Crack limiting velocity

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We address the question of how a dynamic crack can approach zero velocity. Continuum theories usually do not explicitly include the radiation of energy away from the crack tip. We show that its inclusion leads to the prediction of crack velocity that increases smoothly (though sharply) from zero. We then connect an older, simple model of crack propagation (''atoms on rails'') to a recently proposed single-particle model and show how the disappearance of lattice trapping leads to a smooth low-velocity limit. [S1063-651X(97)00307-3]

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I. INTRODUCTION

Recent discrete lattice and Barenblatt models of dynamic brittle cracks raise the question whether a crack velocity smoothly approaches zero as the load is decreased from large values to the Griffith point [1–3]. This problem is independent of crack behavior at the other end of the scale, where the upper limit of crack velocity appears to be associated with instabilities caused by crack branching and dislocation formation [1,2]. This low-end behavior is as interesting as that at the high end, however, because the standard continuum solution for a steady-state moving crack [4] makes definite predictions about it. If a crack in a lattice exhibits unpredicted unstable behavior at the low end in contradiction to the continuum results, then one must explain how and why the discrete lattice effects can be so important.

This paper addresses cracks in lattices, where it will be assumed that a unique cleavage plane is forced by the surface energy anisotropy of the lattice. Thus, because they assume amorphous media with isotropic surface energy, the works of Ching, Langer, and Nakanishi [3] and Lund [5] are not directly relevant.

Expectations about the behavior of dynamic cracks are dominated by the boundary conditions of the problem. Marder and Gross [1] work in the strip geometry, whereas the large-scale computer simulations [2] assume effectively ''infinite'' systems where the crack tip is not in communication either with its other end or with boundaries in the system. The continuum predictions for these two geometries are quite different and will be summarized in Sec. II, where we also present results for a continuum version of the one-dimensional (1D) discrete model of Marder and Gross [1]. However, in each case, we are left with questions about how the atomicity of the problem can explain observed deviations from the continuum predictions.

The analytic description of dynamic fracture is quite abstruse and simulations of the ''infinite'' system require extensive programming and computer time. To surmount some of this barrier to understanding the physical picture, it is our purpose here to extend the kind of thinking already begun in an earlier paper [6], where a very simple model was developed with which one could address the underlying mechanisms of some of the dynamic crack physics without invoking the very complex machinery of the real thing. Here we will present two additional simple discrete models that can be studied completely analytically, one for each geometry. These results will be presented in Secs. III and IV. A concluding discussion is presented in Sec. V.

II. CONTINUUM LIMIT AND BOUNDARY CONDITIONS

A. Strip geometry

In the first type of boundary condition, used extensively by Marder and Gross, in both its theoretical and its experimental implementations, the system is a strip of finite width and infinite length with a semi-infinite crack running down its middle (on the x axis). The strip is loaded on its edges in ''fixed grips.'' That is, the edges of the strip at $y=\pm L$ are displaced by amount $\pm 2u_0$ everywhere. (The factor of 2 has no particular significance and is chosen for consistency with later discussion.) This creates a constant strain in the strip far ahead of the crack tip for large positive x. It is usually assumed that the strain far behind the crack is fully released and that the material there is again at rest for large negative x. It is easily seen [4] that this system has only two steady-state velocities: zero and the Rayleigh speed. Liu and Marder [7] have shown further that if one sets up such a system at the Griffith load and then at time $t=0$ increases the load slightly, the crack slowly increases its velocity from zero to the Rayleigh limit for all loads greater than the Griffith load. These solutions, however, are built on the proposition that the material far away from the crack tip, either ahead or behind it, is at rest.

The reasoning is as follows. Each vertical element far ahead of the crack contains a strain energy density E_e per unit length along the center line x, given by the load. As the crack grows by one atom spacing, the elastic energy of one vertical row of atoms through the strip is available to break the bonds. Thus Griffith equilibrium is set by the condition

$$E_e=2\gamma. \tag{1}$$

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Since the usual assumption is that the system relaxes completely behind the crack with no time-dependent displacements, there is no way for excess energy to be absorbed and the crack has no stable velocity greater than zero.

But these boundary conditions, as stated, are inconsistent because if the load is above the Griffith value, then the excess energy is available to generate waves behind (and in front of) the crack. Physically, the material just behind the crack tip that is released after bond breaking will accelerate toward its equilibrium position and kinetic energy in the form of a wave will be generated to reflect back and forth between the fixed boundaries at $y=\pm L$, with excitation of associated Rayleigh waves. Thus any excess energy can be absorbed in these waves and again, from energy conservation alone, a load-velocity law can be a smooth function of the load and go to zero smoothly as the load goes to the Griffith load. This demonstration does not prove that the velocity law is smooth in the vicinity of zero, only that energy conservation is consistent with it.

