HYPERELASTICIY IN DYNAMIC FRACTURE: THE CHARACTERISTIC ENERGY LENGTH SCALE

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ABSTRACT

A fact that has been neglected in most theories of brittle fracture is that the elasticity of a solid should depend on its state of deformation: metals tend to soften and polymers tend to stiffen as the strain approaches the state of materials failure. It is only for infinitesimal deformation that the elastic moduli can be considered constant and the elasticity of the solid linear. We show by large-scale atomistic simulations that hyperelasticity, the elasticity of large strains, can play a governing role in the dynamics of fracture and that linear theory is incapable of capturing all phenomena. We introduce a new characteristic length scale for the energy flux near the crack tip and demonstrate that the local hyperelastic wave speed governs the crack speed when the hyperelastic zone approaches this energy length scale. The new length scale, heretofore missing in the existing theories of dynamic fracture, helps to explain recent observations of super-Rayleigh and supersonic fracture in computer simulations and experiments.

1. INTRODUCTION

We show by large-scale atomistic simulation that hyperelasticity, the elasticity of large strains, can play a governing role in the dynamics of brittle fracture. This is in contrast to many existing theories of dynamic fracture where the linear elastic behavior of solids is assumed sufficient to predict materials failure [1]. Some experiments [2-4] as well as many computer simulations [5, 6] have shown a significantly reduced crack propagation speed in comparison with the theoretical predictions. Such discrepancies between theories, experiment and simulations can not solely be attributed to the fact that real solids have imperfections, as similar discrepancies also appear in molecular-dynamics simulations of cracks traveling in perfect atomic lattices. It was recently proposed that hyperelastic effects at the crack tip play an important role in the dynamics of fracture [3, 7]. In contrast, it is not generally accepted that hyperelasticity should play a significant role in dynamic fracture. This is because the zone of large deformation is highly confined to the crack tip, so that the region where linear elastic theory does not hold is extremely small compared to the extensions of the specimen [1]. Here we use molecular-dynamics simulations [5, 8-10] in conjunction with continuum mechanics concepts [1] to prove that hyperelasticity is crucial for understanding dynamic fracture. The studies show that local hyperelasticity around the crack tip can significantly influence the limiting speed of cracks by enhancing or reducing local energy flow, even if the zone of hyperelasticity is small compared to the specimen dimensions. The hyperelastic theory drastically changes the concept of the maximum crack velocity in the classical theories. For example, the classical theories predict that mode I cracks are limited by the Rayleigh-wave speed and mode II cracks are limited by longitudinal wave speed. In contrast, both super-Rayleigh mode I and supersonic mode II cracks are allowed by hyperelasticity [8]. We find that there exists a characteristic length scale associated with energy flow near the crack tip that explains supersonic crack motion: Hyperelasticity completely dominates crack dynamics if the size of hyperelastic region approaches this characteristic length.

2. SIMULATION METHOD AND ATOMISTIC MODEL

We consider a crack in a two-dimensional simulation geometry with slab width l_x propagating in a triangular hexagonal lattice (details see [11]). To avoid crack branching, a weak fracture layer is introduced so that atomic bonds across the prospective crack path snap at a critical atomic snapping distance r_{break}, while those in the rest of the slab never break. The snapping distance is used to adjust the fracture surface energy γ [11]. We adopt a biharmonic interatomic potential composed of two spring constants k_0 and $k_1 = 2k_0$ serving as a simplistic model of hyperelasticity common to a large class of real materials [11]. We consider two "model materials", one with elastic stiffening and the other with elastic softening behavior. The spring constant k_0 is associated with small perturbations from the equilibrium distance r_0, and the second spring constant k_1 is associated with large bond stretching ($r > r_{on}$). Harmonic systems are obtained if r_{on} is chosen to be larger than r_{break}.

