Ideal Brittle Fracture of Silicon Studied with Molecular Dynamics

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Dynamic fracture experiments measure *crack velocity* versus *energy flux to the tip*. We report here the first calculation of this quantity in a realistic setting, using molecular dynamics to study silicon. The results require relating the short length and time scales of simulations to the long length and time scales of experiments. [S0031-9007(97)05122-3]

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Silicon is very brittle and a wafer dropped on the floor easily shatters. A clue to explaining why comes from static cracks. Even at room temperature, static cracks in silicon can have tips that are atomically sharp [1], and there is every reason to believe that crystals can be severed very efficiently by the propagation of such sharp cracks. Relations between crack speed and energy consumption have been measured, mainly in brittle plastics [2], but have never realistically been calculated.

The only full characterization of how things break at the atomic level has been obtained in an *ideal brittle* crystal, which is a lattice of atoms in which forces between nearest neighbors rise linearly with separation up to a critical distance, after which they fall immediately to zero. That is, nearby atoms attract each other according to Hooke's law, until they separate too far, at which point the bond between them instantly snaps. Slepyan [3,4] first showed that cracks in crystals of this type can completely be described analytically. A summary of some of the most important results [5,6] is as follows: (i) Moving cracks can naturally evolve to steady states in which patterns of atomic motion repeat indefinitely, and the crack leaves behind atomically flat surfaces. (ii) Cracks in steady state emit surface phonons whose phase velocity equals the crack velocity [3]. (iii) When energy flux to the crack tip falls below a lower critical value, crack motion becomes impossible. This lower critical value is larger than the value one would deduce from considering energy conservation [7], and the minimum allowed crack speed is on the order of 20% of the transverse sound speed, rather than zero. (iv) If energy flux to the crack passes an upper critical value, the tip goes unstable, is no longer atomically sharp, and the system's dynamical behavior rapidly becomes very complex.

These qualitative findings have been limited to the very special models that could be solved by hand. There was no persuasive argument that cracks in real materials should behave similarly, no determination whether ideal brittle fracture is a pathological feature of an artificial model, or whether it is a broad universality class. We therefore decided to check how much of the scenario would be preserved in three-dimensional molecular dynamics simulations of silicon, employing realistic two- and three-body potentials. All the features of the idealized lattice models carry over to the realistic case, although cracks in silicon act in a hysteretic way we had not anticipated from the analytical work.

Why silicon?—We concentrate on simulations of silicon because it is very brittle, and its physical properties are well known. In equilibrium it adopts the diamond crystal structure, and the elastic moduli, phonon dispersion relations, and even fracture energies across various crystal planes have all accurately been measured. We learned not to take such information for granted during an earlier round of simulations of silicon oxide in the β-cristobalite structure. After discouraging experiences in which well-respected atomic potentials [8] caused the well-known equilibrium crystal to explode, we learned that the crystal structure ensconced in the literature for seventy years was incorrect, and that its replacement remains controversial [9]. Studies of silicon do not involve such difficulties. Classical interatomic potentials have carefully been constructed to reproduce correctly a variety of equilibrium properties [10]. The only drawback of these potentials is that since the bonding between silicon atoms is strongly covalent, computationally demanding three-body interactions are necessary just to keep the crystal stable. The contribution to the total energy of these three-body terms is generally less than 0.1%, and they serve mainly to ensure that the energies of face-centered and body-centered cubic structures are raised far above the energy of diamond.

Microscopic and macroscopic scales.—The study of fracture is difficult because crack tips always involve phenomena on atomic scales, while the crack grows to macroscopic lengths. The connection between microscopic and macroscopic scales is made as simple as possible by considering a strip geometry.

The predictions of fracture mechanics—the long wavelength elastic theory of crack motion—are complicated for short cracks moving in large plates [11]. However, for a long crack moving at steady velocity in a strip whose upper and lower boundaries are held rigid one can deduce the energy consumed by the fracture in a trivial way. If elastic energy G is stored per unit area far ahead of the crack tip, then the crack consumes energy G per unit area

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during *steady* motion, since far behind the crack tip all the elastic potential energy has been relieved. This conclusion rests upon symmetry, and does not even demand strains ahead of the crack tip to be so small that linear mechanics be applicable. Steady velocity $\vec{v}$ and a corresponding energy flux G are achieved in the long time limit, the natural scale in experiments as well as in analytical calculations, where the crack tip reaches dynamic equilibrium with waves reflecting from top and bottom boundaries. According to fracture mechanics, the relationship between energy flowing to a crack tip and crack velocity is, for a given lattice direction, universal. Having obtained the relation in a strip, we know it for any of the vast range of geometries to which fracture mechanics is applicable, such as a long crack in a large plate [2].