But one can go further with a continuum version of the 1D discrete strip model introduced by Gross and Marder [1]. In this simple model, we assume two infinitesimally thin stiff foils connected to one another with a nonlinear stress function $f(u_y)$ and to substrates above and below, respectively, with linear springs, such that each foil satisfies the following equation under time-independent static conditions:

$$0=f(u_y^0)+A\frac{d^2u_y^0}{dx^2}+B(2u_0-u_y^0), \tag{2}$$

where A is the stiffness coefficient in a foil and B is the spring constant connecting the foil to the substrate. A crack is assumed to exist between the two foils, so that under fixed grips load, $u_y^0(x)$ is the vertical displacement from the equilibrium position, relative to the centerline of the configuration, of the upper foil as a function of the distance along the strip and u_0 is the displacement of the upper foil from its equilibrium position relative to the centerline of the configuration at $x=+\infty$. Since the problem contains no x displacement, henceforward, we drop the subscript y on the u's. To the left of the crack, the bonds are fully broken, so f goes to zero at $x=-\infty$ and the foils relax to their equilibrium position relative to the substrates. The centerline is a line of symmetry in the problem, so the lower foil has a displacement of $-u^0(x)$ and at $x=+\infty$ far to the right of the crack the upper substrate is displaced relative to the lower by the distance $4u_0$ from their equilibrium separations without load. (This assumes that the ''spring'' constant between the foils for small displacement is half as stiff as that between the foils and the substrates.) For the time-dependent moving crack problem, the equation of motion for one of the foils is

$$0=f(u)+A\frac{\partial^2 u}{\partial x^2}+B(2u_0-u)-\rho\frac{\partial^2 u}{\partial t^2}, \tag{3}$$

where now $u(x,t)$ is the time-dependent displacement of the upper foil and ρ is the mass density in a foil.

We do not attempt a full-scale solution for this nonlinear crack, which would perforce be numerical. Rather we finesse the analysis by making plausible physical assumptions in an attempt to gain information about the velocity law in the limit of small velocities. We first suppose that the static crack has a smooth solution given by the function $u^0(x/w)$, which is a functional of the nonlinear force law $u^0\{f(y)\}$. [The force function is obtained, of course, if the displacement function is known, by direct substitution into Eq. (3).] The displacement function is written so that it scales with a parameter w, which is interpreted as the width of the Barenblatt cohesive zone of the crack.

At small velocities, the moving crack must be very close to a rigidly translating static crack and we thus assume a solution of the form

$$u(x,t)=u^0\left(\frac{x-vt}{w}\right)+u^1(x,t), \tag{4}$$

where the second term is a perturbation from the (known) uniformly translating static crack. After substitution into the equation of motion and remembering that u^0 is a solution of Eq. (2), u^1 satisfies the equation

$$\frac{\partial^2 u^1}{\partial x^2}-g(x)u^1-\frac{1}{c^2}\frac{\partial^2 u^1}{\partial t^2}=\frac{v^2}{c^2}\frac{d^2u^0}{dx^2}, \tag{5}$$

where $c^2=A/\rho$. In this equation an expansion of f is made,

$$f(u)\approx f(u^0)+u^1\frac{df(u^0)}{du^0}+\cdots, \tag{6}$$

where $f(u^0)$ and $df(u^0)/du^0$ are known functions of x once the static solution is known. Then $g(x)$ in Eq. (5) is the collected set of terms linear in u^1 resulting from the substitution in the equation of motion. Equation (5) is a homogeneous wave equation with a curious dispersion relation in the regions both far ahead and behind the crack and thus represents the radiated waves generated by the moving crack. In the core, the source of the radiation is the term on the right-hand side in Eq. (5), which contains the coupling to the translating crack u^0 through its second derivative. Since this source term is proportional to $(v/c)^2$, the radiation is a small perturbation at small velocities, as desired. Of course, one must allow for special force laws for which the moving crack is a soliton, wherein no radiation is generated, but if they exist for this model, they are unusual cases and not considered further.

There is a problem with Eq. (5), which is a special feature of the 1D strip crack tied to a substrate. The term in $g(x)$, which derives ultimately from f and B in Eq. (3), gives a dispersive character to the waves such that the wave group velocity for very long waves goes to zero. This means that a crack with finite velocity would be supersonic, relative to some very long wavelengths. Thus, for the physical picture to be valid, the moving crack must generate radiation with wavelengths much shorter than the critical wavelength where the wave and crack velocities are equal. The effective frequency of a radiated wave will be given by the ratio v/w, so for the physical picture to be valid, this ratio must be sufficiently high. The catastrophe is avoided in the true limit of $v\rightarrow 0$ because of the factor $(v/c)^2$ in the driving term on the right-hand side of Eq. (5): thus, in that limit, no radiation is emitted. Having pointed out the problem, we ignore it in the following by tacitly assuming that the core is always sharp enough. The problem will also not be a feature of any system where the strip is sufficiently wide and properly 2D.

An equivalent way to consider the problem thus posed is to view the moving crack as generating a localized region of kinetic energy in its core. A part of this energy will move coherently with the crack, but part must be radiated in nonsoliton cases. If the system is in steady state, then the radiation rate from the moving core must be a fixed fraction of the total kinetic energy in the core. Since the kinetic energy of the rigidly translating crack is (note there are two foils)

$$\mathcal{T}=\rho\int_{-\infty}^{\infty}\dot{u}^2dx=\frac{\rho v^2}{w^2}\int_{-\infty}^{\infty}\left(\frac{du^0(x)}{dx}\right)^2dx, \tag{7}$$

the energy balance at the crack core (in the Griffith sense) becomes

$$E_e=2\gamma+C(w)\frac{v^2}{w^2}. \tag{8}$$

Here C is a constant, which depends on the form of the force law, but the major dependence on w has largely been removed by means of the assumed way the static crack scales with w. E_e is the elastic energy density in the loaded and stretched system far to the right of the crack. E_e is given by the relation

$$E_e=\frac{3}{2}Bu_0^2 \tag{9}$$

under the assumption noted above that the spring constant between the foils is half that between the foils and the substrates.