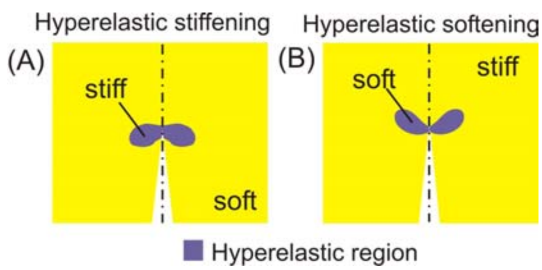

Figure 1: Plots (c) and (b) show the shape of the hyperelastic region for the stiffening and softening case.

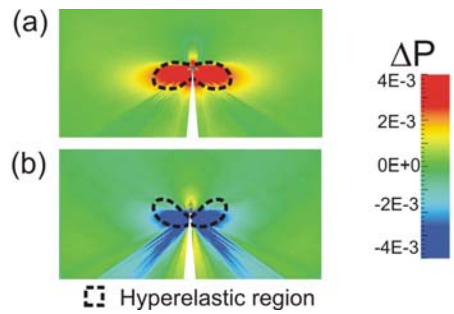

Figure 2: Change of energy flow due to hyperelastic stiffening (a) and softening (b) effect, according to equation (3).

3. CRACK SPEED AND ENERGY FLOW

We show that a localized, small hyperelastic region around the crack tip can have significant effects on the dynamics of crack propagation. In the simulations, the slab is loaded with 0.32 percent strain in mode I. The strain energy density far ahead of the crack tip is given by

$$S = \varepsilon_{xx}^2 l_x E / (1-\nu^2) / 2 , \tag{1}$$

where E is the Young's modulus at small strain. The linear elastic expression of strain energy density is valid because material far ahead of the crack is strained always below the onset threshold of the bilinear law, that is, it remains in the linear elastic regime of material response. According to the linear theory of fracture [1], the crack speed should satisfy the dynamic energy release rate equation

$$A(v / c_R) = 2\gamma / S \tag{2}$$

where the function $A(v / c_R)$ is a universal function of crack velocity. Linear theory predicts that crack velocity should depend only on the ratio S / γ. Our strategy is to focus on the prediction from linear theory that crack velocity depends only on the ratio S / γ. In the harmonic systems, since $S \propto E$ and $\gamma \propto E$ [11], we choose the parameter r_{break} to be identical in all cases. In the biharmonic systems, we adjust the parameter r_{break}, at given values of r_{on}, E_0 and E_1, to always keep S/γ constant.

We choose $r_{break} = 1.17$ for the harmonic systems, and the crack achieves the same propagation velocity around 80 percent of the Rayleigh wave speed, consistent with linear theory. For the biharmonic systems, we choose $r_{on} = 1.1275$ and $r_{break} = 1.1558$ in the stiffening case, and $r_{break} = 1.1919$ in the softening case (then S/γ =const.). In contrast to the linear theory prediction, we find that the crack speed is about 20 % larger in the stiffening system and 30 % smaller in the softening system. These deviations can not be explained by the linear theory: The fact that we change the large-strain elasticity while keeping the small-strain elasticity constant indicates that hyperelasticity is affecting crack dynamics! The region occupied by atoms having a local maximum principal strain $\varepsilon_1 > (r_{on} - r_0)/r_0$ defines the hyperelastic area A [11, 12]. Fig. 1a shows the hyperelastic area in the case of a stiffening material, and Fig. 1b shows the hyperelastic area in the case of an elastically softening material. The hyperelastic effect is highly localized to the crack tip (the pictures show a portion of the simulation slab near the crack tip).

