Dynamical extraction of a single chain from a discrete lattice

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Abstract

We consider a nontrivial anti-plane shear fracture problem for a double-crack configuration where the remote external load is applied to the extracted mass-spring chain and the displacement field is symmetric with respect to the central axis between the cracks. An analytical solution obtained for the steady-state problem describes the displacement fields, stresses, local and global energy release rates and the dissipation. The double-crack configuration differs considerably from the classical problem of fracture in a lattice: the load is applied to the extracted chain rather than the outer domain as in the classical fracture problems. In the corresponding Wiener–Hopf equation, this leads to a special type of kernel, which is not typical for fracture problems.

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1. Introduction

This paper addresses a lattice model describing the propagation of a symmetric fault shown in Fig. 1. In the frame of the anti-plane shear formulation, a semi-infinite “inertial thread”, i.e. the chain of masses connected by massless bonds, is removed from the lattice plane, and consequently two parallel lines of broken bonds are being formed. A remote force is applied to the above-mentioned “inertial thread” to provide energy sufficient for the propagation of the fault. The corresponding continuous analogue is also considered below; it involves a pair of the propagating semi-infinite parallel cracks, with the remote external load being applied to the strip between the cracks. Note that in contrast with the continuous formulation the lattice model allows for the determination of dissipation in the form of the structure-associated waves radiated by the fault propagating in this elastic structure.

In the formulation, we assume that the longitudinal strength of the extracted chain, or that of the continuous strip, is sufficient to withstand the load required for the extraction. For the case when a single chain is extracted from the lattice, this implies that the strength of the longitudinal bonds must be larger than the strength of the bonds in the transverse direction [the corresponding strength ratio is determined by Eq. (18)]

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in the main text of the paper. As to the bond stiffness, we assume that it is the same for all the bonds within
the lattice.

We consider a steady-state problem for a subcritical crack speed $v$. In the main analysis, the speed is
considered as a given constant, and the energy release rate corresponding to this crack propagation speed is
obtained in the analytical form. Furthermore, given that the energy release rate exceeds its critical value, we
can determine the speed intervals corresponding to a stable crack propagation and evaluate the crack speed as
a function of the applied force.

We note that in the classical case of an opening-mode dynamic fracture, when an external load is applied
outside the strip, the double-crack configuration is unstable: as a crack leaves the other one behind it
also shields the slower crack and further reduces its speed. On contrary, in the considered symmetric problem,
the situation is quite the opposite, and the symmetric fault configuration is stable with respect to the crack
speeds.

One of the essential peculiarities of this problem is related to the validity of the steady-state formulation. It
is assumed that the steady-state solution is the limit $t \to \infty, \eta = x - vt = \text{const}$ of the solution to the
 corresponding transient problem with zero initial conditions, that is, the causality principle is adopted here,
following Slepyan (2002, pp. 91–94). However, in the case of the subcritical speed, the solution to the
 corresponding transient problem with zero initial conditions has no such a steady-state limit: the displace-
 ments in the outer domain (e.g., the domain outside the extracted chain or the loaded strip in the
homogeneous model) grow as $\ln t$ when $t \to \infty$. At the same time, a steady-state displacement field as the
solution to the corresponding steady-state problem (considered without invoking the causality principle) exists
and is determined up to an arbitrary additive constant. It shows how the displacements vary in the space. This
issue of convergence does not concern the strain and the particle velocities, which have finite limits.

The analysis of the above-mentioned effects in the lattice problem is the main motivation for the current
study. Physically, this problem is related, in particular, to a model of pulling out a thread from fabric, where
the propagation of the fault is accompanied by rupture of some of retaining bonds. Such a process can be used
to increase the energy consumption under a tensile impact where the tensile force level is given a priori. Here,
we discuss the simplest model where a single chain is extracted from the lattice; it is worthy to note, however,
that the related problem on the extraction of a lattice strip consisting of a finite number of chains can be solved
using the same method.

