude of the oscillations behaves like \( T \Delta x = \Delta xc \) close to threshold, which is consistent with a supercritical Hopf bifurcation, as exper-
mentally observed in [15]. The tip velocity and periodicity of the tip oscillation decreases significantly when \( \Delta_x - \Delta_{x_c} \) is increased; this differs from results in [5] where the wavelength significantly decreases when \( \Delta_x - \Delta_{x_c} \). This may be due to non-linear elasticity effects present in the experiment.

We also performed numerical simulations with biaxial strain and \( \alpha = 0 \). The results obtained did not differ significantly from that observed for \( \alpha = 1.5 \). This is somewhat surprising, since the simplest interpretation of the oscillations observed here suggests that the mechanism is at least partially similar to the one underlying oscillations of a quasi-static crack propagating in a thermal gradient [13, 14]. In that case, theoretical work has explained the transition to an oscillating crack using a (modified) principle of local symmetry [15, 16]; changing the tip direction induces a mode II component which causes further deviation from the original line. We have already shown that this principle does not apply for a symmetric model for pure mode-II loading. Perhaps the explicit breaking of the symmetry by the mode-I part of the driving is enough to suppress the unphysical compressional breaking for the case of \( \alpha = 0 \), and hence this model still exhibits the Hopf bifurcation. In support of this, we verified that even in this case, a crack tip with damped dynamics will obey the principle of local symmetry, if in addition to a pure mode II load one adds a small mode I extension. We should note, though, that we never observe oscillations with damped dynamics, even when \( r \) was set to very close to \( \Delta_y \), i.e. close to hydrostatic strain. However increasing \( \tau \) (up to 50), i.e. increasing the dissipation at the crack tip did not affect significantly either the instability wavelength of the oscillating crack or the threshold but did reduce the crack speed (from 0.362 to 0.05 (\( \tau = 50 \))). Also, changes in \( \Delta_y \) (\( \Delta_y = 12, 14 \), with \( \tau = 20 \) to avoid branching) did not affect significantly the wavelength of the oscillating crack but did change the threshold. Interestingly, the wavelength scales linearly with \( W \). Hence, it seems that the saturation of the amplitude is governed by the interaction of the tip with the sidewall. Underlying the actual instability is perhaps the simple fact that an oscillating crack will alleviate extra elastic energy under biaxial strain.

In summary, this paper shows that the extension of the KKL phase field model of crack propagation to full vector elasticity qualitatively reproduces the different instabilities observed when considering the propagation of cracks. One should note that with an extremely simple model based on generic physical considerations we were nonetheless able to reproduce the variety of observed patterns. This lends us confidence in the entire modeling approach and suggests that we proceed in two complementary directions. First, we can continue to investigate the phenomenology of KKL, specifically looking at the interaction of different cracks (the phase field method can easily deal with intersecting interfaces) and also truly three-dimensional effects [17]. At the same time, it is time to begin understanding how to combine this method with microscopic interaction data about specific materials so as to enable the building of more quantitatively reliable models of dynamic fracture.

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[1] J. Fineberg and M. Marder, Phys. Rep. 313, 2 (1999).
[2] D. Kessler and H. Levine, Phys. Rev. E 68, 036118 (2003).
[3] A. Karma, D. Kessler, and H. Levine, Phys. Rev. Lett. 87, 045501 (2001).
[4] A. Karma and A. Lobkovski, Unsteady crack motion and branching in a phase field model cond-mat/0401056.
[5] R. Deegan, P. Petersen, M. Marder, and H. Swinney, Phys. Rev. Lett. 88, 014304 (2002).
[6] I. S. Aranson, V. A. Kalatsky, and V. M. Volokur, Phys. Rev. Lett. 85, 118 (2000).
[7] L. Eastgate, J. Sethna, M. Rauscher, T. Cretegny, C.-S. Chen, and C. Myers, Phys. Rev. E 65, 36117 (2002).
[8] M. Adda-Bedia, Brittle fracture dynamics with arbitrary paths: III. The branching instability under general loading (2003).
[9] L. Freund, Dynamic Fracture Mechanics (Cambridge University Press (UK), 1990).
[10] J. Fineberg, S. P. Gross, M. Marder, and H. L. Swinney, Phys. Rev. Lett. 67, 457 (1991).
[11] K. Ravi-Chandar and W. G. Knauss, Int. J. Fracture 25, 247 (1984).
[12] B. Lawn, Fracture of Brittle solid, second edition (Cambridge University Press (UK), 1993).
[13] M. Adda-Bedia and Y. Pomeau, Phys. Rev. E 52, 4105 (1995).
[14] A. Yuse and M. Sano, Nature 362, 329 (1993).
[15] J. Hodgson and J. Sethna, Phys. Rev. B 47, 4831 (1993).
[16] E. Bouchbinder, H. Hentschel, and I. Procaccia, Phys. Rev. E 68, 036601 (2003).
[17] E. Sharon, G. Cohen, and J. Fineberg, Nature 410, 68 (2001).