Supersonic crack propagation in a class of lattice models of Mode III brittle fracture

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We study a lattice model for mode III crack propagation in brittle materials in a stripe geometry at constant applied stretching. Stiffening of the material at large deformation produces supersonic crack propagation. For large stretching the propagation is guided by well developed soliton waves. For low stretching, the crack-tip velocity has a universal dependence on stretching that can be obtained using a simple geometrical argument.

The determination of crack-tip velocities in brittle fracture is one of the unsolved problems in fracture mechanics\cite{1, 2}. Spontaneous crack propagation typically occurs when some energy balance condition is satisfied. This is usually known as the “Griffith’s criterion” and it states roughly speaking, that the available elastic energy has to be larger than the energy necessary to create new surface in the material upon crack advance. We will define the excess elastic energy (EEE) as the difference between the available elastic energy and the (static) crack-surface energy. When the EEE is positive a dynamic regime is achieved. The nature of this regime depends on the value of the EEE\cite{1, 2, 3}. If the EEE is low, a stationary regime is usually observed, in which the crack velocity is a well defined (material dependent) function of the EEE, and if the geometric configuration is symmetric with respect to the crack, crack propagation occurs along a straight line. For larger values of the EEE, crack path oscillations, crack branching and other phenomena typically occur.

We will focus here in the low EEE regime. Even in this relatively simple case, the prediction of crack-tip velocity as a function of material parameters, sample geometry and strain conditions is a challenging problem. Linear elastic fracture mechanics (LEFM)\cite{1, 2} suggests that the crack-tip velocity $V$ should be a univocus function of the EEE and material characteristics. Among these, microscopic details of the process zone must be included in general. Another most important prediction of LEFM is the impossibility that the value of $V$ exceeds the Rayleigh velocity of the material, which is typically somewhat lower than the shear sound velocity. There is some experimental evidence that challenges this prediction.\cite{3} In addition, it has been recently shown that elastic stiffening at large deformation can unambiguously produce cracks running faster than the shear sound velocity in simulations of mode I (opening) propagation.

Here we analyze the dependence of crack tip velocity upon model parameters in a class of piece-wise harmonic lattice model for mode III fracture. We find supersonic propagation and study its characteristics. We find a remarkable regime in which the crack-tip velocity can be accurately predicted on the basis of a geometric argument, and is independent of most of the model parameters.

We model a stripe of material, laterally stretched in the out-of-plane direction, with a crack propagating along the mid line. This geometry is particularly adequate to study stationary crack propagation as the system looks identical upon extension of the crack. This kind of models have been studied before, for instance in Refs. \cite{4, 5}. The model consists of a discrete square lattice. At each node a mass is placed, and the links to nearest neighbor sites are modeled by piece-wise linear springs. The full lattice forms a rectangular system, to which out-of-plane fixed-displacement lateral boundary conditions are applied. We take the horizontal $x$ axis along the stripe. This is also the crack propagation direction. The out-of-plane displacement of the masses (the only one which is non-zero) is noted by $u$. The equation of motion of a mass at the discrete position $i, j$ in the lattice is simply

$$\frac{d^2u_{i,j}}{dt^2} = \sum_{[i', j']} F(u_{i', j'} - u_{i,j})$$

where $[i', j']$ are the neighbor sites to $i, j$ and the function $F$ specifies the force law of the corresponding spring: $F(x) = x$ for $x < u_{nl}$, and $F(x) = \gamma x$ for $x > u_{nl}$ for intact springs, and $F(x) = 0$ for broken springs. Note that the low deformation spring constant and mass of the particles have been set to 1 (this sets the wave velocity to 1, also), and that $u_{nl}$ is the critical stretching at which the spring constant changes from 1 to $\gamma$ ($\gamma > 1$).

Springs are assumed to break irreversibly when the stretching is larger than a fixed threshold value $u_{bk}$. To avoid crack branching, which may occur under certain conditions, we allow to break only the vertical springs in the center of the stripe (for low stretching this procedure is not necessary, see below). For symmetry reasons we simulate only the upper half of the stripe, and $N_y$ will denote the number of rows in this half system. The boundary condition at the bottom border is $u_{i,1} = -u_{i,0}$, whereas at the upper border we have $u_{i,N_y+1} = (N_y + 1/2)\delta$, where $\delta$ is the nominal stretching applied to each vertical spring. We always keep $\delta < u_{nl}$, not to force the system in the non-linear regime with the uniform applied strain. Along the $x$ direction, we take
the boundary conditions as follows: $u_{Ny,j} = (j - 1/2)\delta$ and
$u_{0,j} = (Ny + 1/2)\delta$. These conditions correspond to those that
should be valid at $x \to \pm \infty$. By enforcing them at a finite $x$-position
some error is introduced, but we check that this error is small if $N_x$ is
large enough. The crack tip is initially placed at an $x$ position close
to the right border of the system, by seeding the simulations with
an appropriate initial condition. Along the simulation the crack advances in the positive $x$
direction. Each time we detect that a new spring ahead of the crack has broken, we shift all system coordinates
and velocities one unit to the left. In this way the crack tip is always
maintained at the same position with respect to the lattice, and the instantaneous crack-tip velocity is
determined as the inverse of the difference in consecutive
times of spring breaking. Reported values correspond to
averaging over long simulation times, after dependences
on initial conditions have died out.

