CONTINUUM AND ATOMISTIC MODELING OF DYNAMIC FRACTURE AT NANOSCALE

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ABSTRACT

Crack branching and instability phenomena are believed to be closely related to the circumferential or hoop stress in the vicinity of the crack tip. In this paper we show that the hoop stress around a mode I crack in a harmonic solid becomes bimodal at a critical speed of about 73 percent of the Rayleigh speed, in agreement with the continuum mechanics theory. Additionally, we compare the energy flow field predicted by continuum theory with the solution of molecular-dynamics simulations and show that the two approaches yield comparable results for the dynamic Poynting vector field. This study exemplifies joint atomistic and continuum modeling of nanoscale dynamic systems and yields insight into coupling of the atomistic scale with continuum mechanics concepts.

1. INTRODUCTION

Many phenomena associated with rapidly propagating cracks are not thoroughly understood. Experimental work [1-3] and computer simulations [4] as well as theoretical investigations [5] have shown that initially straight cracks start to become unstable upon a critical speed of about 30 percent of their limiting speed, the Rayleigh velocity [6]. In contrast, it was proposed based on the linear elastic continuum theory that cracks become unstable at about 73 percent of the Rayleigh speed (speed of surface waves) [6, 7].

Up to date, it remains unclear what is the governing stress measure governing branching and crack instabilities at the atomic scale. Continuum formulations often use a material instability criterion similar to the principal stress to determine in which direction the material will fracture (e.g. [8]). It remains controversial if such a criterion can be accepted at the atomic scale, as the breaking of single atomic bonds is expected to govern the dynamics of cracks. Yoffe [7] proposed that crack propagation should become unstable when the circumferential or hoop stress near a crack tip has a maximum at angles off the propagation direction. She showed that for low velocities, the hoop stress has a maximum ahead of the crack tip, but for velocities larger than about 73 percent of the Rayleigh speed, the hoop stress maximum is at off-angles of about 60 degrees, potentially causing the crack to change direction.

Atomistic simulations can successfully address many issues of dynamic fracture by providing an *ab initio* description of the fracture process [4, 9-12]. Here we use large-scale atomistic simulations to study the near-crack elastic fields in mode I dynamic fracture and to compare the discrete atomistic and the continuum mechanics viewpoints. The studies reported here are the first in a series of computer experiments where the crack instability is investigated. The main objective of this work is to show that the continuum mechanics prediction of a bimodal hoop stress field is reproduced quantitatively in molecular dynamics (MD) simulations. Since we focus on the deformation field near rapidly propagating cracks even beyond the instability speed, we constrain the crack to propagate along a one-dimensional prescribed fracture path modeled by a weak Lennard-Jones cohesive bonding. In the rest of the slab, atomic bonds are described by a harmonic potential and never break.

The plan of this paper is as follows. We start with an elastic analysis of a Lennard-Jones lattice as well as a harmonic lattice. We then show that in MD simulations of cracks traveling in perfect harmonic lattices the hoop stress becomes bimodal at about 73 percent of Rayleigh speed, in agreement with the continuum theory. In addition, we report comparison of continuum theory with MD simulation of the strain energy field near the crack tip as well as the energy transport field near rapidly moving cracks.

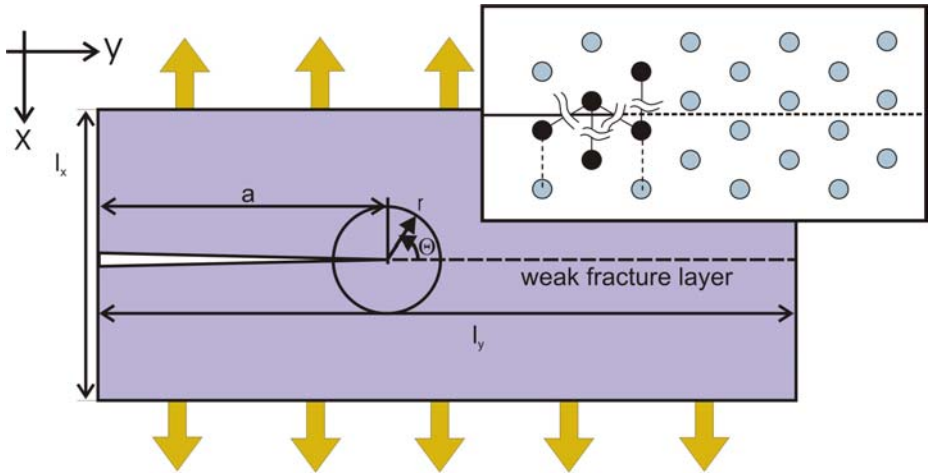

Figure 1: Geometry of the simulation slab under mode I loading. The plot also depicts the crack orientation and the bond breaking process at the crack tip.

