Study of three-dimensional crack fronts under plane stress using a phase field model

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Abstract – The shape of a crack front propagating through a thin sample is studied using a phase field model. The model is shown to have a well-defined sharp interface limit. The crack front is found to be an ellipse with large axis equal to the width of the sample and small axis being a function of the Poisson ratio and of the width of the sample. Numerical results also indicate that the front shape is independent of the crack speed and of the sample extension perpendicular to its width.

When a crack grows in an elastic medium under increasing load, one would expect, according to the Linear Elastic Fracture Mechanics (LEFM) theory, that its speed increases and reaches asymptotically the Rayleigh wave speed \([1]\). Experimentally it has been found that at small loads (and therefore low crack speeds) the theory accounts well for the crack speed. But for higher loads (and for higher crack speeds) the observed phenomena are not predicted by the LEFM. Indeed, above a critical speed that is approximately equal to half the Rayleigh wave speed, the crack speed as a function of time starts to be irregular \([2,3]\) and the crack surface presents marks indicating the growth of secondary crack branches. The theoretical effort to predict this instability in the framework of the LEFM has not been successful yet even though it has been possible to determine a minimal speed below which the branching can not occur \([4,5]\). While experiments have allowed to describe the departure from the LEFM theory they have not been able to give a clear description of the mechanisms leading to the instabilities. This is mainly due to the fact that crack fronts are rapidly moving objects over a long distance compared to the scale at which the instability is assumed to take place (the process zone). In addition to this issue, experiments are limited to the observation of the surface of the sample \([3,6]\) while it is likely that the instability mechanism occurs in the thickness of the sample \([7,8]\). In fact, the theoretical study of propagating cracks has been mostly limited to two-dimensional cases and there is no widely accepted law of motion for the crack front in 3D.

Hence, models where the breaking mechanism occurring in the process zone is described in a simplified way are appealing since their use in numerical simulations would give access to real time observations of the crack front and will hopefully allow to have a better understanding of the branching mechanism. One possible candidate would be the phase field model of crack propagation \([9]\). It was originally presented in \([10]\) for mode-III cracks and then extended to mode I and II \([11–15]\) and more recently used in the study of the propagation of a tridimensional crack under mixed mode loading \([16]\). In this model of fracture, elastic energy is converted into surface energy through the evolution of a phase field that governs the elastic constants in the medium (for a review of phase field models of crack propagation see \([17]\)). This approach has the advantages that no law of crack propagation is needed (since the crack propagation is due to the evolution of the phase field) and that, numerically, its implementation is straightforward without the need of any complex interface tracking approach (this is especially advantageous in 3D where surface tracking is involved). Here, after briefly presenting the model and the numerical setup, I present the study of a single crack front propagating through a thin sample under plane stress conditions at its sides (see fig. 1). This work aims at solving a long-standing question dating back to the work of Benthem \([18]\) where it was shown that, contrarily to what is happening in the quasi–two-dimensional situation of plane strain, a crack front could not be a straight line in a thin sample since the singularity at the crack front combined with the plane stress condition would lead to infinite displacement in the direction of the front (z-direction in fig. 1). Since

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The free energy responds to an intact (respectively, entirely broken) material. The case $\phi = 1$ (respectively, $\phi = 0$) corresponds to an intact (respectively, entirely broken) material. The free energy from which the evolution equation of the phase field and of the elastic field derive writes

$$
\mathcal{F} = \iiint dV \frac{w_\phi D}{2} (\nabla \phi)^2 + \frac{1}{w_\phi} V_{DVW}(\phi) + \frac{1}{w_\phi} g(\phi) \left( \frac{\lambda}{2} (\epsilon^2) + \mu \epsilon^2 \right),
$$

where $\epsilon$ is the symmetric rank-2 strain tensor ($\epsilon_{ij} = (\partial_i u_j + \partial_j u_i)/2$ with $u_i$ the displacement field of the material. The functions are: $V_{DVW}(\phi) = \phi^3 (1 - \phi)^2$ and $g(\phi) = 4\phi^3 - 3\phi^4$. $w_\phi$ is a parameter that sets the interface width (which is proportional to $w_\phi$) without changing the fracture energy $\gamma = \sqrt{2w_\phi D} \int_0^1 d\phi \sqrt{\frac{1}{w_\phi} (V_{DVW} + (1-g)\epsilon^2)}$ [9].

