MOLECULAR-DYNAMICS SIMULATIONS OF FRACTURE: AN OVERVIEW OF SYSTEM SIZE AND OTHER EFFECTS

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ABSTRACT

We have studied brittle and ductile behavior and their dependence on system size and interaction potentials, using molecular-dynamics (MD) simulations. By carefully embedding a single sharp crack in two- and three-dimensional crystals, and using a variant of the efficient sound-absorbing reservoir of Holian and Ravelo [Phys. Rev. B **51**, 11275 (1995)], we have been able to probe both the static and dynamic crack regimes. Our treatment of boundary and initial conditions allows us to elucidate early crack propagation mechanisms under delicate overloading, all the way up to the more extreme dynamic crack-propagation regime, for much longer times than has been possible heretofore (before unwanted boundary effects predominate). For example, we have used graphical display of atomic velocities, forces, and potential energies to expose the presence of localized phonon-like modes near the moving crack tip, just prior to dislocation emission and crack-branching events. We find that our careful MD method is able to reproduce the ZCT brittle-ductile criterion for short-range pair potentials [static lattice Green's function calculations of Zhou, Carlsson, and Thomson, Phys. Rev. Letters **72**, 852 (1994)].

We report on progress we have made in large-scale 3D simulations in samples that are thick enough to display realistic behavior at the crack tip, including emission of dislocation loops. Such calculations, using our careful treatment of boundary and initial conditions - especially important in 3D - have the promise of opening up new vistas in fracture research.

INTRODUCTION

Insufficient understanding of the brittle *vs.* ductile behavior of materials has hindered the development of new materials with high strength and toughness. One of the reasons is that these mechanical properties are influenced by material structures at several different levels, including electronic structure, crystal structure, external environment, and imperfections like cracks, dislocations and interfaces. Combining atomistic, microstructural, and continuum theories is an effective way of exploring these mechanical properties. A valuable key to the toughness problem is to distinguish between an intrinsically brittle material and an intrinsically ductile one. In 1974, Rice and Thomson [1] proposed a semi-quantitative criterion for determining the intrinsic ductile

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vs. brittle behavior of materials in terms of the competition between dislocation emission from crack tips and crack cleavage. Rice has recently improved this model by including some atomistic features into the continuum elastic theory [2].

To gain a comprehensive understanding, however, it is very important to perform large-scale molecular-dynamics (MD) simulations, partly because the strain fields of cracks and dislocations are long-range in character, and partly because moving cracks generate sound waves, which are reflected from (or transmitted through) boundaries. We have developed a massively parallel MD code called SPaSM, which is capable of treating millions of atoms [3,4] and absorbing sound waves and mobile dislocations in boundary regions [5]. With these careful MD simulation techniques, we are able to study many aspects of cracks which have been unobtainable to date. For example, in 2D, we can reproduce the criterion for the brittle-ductile transition for short-range pair potentials [6], and we see dramatic differences between static and dynamic fracture. Moreover, we find that dynamic cracks can significantly facilitate dislocation emission, and that crack branching is initiated by dislocation nucleation. The bond-breaking energy released from a dynamic crack accumulates at the crack tip and strongly excites local phonons on each side of the crack. This is one of the key features of a dynamic crack and has a profound effect on crack instability [7].

Crack-tip fronts in real 3D materials are not always straight; moreover, dislocation nucleation can be a thermally activated process that is dependent on the length scale of the crack front. Ledges and other defects on crack fronts can serve as "easily operated" dislocation nucleation sources [8], which have been experimentally confirmed [9]. Although experimental techniques such as High Resolution Transmission Electron Microscopy are getting more powerful, it is still a challenging task to observe 3D, dynamic, atomistic processes such as dislocation nucleation and emission from a crack tip.

Recently we have performed large-scale 3D MD simulations on a crack in the fcc lattice, similar to the system investigated by deCelis, Argon, and Yip with quasi-3D MD [10]. We have observed blunting half-dislocation loops emitted from both fronts of an embedded crack, at an initial temperature of almost zero. Preliminary results on cracks and dislocations (including jogging dislocations along slip planes that are at an angle to the crack front) are discussed, along with new visualization techniques that are particularly effective in 3D.

