INFLUENCE OF MICROSTRUCTURE ON DYNAMIC FRACTURES

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ABSTRACT

The continuum theory of fracture has many great successes, but there are certain questions it cannot obviously answer. One of these questions concerns the direction of crack motion. Crack directions are usually thought be chosen by the principle of local symmetry. The goal here is to examine carefully a case where one might expect the principle of local symmetry to hold, and to show that it does not. The setting for the study is a molecular dynamics simulation of fracture with very simple force laws contrived so that at large length scales it completely replicates isotropic continuum elasticity. Because at a macroscopic level, this numerical material cannot be distinguished from a continuous isotropic solid, one might believe that a crack moving in it should obey the principle of local symmetry when it chooses directions. However, that is not correct. At small length scales, the solid is crystalline, and the crack is confined to crystalline planes in a fashion that the principle of local symmetry cannot predict. These arguments do not show that the principle of local symmetry is generally incorrect, but they do show that it does not hold in at least one case that can be studied carefully.

1. INTRODUCTION

Much of the theory of dynamic fracture concerns cracks that are assumed to move along a straight lines[1, 2]. There are many cases where they do not; for example, when much more energy is supplied to an object than needed to drive a single crack, in which case repeated branching usually shatters the body into many pieces. There are cases where single rapidly running cracks do not travel in straight lines, as in cracks running along pressurized pipelines. As a matter of principle, it would seem impossible to call the theory of dynamic fracture complete unless one can predict the shapes of crack paths, and not just their speeds on straight lines.

Before one can predict crack paths, it is necessary to decide what features of a solid are relevant. One possibility is that macroscopic elastic properties are all one really needs to know. If this were correct, then all cracks traveling under identical loading conditions in elastically isotropic solids would move in the same way. The rule universally used to predict crack directions is the principle of local symmetry[3, 4], which says that cracks travel in such a direction that K_{II} vanishes with no reference to the structure of the material at all. However, it would seem natural for material microstructure to be able to influence the direction of crack motion. When cracks cleave crystals, one expects them to travel preferentially along crystalline planes. Careful experiments on quasi-static cracks in silicon loaded through thermal gradients show their behavior to be quite different from similarly loaded cracks in glass[5]; for example, when slowly driven thermal cracks in glass begin to exhibit oscillating paths, the transition between straight and oscillating motion is supercritical[6, 7], while in silicon single crystals it is subcritical and hysteretic.

However, the existing experimental data leave room for arguments about what factors are really important for crack motion. Silicon is crystalline at small scales, but it is also macroscopically orthotropic rather than isotropic. Perhaps the elastic properties of silicon alone are enough to explain the differences between crack paths in silicon and glass; in a material that is not isotropic, the principle of local symmetry need not apply. Therefore, it would be useful to have a case in which the separate influence of macroscopic elasticity and microstructure can be disentangled. This goal has not yet been carried out with laboratory experiments, but it is fairly easy to achieve with numerical experiments, as this article will describe. The numerical experiments are performed on simple model systems, using classical molecular dynamics. The point of view regarding these systems is that they could be realized in the laboratory if only there happened to be atoms with such simple interactions. At any rate, the principles of fracture mechanics should apply to these numerical systems as well as to any laboratory sample, and if they do not, then the principles of fracture mechanics are not as

general as one think. Numerical computations have the great advantage that boundary conditions of fracture samples can be controlled with a precision that is simply impossible in the laboratory, and cracks can be followed with great precision as well. Sometimes such computations are dismissed on the grounds that they describe such small numbers of atoms that they have nothing to say about macroscopic materials. However, scaling arguments allow one to relate small samples to macroscopic ones[8], and thus the conclusions from the computations have macroscopic implications.

2. IDEAL BRITTLE CRYSTAL

The material in which I will investigate crack motion is an ideal brittle triangular crystal with equilibrium lattice spacing a in which atoms obey the equation of motion (1)

$$m\ddot{\vec{u}}_i = \sum_j \left[\vec{f}(\vec{u}_{ji}) + \vec{g}(\dot{\vec{u}}_{ji}, \vec{u}_{ji}) \right], \tag{1}$$

with $\vec{u}_{ji} \equiv \vec{u}_j - \vec{u}_i$. The functions $\vec{f}$ and $\vec{g}$ have the specific forms

$$\vec{f}(\vec{r}) = \kappa \hat{r}(r-a)\theta(r_c - r); \;\; \vec{g}(\dot{\vec{r}}, \vec{r}) = \beta \dot{\vec{r}} \theta(r_c - r). \tag{2}$$

Atoms interact with a central force f that varies linearly around the equilibrium spacing of length a, and whose scale is set by κ. If the distance between atoms increases to more than r_c, the force drops abruptly to zero. In addition, atoms experience Kelvin dissipation g; its scale is set by β, is proportional to the relative velocities of neighbors, and also drops to zero when the distance between neighbors exceeds r_c.