When Eq. (8) is inverted, the velocity law for the crack becomes

$$v=w\sqrt{\frac{E_e-2\gamma}{C(w)}}. \tag{10}$$

This relation is obviously only valid in the low-velocity continuum limit for steady-state velocity v and yields a nonsingular behavior in the vicinity of $v=0$. It shows a square-root dependence on the excess load over the Griffith value. It obeys all physical requirements in that for very wide cohesive zones, the crack produces little radiated energy (when the w dependence of C is not too drastic). Also, near $v=0$, the slope of the velocity function is very steep because the crack must pick up significant velocity and kinetic energy before radiation can be important.

We note that although the presentation here is quite general, the physical assumption is made that a true steady state is achievable. It is this assumption that makes it possible to write the generalized Griffith relation, and if no such solution of Eq. (5) is possible, then the whole physical picture of uniformly moving cracks breaks down. However, the general form of Eq. (5) makes one optimistic that steady-state solutions do exist for a wide class of force laws, and for all these cases, then a velocity law of the form (10) is valid. We believe the most probable violation of the steady-state crack assumption would arise if storage modes for the moving crack can exist, but we believe these are more plausible for the crack in a discrete lattice and return to a discussion of this point in the Conclusion.

The reason for going through this 1D strip case, even with its inadequacies, is that the physics that leads to the well-behaved limit at low velocity should be instructive in other cases where the analysis is even more intractible. That is, when one can build first-order solutions out of the rigidly translating static crack, then the velocity law should be well behaved in the zero-velocity limit and have the general character displayed by Eq. (10). We have pointed out that violations are expected if the crack can possess storage modes when it moves, but we believe these are probably not a feature of the continuum.

B. Infinite 2D geometry

In the second boundary condition, the crack is assumed to be long (or even semifinite in length) and to be embedded in an infinite medium. In steady state, the load must be imposed in such a manner that the crack experiences a constant applied K field in the static limit. For actual cracks, these conditions may be difficult to achieve, but they can often be approached for finite lengths of time. It is required that there be a time interval during which no communication is possible with the other end of the crack or with boundary surfaces. Also, any additional crack growth during the interval must be small compared to the initial crack length. Limiting times are set by the time for sound waves to reach the crack tip either from the other end of the crack or from the boundaries. But even if these conditions are difficult to achieve in simulations or in experiment, mathematically, these boundary conditions lead to a well-posed problem, which has received much attention. See the review by Freund [4].

The result of the analysis is that the dynamic driving force on the crack $\mathcal{G}$ is nearly linearly related to the crack driving force that would have been calculated from the loads for the crack if it were static $\mathcal{G}_0$,

$$\mathcal{G}=(1-v/c)\mathcal{G}_0, \tag{11}$$

where v is the (steady-state) velocity of the crack and c is the Rayleigh surface wave speed in the system. This linear relation is not strictly valid, but as an approximation, is ''good enough'' for our purposes. Further, in this same system, if the crack is in steady state, then $\mathcal{G}$ is a constant of the motion and the J integral for the crack tip is independent of the path of integration. This means that $\mathcal{G}$ is the energy that is absorbed at the crack tip by nonmechanical means, presumably by breaking the bonds there. Thus the steady-state dynamic brittle crack also satisfies the Griffith relation

$$\mathcal{G}=2\gamma, \tag{12}$$

which, in terms of the experimentally determined load P, is

$$\frac{v}{c}=1-\frac{2\gamma}{\mathcal{G}_0(P)}. \tag{13}$$

For positive v, this relation shows that the velocity starts at zero for $\mathcal{G}_0=2\gamma$ and asymptotically builds to c for large values of $\mathcal{G}_0$. Since $\mathcal{G}_0\propto P^2$, the velocity curve is an increasing quadratic hyperbola as a function of the load. Thus, as the load drops from large values to the Griffith load, the velocity goes smoothly to zero, according to the continuum theory with the ''infinite'' system boundary conditions.

The physical content of the solutions for either set of boundary conditions is straightforward. In the quasistatic limit, as the crack grows, it absorbs energy from the loading system $\mathcal{G}_0$ in just the amount necessary to break the bonds, so the Griffith relation is simply a statement of energy conservation. Likewise, in the dynamic case, as the crack grows, new material at rest ahead of the crack must be accelerated to an increasing kinetic energy behind the crack. In the strip case, waves are generated by the breaking bonds at the tip. In the infinite case, the crack opening behind the crack increases from the tip with distance as $\sqrt{x}$, so as the crack moves, more and more material is accelerated and the energy of the crack displacement field continuously increases. In either case, this energy must come ultimately from the load system. Thus, in the case of a moving crack, the load system must supply a displacement field kinetic energy as well as bond breaking energy, and this means that additional load is required to move the crack at a finite velocity over and above the Griffith load in the continuum limit. Thus this additional dynamic energy is a smooth function of the crack velocity, at least for velocities much less than the Rayleigh speed, where shock and relativistic effects are expected to occur. (This argument is exactly that of Mott in his early treatment of the moving crack [8,4], which is valid in the low-velocity regime.)

C. Discrete lattices

These continuum results are to be compared with the results for the analytic solutions given by Marder and Gross [1] and to molecular-dynamics simulations [2,9–13]. We consider first the strip.