2. ATOMISTIC MODELING

Recent two decades have witnessed increasing research on MD simulations in materials science. Using huge supercomputers to break tiny nano-crystals has become an unforeseen fruitful combination. [4, 9-12]. The success of atomistic simulations of brittle fracture is partly due to the fact that the time and length scales involved in brittle dynamic fracture is perfectly suitable for MD simulations. Fracture is a process occurring on the order of sound speeds and a crack moves through a crystal with nanometer dimensions in a few picoseconds.

The basis of our simulations is the atomic interactions of a simple rare-gas solid accurately described by the Lennard-Jones 12:6 (LJ) potential. All quantities are expressed in reduced units. Lengths are scaled by the LJ-parameter σ=1, and energies are scaled by the parameter ε=0 which is the depth of the minimum of the LJ potential. The mass of each particle is m=1. Such a two-dimensional lattice behaves as a brittle solid [4].

The LJ potential is highly nonlinear [4, 5]. To rule out nonlinear effects, we linearize the LJ potential around the equilibrium distance $r_0 = 2^{1/6} \approx 1.12246$ and define a harmonic potential

$$\phi(r) = a_0 + \tfrac{1}{2} k(r - r_0)^2 \tag{1}$$

with spring constant k=72/$2^{1/3}$ ≈ 57.15 and $a_0 = -1$.

To avoid crack branching or wiggling [4, 5], we constrain the crack to propagate along a one-dimensional fracture path. The slab geometry and orientation of the two-dimensional hexagonal lattice is shown in Figure 1. To apply loading to the system, we displace the outermost

rows of atoms in the slab according to a prescribed strain rate $\dot{\varepsilon} = 0.00001$ and establish an initial linear velocity gradient in the slab. Note that the strain rate is given in reduced units defined by the LJ potential. Boundaries are held fixed at their current position to stop loading. The interactions across the weak layer are defined by the LJ potential, while the potential is defined by equation (1) in the rest of the slab. A horizontal slit is cut midway along the left-hand vertical slab boundary, serving as a source for further crack extension. The crack is oriented orthogonal to the close-packed direction of the triangular lattice, and the slab is initialized with a temperature T ≈ 0 K.