In general, crystals have anisotropic elastic properties at large scales. However, the triangular lattice is an exception. The macroscopic elastic theory of this crystal is homogeneous and isotropic, with Young's modulus $Y = (5\sqrt{3}/4)(\kappa/a)$ and Poisson's ratio $\nu = 1/4$.

The Kelvin dissipation also deserves comment. In a macroscopic theory of fracture, Kelvin dissipation is forbidden, because a moving crack tip singularity in a material with such a dissipative term dissipates an infinite amount of energy. In a microscopic theory, such terms are expected and natural. The resolution of this apparent conflict is that in the continuum limit, the magnitude of the dissipate term in Eq. (1) must go to zero in just such a way as to keep the total dissipation in the vicinity of the tip finite.

The geometry in which I will study cracks is depicted in Fig. 1.

3. SOLUTIONS OF MODEL

Fracture properties of this model can be obtained analytically in the limit $r_c \to 1$, which means that bonds snap when they are stretched just a tiny distance above their equilibrium length. First, one can find that for fracture first to be energetically possible, one rigidly raises the top of the crystal above its equilibrium position by a vertical distance y_c

$$y_c = \frac{2}{\sqrt{3}}(r_c - a)\sqrt{N-1}. \tag{3}$$

In addition, in the limit $r_c \to a$ steady state cracks in this crystal are described by exact analytical solutions[9–12]. The most important observation to extract from these solutions is that the natural dimensionless measure of how much one has loaded the crystal is obtained by rigidly displacing its upper surface a distance δ_y and then forming the ratio

$$\Delta \equiv \delta_y / y_c. \tag{4}$$

That is, Δ is a variable proportional to the strain applied far ahead of the crack. It equals 1 when the crystal has been loaded precisely to the Griffith point where fracture first becomes possible. The

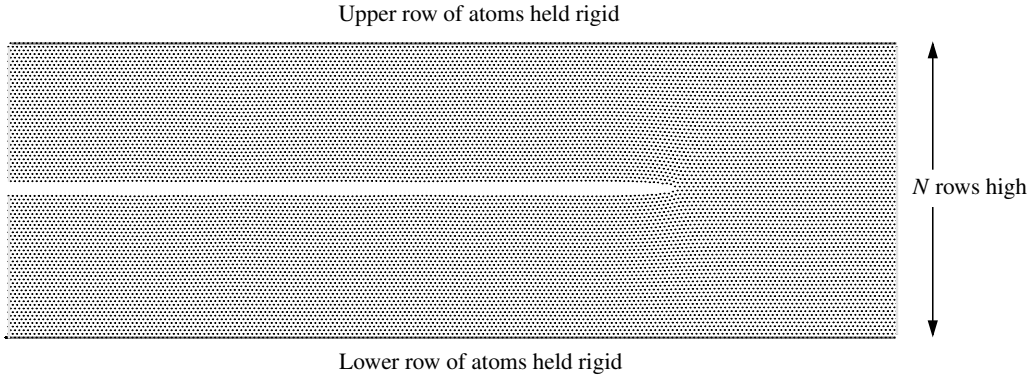

Figure 1: Setting for numerical experiment to find steady crack states. Atoms are originally arrayed in triangular lattice 80 rows high, and three times as long as it is tall. Primitive vectors for the equilibrium lattice are $a(1\ 0)$ and $a(1/2\ \sqrt{3}/2)$. The crack tip is defined as the location of the rightmost atom whose nearest vertical neighbor is at distance greater than $2.5a$. When the crack tip approaches within $60a$ of the right boundary, 10 columns of new crystal are attached to the right boundary, and the same amount discarded from the left hand side. In the discussion leading to Eq (4), top and bottom rows of atoms are held rigid and stretched vertically apart by a distance δ_y. To produce Figure 3,the top boundary is also slid horizontally relative to the bottom by an amount δ_x.