The discrete 1D strip model developed by Marder and Gross is the most transparent case to consider and the result for the 1D bond snapping model is that all velocities in the vicinity of zero are forbidden. (In the bond snapping force law, the force function f used above in the continuum analog becomes a sharp saw tooth with infinite negative slope.) There are two reasons for this. First, velocities that have a negative slope as a function of load are unstable and not allowed. Second, if the solution for small velocity is examined carefully, it is found that the crack tip bond oscillates from a bound to a broken state, which is inconsistent with the assumed solution. The velocity must build to a significant fraction of the Rayleigh velocity before the solution becomes regular. This solution for the discrete 1D strip model is inconsistent with the continuum solution obtained above. The snapping bond solution is sufficiently singular relative to the smooth Barenblatt solution that it is impossible to make one case the limit of the other. But one suspects that the singular character of the snapping bond release is important, and this aspect will be explored in Sec. III.

How about the infinite system case? Zhou *et al.* [2] show that when the crack system is loaded with care, the velocity builds quickly to a significant fraction of the Rayleigh velocity and runs smoothly for a long distance before it finally becomes unstable. Although these results are incomplete in

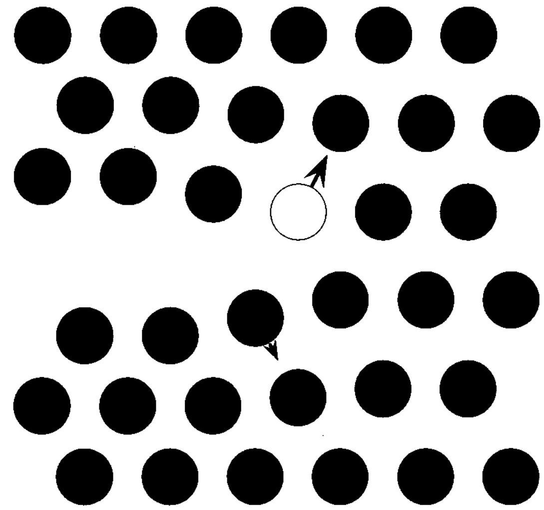

FIG. 1. Schematic of a crack in a uniaxially strained (in the vertical direction) triangular 2D lattice, which is six close-packed rows of atoms from top to bottom. The crack-tip atom is unshaded; the bond with its neighbor (shown moving down and to the right) has just broken, sending the crack-tip atom up and to the right. Its bond with the next atom in line will be stretched and broken in time t_{break}, so that this ''iceskating'' advances the crack one nearest-neighbor distance r_0 in a time $2t_{break}$, with a steady-state crack velocity of $v_{crack}=r_0/2t_{break}$.

the sense that the strain is still increasing above the Griffith load after the crack starts to run, the initial velocity is quite high and suggests that the crack resists motion at near zero velocity. Indeed, if the strain rate is insufficient, the crack velocity is unstable in the sense that the velocity surges to a high value and then back to zero, with complete arrest of the crack. This behavior is suggestive that low-velocity crack advance is unstable, although these simulations require further study with a variety of loading regimes near Griffith in order to explore adequately the stability of the crack at low velocity. Thus, again (but with less confidence), the lattice results do not follow the continuum predictions.

The most important difference between the continuum and lattice descriptions is the existence of lattice trapping in the discrete case. Thus we will be interested in learning how lattice trapping effects might bear on low-velocity instabilities. In particular, the analytic models of Marder and Gross [1] assume bond snapping force laws that lead to very high lattice trapping, which might reasonably be expected to play a role. However, the large-scale simulations of Zhou *et al.* [2] use much softer force laws, with lattice trapping loads that are only a few percent of the Griffith load.

III. A SIMPLE LATTICE STRIP MODEL

Holian, Blumenfeld, and Gumbsch [6] have developed a simple version of a strip crack with only a small number of atom rows (4,6,8, . . . ; see Fig. 1). The idea is if the strip is very narrow, then the crack degenerates into ''pure core,'' in which case only a few atoms are involved in crack growth, and the analysis is vastly simplified to only a few pairs of atoms. Here we take this idea one step further, to the stage where one can write down a fully analytic solution without

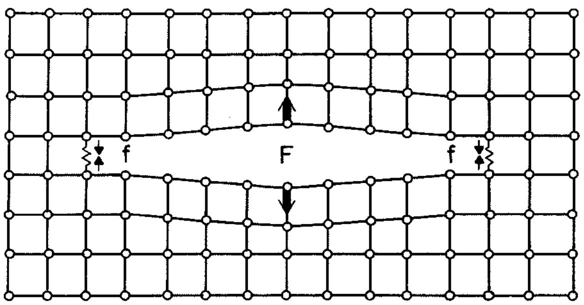

FIG. 2. Schematic of a square 2D lattice with a crack. The lattice points are allowed to displace only in the vertical or Y direction (''atoms on rails''). The force laws are composed of nearest-neighbor stretching forces and nearest-neighbor bending bonds as given in the text. The crack is formed by cutting the stretching bonds on the cleavage plane from $X=-L$ to $X=+L$ and nonlinear bonds attached to the last cut bond. The force in the nonlinear bond is f and the forces loading the crack at its center are F.

appealing to the full sophistication of the analysis invoked by Marder and Gross [1] for their 1D model. Since the physics of such simple models is so transparent and yet still contains the essence of the behavior of the more complex system, they are worth pursuing. In particular, we will develop a prediction of the crack velocity in terms of the bonding at the tip.