The evolution equation of the displacement field writes

$$
\partial_t u_i = -\frac{\delta \mathcal{F}}{\delta u_i},
$$

so that, if the phase field is uniformly equal to 1, one retrieves the wave equation for a solid of density 1 and that the region where the phase field is equal to zero cannot transmit any stress. The evolution equation of the phase field is

$$
\tau \partial_t \phi = -\frac{\delta \mathcal{F}}{\delta \phi}/\beta,
$$

where $\beta$ is a constant kinetic coefficient that measures the dissipation at the crack tip (see [15]) and $\tau$ is a variable kinetic coefficient that is equal to 1 except in the following cases:

- it goes to zero if the r.h.s. of eq. (3) is positive, so that the phase field can only decrease (breaking is irreversible);

- $\tau$ is $\max(0, (A + g'(\phi)K_{Lam}e(\epsilon^2))/A)$ with $A = -\delta \mathcal{F}/\delta \phi$ if $\epsilon^2 < 0$ so that the compression energy does not contribute to crack growth.

One should note that these kinetic modifier, even if they may prevent the system from reaching a global minimum (in the same way as actual irreversibility does) do not lead to an unphysical increase of the free energy. As previously mentioned these equations have already been used to describe the growth of a crack in a 2D set up. Here I use them to study the crack growth in a 3D set-up considering a plate under plane stress condition:

$$
\sigma_{zz} = \sigma_{yz} = \sigma_{xz} = 0,
$$

which translates in

$$
\epsilon_{zz} = 0, \quad \epsilon_{yz} = 0 \quad \text{and} \quad \epsilon_{xz} = -\lambda \ast (\epsilon_{xx} + \epsilon_{yy})/\lambda + 2\mu
$$

with a no-flux boundary condition for the phase field, so that surface terms $\iiint \delta \phi \nabla \cdot dS$ do not contribute to the change in the free energy.

The simulations were performed using finite differences (using a scheme that derives from a discretized free energy)

\[\text{since such a boundary condition is not the more generic one for a crack front intersecting the boundary of the material with a finite angle, simulations using a different boundary condition that allows the intersection of the crack front with an angle were performed without noticeable change in the crack front shape.}\]
to compute the derivatives and the time stepping was performed using a simple forward Euler scheme. The grid spacing was taken equal to \( dx = 0.3 \) and \( dx = 0.15 \) to check that discretisation effects are negligible.

In this model, the crack surface can be seen as the \( \phi = 0.5 \) isosurface and the coordinate system is the elastic body at rest. Hence, the crack surface in the \( x0y \)-plane corresponds to a single thin finger using the present coordinate system. To retrieve the laboratory frame, one needs to apply the coordinate change: \( x \sim x + u_x(x, y, z), y \sim y + u_y(x, y, z), z \sim z + u_z(x, y, z) \). Using this coordinate change, one retrieves the parabolic crack front opening far from the tip (see [20] for the effects of a non-linear elastic zone at the crack tip). The crack front was taken as the set of points of higher \( x \) of the isoline \( \phi = 0.5 \) in each \( x0y \)-plane (see fig. 1) and it was a line in the \( y = 0 \) plane.

Numerical simulations showed that in the case of a single crack the points were located at the middle of the sample (\( y = 0 \)). While the crack front reached a steady shape after a transient regime when the crack speed was below the branching threshold, in the quantitative study an averaging procedure (usually over 5 to 10 snapshots of the front equally spaced in time) was used to reduce the discretisation effects.