Comparing the continuum and the lattice models we also note a paradox occurring in the two-crack
configuration in the infinite elastic plane. The finite energy release rate can be maintained at a constant level as
the strip width and the force magnitude both tend to zero. Consequently, we arrive to the conclusion that a
“fault” generating a finite energy release rate propagates under the action of a zero force. Such a paradox is
inherent to continuum models. For example, if the Barenblatt cohesive forces neutralizing the crack-tip
singularity are tightened to a point, the total force appears to be zero, while the energy rate produced by this
zero force remains equal to a nonzero constant. In connection with this paradox, we have to stress, however,
that the energy flux density tends to infinity as the corresponding size (for example, the strip width) tends to
zero, and the realizability of such a situation is always questionable. Such a paradox is explicitly resolved using
the solution of the corresponding lattice problem.
We also mention another paradox associated with the continuum formulation in a different physical context. The classical Peierls–Nabarro model (see Peierls, 1940; Nabarro, 1947) involves a hypersingular integral equation describing a displacement jump across the glide plane—within a continuum approach any nonzero constant stress, represented by a constant term in the right-hand side of the equation, is sufficient to move the dislocation all the way to infinity.

There is a large, steadily increasing stream of papers on fracture in lattices. Numerical simulations of atomic lattices were initiated by the work of Thomson et al. (1971) and Ashurst and Hoover (1976), and still receive substantial attention in the modern literature (see, for example, Wang et al., 2004; Zhu et al., 2006 and references therein). The first analytical solution for a mass-spring 2D lattice model was obtained in Slepyan (1981). Such lattice models were then studied in Kulakhmetova et al. (1984), Marder and Liu (1994), Marder and Gross (1995), Marder and Fineberg (1996), Kessler (1999, 2000), Kessler and Levine (2001, 2003), Slepyan (2000, 2001a,b, 2005), Heizler et al. (2002), Slepyan and Ayzenberg-Stepanenko (2002, 2004, 2006). The main analytical results on this topic are summarized in Slepyan (2002). Beam-like lattices were studied in Herrmann et al. (1989), Tzschichholz et al. (1994), Chen et al. (1998), Astrom and Timonen (1996), Gibson and Ashby (1997), Schmidt and Fleck (2001), Skjetne et al. (2005), Lipperman et al. (2005).

A symmetric problem for a double-crack configuration considered in the present paper differs substantially from the above-mentioned studies. The main difference is that the load is applied to the extracted chain (or the strip between the cracks) rather than the outer domain as in the classical fracture problems. In the corresponding Wiener–Hopf equation, this leads to a special type of the kernel, which is not typical for fracture problems.

The plan of the paper is as follows. The formulation of the lattice problem and the analysis of the solutions to the corresponding Wiener–Hopf equation and evaluation of the local and global energy release rates are included in Section 2. Section 3 deals with the continuum model for a double-crack configuration. In particular, we address an apparent paradox which occurs in the limit case as the distance between the parallel cracks tends to zero. Finally, Section 4 includes the concluding discussion.

2. Lattice problem

We consider a steady-state dynamic problem for a square lattice where a chain of connected particles is extracted from the lattice by a remote force. This can be thought of as two parallel crack propagation; these “cracks” bound the extracted chain, Fig. 1. The particle displacements are symmetric relative to the line, and the stress within the chain forces the cracks to propagate. In the macrolevel description of the state, where the structure-associated oscillations are ignored, the line is expected to have a constant slope proportional to the remote force. We start with the dynamic lattice equations:

$$\begin{align*}
\ddot{u}_{0,m} &= u_{0,m+1} + u_{0,m-1} + 2u_{1,m} - 4u_{0,m} - 2(u_{1,m} - u_{0,m})H(-\eta), \\
\ddot{u}_{1,m} &= u_{1,m+1} + u_{1,m-1} + 2u_{2,m} + u_{0,m} - 4u_{1,m} + (u_{1,m} - u_{0,m})H(-\eta).
\end{align*}$$