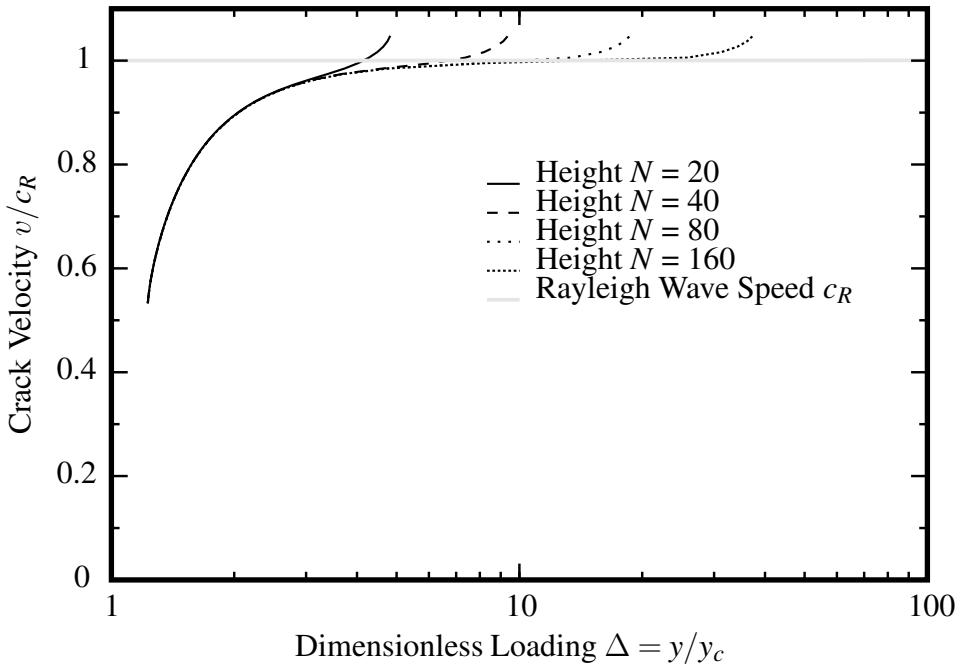

Figure 2: Relationship between velocity v and dimensionless loading Δ for lattice strips of varying height N in pure tension. The calculations are performed in the limit $r_c \to a$ with Kelvin dissipation $\beta = 0.01$ with the Wiener–Hopf technique[9–11]. The left–hand portions of the curve are almost completely independent of system height. The cracks are presumed to travel along a weak interface that precludes transverse instabilities, and therefore the curves continue up and through the Rayleigh wave speed c_R. Were the curves to be terminated at the points where cracks become unstable in homogeneous crystals, they would be nearly indistinguishable.

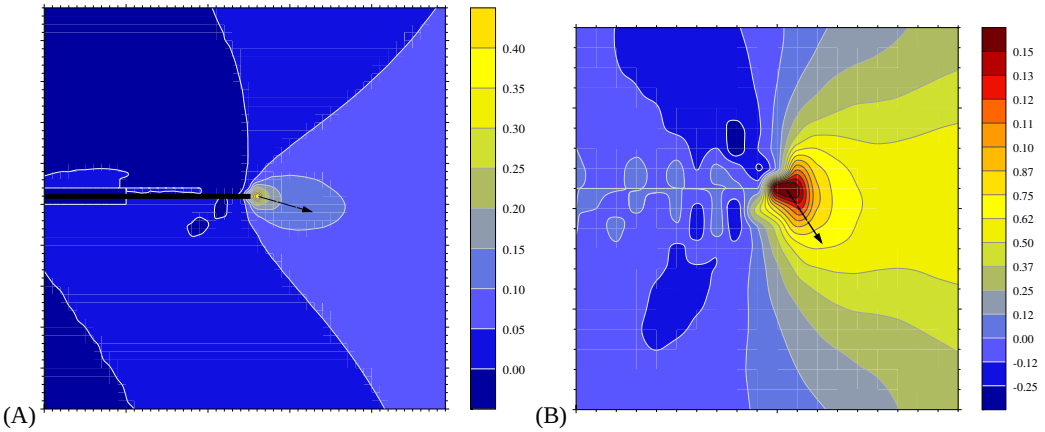

Figure 3: Color contour plots of tensile stress field $\sigma_{\theta\theta}$ surrounding crack tips in strips with rigid vertical tensile (δ_y) and horizontal shear (δ_x) displacements of upper and lower boundaries, computed from solutions of Eq. 1. Arrows show directions the cracks should turn according to local symmetry. Instead, they travel stably forever along the horizontal axis. The circular stress islands to the left of the crack result from averaging over high–frequency waves emitted by the crack and traveling left to right. (A) System $N = 150$ rows high, $\delta_y/y_c = 1.29$, $\delta_x/\delta_y = .23$, $r_c = 1.2$, force constant $\kappa = 1$, and Kelvin dissipation $\beta = 2$, resulting in a crack velocity $v/c_R = .01$. (B) As in (A), but $N = 200$ rows high and Kelvin dissipation $\beta = .02$, resulting in a crack velocity $v/c_R = .83$. The smaller value of β is completely responsible for the larger crack speed. The larger system is chosen because details of the fast–moving crack are more difficult to resolve.