RESULTS

Since cracks and mobile dislocations move at appreciable fractions of sound velocities, and since stresses relax by sound waves, it is only natural that dynamic processes accompanying crack propagation impose severe temporal limitations on molecular dynamics simulations, where the inherent length scale is made very small by computer-memory limitations. If, for example, sound

waves are permitted to pass through periodic boundaries or reflect from free boundaries, they will eventually return to the region ahead of the crack and impose artificial stresses long before they would have done so in a truly macroscopic sample. For this reason, Holian and Ravelo [5] devised smooth impedance-matched, acoustic-absorbing reservoir regions, where atoms are subjected to artificial viscous damping, which is gradually ramped up from zero at the reservoir-sample interface to a value that critically damps high frequency sound waves. Thus, the whole spectrum of quasiharmonic phonon frequencies of traveling waves is damped out. Other methods of damping that do not use this impedance matching make the reservoir-sample boundary look like a hard wall and reflect a significant fraction of the sound-wave amplitude. A modification of this reservoir approach has been proposed [11], wherein an embedded crack is surrounded by an elliptical "stadium," defined by the function $0 \le f \le 1$ ($f = 0$ in the sample region):

$$f(r) = \min\left(1, \max\left(0, \frac{(x/L_x)^2 + (y/L_y)^2 - (a/L_x)^2}{1/4 - (a/L_x)^2}\right)\right) , \qquad (1)$$

where L_x and L_y are the widths of the entire computational cell, and a and b are the x- and y-axes of the inner sample region, such that $a/L_x = b/L_y$. The temperature in the reservoir region can then be defined by $kT = \Sigma\, m|u|^2 f / (2\Sigma f)$ ($\mathbf{u}$ is particle velocity, and the sum extends over all atoms in the system), with viscous damping coefficient $\gamma = 2\omega_E(1-T_o/T)$ controlling the long-time average of the temperature to be T_o, the initial sample temperature.

In addition to this gentle boundary treatment, the embedded crack itself can be made atomistically sharp, with initial atomic displacements chosen to be nearly the final relaxed values for the critical Griffith strain, according to the continuum elastic solution [11]. Nonlinear relaxation occurs in a tiny region (only two or three atomic spacings away from the crack tip), generating small-amplitude sound waves that are only barely perceptible. Slight additional overstrain can then be achieved by applying a homogeneous strain rate (in the x-direction) $\dot{\varepsilon}_{xx}$ appropriate to adiabatic expansion; the Hamiltonian equations of motion for the atomic coordinates $\mathbf{r}$ and thermal velocities (relative to the imposed strain rate) $\mathbf{u}$ are then given by [11]

$$\begin{aligned} \dot{\mathbf{r}} &= \mathbf{u} + \dot{\varepsilon}_{xx}\, x\, \hat{\mathbf{x}} \\ \dot{\mathbf{u}} &= \frac{\mathbf{F}}{m} - \dot{\varepsilon}_{xx}\, u\, \hat{\mathbf{x}} - \gamma\, \mathbf{u}\, f \quad . \end{aligned} \qquad (2)$$

(Note that viscous damping is *not* applied in the sample, but only in the reservoir.) The result is the gentlest driving possible, with relaxation waves from free surfaces eliminated entirely when periodic boundary conditions are used along with constant boundary velocities $u_p = \pm\dot{\varepsilon}_{xx} L_x$. Homogeneous strain-rate loading, coupled with the sharp-crack initial condition, as opposed to a

blunt notch, allows MD simulations to recover very reproducibly the continuum Griffith criterion for initiation of crack motion. This loading is also preferable to applying constant stress at the boundaries, since the latter invariably introduces perturbing stress waves into the sample region.

When we used these gentle initial and boundary conditions in 2D fracture simulations, we were able to drive a long crack (whose Griffith strain was well below 1%) so delicately that it eventually came to a halt and then receded in length. We were able to determine very precisely the dislocation emission criterion by MD, which compared very favorably with earlier static lattice Green's function calculations by Zhou, Carlsson, and Thomson [6]. We also saw from a series of simulations under a variety of loadings that: (1) dynamic cracks accelerate rapidly to an approximately steady velocity; (2) bond-breaking energy leads to a gradual buildup of a local phonon field near the crack tip; (3) when a critical excitation level is reached, dislocation emission is observed, almost regardless of the interatomic potential (as long as it is longer-ranged than nearest neighbors only); (4) branching is initiated by dislocation emission in almost every case - for the stiffest pair potentials, dislocations cannot even escape the crack; (5) branches zigzag, turning back toward the initial direction of propagation (along the natural cleavage direction; if the strain is contrary to the natural direction, i.e., not along a slip plane in 2D, then the crack behaves in an erratic manner with a diminished rate of dislocation emission). In Figure 1, we show a sequence of snapshots of dynamic crack propagation and branching.

