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CONTINUUM AND ATOMISTIC STUDIES OF INTERSONIC CRACK PROPAGATION

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ABSTRACT

Mechanisms of intersonic crack propagation along a weak interface under shear dominated loading are studied by both molecular dynamics and continuum elastodynamics methods. Part of the objective is to test if continuum theory can accurately predict the critical time and length scales observed in molecular dynamics simulations. To facilitate the continuum-atomistic linkage, the problem is selected such that a block of linearly isotropic, plane-stress elastic solid consisting of a two-dimensional triangular atomic lattice with pair interatomic potential is loaded by constant shear velocities along the boundary. A pre-existing notch is introduced to represent an initial crack which starts to grow at a critical time after the loading process begins. We observe that the crack quickly accelerates to the Rayleigh wave speed and, after propagating at this speed for a short time period, nucleates an intersonic daughter crack which jumps to the longitudinal wave speed. The daughter crack emerges at a distance ahead of the mother crack. The challenge here is to test if a continuum elastodynamics analysis of the same problem can correctly predict the length and time scales observed in the molecular dynamics simulations. We make two assumptions in the continuum analysis. First, the crack initiation is assumed to be governed by the Griffith criterion. Second, the nucleation of the daughter crack is assumed to be governed by a peak of shear stress ahead of the crack tip reaching the cohesive strength of the interface. Material properties such as elastic constants, fracture surface energy and cohesive strength are determined from the interatomic potential. Under these assumptions, it is shown that the predictions based on the continuum analysis agree remarkably well with the simulation results.

KEYWORDS

Continuum, Atomistic Models, Intersonic Crack Propagation

INTRODUCTION

This paper is a study of intersonic crack dynamics using both atomistic and continuum methods, with emphasis on the linkage between "mechanics" and "physics" modeling of fracture. Continuum mechanics is limited by its coarse view of physical phenomena and various assumptions adopted in its constitutive laws. On the other hand, atomistic methods, such as molecular dynamics (MD), is limited not just by the large number of degrees of freedom involved but also the time scale. There are only a few classes of problems to which

continuum and atomistic approaches can both be applied and the results directly compared. One of such problems is the simulation of dynamic crack propagation in a nanometer size crystal. The system is large enough for the continuum methods of dynamic fracture mechanics [1,2] to be applicable. On the other hand, the emergence of large scale parallel computers have also allowed MD simulations of crack propagation for system sizes reaching 1 billion atoms and time scales approaching nanoseconds [3]. Atomistic simulations provide an ab initio investigation of fracture by which the validity of continuum methods can be tested. Continuum mechanics analysis provides a conceptual framework in which MD simulation data can be analyzed and understood. It is in this spirit that we conduct a joint continuum and atomistic investigation of intersonic crack propagation along a weak interface.

Our present study is motivated by recent experiments on intersonic crack propagation by Rosakis et al. [4] who investigated shear dominated crack growth along weak planes in a brittle polyester resin under far field asymmetrical loading. They observed crack propagation as fast as the longitudinal wave speed. This experiment is interesting because it has been widely believed that a brittle crack cannot propagate faster than the Rayleigh wave speed. The origin for this belief stems from the vanishing of crack tip energy release rate and stress singularity at the Rayleigh wave speed predicted by continuum mechanics. The late arrival of laboratory experiments on intersonic fracture [4] is due, in part, to the fact that a crack in elastic homogeneous and isotropic solids always kinks or branches out, deviating from the initial crack plane and having a zigzag crack path, once the crack tip velocity exceeds only 0.3 ~ 0.4 of the shear wave speed [1, 5, 6]. A wavy crack instability occurs at low crack velocities and prevents an exploration of the full range of possible velocities. In fact, the only possibility of attaining intersonic crack propagation is to introduce a weak path (a layer of lower toughness) so that crack growth is confined to this path. Although the experiments of Rosakis et al. [4] have shown convincingly that a shear dominated crack can propagate with velocity up to the longitudinal wave speed, the question of whether such a crack has been accelerated from a subsonic crack or is nucleated directly as an intersonic crack has not been fully resolved by experiments.