The first subscript stands for the number of the horizontal layer, whereas the second subscript denotes the number of the node within the layer. The problem is normalized in such a way that the lattice spacing, stiffness of bonds and the mass of particles are taken as natural units. The Fourier transform on \(\eta = m - vt\) leads to the equations:

$$\begin{align*}
(2 + h^2)u_0^F - 2u_1^F &= -2(u_{1-} - u_{0-}), \\
u_0^F + (2 + h^2 - \lambda)u_1^F &= (u_{1-} - u_{0-}),
\end{align*}$$

where

$$\begin{align*}
\lambda &= \frac{u_0^F}{u_1^F} = \frac{r - h}{r + h} = \frac{(r - h)^2}{4}, \\
h &= \sqrt{2(1 - \cos k)^2 + (0 + ikv)^2}, \quad r = \sqrt{h^2 + 4},
\end{align*}$$
and the expression for \( \lambda \) is derived in Slepyan (2002, p. 394). Here \( v \) is the normalized crack speed. These two equations can be solved with respect to \( u_0^F \) and \( u_1^F \)

\[
\begin{align*}
    u_0^F &= -\frac{2(r + h)}{r^2 + rh - 2}(u_1 - u_0), \\
    u_1^F &= \frac{2h}{r^2 + rh - 2}(u_1 - u_0) - 2.
\end{align*}
\]

(3)

The asymptotes for \( k \to 0 \) are

\[
    \frac{2(r + h)}{r^2 + rh - 2} \to 1, \quad \frac{2h}{r^2 + rh - 2} \sim \frac{1}{2} \sqrt{1 - v^2}(0 + i k)(0 - ik).
\]

(4)

It follows that

\[
    Q^F = (u_1 - u_0)^F = \frac{2(r + 2h)}{r^2 + rh - 2} Q^-.
\]

(5)

Thus, we come to a homogeneous Wiener–Hopf type equation of the form

\[
    Q_+ + L(k)Q_- = 0
\]

(6)

with

\[
    L(k) = \frac{h^2(r + h)}{r^2 + rh - 2}.
\]

(7)

Note that

\[
    r + h \neq 0, \quad r^2 + rh - 2 \neq 0
\]

(8)

and hence real zeros and singular points of the function \( L(k) \) coincides with those of \( h \) and \( r \), respectively.

For subcritical speeds, \( 0 \leq v < 1 \), the kernel \( L(k) \) possesses the following features:

\[
    L(k) \sim \frac{1 - v^2}{2} k^2 \quad (k \to 0), \quad L(k) \to 1 \quad (k \to \pm \infty), \quad \text{Ind} L(k) = 0.
\]

(9)

This allows for the factorization as

\[
    L(k) = L_+ L_-,
\]

\[
    L_+ = \exp \left[ \pm \frac{1}{2} \pi i \int_{-\infty}^{\infty} \frac{L(\xi)}{\xi - k} \, d\xi \right] \quad (\pm \Im k > 0),
\]

\[
    L_+ \to 1 \quad (k \to \pm \infty), \quad L_+ \sim \sqrt{\frac{1 - v^2}{2}} R^{\pm 1}(v)(0 \mp ik) \quad (k \to 0),
\]

\[
    R(v) = \exp \left[ \frac{1}{\pi} \int_{0}^{\infty} \frac{\text{Arg} L(k)}{k} \, dk \right].
\]

(10)

We now divide Eq. (6) by \( L_+ \). The function \( L_+ \) has a zero at \( k = 0 \), and we proceed to the inhomogeneous equation according to Slepyan (2002, Section 11.5.1), by introducing the delta-function (as the generalized limit of its standard analytical representation) in the right-hand side of the factorized equation:

\[
    \frac{Q_+}{L_+} + L_- Q_- = \frac{C}{0 - ik} + \frac{C}{0 + i k},
\]

(11)

where \( C \) is a constant. In terms of the one-sided Fourier transforms the required solution is

\[
    Q_+(k) = \frac{CL_+}{0 - ik}, \quad Q_-(k) = \frac{C}{(0 + i k)L_-} \sim \sqrt{\frac{2}{1 - v^2}} \frac{CR(v)}{(0 + i k)^{2}} \quad (k \to 0).
\]

(12)

In terms of the original functions, we obtain

\[
    Q(0) = \lim_{s \to -\infty} s Q_+(i s) = C, \quad Q(\eta) \sim C \sqrt{\frac{2}{1 - v^2}} R(v)(-\eta) \quad (\eta \to -\infty).
\]