We note that crack velocity is not the only diagnostic that determines when branching occurs; in fact, a crack can travel for some time at a relatively steady velocity before it slows down and then branches. The dynamic buildup of phonon amplitude is also an important part of the dynamic crack propagation process.

In order to visualize dynamic cracks, we have colored the atoms according to their velocities, forces, and potential energies. The first two methods are particularly useful for demonstrating the localized phonon field buildup in a region within a few lattice spacings of the crack tip. Plotting atoms according to their potential energies is especially useful for showing the local structures near the crack tip, with a somewhat more subtle display of the phonon field. For example, with a movie of atom potential energies, we can clearly see crack surfaces and dislocation cores, and the incipient events leading to their formation and emission. (See Figure 1.) In 3D, the effects are even more dramatic, since we can render bulk atoms (with the lowest potential energies) invisible, leaving dislocation loops and crack surfaces exposed to view.

In our recent preliminary 3D simulations, we have used our potential-energy visualization technique to see both blunting and jogging dislocations being emitted from the crack tip, as shown in Figure 2. Almost two million atoms were used in these calculations, and even so, the size was only marginally adequate. Nevertheless, the systems were over an order of magnitude larger in the thickness dimension (along the axis of the elliptical-cylindrical crack) than those of earlier

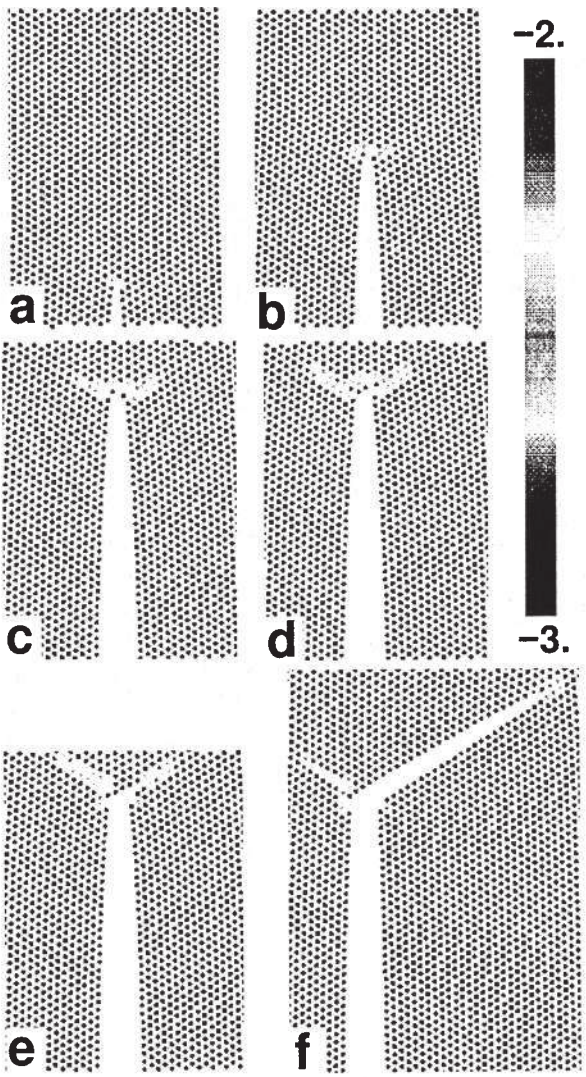

Figure 1. Dislocation emission and crack branching sequence for a 2D dynamic crack (increasing time from a-f, up to 100 vibrational periods). The full computational cell (not shown here in its entirety) includes about 400,000 atoms interacting via the Morse pair potential ($\alpha = 6$). The initial half-crack length is 240 lattice spacings. Particles are colored by a rainbow ranging from deep blue for a minimum potential energy of -3.0 (bulk) to bright red for a maximum value of -2.0 (free surface), indicated by the color bar (shown here in grayscale).