In order to relate samples of different size to one another, let G_c be the Griffith energy density [7,11], that is, twice the crack surface energy density, a lower bound on the energy per unit area required for a perfectly efficient crack to propagate along a certain plane. In our numerical silicon, $G_c = 3.3\ \mathrm{J/m^2}$ for cracks along (110), and $G_c = 2.7\ \mathrm{J/m^2}$ for cracks along (111). Define a dimensionless measure of loading

$$\Delta = \sqrt{G/G_c}\,, \tag{1}$$

where G is the energy stored per unit area ahead of the crack. According to analytical solutions for the ideal brittle solid, the relationship between Δ and crack velocity becomes independent of the height of the strip (number of planes along z) for surprisingly small strips; a strip 80 atoms high has for all practical purposes reached the infinite limit. This very rapid convergence of the main quantity of physical interest allows us to obtain physically meaningful results from simulations that by today's standards [12–15] involve small numbers of atoms. Because of the long time scales required for steady states, we therefore need to make the system as small as possible along z, Fig. 1, and to carry out very long runs.

Design of simulations.—In the simulations indicated in Fig. 1, the crack runs along x, exposing either (111) or (110) planes. Three separate boundary conditions are employed.

x-y planes.—Two layers of atoms at the top and bottom of the strip are held rigid during the simulation. By pulling them apart, elastic energy of any desired amount can be stored ahead of the crack tip. Sometimes the distance between top and bottom layers is held fixed during the whole simulation, while other times it is increased or decreased adiabatically.

y-z planes.—We want to model a crack in an infinitely long strip. To accomplish this aim with a finite number of atoms, we use two techniques at these boundaries. First, whenever the crack tip approaches within 150 Å of the right-hand boundary, we paste new crystal onto the right-hand side, and cut broken crystal from the left. Second, to prevent elastic waves from informing the crack tip that it lives in a strip of finite extent, we create energy absorbing regions 20 Å thick at both the left and right ends—though this is not important for the region ahead of the crack tip, which remains practically undisturbed until the crack goes unstable.

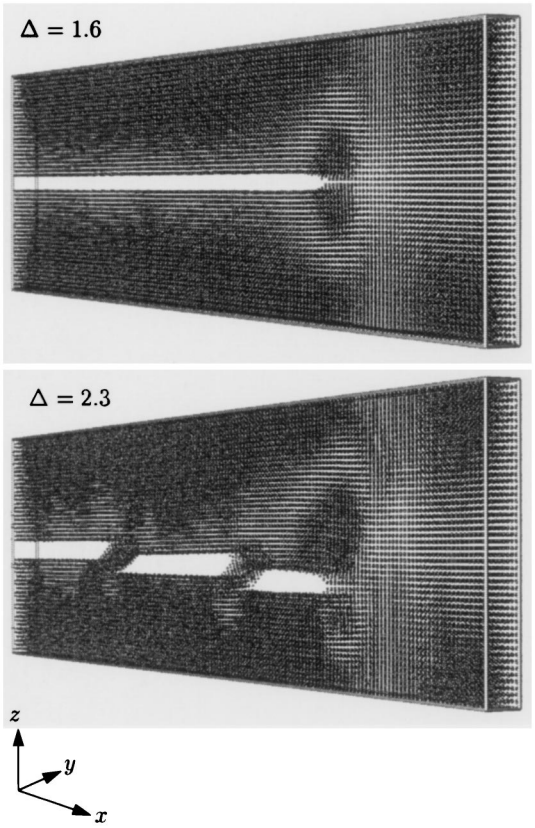

FIG. 1. Visualizations of the simulations, showing a stable steady-state crack at 6.24% strain, top, and an unstable crack at 8.97% strain, bottom, along (111). Animations can be seen at http://chaos.ph.utexas.edu/~marder/Crack/.

x-z planes.—Across these boundaries, we employ periodic boundary conditions. This choice enables us correctly to describe the flux of energy to the crack tip in a macroscopic sample. Nakamura and Parks [16] have shown that in a plate of thickness d, at distances from the crack tip much smaller than d, the appropriate elastic solutions are found to be those with such periodic boundary conditions.