(13)

Thus, according to Eq. (5), \( C \) is the limiting “crack-tip opening”, that is the limiting strain of the bond.
Referring to Eq. (3) the Fourier transforms of the displacements are

\[ u_0^F = -\frac{2(r+h)}{r(r^2+rh-2)}Q_-, \]
\[ u_1^F = \frac{2h}{r(r^2+rh-2)}Q-. \]  

This yields

\[ u_{0-} \sim -Q_- (k \to 0), \quad u_0(\eta) \sim \sqrt{\frac{2}{1-v^2}}CR(v)\eta \quad (\eta \to -\infty). \]  

This result corresponds to the formulation where a remote force

\[ P = -u_0' = -\sqrt{\frac{2}{1-v^2}}CR(v) \]

is applied to the extracted line at a fixed coordinate far from the moving point \( \eta = 0 \). Then the constant \( C \) and the function \( Q_- (k) \) can be re-written in the form

\[ C = -\frac{P}{R(v)}\sqrt{\frac{1-v^2}{2}}, \quad Q_- (k) = -\frac{P}{(0+ik)L_-} - \frac{P}{(0+ik)^2} (k \to 0). \]

It follows that

\[ Q(\eta) \sim P\eta, \quad u_0(\eta) \sim -P \eta \quad (\eta \to -\infty), \quad Q(0) = \frac{P}{R(v)}\sqrt{\frac{1-v^2}{2}}. \]

Hence the local energy release rate (for both cracks)

\[ G_0 = \frac{1}{2}Q^2(0) = \frac{(1-v^2)P^2}{2R^2(v)}, \]

whereas the global energy release is

\[ G = \frac{Piu_0}{v} - \frac{(u_0')^2}{2} - \frac{(\dot{u}_0)^2}{2} = \frac{(1-v^2)P^2}{2}, \]

and the energy release ratio is

\[ \frac{G_0}{G} = R^{-2}(v). \]

This dependence is plotted in Fig. 2. The limiting value, \( v \to 0 \), corresponding to a quasi-static crack growth can be obtained using the discrete Fourier transform. It is found that

\[ \frac{G_0}{G} = \exp \left[ \frac{1}{\pi} \int_0^\pi \ln L(k) \, dk \right] \approx 0.231 \quad \text{when} \quad v = 0. \]

This value is marked in Fig. 2 by a dashed line. Note that the difference, \( G - G_0 \), is the energy dissipation rate which is inherent to fracture of a lattice. The last relation in Eq. (18) defines the ratio between the limiting stresses in the extracted chain and in the transverse breaking bonds.

Note that when the bond strength is not a time-dependent quantity, the low-speed steady-state regime, 0 < \( v < 0.45 \), cannot be realized since the elongation reaches the critical value first, before the expected time at \( \eta > 0 \) (see Marder and Gross, 1995).

Now consider the domain outside the extracted line. The function \( u_1^F \) (see Eq. (19)) has the asymptotic representation:

\[ u_1^F(k) \sim -\frac{\sqrt{1-v^2}(0+ik)(0-ik)P}{2(0+ik)^2} = -\frac{1}{2} \frac{1-v^2P}{0+ik} S^F(k) \quad \text{as} \quad k \to 0, \]
where

$$S^F(k) = \sqrt{\frac{0 - ik}{0 + ik}} = -i \text{sign } k$$

(24)

and hence it is the Fourier transform of

$$S(\eta) = -\frac{1}{2\pi} \left( \frac{1}{\eta - i0} + \frac{1}{\eta + i0} \right) = -\frac{1}{\pi} V.p.\frac{1}{\eta},$$

(25)

where $V.p.(1/\eta)$ is a generalized function; it means the Cauchy principal value for an integral of a product of this function with another one. At the same time, the original of $1/(0 + ik)$ is the Heaviside unit step function $H(-\eta)$. Thus

$$\frac{du_1(\eta)}{d\eta} \sim -\frac{\sqrt{1 - v^2} P}{2\pi} V.p.\frac{1}{\eta} \ast \delta(\eta) = -\frac{\sqrt{1 - v^2} P}{2\pi} V.p.\frac{1}{\eta}.$$  

(26)

This long-wave asymptote corresponds to the solution of the homogeneous medium considered below.