Results are discussed as follows. First, the shape of the crack front in the case of thin samples is described. Then the dependence of the crack front on the phase field interface thickness is discussed from a quantitative point of view and the model is shown to converge toward a well-defined limit when the interface thickness is decreased toward 0. Finally, the dependence of the crack front on relevant physical parameters is discussed. The physical parameters considered here are the geometry of the sample: that is the ratio \( T/W \) and the actual value of \( T \), the Poisson ratio of the material \( \nu = \lambda/(2(\lambda + \mu)) \), the load applied to the material that is directly related to the crack speed and the kinetic coefficient \( \beta \) that governs dissipation at the crack tip.

Before describing the crack front, the change in crack speed is briefly discussed. When considering a single crack propagating in a thin plate (the quantitative meaning of thin will be precised later), one expects to retrieve the results one would get from a 2D computation. Indeed, in both cases, the crack propagation can be described as transforming elastic energy stored in the material at rest into kinetic energy (in elastic waves) and surface energy. Only a little slowdown of the crack due to the additional degree of freedom along the \( z \)-axis (along which the elastic wave will also propagate) is expected. Simulations have shown that this is the case and that there is very little difference between the speed computed using 3D simulations and the speed computed using 2D simulations provided the elastic coefficients are rescaled to take into account the zero-stress condition.

As already shown ([19]) the zero-stress condition implies that the crack front cannot be flat. Numerical results show that this is actually the case and the crack front is not flat and presents a noticeable curvature at its tip. A fit of the crack front using various possible test functions (such as power laws) indicated that the best fit is an ellipse with large axis equal to the half-thickness of the sample, \( T/2 \), and small axis \( \epsilon T \), where \( \epsilon \) is a real constant (see fig. 2). The equation of the ellipse in the following will write

\[
1 = \frac{x^2}{(T/2)^2} + \frac{x^2}{(\epsilon T)^2}, \quad y = 0.
\]  

It should be noted here that since \( T \) is fixed, there is only one adjustable parameter for the fit: \( \epsilon \) which is \( a \) priori a function of other parameters describing the system (load, elastic constants and geometry of the sample). This fit was valid only for thin samples where \( W/T \) was approximately larger than 5. For thicker samples the crack front was no longer elliptical and its shape will only be briefly discussed here.
In phase-field simulations, the role of the interface thickness has to be measured and one needs to show that a proper sharp interface limit exists when the interface thickness goes to zero keeping other parameters constant (including the surface energy). In our model, this can be done by varying \( w_\phi \) and one can easily show that the interface thickness is proportional to \( w_\phi \) while the surface energy is kept unchanged \([9]\). Simulations using various values of \( w_\phi \) (namely 1, 2, 3 and 4) have shown that the value of \( \epsilon \) converges toward a well-defined limit when \( w_\phi \) goes to 0 (see fig. 3). Moreover, they show that the relative error made when considering the case \( w_\phi = 1 \) is of the order 10\%. This indicates that the model has a well-defined limit when \( w_\phi \) is decreased toward 0. One should note that when \( w_\phi \) is decreased both the phase field interface thickness and the phase field process zone size are going toward zero and that the model has not a well-defined sharp interface limit as solidification models do. Nevertheless, the fact that the size of the process zone decreases proportionally to the interface thickness is coherent with the LEFM theory where the process zone is a point. In the following all the results considered were obtained using \( w_\phi = 1 \).

I now turn to the study of the dependence of \( \epsilon \) on the different parameters characterizing the physical system. First a system where the geometry \((W, T)\), the elastic constants \((\lambda, \mu\) and more importantly \(\nu\)) and the fracture energy are fixed while the crack speed is varied is considered. The variation in the crack speed can be achieved either by changing the load or by changing the dissipation \((\beta)\) at the crack tip. As can be seen in fig. 2(d), changing the value of \( \beta \) does not affect significantly \( \epsilon \). Varying the load did not change the value of \( \epsilon \) for a wide range of crack speeds \((0.05 \ c_e \ to \ 0.4 \ c_e\) close to the threshold speed at which the branching instability occurs).