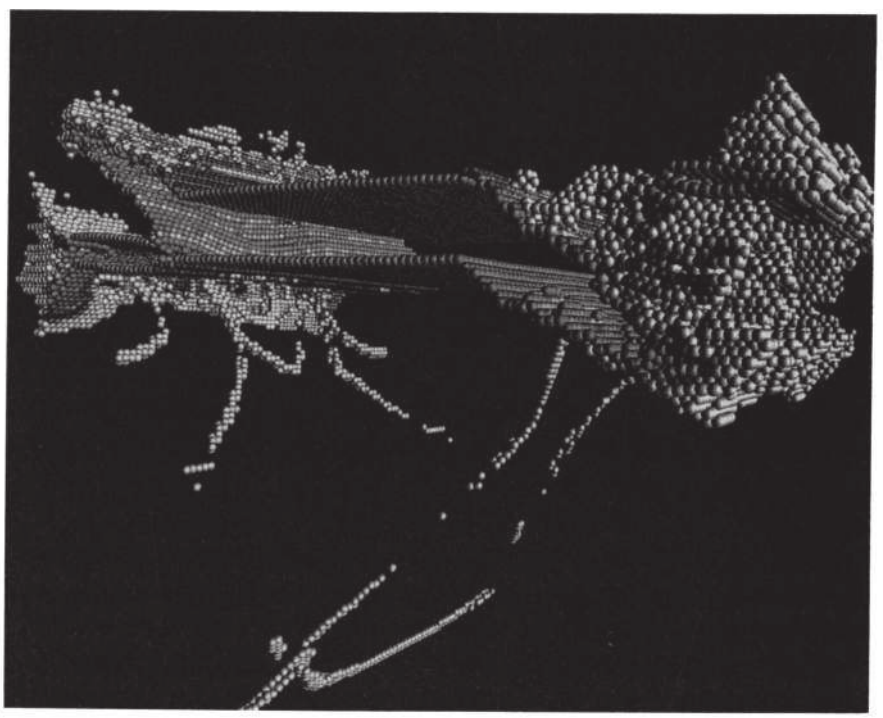

Figure 2. Blunting half-dislocation loops (3D) generated from crack fronts along {111} planes, and crack branching, also along {111} planes. The full periodic-boundary-condition computational cell includes 1.7 million atoms interacting via the Morse pair potential ($\alpha = 7$). The initial half-crack length is 20 lattice spacings. Particles are colored by potential energy (shown here in grayscale). To visualize dislocation loops, only particles with local potential energy above a certain value are shown. The crack plane is (010) and crack fronts are along the [101] direction.

generations of computers [10]. Generally speaking, as the potential is made softer and longer-ranged, the number of jogging dislocations diminishes, while the number of blunting dislocations increases. Jogging dislocations, originating at the junction of the elliptical-cylinder crack and a free surface, are emitted along slip planes that intersect the crack tip, while blunting dislocations are emitted along slip planes that are coincident with the tip. [The stiffness of the potential is exemplified by the Morse potential form: $\varphi(r) = e^{-2\alpha(r-1)} - 2e^{-\alpha(r-1)}$, where length is measured in units of nearest-neighbor distance r_0 and energy in well-depth ε; the stiffness parameter α is then the ratio of bulk modulus to cohesive energy, and the reduced force constant is $2\alpha^2$.]

Our preliminary 3D calculations utilized the sharp-crack initial conditions and adiabatic expansion boundary conditions, with very low initial temperatures. We saw significant differences between fully periodic boundary conditions and partially free boundary conditions, both in the kinds of dislocations generated and in their shapes.

It will be important in future 3D MD simulations to explore the effects of initial temperature, crack geometry, interaction potential (particularly, embedded-atoms method - EAM - many-body potentials), and system size, as well as utilizing the "stadium" reservoir treatment we have developed in 2D. Already, 3D simulations of crack propagation have revealed a richness of features that could only have been guessed at a few years ago.

CONCLUSIONS

We have studied dynamic cracks using large-scale molecular-dynamics simulations in both 2D and 3D. By setting up initial conditions that are close to those in traditional fracture mechanics treatments, and by absorbing unwanted sound-waves generated at the crack tip, we have been able to compare MD simulations to quasi-static methods. We see differences, however, between the static view and dynamic cracks, namely a gradual buildup of phonon content that is highly correlated in time and intimately associated with the moving crack tip. In dynamic cracks, this buildup then leads to dislocation emission and branching. By coloring atoms according to their potential energy, much of the structure of crack tips and emitted dislocation loops can be seen, even in 3D. We believe that large-scale MD simulations with careful treatments of boundary and initial conditions - especially important in 3D - have the promise of opening up new vistas in fracture research.

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