In order to connect well with the model in Sec. IV, we outline a simplified model for 2D fracture, namely, ''atoms on rails,'' where the atomic motion is restricted to be orthogonal to the crack plane (line in two dimensions). The atoms are placed on a rectangular lattice (shown in Fig. 2) and labeled by the integer i in the x direction (crack propagation direction; the lattice constant is unity) and j in the y direction (applied load or strain direction; the lattice constant is $1+\epsilon$, where ϵ is the vertical strain in the lattice). The positions of atoms in the vertical direction are denoted by $Y_{i,j}$ and displacements of atoms from these rectangular lattice sites are denoted by $y_{i,j}$. The compressive nearest-neighbor interaction between atoms in the vertical direction is characterized by a central pair potential $\phi(|Y_{i,j}-Y_{i,j\pm 1}|)$; for simplicity, we set $\phi(1)=0=\phi'(1)$ and $\phi''(1)=1$ (in tension, we can impose a discontinuous snapping-bond potential or a smooth cutoff, if we choose). There is no motion in the x direction, but a linear bending force is applied between nearest neighbors with the same value of j, with bond-bending force constant B. Thus the force on atom i,j is given by

$$f_{i,j}=\phi'(|Y_{i,j}-Y_{i,j+1}|)-\phi'(|Y_{i,j}-Y_{i,j-1}|)+B(y_{i+1,j}-2y_{i,j}+y_{i-1,j}). \tag{14}$$

We can simplify the problem by imagining that the crack propagates in a strip four rows high, where the top and bottom rows of atoms are fixed and the middle two rows are free to move. By assuming that the motion of these two rows is mirror symmetric about the crack plane, we can reduce the crack propagation problem even further, namely, to the dynamics of a one-dimensional chain. Atoms i are located above the mirror plane $(Y=0)$ at $Y=y_i+(1+\epsilon)/2$, with mirror image particles at $-Y_i$, and fixed neighbors above, located at $Y=3(1+\epsilon)/2$. Thus, in terms of vertical displacements y_i along the chain, the force on atom i is now given by

$$f_i=\phi'(1+\epsilon-y_i)-\phi'(1+\epsilon+2y_i)+B(y_{i+1}-2y_i+y_{i-1}). \tag{15}$$

The equation of motion is then $m(d^2y_i/dt^2)=f_i$ for $i=0,\pm 1,\pm 2,\ldots$.

We can introduce a mirror-symmetric crack of length $2L+1$ by specifying that particles $i=-L$ to $+L$ have displacement $y_i=\epsilon$ and for all others $y_i=0$. For all particles except L and $L+1$, the force is zero, assuming that $\phi'(1+3\epsilon)=0$ (broken bond between mirror-image partners); $f_L=-B\epsilon$ and $f_{L+1}=+B\epsilon$. (By an iterative relaxation process, we can make the crack tip assume an equilibrium, zero-force initial configuration. However, for a dynamic crack moving at a steady-state velocity, this nonequilibrium crack-tip force field is probably not too far from reality.)

We can now propose a single-particle Einstein model for the steadily propagating crack. By this we mean that we can calculate the steady crack velocity by assuming that the crack-tip atom $L+1$ moves under the influence of its fixed neighbor in the row above and its immobilized neighbors behind (L) and forward $(L+2)$. Thus the force on the Einstein atom $(L+1)$ is (dropping the atom number for simplicity)

$$f=\phi'(1+\epsilon-y)-\phi'(1+\epsilon+2y)+B(\epsilon-2y). \tag{16}$$

Since $y(t=0)=0$, the force on the atom is initially upward: $f=B\epsilon$. We record the time t_{break} it takes to break the bond between the Einstein atom and its mirror image; the crack will then have advanced by one lattice spacing, so that the crack velocity is

$$v_{crack}=\frac{1}{t_{break}}. \tag{17}$$

If we linearize the potential ϕ such that $\phi'(1+y)=y$, then

$$f=-(3+2B)y+B\epsilon=-\omega^2(y-y_0); \tag{18}$$

hence

$$\omega^2=3+2B,$$

$$y_0=\frac{B}{3+2B}\epsilon. \tag{19}$$

At the critical lattice-trapping strain ϵ_{crit}, the bond between the Einstein atom and its mirror-image partner is broken when the maximum interaction range r_{max} is

$$r_{max}=1+\epsilon_{crit}+2(2y_0)\rightarrow\epsilon_{crit}=(r_{max}-1)\frac{3+2B}{3+6B}. \tag{20}$$

The Einstein model for atoms on rails predicts a zero steady-state crack velocity for strains below this lattice-trapping value; for strains just above this, the velocity starts at

$$v_{crit}=\frac{1}{\tau/2}=\omega/\pi=\frac{\sqrt{3+2B}}{\pi}. \tag{21}$$

The Griffith strain ϵ_G for a system w rows of atoms wide is obtained from equating the elastic strain energy far in front of the crack to the energy of the relaxed system with a broken bond across the cleaved surface far behind the crack tip:

$$(w-1)\phi(1+\epsilon_G)=\phi(r_{max})\rightarrow\epsilon_G=\frac{r_{max}-1}{\sqrt{w-1}}\quad\text{(harmonic)}$$

$$\rightarrow\frac{\epsilon_{crit}}{\epsilon_G}=\frac{3+2B}{3+6B}\sqrt{3}\quad(\text{for } w=4). \tag{22}$$

