action. Such experimental information would facilitate further elaboration of the simple theory described here, such as the introduction of many-body interactions or couplings to other (elastic, electronic) degrees of freedom.

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[14]In this work, "*nonpure* stage" refers to a *single-phase*, ordered, periodic sequence of layers (e.g., three empty, one filled, two empty, one filled...) and not to a *mixed* phase of pure stages.

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Computer Simulation of Crack Propagation

Arthur Paskin and A. Gohar
Queens College of the City University of New York, Flushing, New York 11367

and

G. J. Dienes
Brookhaven National Laboratory, Upton, New York 11973

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Computer simulations of crack properties were performed on a two-dimensional triangular lattice with a Lennard-Jones interatomic interaction. The use of a long-range potential and an unconstrained sample revealed novel features compared to earlier simulations. The Griffith energy treatment for fracture was found wanting. This system is brittle at low stresses in agreement with the Rice-Thomson criterion and shows dislocation formation at elevated stresses.

Brittle fracture is an important material property and yet has received relatively little attention with respect to the underlying atomic mechanisms. Indeed, it is only with the advent of modern computers that dynamic investigations became possible.[1-3] Prior to these recent developments essentially all approaches were based on continuum mechanics,[4] and elastic statics.[5] Griffith has shown how energy criteria and continuum mechanics can be combined to yield a critical

stress for crack propagation. The Griffith criterion for the initiation of crack motion is derived from conservation-of-energy concepts with the additional key assumption that the change in elastic energy is equal to half of the external work done as the crack moves. The crack may propagate in a brittle or ductile manner. Rice and Thomson[6] have derived criteria for brittle fracture in terms of dislocation emission. Computer simulation of the atomic responses permits one to investigate systematically the above criteria. Our dynamic simulation studies were performed at constant applied load on an unconstrained two-dimensional triangular lattice using the Lennard-Jones potential for the interatomic interaction. The main difference between ours and earlier dynamic calculations is that the external surfaces along and perpendicular to the crack are free to move and thus there are no boundary restrictions on dislocation motion.

Our system consists of a triangular array of 5284 atoms arranged in 39 rows, as shown in Fig. 1(a). The mirror symmetry about the central vertical axis is used to reduce the computation. The 6-12 Lennard-Jones potential, in the form

$$\varphi_{ij}(r_{ij}) = \epsilon[(d/r_{ij})^{12} - 2(d/r_{ij})^{6}]$$

with all energies measured in units of ϵ and distances in units of the equilibrium spacing d, was used to calculate the forces between atoms which are initially near neighbors. Subsequent to the introduction of the crack (which can produce considerable atomic displacements and local structural deformation) forces are calculated between all atoms that are within 1.6 times the original near-neighbor distance, i.e., $1.6d$ is the "searching range" for the force calculation. This is well beyond the maximum force (at $1.11d$) and is slightly less than the second-neighbor equilibrium distance. Further, when the nth bond is stretched to $1.11d$ the $(n-1)$th bond is still within the range of the potential. The molecular dynamic properties of the crack behavior are studied by solving Newton's equation using the Verlet scheme.[7] The atomic positions, velocities, and forces as well as the total energy, work, potential energy, and modulus of elasticity were monitored throughout the calculations. The time step in the calculation was chosen to give one part in 10^6 accuracy in the energy.

In these calculations the system was brought to equilibrium under a given constant external force, σ (in units of ϵ/d), before the crack was inserted (see Fig. 1). The external force is applied to the individual atoms of the uppermost row and the lowermost row. All external boundaries were free to move. Equilibrium at zero temperature was obtained by inserting critical damping into the equations of motion. A crack was created by cutting[1,2] the bonds between a given number of atoms in the 19th and 20th rows, i.e., the interatomic potential for these atoms was set at zero. These conditions correspond to the insertion of a very thin knife to create the crack. There was no damping subsequent to the creation of the crack. Consequently, the system acquired some kinetic energy which was also monitored. The long range of the potential, the boundary conditions, and the continuous monitoring of the atoms within the searching range regardless of their