A two-dimensional MD simulation was conducted to investigate the mechanisms of shear crack propagation along a weak interface joining two harmonic crystals [7]. The atomic bonds of the harmonic crystals are characterized by the harmonic interatomic potential with infinite cohesive strength. Crack propagation is forced to propagate along the interface which is characterized by the Lennard-Jones (LJ) potential. The two-dimensional crystal with pair interatomic potential assumes a triangular atomic lattice and behaves as a linear elastic isotropic sheet deforming under plane-stress conditions. Loaded by linearly increasing shear displacements along the boundary of the simulation block, a pre-existing notch is introduced to represent an initial crack which starts to grow at a critical time after the loading process begins. The main results in [7] can be briefly summarized as follows. A mode I crack never exceeds the Rayleigh wave speed. In comparison, a mode II crack initiates at a critical load level and accelerates very quickly to the Rayleigh wave speed. It travels at the Rayleigh speed for a short while and nucleates an intersonic daughter crack ahead of its tip. The daughter crack propagates near the longitudinal wave speed.

The objective of this paper is to test if continuum theory can accurately predict the critical time and length scales observed in molecular dynamics simulations [7]. We apply the dynamic elasticity methods [1] to solve the crack propagation problem subject to identical geometry and loading conditions in the molecular dynamics simulation. We determine material properties including Young's modulus, Poisson ratio, wave speeds, surface energy and cohesive strength from the interatomic potentials used in the atomic simulation. This precise knowledge of material properties allow us to use the simulation results to test the validity of continuum theories of fracture. We make two assumptions in the continuum analysis. First, the crack initiation is assumed to be governed by the Griffith criterion.

Second, the nucleation of the daughter crack is assumed to be governed by a peak stress ahead of the crack tip reaching the cohesive strength of the interface. Under these assumptions, we show that the predictions based on the continuum analysis agree remarkably well with the atomic simulation results.

ATOMIC SIMULATION RESULTS

The atomic simulation of intersonic shear fracture is based on molecular dynamics which is a computational method [8, 9] for predicting the motion of a given number of atoms by numerically integrating Newton's law for each atom. In the MD simulation, the mutual interactions among atoms are described by a continuous potential function. The details of MD simulations of intersonic shear fracture can be found in [7]. Here we briefly discuss the most relevant results that will be compared to the continuum analysis.

In accordance with the objective of studying crack propagation along a weak interface in a linear elastic isotropic solid, we consider a two-dimensional atomic lattice characterized by a pair potential. Atoms across a weak interface line are assumed to interact according to the LJ potential, $\varphi = 4\left(r^{-12} - r^{-6}\right)$. All results are expressed in terms of reduced units: lengths are scaled by the value of the interatomic separation for which the LJ potential is zero, energies are scaled by the depth of the minimum of the LJ potential, and mass is scaled by the atomic mass. A cut-off distance equal to *2.5* is assumed for the LJ potential. Atoms in the adjacent crystals are assumed to interact according to the harmonic potential $\varphi = k(r-d)^2/2$, where $d = \sqrt[6]{2}$ and $k = \varphi''(d) = 72/\sqrt[3]{2}$ such that the materials are elastically homogeneous across the interface. We note that the harmonic crystal has infinite fracture strength due to linear interactions among nearest neighbors. The only fracture path in this linear elastic homogeneous and isotropic solid is along the interface which has a finite cohesive strength associated with the LJ potential.