For strains that are not too large compared to the Griffith value, the above harmonic analysis can be extended to obtain the crack velocity as a function of strain. The motion in the harmonic well can then be written as

$$y(t)=y_0(1-\cos\omega t), \tag{23}$$

so that

$$v_{crack}=\frac{\omega}{\cos^{-1}[1-(r_{max}-1-\epsilon)/2y_0]}. \tag{24}$$

In the triangular lattice, this single-particle Einstein model exhibits two phases in the forward motion of the crack: first a movement toward one side of the crack and then a movement toward the other side, hence the name ''Einstein ice-skater'' model. The analysis proceeds similarly to the model outlined here in the square lattice, where we have transformed the bond-breaking motion into a single mirror-symmetric phase that is perpendicular to the crack propagation direction. The result for the triangular lattice is

$$\frac{v_{crack}}{c_s}=\frac{4}{3\cos^{-1}(5-4\sqrt{3}\epsilon_G/\epsilon)}, \tag{25}$$

where $\epsilon_{crit}/\epsilon_G=2/\sqrt{3}$ and $v_{crit}/c_s=4/3\pi=0.424$ (c_s is the shear-wave speed in the triangular lattice, which is also very close to the Rayleigh-wave speed).

The conclusions we get from these simplifications of steady-state crack propagation are (1) there is lattice trapping in narrow strips, and (2) the velocity quickly jumps from zero to a sizable fraction of the shear-wave or Rayleigh-(surface) wave speed. Numerical modeling is required for anharmonic interactions, and the result is a reduction of the crack speed, even for anharmonic systems with sound speeds identical to those of their harmonic-system counterparts. The reduction comes about because of the softening of the effective force constant in the expansion (beyond the attractive minimum of the pair potential). With increasing strain, over and above the Griffith value and the somewhat higher lattice-trapping value, the harmonic-system crack velocity quickly approaches the shear-wave speed, while the anharmonic systems show much more gentle variation with increasing strain. This feature too is a result of the softening of the attractive forces in expansion. All in all, these simple models of steady crack propagation contain significant insight into the physics of dynamic brittle fracture.

IV. A SIMPLE INFINITE LATTICE CRACK MODEL

In this section we revisit the atoms-on-rails model of a crack moving in an infinite system. We are not able to develop a fully dynamic solution, but rather show that one can construct a lattice model that has zero lattice trapping and demonstrate that such a crack has a smooth transition from zero to small finite velocities. We do this by showing that it is possible to choose a special set of bonding forces at the crack tip, which leads to the desired crack property. The model is based on an extension of earlier work on quasistatic cracks analyzed by lattice Green's functions [14]. The notation is the same as in Sec. III; however, the lattice is infinite in both dimensions. The atoms are on the square lattice sites denoted by (i,j) with i and j integers. The crack is constructed by cutting the bonds crossing the cleavage plane between the planes $(i,0)$ and $(i,-1)$ with the crack tips (last cut bond) at $(x=\pm L)$. See Fig. 2. The lattice is connected by the same linear force law as before with both stretching and bending springs [Eqs. (14) and (18)] with the stretching spring constant chosen to be unity for convenience. The crack is loaded by external forces $\pm F$ exerted on the atoms facing one another across the cleavage plane at $x=0$.

Nonlinearity is introduced into the problem by reconnecting the last pair of broken atoms at the crack tip with a stretching bilinear force law of the form

$$-f_L=2y_L,\quad y_L<y^0 \tag{26a}$$

$$-f_L=-f_0-\kappa(y_L-y^0),\quad y^+>y_L>y^0, \tag{26b}$$

where y_L is the vertical displacement of the atom at $(L,0)$ and it is assumed that the (vertical) displacements in the lattice are mirror symmetric across the cleavage plane everywhere. Thus, from Eq. (14), the linear part of the stretching force on the atom at the crack tip due to the reattached bond, in the two-index notation of the 2D lattice, is given by $-f=(y_{L,0}-y_{L,-1})=2y_{L,0}=2y_L$, which explains the factor 2 in Eq. (26a). Similar considerations apply to the release part of the force, where $y^+>y_L>y^0$. The linear form of the bending bonds is not affected by the crack, of course.

Analysis of the cracked lattice proceeds by means of the lattice Green's functions that have been worked out for this lattice [14]. Since we will only use applied load forces exerted as vertical dipoles on nearest neighbor atoms, instead of the Green's functions, we define the related response functions for the cracked lattice as follows. The response function g_{ij} corresponds to the displacement at atom position $(i,0)$ on the upper cleavage plane for a point force acting at the position $(j,0)$ on the upper cleavage plane in a positive y direction and an equal negative force at the atom on the site just below it on the lower cleavage plane at $(j,-1)$. It is necessary to define the response functions only for the atoms on the upper side of the cleavage plane at position $(i,0)$. With these response functions for the system, if a load dipole is applied at the center of the crack F and a second bonding dipole force f is applied at the atom pair located at L (see Fig. 2), then the response of the total system can be written in terms of the displacements and forces acting on the atoms at $x=0,L$:

$$Y_0=g_{00}F+g_{0L}f, \tag{27a}$$

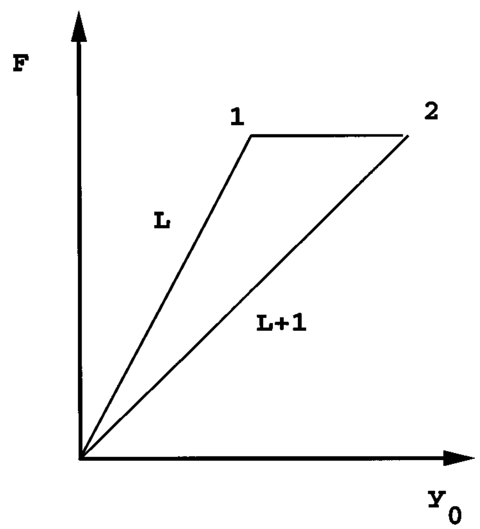

FIG. 3. Two straight lines through the origin, corresponding to the response of a fully linear lattice (no nonlinear bonds) for cracks of half length L and $L+1$. The ordinate is the load F applied to the center of the crack and the abscissa is the displacement y_0 of the atom at the center of the crack. If the atoms have a bilinear force law, then for a crack of half length L, as the bond at the tip extends, it reaches the limit of its linear portion at y^0 at the point in the diagram labeled 1 and further extension occurs on its ''back side.'' When the bond at the tip is extending on the back side, the response function is assumed to be flat, until the bond finally breaks at the same time as the response curve meets the linear lattice function again for $L+1$ at the point labeled 2.