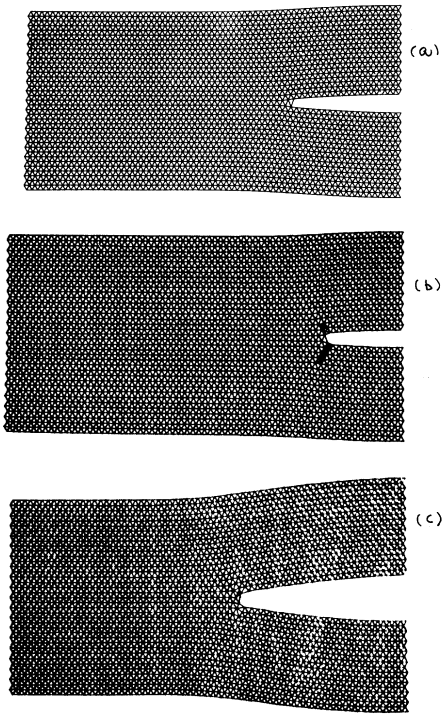

FIG. 1. A two-dimensional triangular lattice with a crack. Because of mirror symmetry the entire sample can be obtained by reflection about the right-hand side of this figure. Forces are applied to atoms in the 1st and 39th rows (applied σ). Lines are drawn between atoms that are less than $1.6d$ apart. (a) Clean brittle fracture at $\sigma = 0.5$ and $L_0 = 39$ (L_0 is the number of initially broken bonds for the half sample). (b) Incipient dislocation formation at $\sigma = 1.3$ and $L_0 = 19$. The extra lines designate the atoms that have moved into the range of interaction. (c) Dislocation formed at the lower end of the crack tip at $\sigma = 1.3$ and $L_0 = 39$. This dislocation later on propagated to the surface.

original position allowed the system to deform freely.

As the crack moves under a constant load, applied to both horizontal surfaces, conservation of energy requires that

$$\Delta W = \Delta E_p + \Delta E_k = \Delta E_e + \Delta E_s + \Delta E_k , \quad (1)$$

where ΔW is the work done on the sample as the crack moves, ΔE_p is the change in total potential energy, ΔE_k is the change in total kinetic energy, ΔE_e is the change in strain energy, and ΔE_s is the change in surface energy of the crack. Conservation of energy was always obeyed in our simulations. ΔE_e is evaluated as $\Delta E_p - \Delta E_s$, where ΔE_s is taken as two bond energies per pair of interacting atoms, i.e., the depth of the Lennard-Jones potential, ϵ, per atom. In the Griffith energy treatment ΔE_k is zero. In order to obtain a quantitative criterion for the stress using Eq. (1) it is necessary to have a relation between ΔW and ΔE_e. If one assumes macroscopic linear elasticity, $\Delta E_e = \frac{1}{2}\Delta W$, and therefore, $\Delta E_e = \Delta E_s$ which is the basic Griffith energy criterion. In order to obtain the critical stress Griffith used the Inglis elastic continuum calculation for ΔE_e.[4]

In the first part of our analysis we concentrate on the validity of the basic energy criterion under constant load conditions. In Fig. 2, ΔW, ΔE_s, ΔE_e, and ΔE_k are plotted versus the relative increase in crack length, $(L - L_0)/L_0$, for two computer simulations at different loads and initial crack lengths. These energy changes were evaluated in the region of early crack motion where ΔE_k is approximately zero and, thus, a direct comparison can be made with the Griffith energy assumption. In these computer simulations $\Delta E_e/\Delta W$ varies all the way from zero ($\sigma = 0.5$, large crack) to 0.75 ($\sigma = 1.3$, medium crack). While one might say that the Griffith energy criterion ($\Delta E_e/\Delta W = 0.5$) is approximately true for the latter, clearly the case of zero initial change in strain energy indicates failure of the elastic mode of brittle fracture. As a matter of fact, the negligible change in strain energy suggests that a rigid tearing mode is a better description of such a fracture. This fracture ($\sigma = 0.5$) exhibited no dislocation formation or bifurcation and was the cleanest example of brittle fracture in our simulations [Fig. 1(a)]. Further, the failure of the Griffith energy criterion for the large crack does not seem to result from a simulation artifact. The Griffith energy criterion was approximately obeyed for the same size crack at a stress about 2.2 times larger. One can estimate

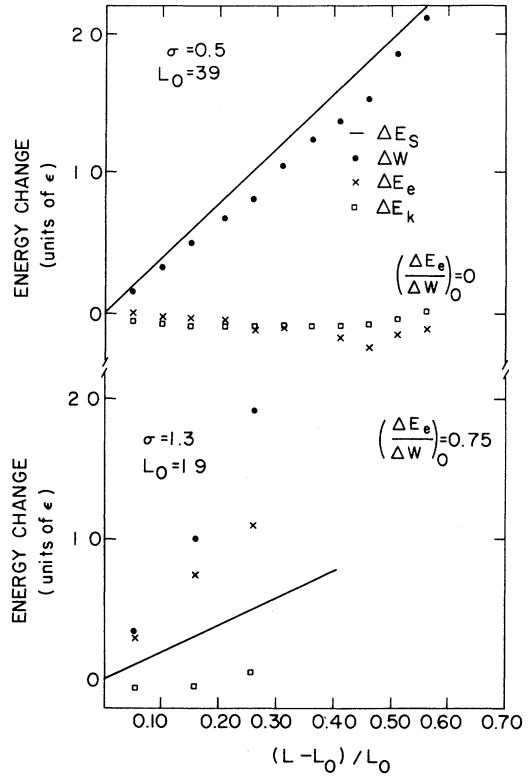

FIG. 2. Changes in energy components as a function of fractional increase in crack length during crack propagation. σ is the applied force (0.5 in the upper figure, 1.3 in the lower) and L_0 is the number of initially broken bonds for the half sample (39 in the upper figure, 19 in the lower). The energy components are ΔW, circles; ΔE_e, crosses; ΔE_k, squares; and ΔE_s as defined in Eq. (1), solid curves.