The total dimension of the simulation system under study is a 2D slab of atoms with *1424* atoms along the horizontal length defining the x_1 direction and with *712* atoms along the vertical length defining the x_2 direction. A horizontal slit of *200*-atom distance is cut midway along the left-hand vertical slab boundary. The 2D crystal has a triangular lattice with the slit parallel to the close packed direction along which atomic spacing is equal to the lattice constant $\sqrt[6]{2}$. To study a shear dominated crack, a shear strain rate of *0.00025* and a tensile strain rate of *0.00005* are imposed on the outer most rows of atoms defining the opposing horizontal faces of the two-dimensional slab. The crack is of mixed mode but dominantly shear. Linear velocity gradients are established across the slab initially. Then the loading process proceeds with constant shear and tensile velocities along the boundary, which leads to eventual failure of the material at the slit tip. The applied strain rates remain constant during the simulation, and the simulation is continued until the growing crack has traversed the total length of the slab. Simulations of a mode I crack is conducted with the same geometrical setup except only an opening strain rate is imposed.

The mode I crack in the atomistic simulations (Abraham and Gao, 2000) quickly approaches a constant velocity equal to the Rayleigh wave speed *4.83* of the harmonic crystal, which shows that the crack velocity is limited by the Rayleigh wave speed, consistent with the classical theories of fracture. The mode II crack initiates at a critical time estimated to be *65* and quickly approaches the Rayleigh wave speed of the harmonic solid. After propagating at the Rayleigh wave speed for a short while, the crack tip jumps to the longitudinal sound speed calculated to be *9*. The time for this velocity jump is estimated to be around *140*.

The mechanism for the mode II crack "jumping" over the forbidden velocity zone is the nucleation of an intersonic daughter crack ahead of the mother crack travelling at the

Rayleigh wave speed [7]. A sharp intersonic crack is nucleated at a small distance estimated to be around *22* ahead of the mother crack. Transverse Mach cones near the daughter crack are observed in atomistic simulations, and the angle of the Mach cone shows that the velocity of the daughter crack is consistent with the longitudinal wave speed. As the daughter crack moves ahead, the mother crack trails behind at the Rayleigh wave speed. The MD simulations demonstrate intersonic crack propagation and the existence of a "mother"-"daughter" crack mechanism for a subsonic shear crack to jump over the forbidden velocity zone. This mechanism is reminiscent of the mechanism of Burridge [10] and Andrews [11] based on continuum theories, although the continuum description cannot provide an ab initio description for crack formation. The birth of the daughter crack cannot be characterized by a critical energy release rate or a critical stress intensity factor near the mother crack because both these quantities vanish at the Rayleigh wave speed. It seems that the only possible mechanism by which the daughter crack can be nucleated is by the finite stress peak ahead of the mother crack and along the weak bonding line, as measured in the stress field and discussed by Burridge [10].

MATERIAL PROPERTIES

Material properties of importance to continuum descriptions of fracture include the elastic moduli, elastic wave speeds, surface energy and cohesive strength. In comparison with a laboratory fracture experiment, atomistic simulations have the advantage of providing a precise knowledge of these material properties from the interatomic potential.

A two dimensional triangular lattice behaves as a plane stress elastic sheet with the shear modulus $\mu = \sqrt{3}k/4$, Young's modulus $E = 2k/\sqrt{3}$, and Poisson's ratio $\nu = 1/3$ [12]. With the atomic mass taken as the unit of mass, the triangular lattice has density $\rho = \sqrt[3]{4}/\sqrt{3}$. The longitudinal, shear and Rayleigh wave speeds are $c_d = 9$, $c_s = 5.20$, and $c_R = 4.83$, respectively.

The fracture surface energy of the material is defined as the energy consumed in breaking atomic bonds as crack grows. For the MD simulations described in section 2, the crack is parallel to the close packed direction and atoms across the interface interact according to the LJ potential with a cut-off distance equal to *2.5*. Accounting for all the atomic interactions, four atomic bonds (2 between nearest neighbors and 2 between next nearest neighbors) are snapped per atom in the fracture process. The fracture surface energy is defined as half of the energy stored in these bonds and is equal to $\gamma = 0.956$ [12].