$$y_L = g_{L0}F + g_{LL}f, \tag{27b}$$

$$y_{L+1} = g_{L+1,0}F + g_{L+1,L}f. \tag{27c}$$

Figure 3 is a graph of the displacement of the center atom of the crack as a function of the load force F. As the force F is increased from zero, the cracked lattice responds linearly, as shown for crack length L. But when the atom at L reaches the critical value y^0, according to the force law, it begins to release and the response of the system changes abruptly. The figure shows a flat response, but in general the slope will be some nonzero value, depending on the crack length and the value of κ. We define the condition of zero lattice trapping to be that shown, with the zero slope. The second linear line through the origin corresponds to a linear cracked lattice of length $L+1$ and we assume that the forces at the crack tip act in such a way that exactly when the horizontal line meets the response line for $L+1$, the force in the bond at L goes to zero and the force in the bond at $L+1$ is at the critical value f_0, where the bond begins its release phase. Thus, as the crack grows from one lattice position to the next, it always has exactly one atom at the tip in its ''core,'' defined as $y^+ > y > y^0$. For this assumption to be valid, as the crack grows from one atom position to another, the crack tip atoms must smoothly execute a ''dance'' along the force law so that as the atom at $L+1$ reaches the critical value y_0 the atom at L must simultaneously reach the next critical displacement y^+. In the figure, the state labeled 1 corresponds to the atom at L reaching y^0, while state 2 corresponds to the same atom reaching y^+ and simultaneously the atom at $L+1$ reaching y^0. Thus, as the system progresses from 1 to 2, the crack grows from one lattice site the next. Such a cracked lattice has a flat response curve and thus exhibits zero lattice trapping. This condition is obviously a stringent one, which will be analyzed below. In passing, we note that if the atom at L is in the flat portion of the force law and the other conditions are also satisfied, the Griffith condition for the crack will be satisfied.

The (total) energy changes that occur when the crack grows from state 1 to state 2 in Fig. 3 is given by

$$\delta E = \int_1^2 F d(2y_0) - F\Delta(2y_0), \tag{28}$$

where the first term is the work done by the external force as it displaces the atom pair at the center of the crack. The second term is the potential-energy change in the load system that supplies the load. If the response of the system is flat from state 1 to state 2, as drawn in Fig. 3, then the energy change $\delta E = 0$ because the first term exactly cancels the second. Thus a flat response from 1 to 2, defined as a state of zero trapping, is also a state where there are no atomic scale excursions in the energy of the system during quasistatic crack growth, an essential physical attribute of the zero trapping system.

From Eq. (27b), $dy_L = g_{L0}dF + g_{LL}df = g_{LL}df$. ($dF = 0$ when the response is flat.) From the force law (26b), $df/dy = \kappa$ and

$$\kappa = \frac{1}{g_{LL}}. \tag{29}$$

Although the criterion (29) ensures that the response of the system is flat, it must be supplemented by a self-consistency condition that the force law ''hands off'' the core atom from one site to the next such that there is always one and only one atom in the release or ''back side'' portion of the force law at all times. That is, the atom at L reaches the displacement $y_L = y^+$ at the same time the atom at $L+1$ reaches the displacement $y_{L+1} = y_0$. Since y^+ is defined from the force law by $-f = 0 = -f_0 - \kappa(y^+ - y_0) = 2y_0 - \kappa(y^+ - y_0)$, then $y^+ = (\kappa+2)y_0/\kappa$. Then, from Eq. (27b), and since $f = 0$ at the point where the crack moves from one site to the next,

$$y^+ = \frac{\kappa+2}{\kappa} y_0 = g_{L0}F. \tag{30}$$

Likewise, from Eq. (27c) we have

$$y_{L+1} = y_0 = g_{L+1,0}F, \tag{31}$$

where we have again used the fact that $f = 0$ at the point where the crack moves from one site to the next. Solving for F from these two equations and substituting for κ from Eq. (29), we obtain the final result

$$g_{LL} = \frac{1}{2}\left(\frac{g_{L0}}{g_{L+1,0}} - 1\right). \tag{32}$$

This condition is written in a form to emphasize the factor $g_{L0}/g_{L+1,0}$, which is always greater than 1. Physically, the ratio must be greater than 1 because the Green's-function elements are proportional to the displacements for any atom in the linear cracked lattice before the nonlinear bonds are reattached. That the crack closes smoothly at the tip means that this ratio must be greater than 1.

We find that from direct calculations of the various Green's functions, Eq. (32) is identically satisfied for all values of the bending spring constant B. Unfortunately, we have not been able to deduce this remarkable result analytically from the form of the Green's functions [14]. But the result implies that self-consistency is automatically satisfied if the back side of the force law is set so that the force in the bond at L goes to zero when the bond at $L+1$ is stretched to $2y_0$. (The factor of 2 reflects the antisymmetry of the displacements below the crack plane.)