3. Related continuum model

Consider an infinite plane containing two parallel cracks $M_U$ and $M_L$, separated by the distance $a$ and propagating with the speed $v$ along the $x$-axis:

$$M_U = \{(x, y) : \eta = x - vt < 0, y = a\} \quad \text{and} \quad M_L = \{(x, y) : \eta = x - vt < 0, y = 0\}.$$  

(27)

For the problem of anti-plane shear, the displacement function $u(\eta, y)$ satisfies the equation:

$$ax^2 \frac{\partial^2 u(\eta, y)}{\partial \eta^2} + \frac{\partial^2 u(\eta, y)}{\partial y^2} = 0, \quad \alpha^2 = 1 - v^2/c^2,$$

(28)

where $c$ is the shear wave speed; for the sake of convenience we will use the normalization $c = 1$.

On the crack faces, we impose the homogeneous Neumann boundary conditions (zero tractions), i.e.

$$\frac{\partial u(\eta, y)}{\partial y} = 0 \quad \text{when } (x, y) \in M_U \text{ and } (x, y) \in M_L.$$  

(29)

The conditions at infinity are defined as follows:

$$u(\eta, y) \sim -C\eta \quad \text{as } \eta \to -\infty \text{ and } 0 < y < a,$$

(30)
and
\[ u(\eta, y) = -\frac{\pi Ca}{4}\ln(\eta^2 + z^2 y^2) + \text{const} \]  \hspace{1cm} (31)
when \( \eta^2 + y^2 \to \infty \) outside the strip between \( M_U \) and \( M_L \). Recall that the causality principle is not taken into account when this solution is constructed.

The above formulation corresponds to two parallel cracks propagating under the action of a force \( P = Ca \) applied at 'minus infinity' within the infinite strip between the cracks (this load is assumed to act at an unmoving point or in an unmoving region far from the crack-tip coordinate \( \eta = 0 \)).

The above problem allows for an explicit closed form solution incorporating a conformal map of \( \mathbb{R}^2 \setminus (M_U \cup M_L) \) into the upper half-plane (see Morse and Feshbach, 1953, p. 229):
\[ z - z_0 = A(w^2 - \ln w), \]
where \( A = -a/\pi, z_0 = -A/2 \).

The solution of the problem (28)–(31) is not differentiable at the vertices of the cracks \( M_U \) and \( M_L \), i.e. the components of \( \nabla u \) are \( O(1/(\eta^2 + y^2)^{1/4}) \) and \( O(1/(\eta^2 + (y - a)^2)^{1/4}) \) singular, as expected for stress near the crack tips.

We note that, under this continuous formulation, the energy is not radiated to infinity, and all the energy produced by the remote force goes to the crack tips. Consequently, the total energy release rate per unit length is represented in the form:
\[ \varepsilon = \varepsilon_f - \varepsilon_s - \varepsilon_k, \]  \hspace{1cm} (32)
where \( \varepsilon_f = -Pu' = P^2/a \) is the rate of the work of the external force applied at minus infinity within the strip, \( \varepsilon_s = \frac{1}{2}(u')^2 = P^2/2a \) is the strain energy rate of the strip, and \( \varepsilon_k = \dot{u}^2a/2 = P^2v^2/2a \) is the rate of the kinetic energy of the strip.

Thus, the energy release rate per unit length for each crack is equal to
\[ G_{\text{crack}} = \frac{1}{2} \varepsilon = \frac{P^2(1 - v^2)}{4a}. \]  \hspace{1cm} (33)
It is evident that the strain at minus infinity
\[ u'(-\infty) = -P/a. \]

Assume that the crack resistance is given as \( G_{\text{crack}} = G_c \). Then the crack speed is determined by equation
\[ v = \sqrt{1 - \frac{4aG_c}{P^2}}. \]  \hspace{1cm} (34)
In particular, it follows that the external force \( P \) should be greater than \( 2\sqrt{aG_c} \) to support the crack growth. In this problem, the crack growth is stable in the sense that the speed \( v \) increases with the increase of the external force \( P \), and \( v \to 1 \) as \( P \to \infty \).