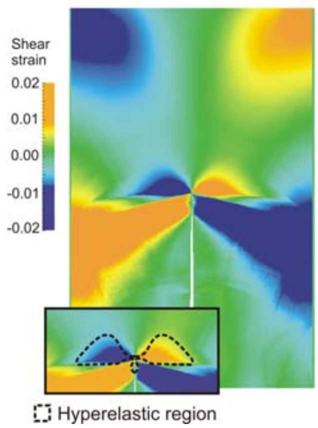

Figure 3: Shear strain field during intersonic mode I crack propagation. The fact that mode I cracks can move faster than the shear wave speed is completely contradicting the existing theories of fracture. This observation suggests that the energy release rate does not vanish for mode I cracks in excess of Rayleigh-wave speed, thus the universal function *A(v/c$_r$)* of linear elastic fracture mechanics theories [1] is incorrect. Intersonic mode I cracking, for the first time observed in computer simulation, was recently verified in experiment [14].

A measure for the direction and magnitude of energy flow in the vicinity of the crack tip is the magnitude of the dynamic Poynting vector [11, 13]. A measure for the change in energy flow is obtained by subtracting the magnitude of the dynamic Poynting vector in the harmonic case from that in the biharmonic case at every point in the slab,

$$\Delta P = P_{biharm} - P_{harm} . \tag{3}$$

If the difference is negative, energy flow is reduced, and if the difference is positive, energy flow is enhanced. Fig. 2a and b shows the energy flow enhancement and reduction in the vicinity of the crack tip for the elastically stiffening bilinear system (a) and for the elastically softening system (b). In each plot, the local hyperelastic zone is indicated by a dotted line. The energy flow in the vicinity of the crack tip is enhanced in the bilinear stiffening case and reduced in the softening case. The plots show that the local hyperelastic effect leads to an enhancement (stiffening system) or reduction (softening system) in energy flow. The higher crack velocity in the stiffening system and the lower velocity in the softening system are due to enhancement or reduction of the energy flow in the vicinity of the crack tip. Steady state crack motion is confirmed by the path-independency of the dynamic J-integral.

An important result is that when sufficient loading is applied to the system, mode I cracks in bilinear stiffening solids can reach speeds beyond the Rayleigh-wave speed. It was shown that the size of the hyperelastic region can be correlated with the crack speed, for different choices of the potential parameter ε_{on} [11]. The larger the hyperelastic region, the higher the crack speed, and for purely harmonic systems the terminal crack velocity is the Rayleigh-wave speed.

Even intersonic mode cracks can be observed, when the stiffening is relatively strong (here $k_1 = 4k_0$). Intersonic mode I cracking is shown in Figure 3. This phenomenon has, motivated by MD simulation results [11], recently been verified in experiment [14]. Our observations can be explained by the concept of the characteristic energy length scale. Another interesting observation is supersonic mode II cracking as depicted in Figure 4. Due to a very small, localized hyperelastic region, the crack breaks through the sound barrier and moves supersonically. These observations can only be understood from the hyperelasticity point of view.

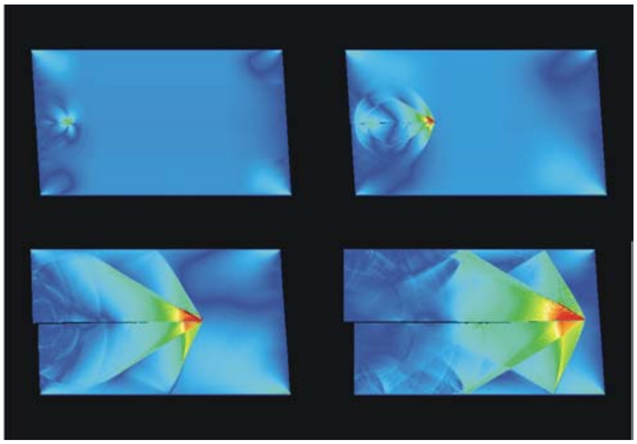

Figure 4: Supersonic mode II cracking. Due to a small, localized hyperelastic zone near the crack tip, the crack breaks through the sound barrier and moves supersonically. The fact that supersonic cracking is possible suggests that the energy release rate does not vanish, a fact that is in clear contrast to the existing theories of fracture.