the critical stress, σ_c, for such a tearing mode of crack propagation by assuming rigid propagation of the changing crack shape to the boundary in calculating ΔW. If all of this work, rather than one half, goes into surface energy, σ_c turns out to be of the same functional form as the Griffith σ_c but is lower by a factor of $\sqrt{2}$. This simple estimate yields, using an effective modulus of $30\epsilon/d^2$, a $\sigma_c = 0.7\epsilon/d^2$ as compared to the simulation value of 0.5. Thus, even though the energy criterion is violated for this fracture mode, the critical stress estimate is approximately valid.

Rice and Thomson[6] consider a material to be brittle if a dislocation generated in the neighborhood of the crack tip cannot escape from the tip region. The critical distance, r_c, at which a straight dislocation is in unstable equilibrium is obtained from considering the following forces: (1) the repulsive force due to the crack stress

field, (2) the attractive image force of the dislocation in the free surface of the crack, and (3) another attractive force arising from the additional surface created by the blunted crack. If r_c is larger than the dislocation core cutoff, r_0, then the material is brittle. For our two-dimensional system application of the Rice-Thomson equations yields $r_c = 1.8d$. From Esbjorn and Jensen[8] r_0 for this system is $1.7d$. Consequently, this two-dimensional Lennard-Jones system is barely brittle according to the Rice-Thomson criterion. In our simulations we find that crack propagation in our system varies from brittle to ductile depending on the applied stress and the detailed dynamics. This suggests that the Rice-Thomson formulation has considerable quantitative validity.

These behaviors are demonstrated by examining the simulation results shown in Figs. 1(a)–1(c). Figure 1(a) represents the same simulation whose energetics are shown in Fig. 2 (top), i.e., a large initial crack with an applied σ of 0.5. This crack propagated in a clear brittle manner with very little distortion at the crack tip. Figure 1(b), corresponding to Fig. 2 (bottom), shows a crack with large directional distortions near the tip indicated by additional atom-to-atom lines connecting atoms which were originally not in range but have now come into range. Such lines of distortion, which may be considered incipient dislocations, are generated and absorbed as the crack propagates. In Fig. 1(c), a large initial crack with $\sigma = 1.3$, the crack propagated to the configuration shown. A dislocation can be seen at the lower end of the crack tip. This dislocation then propagated to the surface and bifurcation occurred. Raising the stress of the crack of Fig. 1(b) to $\sigma = 3.0$ resulted in the immediate formation of dislocations and the subsequent blunting of the tip, i.e., ductile behavior.

These results are in accord with more detailed considerations of the role of the crack tip force in the Rice-Thomson formulation. An increase in the crack tip stress along the slip direction at about $1.7d$ from the tip means that dislocations are more strongly repelled. The attractive dislocation forces are not expected to depend on the applied load or the crack tip velocity. An increase in the crack repulsion force on the dislocation with constant attractive terms favors dislocation generation. A detailed analysis of our simulation data for propagating cracks shows that the stresses along the slip direction at about $1.7d$ increase as a function of increased applied load and increased crack velocity. The velocity dependence results are in accord with earlier continuum mechanical calculations which are used to explain bifurcation.[4] As the applied load is increased above critical, it is not surprising that the stress at a distance from the crack tip increases. Including this stress dependence in the Rice-Thomson formulation, it is found that r_c is approximately proportional to $(\sigma_c/\sigma)^2$ and thus high applied loads, σ, should reduce r_c and produce a tendency towards dislocation emission. As our material is barely brittle at low stresses and low crack velocities, it is not surprising to find dislocation formation and ductility at high applied loads and large crack velocities.

In addition to the results reported here we observe a number of other dynamic and static crack characteristics.[9] For example, the dynamic and static stress profiles at or below the critical stress are similar to one another as well as to the ones obtained by Sinclair in static simulations.[10,11] Further, in an equilibrium simulation achieved by damping, which corresponds to a static simulation, the work done by the applied loads at a $\sigma = 0.5$ after crack creation was 2.1 times the strain potential energy, as expected from linear elasticity theory.[4] This differs drastically from the dynamic behavior. Details will be published elsewhere.

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