We start with an equilibrium sample $614 \times 19 \times 153\ \mathrm{Å}^3$. The number of atoms involved at any stage of the simulation is approximately 94 000, although after numerous cuts and pastes at left- and right-hand boundaries tens of millions of atoms are cumulatively involved. This number is small enough to enable us to follow crack motion for the times ($\sim$10 ns) needed for the cracks to proceed through a succession of steady states between arrest and instability. To initiate the simulation, we pull the two x-y boundaries apart so that Δ as defined in Eq. (1) is 1.6, insert a narrow seed crack running half the sample length,

give an initial velocity to a few atoms near the crack tip, and let Newtonian mechanics take over. The time step used is 4 fs. There are about 30 time steps in the smallest period of vibration in the system, giving very good energy conservation. Decreasing the time step by a factor of 4 shows no change in the dynamics.

Results of calculations in silicon.—We want the calculations to answer the following questions: (i) Are there loads Δ where cracks are attracted to steady states? (ii) Do cracks emit phonons at the predicted frequencies? (iii) Do cracks refuse to travel below a minimum velocity $v_1 > 0$? (iv) Do they go unstable above an upper load Δ_c? The answer to all the questions is yes.

Figure 2 shows the time history of two different atoms just above a (111) fracture surface for $\Delta = 1.6$ and for times greater than 0.24 ns. As anticipated by the theory of ideal brittle fracture, the crack has reached steady state with velocity $v = 3460$ m/s, which means that the vertical displacement $z_{\vec{R}}$ of an atom originally at crystal location $\vec{R}$ is related to the vertical displacement $z_{\vec{R}+n\vec{a}}$ of an atom n lattice spacings $\vec{a} \equiv a\hat{x}$ to the right by

$$z_{\vec{R}+n\vec{a}}(t + na/v) = z_{\vec{R}}(t)\,. \tag{2}$$

For a range of loads Δ, Eq. (2) applies for any pair of atoms, whatever their separation along the crack surface. In order to obtain the perfect periodicity shown in Fig. 2, the crack was allowed to run first for 60 000 time steps so as to come into equilibrium with the waves it sends towards top and bottom boundaries.

Under steady-state conditions as described by Eq. (2), the radiation far from the crack tip must obey

$$e^{[i\vec{k}\cdot(\vec{R}+n\vec{a})-i\omega(\vec{k})\,(t+na/v)]} = e^{[i\vec{k}\cdot\vec{R}-i\omega(\vec{k})t]}. \tag{3}$$

Since $\vec{a}$ and $\vec{v}$ are parallel, it follows that the crack should excite all surface phonons whose frequency $\omega(\vec{k})$ and wave number $\vec{k}$ obey the Cherenkov condition

$$\omega(\vec{k}) = \vec{v}\cdot\vec{k}\,, \tag{4}$$

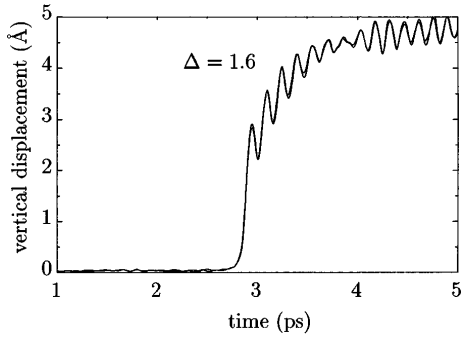

FIG. 2. Height z of two atoms lying on the crack line as a function of time, showing passage of a crack on a (111) plane. The second atom lies 184 Å along x relative to the first, and is displaced backwards by 5.32 ps in time. That the two overlapped curves are almost completely indistinguishable shows the crack has reached steady state, according to Eq. (2), and is emitting phonons in accord with Eq. (4).

so that crack velocity $\vec{v}$ equals phonon phase velocity. Thus, the Cherenkov condition is equivalent to demanding that a propagating wave obey Eq. (2), so Fig. 2 also shows that Eq. (4) is satisfied.