The problem of a super-Rayleigh mode I crack in an elastically stiffening material is somewhat analogous to Broberg's [15] problem of a crack propagating in a stiff elastic strip embedded in a soft matrix (Fig. 5). It was shown that the energy release rate can be expressed in the form

$$G = \sigma^2 h / Ef(v, c_1, c_2)\,, \tag{4}$$

where σ is the applied stress, h is the half width of the stiff layer and f is a non-dimensional function of crack velocity and wave speeds in the strip and the surrounding matrix. The dynamic Griffith energy balance requires

$$G = 2\gamma\,, \tag{5}$$

indicating that crack propagation velocity is a function of the ratio h/χ where

$$\chi \propto \gamma E / \sigma^2 \tag{6}$$

is defined as a characteristic length scale for local energy flux. By dimensional analysis, the energy release rate of our hyperelastic stiffening material is expected to have similar features except that the strip width h should be replaced by a characteristic size of the hyperelastic region r_H. Therefore, we introduce the concept of a characteristic length

$$\chi = \beta\gamma E / \sigma^2 \tag{7}$$

for local energy flux near a crack tip. We find that the mode I crack speed reaches the local Rayleigh wave speed as soon as h/χ gets sufficiently large and verify that the scaling law holds by changing γ, E and σ independently (details can be found in [11]).

The hyperelastic zone characterized by r_H is somewhat similar as the thin stiff strip characterized by *h* [11]. Under a particular experimental or simulation condition, the relative importance of hyperelasticity is therefore determined by the ratio r_H / χ: For small r_H / χ, the crack dynamics is dominated by the global linear elastic properties since much of the energy transport necessary to sustain crack motion occurs in the linear elastic region. However, when r_H / χ approaches unity, as is the case in some of our molecular dynamics simulations, the dynamics of the crack is dominated by local elastic properties because the energy transport required for crack motion occurs within the hyperelastic region.

The concept of energy characteristic length χ immediately provides an explanation how the classical barrier for transport of energy over large distances can be undone by rapid transport near the tip.

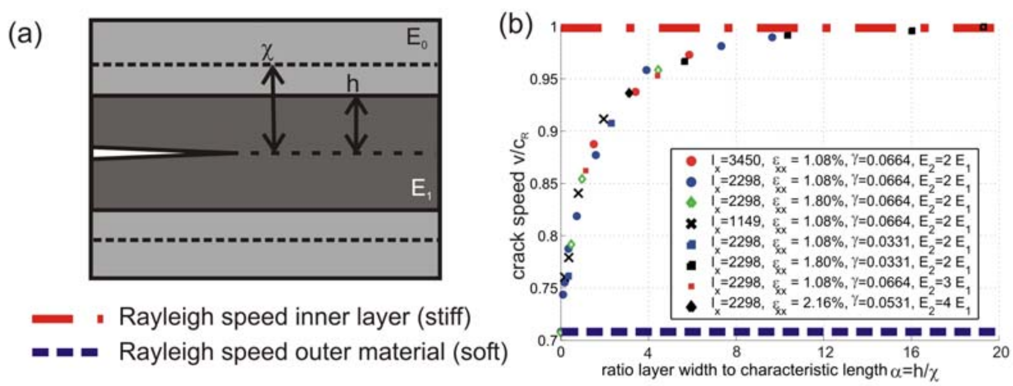

Figure 5: Numerical verification of the characteristic energy length scale in dynamic fracture (Broberg problem [15] of crack motion in a thin stiff strip embedded in a soft matrix, $E_1 > E_0$).

5. DISCUSSION AND CONCLUSIONS

Our studies suggest that hyperelasticity plays a dominating role in the dynamics of cracks, as it has strong impact on energy flow. Figure 6 shows the classical viewpoints of length scales around a dynamic crack tip, compared to the new picture featuring the energy length scale [11]. Our results suggest that the classical, linear elastic theories should be replaced by nonlinear theories of fracture in order to form a comprehensive picture of crack dynamics. Ongoing studies include investigations of the effect of material nonlinearities on the instability dynamics of cracks.