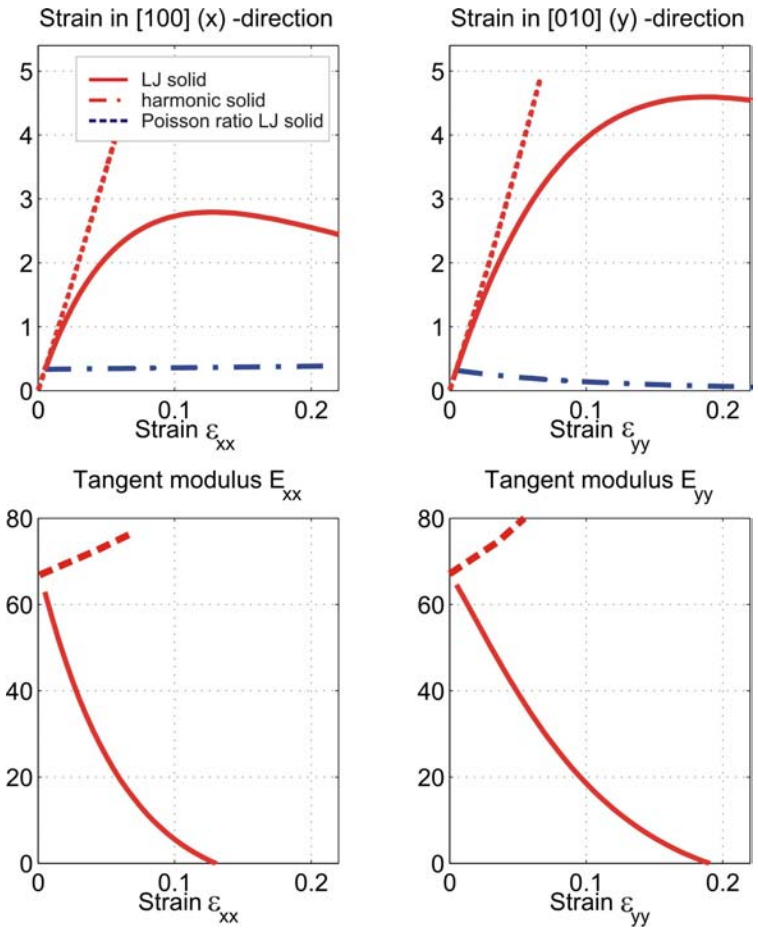

Figure 2: The continuous lines show the elastic properties of the Lennard-Jones solid. The dashed lines show the elastic properties associated with the harmonic potential. The dash-dotted lines in the upper plots show Poisson's ratio.

Figure 2 shows numerical estimates of the elastic properties of a Lennard-Jones solid, where the elastic properties of the harmonic interactions are also included. The systems are loaded uniaxially in the two symmetry directions of the triangular lattice. The plot of the LJ system shows that the *y* direction requires a higher breaking strain than in the *x* direction (about 18 percent versus 12 percent). The tangent Young's modulus drops significantly from around 66 for small strain until it reaches zero when the solid fails. Poisson ratio remains around 1/3, but increases slightly when

loaded in the x direction and decreases slightly when loaded in the orthogonal direction. The Young's modulus E with harmonic interactions increases with strain, and coincides with the value of the LJ solid for small strains. It can also be shown that the harmonic solid is isotropic for small strains, with Poisson's ratio close to 1/3 similar to the LJ solid.

Exact knowledge of the elastic properties (see further details in [8]) allows calculating the wave speeds, which will be critical in comparing the deformation field near the moving crack tip to the continuum theory prediction. The Ralyeigh-wave speed is found to be c_R=4.8, the longitudinal wave speed is found c_l=9 and the shear wave speed is determined to be c_s=5.2.

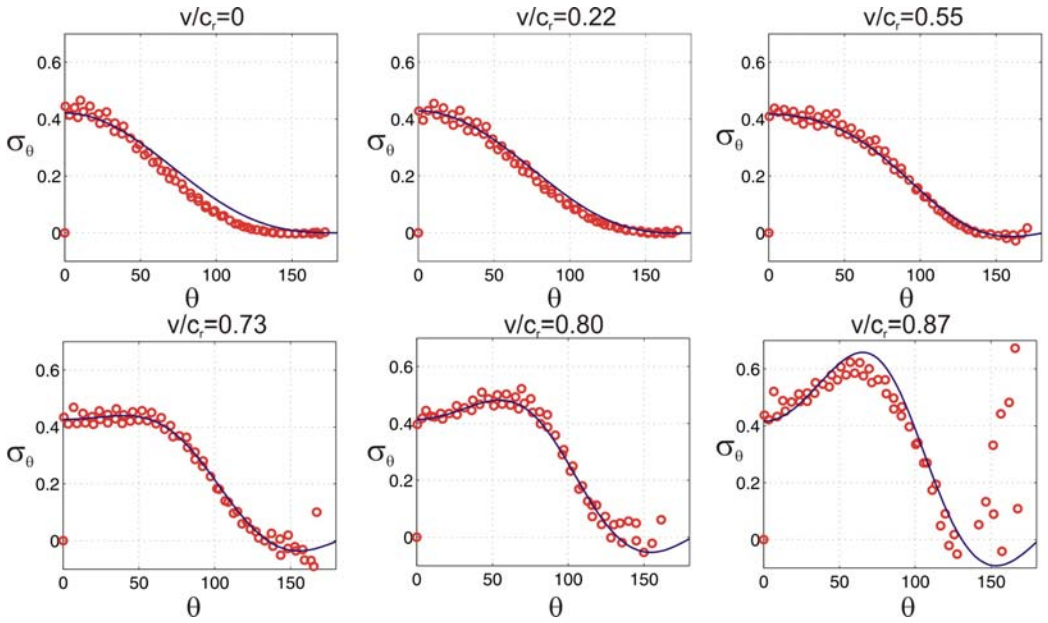

Figure 3: Comparison between hoop stress from MD simulation with harmonic potential (dots) and the prediction of the continuum mechanics theory (continuous line). The crack speed with respect to the Rayleigh velocity is indicated in each subplot.