analytical solutions demonstrate that if one measures crack speed v and plots it as a function of loading Δ, the results become independent of system height N to better than 1% for surprisingly small values of N, on the order of $N = 50$, as shown in Figure 2. This statement is true so long as the crack speed is not too large. Continuum theory predicts that cracks in tension cannot exceed the Rayleigh wave speed c_R, which for this model equals $.563\sqrt{\kappa a^2/m}$. Figure 2 shows that crack speed is practically independent of system height for $N > 50$ and $v < .9c_R$.

The model Eq. (1) is more realistic when $r_c = 1.2a$ than in the limit $r_c \to a$, since atomic bonds in real brittle materials actually give way when extended by about 20%. For $r_c = 1.2$, analytical techniques are no longer available to provide exact solutions. However, the scaling properties provided by the analytical solutions continue to hold. The relationship between crack speed v and loading Δ is practically independent of system height N once N reaches a value of around 50. As a result one can accurately predict the relationship between crack velocity v and loading Δ up to the macroscopic limit by performing computations in systems of microscopic dimensions.

Having established that microscopic computations have a legitimate macroscopic interpretation, I will now set out to show that the principle of local symmetry does not always correctly predict crack paths. Instead there is an interplay between the direction preferred by far–field stresses, and the direction preferred by microstructure. This conclusion comes from seeding cracks on the centerline of strips as in Figure 1, but then loading them with a mixture of tension and shear. The top and bottom boundaries are displaced vertically by distance δ_y and horizontally by distance δ_x.

The main result is represented in Figure 3. This figure shows contours of the tensile opening stress surrounding crack tips moving at two different speeds in a crystal. The contours are tilted away from the horizontal axis. The principle of local symmetry predicts that a crack tip surrounded by such stress fields should rapidly turn and move toward the tip of the largest lobe. However, the cracks move steadily and stably along the horizontal axis forever. These cracks follow crystal planes, not external stress fields. It should be emphasized that the macroscopic elastic properties of a triangular crystal are completely isotropic. Only the presence of atomic–scale planes can explain the failure of the cracks to follow the directions predicted by local symmetry.

To check the principle of local symmetry, it is necessary to compute the continuum elastic fields

surrounding these cracks. This task has been performed in two ways, which agree. First, the elastic stress fields were computed directly from the positions of atoms in the simulation by taking binned spatial averages in volumes V_0 where $\vec{f}_{ij}$ is the force between atoms i and j[13]. Second, the system was viewed as a fracture in a continuous elastic strip, and the stress fields around the crack tip were computed exactly with techniques of fracture mechanics[14].

The cracks in Fig 3 travel in lattices where the upper boundary is rigidly displaced by amounts (δ_x, δ_y), where $\delta_x/\delta_y = \tan(.073\pi)$. Fracture mechanics calculation predicts that tensile stresses are maximal at angles of $\theta = -16^\circ$ (case (A)) and $\theta = -57^\circ$ (case (B)) to the x axis. Therefore, the principle of local symmetry predicts that the crack in (A) should quickly turn and travel at an angle of -16°, and the crack in (B) should quickly turn along an angle of -57°. The arrows in Fig. 3 show these directions of crack motion as predicted by the principle of local symmetry. Stress contours, computed directly from spatial averages over interatomic forces, indeed have lobes in the directions continuum theory predicts. But the cracks do not move in these directions. Instead, they travel endlessly along the crystal planes defined by the x axis.

4. CONCLUSIONS

The calculations described here show that it is possible to have a homogeneous isotropic elastic solid where cracks are trapped along crystal planes, and cleave them rather than choosing directions that would be expected from the principle of local symmetry. This does not mean that the principle of local symmetry is always wrong; in amorphous materials where it is hard to see what else could be true, the principle of local symmetry appears to agree with experiment[15]. It seems likely that there should exist a generalization of the principle of local symmetry that uses information about the anisotropy of crystalline fracture energies to obtain an improved equation of motion. However, preliminary attempts to obtain such a rule have not been successful[16]. Thus it is not yet possible to say that the physical laws governing the direction of crack motion are understood.

5. ACKNOWLEDGEMENTS

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