6. ACKNOWLEDGMENTS

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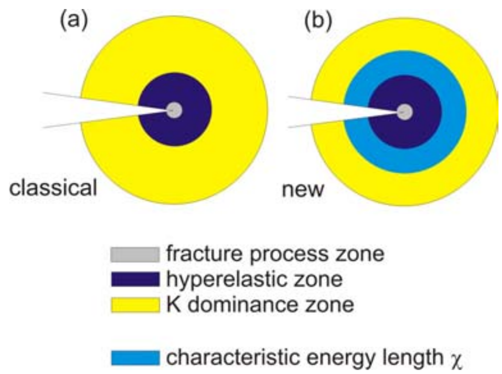

Figure 6: The characteristic energy length scale in dynamic fracture, in comparison with classical length scales. In the classical picture, there exist only the fracture process zone, the *K* dominance zone and the zone of large deformation (hyperelastic zone). With the new concept of the characteristic energy length scale χ, the relative importance of hyperelasticity becomes obvious: It dominates once the size of the hyperelastic zone approaches that of the characteristic energy length scale.

7. REFERENCES

1. Freund, L.B. *Dynamic Fracture Mechanics* (Cambridge University Press, 1990).
2. Fineberg, J. Gross, S.P., Marder, M., and Swinney, H.L. Phys. Instability and Dynamic Fracture. Rev. Lett. **67**, 141-144 (1991).
3. Ravi-Chandar, K. Dynamic Fracture of Nominally Brittle Materials. Int. J. of Fract. **90**, 83-102 (1998).
4. Cramer T., Wanner A., Gumbsch, P. Energy Dissipation and Path Instabilities in Dynamic Fracture of Silicon Single Crystals. Phys. Rev. Lett. **85** (4): 788-791 (2000).
5. Abraham, F.F., Brodbeck, D., Rudge, W.E., Xu, X. Instability Dynamics of Fracture: A Computer Simulation Investigation. Phys. Rev. Lett. **73**, 272-275 (1994).
6. Falk, M.L., Needleman, A. and Rice, J.R. A Critical Evaluation of Cohesive Zone Models of Dynamic Fracture. Journal de Phys. IV France **11**, 5-43-50 (2001).
7. Gao, H. A Theory of Local Limiting Speed in Dynamic Fracture. Mech. Phys. Solids **44**, 1453-1474 (1996).
8. Abraham F.F et al. Simulating Materials Failure by using up to one billion atoms: Brittle Fracture. Proc. Nat. Acad. Sci. **99**, 5777-5782 (2002).
9. Abraham, F.F., Gao, H, How Fast Can Cracks Propagate? Phys. Rev. Lett. **84**, 3113-3116 (2000).
10. Rountree, C.L. et al. Atomistic Aspects of Crack Propagation in Brittle Materials: Multimillion Atom Molecular Dynamics Simulations. Annu. Rev. Mater. Res. **32**, 377-400 (2002).
11. Buehler, M.J., Abraham, F.F., Gao, H. Hyperelasticity Governs Dynamic Fracture at a Critical Length Scale. Nature **426**, 141-146 (2003)
12. Zimmermann, J. *Continuum and atomistic modeling of dislocation nucleation at crystal surface ledges.* PhD Thesis, Stanford University (1999).
13. Fratini S., Pla O., Gonzalez P., Guinea F., and Louis E. Energy Radiation of Moving Cracks. Phys. Rev. B. **66**, 104104 (2002).
14. Petersan, P.J., Deegan, R.D., Marder, M., Swinney, H.L. Cracks in Rubber under Tension Break the Shear Wave Speed Limit. Under submission, preprint available at: http://arxiv.org/abs/cond-mat/0311422
15. Broberg, K.B. Dynamic Crack Propagation in a Layer. Int. J. Sol. Struct. **32** (6-7), 883-896 (1995).