The cohesive strength of the weak interface under shear dominated loading is calculated as follows [13]. The cohesive failure of a single atomic bond is defined as the state when the interactive force between two atoms reach the maximum, which corresponds to $\varphi''(d_m) = 0$ and $d_m = \sqrt[6]{26/7}$ is the critical bond length at failure. Balance of forces parallel and normal to the interface gives the relation $\tau_{int} + 0.577\sigma_{int} = 2.04$ between shear and normal stresses along the interface at the cohesive limit, which is the cohesive strength criterion and has a strong coupling between shear and tensile stresses.

CONTINUUM ANALYSIS OF CRACK INITIATION AND PROPAGATION

The aforementioned entire process of crack initiation and propagation is studied via a transient, continuum analysis of dynamic fracture [13]. It is shown that the continuum analysis, in conjunction with the Griffith criterion, can determine the critical time for crack initiation rather accurately. The location and time at which the daughter crack is nucleated

are also determined rather accurately by the continuum analysis, together with a cohesive strength criterion.

An infinite plane-stress solid containing a semi-infinite crack on the negative x_1 axis is subjected to constant remote shear stress rate $\dot{\tau}_0$ and tensile stress rate $\dot{\sigma}_0$ normal to the crack. Consistent with the atomistic simulations, an initial velocity field at time $t = 0$ corresponding to the constant remote stress rates is imposed such that there are no waves coming from the remote field. The deformation field can be decomposed into the following two sub-problems. First, a uniform deformation field corresponding to constant shear stress-rate $\dot{\tau}_0$ and normal stress-rate $\dot{\sigma}_0$ in the same solid but without the crack; the initial velocity field is consistent with $\dot{\tau}_0$ and $\dot{\sigma}_0$ such that there are no waves from the remote field. The second sub-problem has constant shear and normal traction-rates, $\dot{\tau}_0$ and $\dot{\sigma}_0$, imposed on the entire crack faces (including the new ones generated by crack propagation) in order to negate the crack-face tractions from the first sub-problem. There is no initial velocity field. The crack tip remains stationary until a critical time, $t = t_{init}$, is reached at which the Griffith criterion is met. The crack tip then propagates in the crack plane at the Rayleigh wave speed c_R, consistent with the atomistic simulation discussed in section 2. It should be pointed out that stresses are indeed not singular near a crack tip propagating at the Rayleigh wave speed c_R. Instead, the shear stress has a peak that occurs at a finite distance ahead of the crack tip. Once the peak stress reaches the cohesive strength of the solid, the daughter crack is nucleated.

Griffith Criterion and Crack Initiation

We study first the critical time for crack initiation, $t = t_{init}$, at which the macroscopic crack tip starts to propagate. The plane-stress crack tip energy release rate for a stationary crack subjected to constant remote shear and normal traction-rates $\dot{\tau}_0$ and $\dot{\sigma}_0$ on the crack faces are given in [1]. The Griffith criterion predicts that the crack tip starts to propagate when the crack tip energy release rate reaches twice the surface energy, 2γ, which gives the critical time for crack initiation. Using the shear and normal strain rates in the atomistic studies given in section 2 as well as the elastic constants, wave speeds and fracture surface energy in section 3, we find that the critical time for crack initiation predicted by the continuum elasticity is $t_{init} = 70.3$ in the reduced unit, which is in good agreement with the corresponding result of *65* in the MD simulations. This analysis indicates that the Griffith criterion holds even down to the atomic scale.

Cohesive Strength Criterion and the Nucleation of Daughter Crack

The continuum analysis becomes much more difficult after the crack tip propagates at the Rayleigh wave speed c_R after time $t = t_{init}$. We follow the same method developed by Freund (1990) to solve this fully transient dynamic fracture problem involving both the dynamic crack-face loadings and the crack propagation. We skip details of the solution and present only the shear stress relevant to the nucleation of daughter crack. The shear stress has a very sharp peak at the shear wave front ahead of the moving the crack tip. This maximum shear and normal stresses have been determined in terms of the applied load, time, as well as the elastic constants and wave speeds. Using the cohesive strength criterion in section 3, we have determined the critical time and location for the nucleation of the daughter crack. For the material properties given in section 3 and the imposed strain rates in atomistic simulations (section 2), we find the critical time for the nucleation of the daughter crack predicted by classical elasticity is $t_{nucl} = 120$ in the reduced unit, which is in reasonable agreement with the counterpart of *140* in atomistic simulations. The corresponding location at which the daughter crack is nucleated ahead of the moving crack tip is the shear wave front and is found to be *18.2* in the reduced unit, which is once again in reasonable agreement with the estimate of *22* from atomistic simulations. This indicates that the

cohesive strength criterion seems to govern the nucleation of the daughter crack even down to the atomic scale, leading to intersonic crack propagation.