In the present stripe geometry, the Griffith’s criterion is stated as follows: crack propagation cannot
occur if stretching is lower than some critical value $\delta_G$. Equating the elastic energy far ahead of the crack-tip, to
that far behind it, we find $\delta_G = \sqrt{2t/(2Ny + 1)}$, where
$\Gamma = u_{nk}^2/2(Ny + 1)/2$ is the crack energy
per bond. We see that $\delta_G \to 0$ for $Ny \to \infty$. The EEE per horizontal bond (referred to as $\varepsilon$) is easily calculated
in terms of $\delta_G$ as $\varepsilon = \Gamma[(\delta/\delta_G)^2 - 1]$. As it should,
this quantity vanishes at $\delta = \delta_G$. Note that contrary to the usual assumption in LEFM, in our model the excess
energy $\varepsilon$ is not dissipated at the crack tip, but it is trans-
formed into kinetic energy, that eventually escapes from the left border of the system.

To test the classical prediction in the normal (sub-
sonic) case, in Fig. 1 we show curves for the velocity
as a function of the strain ahead of the medium.

The result agrees with the predictions of LEFM. The velocity
approaches the wave speed for large $\varepsilon$, whereas at low $\varepsilon$
is reduced due to lattice trapping effects. In accordance
also with previous simulations in this kind of models[2],
the instantaneous velocity (Fig. 1 inset) is found to tend
to a constant for large stretching, but it is a fluctuating
function of time in the low stretching regime.

Results change if $\gamma > 1$. In this case different velocity
curves for different stripe widths do not tend to collapse
in the large $Ny$ limit if plotted as a function of $\varepsilon$. Instead,
they do if plotted as a function of the unperturbed value $\delta$
of the strain ahead of the crack. This is an important
result: since the propagation is supersonic, the crack can respond only to the local state of the medium, and
the velocity must be independent of the system width if this
is large enough. In Fig. 2 we plot the velocity dependence
on $\delta$ for different system parameters. We clearly see the supersonic propagation, which occurs for any $\delta > 0$ if $Ny$
is large enough.

To analyze these results, it is convenient to solve first the following formal problem. Consider a perfectly har-
monic, infinite and continuous system, stretched some
fixed amount $\delta$ per unit length in the y direction. Suppose
that by some external mean we force a crack to prop-
agate along the $x$ direction at some velocity $V$, which is
arbitrary, with the only condition $V > 1$. The displace-
ment field $u(x, y)$ is found to be simply:

$$u(x, y) = y\delta$$

outside the Mach’s cone.
\[ u(x, y) = \pm \frac{x\delta}{\sqrt{V^2 - 1}} \] inside the Mach’s cone, for \( y \leq 0 \).

Here, the crack tip is located at \( x = 0, y = 0 \), and the Mach’s cone half-angle \( \theta \) is given by \( \sin \theta = 1/V \). Note that inside the Mach’s cone this solution has a constant value of \( |du/dx| \), given by \( |du/dx| = \delta/\sqrt{V^2 - 1} \). In the case in which the same problem is solved (numerically) on a discrete square lattice (inducing the propagation by breaking bonds at a fixed rate \( V \)), an oscillation close to the border of the Mach’s cone is found, and the maximum stretching \( |\Delta u|_{\text{max}} \) of a spring in the system is enhanced by a constant factor. It is found to be \( |\Delta u|_{\text{max}} \approx 1.26 \delta/\sqrt{V^2 - 1} \). Note that \( |\Delta u|_{\text{max}} \) diverges when \( V \to 1 \) no matter how small \( \delta \) is.

In Fig. 3 we see the actual results from the simulations in the non-linear model. At low \( \delta \) (upper panel) the \( u_{ijkl} \) function looks roughly similar to that given by Eq. 2 (except for the reflection effects at the lateral borders of the system). We find a number of spatial positions at which the non-linear threshold is exceeded. This is quite reasonable, otherwise we should not expect any supersonic propagation. In addition, it is found that the instantaneous crack tip velocity is a fluctuating function of time, typically around \( \pm 10 \% \) of the mean value. This fluctuation is accompanied by a change in the location of the points at which the non-linear threshold is exceeded. In spite of this, the mean velocity can be determined to a high precision by averaging over a long simulation time. Upon increasing \( \delta \), the non-linear regions tend to arrange in the form of solitons, that eventually (for \( \delta/u_{nl} \) between 0.7 and 0.75 in Fig. 3) go outside the Mach’s cone. There are five solitons at \( \delta/u_{nl} = 0.75 \) in Fig. 3 and this number reduces as \( \delta \) increases. For the largest \( \delta \) values studied, typically a single soliton is observed, which drives the supersonic propagation. We have carefully verified that the solitons in front of the crack tip are simply the non-linear solitary waves corresponding to the present non-linear elastic system, i.e., they are the analogous of the solitons appearing for instance in the well known Toda lattice. In the regime of solitons-driven propagation the instantaneous velocity is constant. The transition between the low-\( \delta \) and the soliton driven regimes is found to be abrupt, with some hysteresis upon increasing/decreasing \( \delta \), and with a small but clearly observable jump in the velocity (not appreciable in the scale of Fig. 4).