In order to find fracture speed v as a function of the loading parameter Δ, we adiabatically decrease the separation between the x-y boundaries while allowing the simulation to run. The crack tip is precisely located every second time step, showing clearly every single bond-breaking event. In order to estimate just how slow the strain rate must be to achieve the adiabatic limit, we carried out numerical simulations of the analytically solvable models. We compared numerical and analytical results, arriving at the criterion that the dimensionless strain rate $\dot{\epsilon}h_z/c$ should be much less than one, where $\dot{\epsilon}$ is the strain rate, $c = 5500$ m/s is a sound speed, and $h_z = 153$ Å is the height of the sample along z. We employ low rates $\dot{\epsilon} < 100\ \mu\text{s}^{-1}$, or $\dot{\epsilon}h_z/c < 10^{-4}$. Prior molecular dynamics simulations of fracture have been carried out with strain rates of order 10^4 times greater, for which steady states are unattainable and the crack very rapidly goes unstable. In laboratory experiments [17], $\dot{\epsilon}h_z/c \sim 10^{-8}$.

Along (110).—The relation between velocity v and load Δ for cracks exposing (110) and traveling along $[1\bar{1}0]$ appears in Fig. 3(a). The crack velocity smoothly decreases as Δ decreases, until at $v_1 = 2256$ m/s and $\Delta = 1.258$, the crack abruptly comes to a halt. Raising Δ again, the crack does not begin to move until $\Delta = 1.366$, a value that is sensitive to residual vibrations in the crystal, but the rising curve then perfectly overlaps the descending one. Crack speed continues to rise smoothly until $v = 3586$ m/s, $\Delta \approx 2.2$, at which

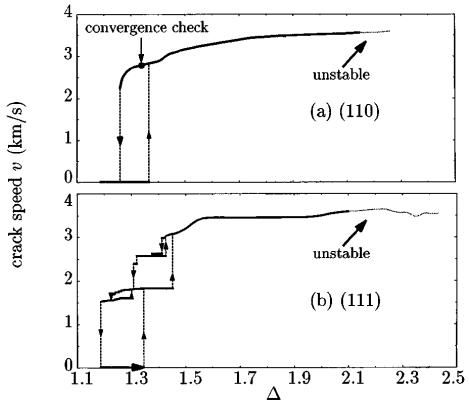

FIG. 3. (a) Relation between crack speed v and loading Δ for crack along (110). As Δ descends, velocity drops abruptly to zero at lower critical value, and as Δ ascends resumption of crack motion is hysteretic. For convergence check, system size was doubled along x and z, and $v(\Delta)$ measured. (b) Same for crack along (111). For $\Delta < 1.44$ the crack is able to expose many different states lying along many hysteresis loops; see Fig. 15 of Ref. [6]. Gray lines show where ideal steady states are unstable.

point steady-state motion becomes unstable. We have not yet investigated the instability in detail, but observe such complicated phenomena as formation of small branches, emission of dislocations, and changes in the plane of propagation.

Along (111).—The relation between velocity v and load Δ for cracks along (111) and traveling along $[01\bar{1}]$ appears in Fig. 3(b). For $1.44 < \Delta < 2$, the crack has stable steady states, and for $\Delta > 2$ it goes unstable in a similar manner to cracks along (110). However, for $1.175 < \Delta < 1.44$ the dynamics of the crack exhibits a number of interesting features we have not seen previously, and for which we do not now have a complete theoretical description. There is a variety of different dynamical states available for each value of Δ, where the crack travels at different speeds. Each of these states corresponds to a plateau in $v(\Delta)$; Δ can change by as much as one fifth of the amount needed to go from arrest to instability and the crack velocity does not alter within numerical resolution. When the crack finally decides to accelerate out of the plateau, it may jump by over 1 km/s and reach an upper plateau to within a few m/s. On cyclical loading the same plateaus are always reached. All of these transitions are hysteretic, as depicted in Fig. 3. The different states emit noticeably different phonons; on a given plateau, the phonon frequencies appear fixed and their amplitude changes, while between plateaus the frequencies change, in accord with Eq. (4). All these phenomena are easily disguised if strain rates are too high. Resolving all the fine structure visible in Fig. 3 required $\dot{\epsilon} < 8\ \mu\mathrm{s}^{-1}$, or $\dot{\epsilon} h_z/c < 10^{-5}$.

Naturally, it would be very interesting to know how much of the dynamical scenario we present here actually occurs in nature. Experiments aimed at answering this question are underway. In the current incarnation, they are being performed at room temperature, and we are also carrying out new computer simulations at elevated temperatures. However, new experiments at low temperatures will be required if a detailed comparison between theory and experiment is to be completed.

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