In summary, in such a system, a crack can grow smoothly from one atom spacing to the next without any energy changes except those that smoothly feed energy from the loading system and the elastic regions of the lattice into breaking the core bond. No additional energy is generated in this system. One could use the Mott approach to derive an approximate K/v law in the low-velocity regime, as we did in Eqs. (5) and (6). Such a crack would grow smoothly from zero velocity at the Griffith load. We note that for a crack loaded a finite increment over the Griffith load, the smooth zero trapping property begins to break down, because the construction is valid only exactly at the Griffith load. Above the Griffith value, some additional energy is dumped into the lattice over and above that necessary to move the zero trapped crack. But since the trapping energy increases smoothly with the load, nothing dramatic happens. The K/v law should merely turn up a little above the continuum curve near $v=0$.

V. CONCLUSION

In this paper we have addressed the question of how a dynamic crack will approach zero velocity. There are two quite different styles for setting boundary conditions on dynamic cracks and they lead to very different results. In the strip case, the crack is in equilibrium with the waves returning from the boundaries (but not from its other tip); in the second, a single crack tip is in an effectively infinite medium.

The continuum boundary conditions for the strip model generally do not include a radiation condition at infinity, and this leads to a nonphysical prediction when the crack is loaded above the Griffith value. But we show in a simplified version of the strip that when the medium can radiate its accelerations, a steady-state velocity law is expected, which has a square-root behavior as a function of the excess load over the Griffith load. This means that the steady-state velocity increases with an infinite slope near zero overload, but otherwise in a smooth fashion with load. This fast increase of the velocity near zero overload will of course make it difficult to control the crack at slow velocity, but otherwise the low-velocity regime is well behaved.

For infinite systems, the continuum theory predicts a velocity law that approaches the sound velocity asymptote as the inverse square of the load [Eq. (13)]. This velocity law also grows faster near zero velocity than elsewhere, but is much better behaved than that for the strip.

In the two different geometries, we have introduced two simple lattice crack models where the atoms are free to move only in the direction normal to the crack plane (atoms on rails). In the strip, the lattice contains only two rows of movable atoms, with the crack running between the two rows. Analytic results are possible for bond-snapping linear force laws and the velocity is nonzero only above a critical velocity, which depends on the lattice trapping level. For fully nonlinear force laws, numerical results are easily calculated, which show that as the lattice trapping is decreased, the critical velocity also decreases towards zero. Thus the critical velocity observed previously in strip models is purely a function of the lattice trapping, and as the trapping is decreased, the crack reverts to the behavior predicted by the continuum model.

In the infinite lattice, we have shown that with the same atoms on rails it is possible to find a bilinear force law that has strictly zero lattice trapping and that as the load is increased above the Griffith value this lattice again exhibits a smooth increase above zero velocity. Thus, in both cases, any critical velocity observed is associated with lattice trapping.

The paper addresses the problem of the steady-state velocity of a crack and leaves the question of how a crack that is initially at rest might achieve its steady state if there is lattice trapping. In this case, the crack must be overloaded above the Griffith value before any state of motion is possible at all. This is the problem so aptly dubbed ''starting the crack'' by Eshelby [15]. According to the continuum solutions, we would expect, if the crack has no field inertia, that once the trapping limit is exceeded and the crack can move, it will achieve the equilibrium steady state immediately and thereafter move at a fixed velocity. But if the crack has a field inertia, which may be the case for a discrete lattice, then it is likely that the crack velocity will exhibit a transient oscillation. Moreover, with such oscillations, if the cracked lattice cannot support a crack motion less than some critical value because of trapping, then the transient will die, even though the lattice trapping limit is exceeded. This problem could be explored by first preparing a crack in a steady-state motion and then lowering its load below the lattice trapping value into the regime it would not be able to achieve ''from below.'' We suggest that such a hysteretic behavior should be associated with a finite field inertia for the crack and that this in turn might be associated with a magnification of the velocity regime denied the crack as it is loaded slowly from below its trapping value. Such a behavior might have been observed in the simulations of Zhou *et al.* [2] and Gumbsch *et al.* [13], but the simulation results should be reaffirmed. In any event, we should point out that, for zero initial temperature, it may be almost impossible to observe crack propagation at very low velocities by molecular-dynamics simulations simply because of the long times required to see the launching of the crack.

A further consideration for the problem of starting the crack is to assess the role that any storage modes might play (if they exist). We commented on such a possibility in discussing the strip continuum problem. In that case such a storage mode would be equivalent to the proposal made by

Gao [16] that the upper limiting speed of the crack is in part determined by the locally diminished elastic wave speed in the vicinity of the crack tip. If the crack moves faster than the local wave speed, then energy will build up, which will lead to unstable behavior. But we would not expect such an effect to play a role in bunching energy near the crack tip when the velocity is near zero and below any locally diminished wave speed. (We noted in the 1D model of Sec. II that the special dispersive character of the model leads to zero velocity waves for infinite wavelength, which is a special case of Gao's mechanism, but this is a very special feature of this model and thus not a general phenomenon.) But for the discrete crack, actual local modes might exist, which, moving with the crack, could become excited and give rise to important effects even at relatively low velocity [2]. This is a mechanism that deserves additional study not only for its role in the velocity law, but as a mechanism for generating instabilities in the crack behavior.

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