Based on formula (33), we can mention three different cases when \( a \to 0 \):

- Assume \( P = \text{const} \). Then the crack speed tends to the critical value, which is equal to 1.
- Assume \( P/\sqrt{a} \to \infty \). In this case, the energy release rate must tend to zero and hence the crack should stop.
- Finally, let \( P/\sqrt{a} \to \mathcal{P} > 2\sqrt{G_c} \). Then the force \( P \) tends to zero, whereas the energy release rate tends to a nonzero constant sufficient to support the propagating cracks.

Here, we observe the following paradox associated with the proposed continuum model: in the limit when \( a \to 0 \), the united cracks can propagate (as a point singularity) under a nonzero energy flux but zero external force. We would like to emphasize that this paradox is inherent to the continuous model only, and it does not arise in the discrete lattice model.
4. Concluding discussion

Fig. 2 includes the graph of the ratio \( G_0/G \) versus the normalized crack speed \( v \). The computation is based on the analytical formulae (21) and (22), and the local and global energy release rates \( G_0 \) and \( G \) are determined (up to a constant multiplier) by (19) and (20). As expected, the limit of the energy ratio as \( v \to 0 \) coincides with the static result (22), obtained via an independent analysis. The nonzero dissipation at zero crack speed (in this case, the dissipation rate \( G - G_0 \approx 3.33G_0 \)) is caused by the bond-break impulses which take place in the quasi-static crack growth as well.

We remark that the paper does not address the issue of the fracture criterion in the sense that we assume the steady state, and then using the analytical solution obtained here judge on the validity of this assumption. In particular, it follows from the diagram 2 that the propagating crack is stable if the normalized crack speed is larger than about 0.45. Indeed, if one wishes to pursue the study of the fracture criterion, then the physical criterion \( |u_{1,m} - u_{0,m}| > u_c \), for some critical value \( u_c \) can be used for the breaking bond. It is not feasible to reduce the corresponding problem to an analytically solvable functional equation though, but a numerical simulation is indeed possible. This approach would lead to an alteration of the diagram 2 when the normalized wave speed is less than 0.45.

In the framework of the mathematical formulation adopted in the present paper, the highly oscillatory behaviour of the graph for low crack speeds is well understood in the sense that a slow crack generates many dissipative waves of different frequencies and the energy carried by these waves is highly sensitive to the crack speed variation, as discussed in detail for a classical lattice fracture in Slepyan (2002, Fig. 11.2, p. 397). At the other extreme, when the crack speed tends to the critical value \( v_{\text{critical}} = 1 \), which corresponds to a resonance speed, the energy ratio \( G_0/G \) tends to zero, since the energy radiation rate tends to infinity. In contrast to the Mode-III fracture of the lattice (Slepyan, 2002, Fig. 11.3, p. 404), there exists a finite derivative \( d(G_0/G)/dv \) at \( v = 1 - 0 \); mathematically, this reflects the difference in the kernels of the Wiener–Hopf equation for these two cases. A strong jump in the dissipation in the interval \( 0.3 < v < 0.32 \) reflects the fact that a very productive wave mode excited at \( v < 0.3 \) goes out of the excitation as the crack speed varies in this short interval. Note that the minimal dissipation point, \( v \approx 0.45 \), is the lower bound of the stable crack-speed interval \( 0.45 < v < 1 \).

The mathematical model of this paper indicates that the low-speed steady-state regime is not realizable. The last point of the Discussion concerns the realizability of the considered dynamic process. Recall that the strength of the longitudinal bonds must be sufficient to support the double-crack configuration during the extraction. However, if the external forces are applied to the extracted chain not far from the separation point \( \eta = 0 \), but within a region which includes this point, the required strength level of the longitudinal bonds can be dramatically lowered, and the above-assumed extraction process can be realized for a lattice having an isotropic strength.

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