The low \( \delta \) region of the plot in Fig. 2 shows a remarkable independence on model parameters. Actually, this part of the curve can be understood and fitted on the basis of the following heuristic argument. Consider the previously found solution for the harmonic system, Eq. 2. We look for the possibility that this solution is self-maintained in the presence of non-linearities (i.e., when \( \gamma \neq 1 \)), and we analyze in particular the case in which \( \gamma \) is very large. It is then found that the velocity \( V^* \) obtained by requiring \( u_{nl} = |\Delta u|_{\text{max}} \) plays a special role. This velocity is (taking into account the factor introduced by the discreteness of the system)

\[ V^*(\delta) \approx \sqrt{1 + (1.26 \delta/u_{nl})^2}. \] (3)

In fact, if \( V > V^* \), the solution does not explore the non-linear part of the potential anywhere, and then it cannot be self-maintained. On the other hand, if \( V < V^* \), there are regions in the system in which the non-linear threshold is exceeded by a finite amount, but this cannot be acceptable if \( \gamma \) is sufficiently large. Then we expect that the velocity at which the crack propagation stabilizes is precisely \( V^* \). This prediction is plotted on top of the numerical results in Fig. 2. The only parameter of the model on which \( V^* \) depends upon is the non-linear threshold \( u_{nl} \), beyond that the solution is independent of the precise values of \( \gamma \) (assumed large) and \( u_{hk} \). The fitting improves for larger systems as shown in the inset to Fig. 2, where different points for all combinations of the parameters indicated are plotted as a function of \( V^*(\delta_G) \). The continuous lines in Fig. 2 (inset) correspond to the finite size ansatz \( V(\delta) = V^*(\delta) - V(\delta_G) + 1 \). The numerical data follow accurately this trend, and numerical extrapolation for \( N_y \to \infty \) allows to claim that the fitting is better than \( 1 \% \) for \( \delta/u_{nl} \lesssim 0.3 \) for all the parameters studied. This accuracy is remarkably good because, as we already said, the instantaneous velocity in the low \( \delta \) regime fluctuates around the mean value in about \( 10 \% \).

An attempt to predict by the same kind of geometric argument the propagation velocity of intersonic mode I or mode II cracks gives negative results: A theoretical investigation in a purely harmonic system shows that (contrary to the mode III solution 2) the stress fields diverge at the crack tip and are dependent on the boundary conditions at infinity (see 2, pp. 348-355). Then there is not a well defined maximum stress to be used in an argument similar to that presented for mode III. In addition, the consideration of truly supersonic mode I or mode II cracks for totally harmonic springs up to breaking shows that (in opposition to the mode III case) for any fixed velocity all stresses fall below any chosen threshold value if \( \delta \) is taken small enough, and this implies that supersonic propagation cannot occur for arbitrarily low values of stretching. These considerations show that the present mode III problem stands as a very particular but important case in which the crack tip velocity can be predicted on the basis of general arguments.

The simulations that produced Fig. 2 were done by allowing to break only the vertical springs ahead of the crack. However, we can check a posteriori whether other springs overpass the breaking threshold \( u_{hk} \) or not. It is found in general that there is a separating value \( \delta_0 \) below which the previous prescription is not necessary. If all springs are allowed to break, there are no changes in the results for \( \delta < \delta_0 \), whereas other phenomena (typically crack branching) are observed if \( \delta > \delta_0 \). We found \( \delta_0 \)
The non-linear threshold for the vertical springs is moved to infinity, the velocity curves obtained are only slightly modified, the low δ fitting remains good, and in particular propagation remains supersonic. On the other hand, if the non-linear threshold of the horizontal springs is moved to infinity, supersonic propagation completely disappears. Then we arrive at the seemingly paradoxical result that the non-linearities of the springs that actually break are not crucial in determining the propagation velocity. This consideration is important for theoretical arguments since it tells that the present results cannot be explained with an analysis assuming a Barenblatt-type process zone (see [2], ch. 3), since in this case only non-linearities in the vertical links are considered.

In conclusion, we have studied the supersonic propagation of cracks in a lattice model of mode III fracture, in the context of elastic stiffening at large deformation. Crack velocity is found to depend on the local strain ahead of the crack. For large stretching, the crack propagation is driven by solitons formed in the non-linear lattice. In the low stretching regime well developed driving solitons are absent. In this last case the crack velocity can be accurately predicted on the basis of a geometrical argument, and it is found to have a general explicit expression. This stands as one of very few predictions of crack propagation velocities in models of brittle fracture.

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