3. HOOP STRESS FIELD AND DYNAMIC INSTABILITY DURING CRACK ACCELERATION

We calculate the hoop stress field for different crack speeds ranging from 0 to 87 percent of the Rayleigh speed. Figure 3 shows the angular variation of the hoop stress σ_θ, comparing the MD results (dots) with the continuum theory prediction (continuous line). The results show reasonable agreement of the continuum theory prediction [6] and the MD simulation results. The most important observation is that once the crack speed exceeds a critical value of about 73 percent of the limiting Rayleigh-wave speed, the hoop stress maximum shifts from 0 degrees to about 60 degrees, in agreement with continuum theory [6, 7].

In the next step, we wish to focus on the dynamics of cracks in homogeneous materials. Therefore, we relieve the constraint of the weak path. Figure 4 shows a crack moving in a harmonic lattice with snapping bonds along the direction of lowest fracture surface energy, the stable crack propagation direction. The most important result is that the crack initially propagates straight with perfect cleavage where the crack faces are atomically flat. At a velocity of about 73

percent of Rayleigh-wave speed, the crack starts to oscillate and the crack surface roughens. This leads to significantly reduced propagating speeds. Comparing this result to the predictions by the continuum mechanics theories [6, 7], we find good agreement! The analysis of the hoop stress shown in Figure 3 revealed that the hoop stress becomes bimodal upon a critical speed of about 73 percent of Rayleigh-wave speed. An important observation is that at onset of instability, the crack branches at an angle of 60 degrees. Since the hoop stress maximum is at about ±60 degrees, this observation corroborates the notion that the hoop stress governs the instability in harmonic systems!

4. DISCUSSION AND CONCLUSION

In summary, we have shown that the instability speed in harmonic lattices agrees reasonably well with the prediction by linear elastic fracture theory. The observation of branching at an angle of 60 degrees supports the notion that the hoop stress governs this mechanism. We have further exemplified how a systematic comparison of continuum mechanics theories and atomistic viewpoints can be performed. Such studies may be critical in investigating numerous other dynamical materials phenomena at small scales.

Future investigation could focus on the effect of hyperelasticity on the dynamic crack tip instability. Preliminary results suggest that hyperelastic stiffening materials yield an increase in critical instability speed, whereas softening materials show a significant decrease in critical speed where the crack tip instability sets in. In our preliminary studies, we have observed mode I cracks moving mirror-like up to super-Rayleigh speeds, provided that the material is hyperelastic and stiffens with strain. This suggests that hyperelasticity is critical for dynamic fracture, as proposed earlier [12].

5. ACKNOWLEDGMENTS

Most of the simulations were carried out in the Garching Supercomputer Center of the Max Planck Society, we gratefully acknowledge their support.

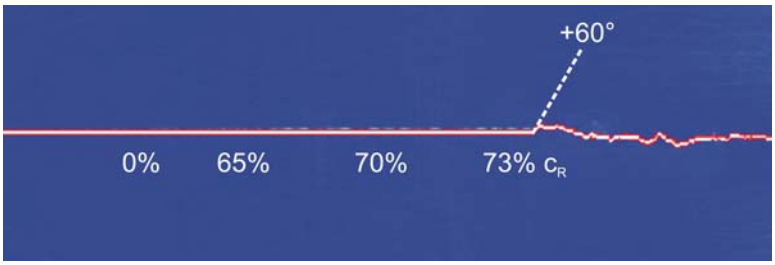

Figure 4: Dynamic crack tip instabilities harmonic system (potential energy indicating the crack surface by the red color). The results illustrate that the crack becomes unstable at about 73 percent of the Rayleigh-wave speed, in agreement with the continuum theory predictions. The observation of the instability can be correlated with the hoop stress becoming bimodal (see Figure 3).

6. REFERENCES

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