In the following, the effects of the parameters describing the mechanical problem \(i.e., \) the Poisson ratio and the geometry of the sample) are investigated.

First for a given geometry sample \((T \ and \ W)\), the value of the Poisson ratio \(\nu\) was varied \((by \ changing \ \lambda \ and \ \mu)\). As shown in fig. 4 the value of \(\epsilon\) is significantly affected by the Poisson ratio. For small values of \(\nu\), the value of \(\epsilon\) is small and the crack front is almost flat as it is expected in the plane strain situation. This is not surprising since for \(\nu\) close to zero, the amplitude of the so-called Poisson effect is small and the difference between plane stress and plane strain condition is small. More precisely, in the limit where \(\nu\) goes to zero, one expects the plane stress and plane strain condition to be equivalent and therefore the crack front is expected to be flat. Here, the limit of \(\epsilon\) when \(\nu\) goes to zero is zero which is in agreement with this prediction.

On the opposite for values of \(\nu\) close to 0.5 (incompressible limit), the value of \(\epsilon\) is much higher and goes toward a finite limit when \(\nu\) goes to 0.5 (its maximal value corresponding to an incompressible material where the difference between the plane strain and plane stress condition should be the highest).

Now I turn to the description of the effects of the sample geometry. All results were obtained for a given Poisson ratio \(\nu = 0.25\) and, in the case of thin samples, various values of the width \(W\) \((80, 160 and 320 space units (su))\) and thickness \(T\) \((from 6 to 60 su)\) of the sample. The value of the width of the crack \(w_\phi\) was kept constant. In the case of thick samples, values of \(T\) equal to \(W\) and larger were used. First the results obtained using thin samples are presented. In this situation, \(T \leq W\), the crack front is half an ellipse and it is completely described by the value of \(\epsilon\). In this situation, it appears that \(\epsilon\) is a function of \(T\) and does not depend on \(W\) as can be seen on fig. 4 where the computed values of \(\epsilon\) are plotted as a function.
of $T$ for two different values of $W$ (160 and 320 su) and collapse well on a master curve. When $T$ goes to zero, one can see that $\epsilon$ converges toward a well-defined finite limit. When $T$ goes to infinity, the behaviour of $\epsilon$ is still not clear since the present data do not allow to determine wether it converges toward a finite limit or wether it decreases toward 0.

When considering thick samples, the use of $u_z = u_x = 0$ as top and bottom boundary conditions leads to the fact that most of the elastic material is under plane strain. Then the system is in a situation where the work of Bazant [19] can be applied. As a result one expects the crack front to intersect the free boundary with a finite angle that is a function of the Poisson ratio. Numerical results are in good agreement with this prediction. Indeed, as can be seen in fig. 3 where half the crack front is plotted, the crack front is V-shaped and intersects the free boundary with a finite angle. Moreover, the value of the angle obtained during numerical simulations is a function of the Poisson ratio and is in good agreement with the prediction of [19].

Hence, this work indicates that the shape of a crack front through a thin sample is half an ellipse that is tangent to its sides. The small axis of this ellipse is, as one would have expected, a function of the Poisson ratio of the material and, more surprisingly, of the thickness of the sample, independantly of its width. Extensive checks on parameters show that the dependence on other parameters of the crack front propagation is not significant. Indeed, simulations have shown that the crack front shape is independent of the crack speed, the dissipation at the crack tip and the width of the sample (provided one stays in the $T \ll W$ regime). In addition, the behaviour of the model was checked against predictions made using the LEFM theory in the case of thick samples [19] and a good agreement was found.

This study stresses one of the main interest of the phase-field modelling of crack propagation in three dimensions: it allows to predict the shape of a crack front without any a priori hypothesis.

Another continuation of this work would be to use the phase field model to understand the branching instability in three dimensions. Indeed, from a qualitative point of view, the phase field model allows to reproduce well three-dimensional branching events (see fig. 5) with a good qualitative agreement with experimental findings [21] as far as the shape of the branch is concerned.

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