CONCLUSIONS

We have studied intersonic shear crack propagation along a weak interface by both molecular dynamics and continuum elastodynamics. The problem selected is a block of linearly isotropic, plane-stress elastic solid consisting of a two-dimensional triangular atomic lattice with pair interatomic potential loaded by constant shearing velocity along the boundary. The fracture process revealed by MD simulations shows the following sequence of events. The initial crack starts to grow at a critical time after the loading process begins. It quickly accelerates to the Rayleigh wave speed and, after propagating at this speed for a short time period, nucleates an intersonic daughter crack which immediately jumps to the longitudinal wave speed. The daughter crack emerges at a critical distance ahead of the mother crack. We solve the continuum elastodynamic problem of the same crack geometry under the same loading history to test if the continuum analysis can correctly predict the length and time scales observed in the atomic simulations. We assume that the crack initiation is governed by the Griffith criterion while the nucleation of the daughter crack is governed by the Burridge-Andrew mechanism of cohesive failure by a peak of shear stress ahead of the crack tip. We determine material properties including elastic constants, elastic wave speeds, fracture surface energy and cohesive strength from the interatomic potential used in the atomic simulations.

The critical time for initial crack growth predicted by the continuum elastodynamics and the Griffith criterion agrees with the atomistic simulation results within *10%*. Also, we find remarkably good agreement between continuum analysis and atomic simulations for the time and location of the nucleation of the daughter crack. From this comparison, we conclude that continuum mechanics can provides not only qualitatively useful insights into the mechanisms of intersonic shear crack propagation, but also gives quantitatively correct predictions for the times and locations of critical atomistic events. Effective linking between continuum and atomistic methods is expected to be a powerful way of studying a wide variety of nanoscale dynamic phenomena.

REFERENCES

1. Freund, L.B. (1990). *Dynamic Fracture Mechanics*. Cambridge University Press, Cambridge, England.
2. Broberg, K.B. (1999). *Cracks and Fracture*. Academic Press, San Diego.
3. Abraham, F.F., Brodbeck, D., Rudge, W.E., Broughton, J.Q., Schneider, D., Land, B., Lifka, D., Gerner, J., Rosenkrantz, M., Skovira, J. and Gao, H. (1998). *Modeling and Simulation in Materials Science and Engineering* 6, 639.
4. Rosakis, A.J., Samudrala, O. and Coker, D. (1999). *Science* 284, 1337.
5. Gao, H. (1993). *J. Mech. Phys. Solids* 41, 457.
6. Abraham, F.F., Brodbeck, D., Rafey, R.A. and Rudge, W.E. (1994). *Phys. Rev. Lett.* 73, 272.
7. Abraham, F. F. and Gao, H. (2000). *Phys. Rev. Lett.* 84, 3113.
8. Abraham, F.F. (1986) *Adv. Phys.* 35, 1.
9. Hoover, W.G. (1986). *Molecular Dynamics*. Springer-Verlag, Berlin.
10. Burridge, R. (1973). *Geophysical J. of the Royal Astronomical Soc.* 35, 439.
11. Andrews, D.J. (1976). *J. Geophys. Res.* 81, 5679.
12. Gao, H. (1996). *J. Mech. Phys. Solids* 44, 1453.
13. Gao, H., Huang, Y. and Abraham F.F. (2001). Continuum and atomistic studies of intersonic crack propagation. *J. Mech. Phys. Solids* (in the press).