

NONLINEAR EFFECTS IN DYNAMIC FRACTURE

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ABSTRACT

A fact that has been neglected in most theories of brittle fracture is that the elasticity of a solid clearly depends on its state of deformation. Metals will weaken, or soften, and polymers 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 concept of a characteristic length scale χ 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 χ , heretofore missing in the existing theories of dynamic fracture, helps to form a comprehensive picture of crack dynamics, explaining super-Rayleigh and supersonic fracture. We further investigate the stability of cracks, and show agreement of the Yoffe criterion with the dynamics of cracks in harmonic systems. We find that softening hyperelastic effects lead to a decrease in critical instability speed, and stiffening hyperelastic effects leads to an increase in critical speed, allowing for straight crack motion up to super-Rayleigh crack speeds. The main conclusion is that hyperelasticity plays a critical role in forming a complete picture of dynamic fracture.

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 first part of 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. In the second part of the paper, we report studies on the crack tip instability, and we show that hyperelasticity also plays a governing role.

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} .

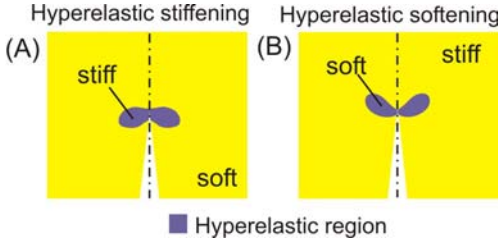


Figure 1: Plots (c) and (b) show the shape of the hyperelastic region for the stiffening and softening case.

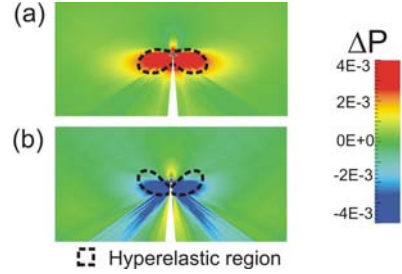


Figure 2: Change of energy flow due to hyperelastic stiffening (a) and softening (b) effect.

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 $S = \varepsilon_{xx}^2 l_x E / (1 - \nu^2) / 2$, 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 $A(v/c_R) = 2\gamma/S$ 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 $S/\gamma = \text{const.}$). 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).

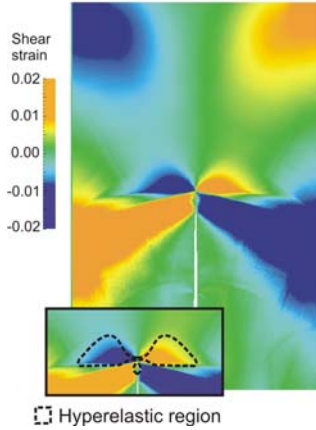


Figure 3: Shear strain field during intersonic mode I crack propagation. The fact that mode I cracks can move faster than the shear wave speed is completely contradicting the existing theories of fracture. This observation suggests that the energy release rate does not vanish for mode I cracks in excess of Rayleigh-wave speed, thus the universal function $A(v/c_r)$ of linear elastic fracture mechanics theories [1] is incorrect. Inter-sonic 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, $\Delta P = P_{biharm} - P_{harm}$. 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 $k_1 = 4k_0$). Inter-sonic 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. 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. 7a). It was shown that the energy release rate can be expressed in the form $G = \sigma^2 h / Ef(v, c_1, c_2)$, 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 $G = 2\gamma$, indicating that crack propagation velocity is a function of the ratio h/χ where $\chi \propto \gamma E / \sigma^2$ 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

$\chi = \beta \gamma E / \sigma^2$ 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]). Under a particular experimental or simulation condition, the relative importance of hyperelasticity is 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.

4. HYPERELASTICITY GOVERNS CRACK TIP INSTABILITIES

In addition the studies on crack speed and energy flow, we report preliminary studies focusing on the effect of hyperelasticity on the instability dynamics of cracks. It is known that cracks in softening materials become unstable at reduced speeds compared to the theoretical prediction of 73 % c_R by the Yoffe criterion [1-3, 7]. Our simulations of cracks in homogeneous materials with linear elastic properties (harmonic potential) show that the instability occurs at about 73 % c_R , in perfect agreement with the prediction by theory (Fig. 4a). We note that the branching angle of 60 degree also matches the theoretical prediction [1], and the instability can be correlated with the development of a bimodal hoop stress as originally proposed by Yoffe (Fig. 4a and b).

As in the previous case, the linear systems now serve as reference system when we probe crack dynamics in nonlinear materials. To test the nonlinear dynamics, we use a similar biharmonic potential as in the previous sections, with the difference that it smoothens close to bond breaking, which leads to smoother crack acceleration (details on the potential will be published in another paper). The results show that cracks become unstable at much lower speeds when softening materials are used (Fig. 5a), and that cracks are stable up to velocities close to the Rayleigh-wave speed in stiffening materials (Fig. 5b). In some simulations with very strong

stiffening effect ($k_1 = 4k_0$), the instability speed is even super-Rayleigh! Such observations can only be understood from the hyperelasticity point of view. We briefly note that analyses suggest that the critical instability speed can be approximated by Gao's model of local limiting speed [7] in softening materials. These results together with detailed modeling will be discussed in a forthcoming publication [16].

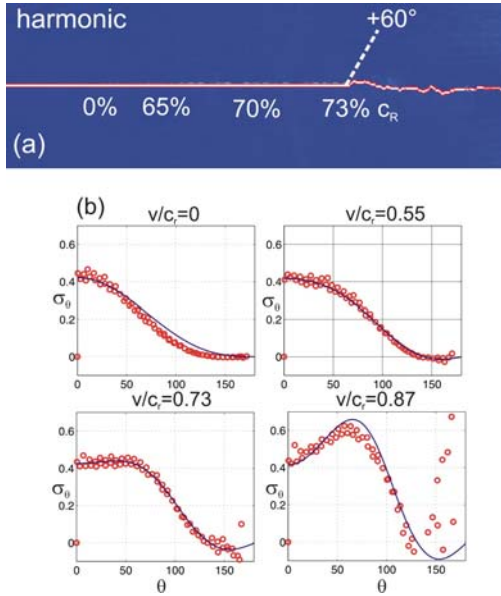


Figure 4: Dynamic crack tip instabilities harmonic system (subplot (a) shows potential energy indicating the crack surface by the red color), Subplot (b) shows the hoop stress in the harmonic systems, becoming bimodal just at the speed when the instability is observed. This observation is in perfect agreement with Yoffe's prediction [1].

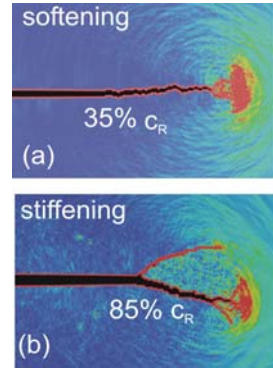


Figure 5: Dynamic crack tip instabilities in (a) softening system and (b) stiffening system. The instability speed is changed dramatically dependent on the large-strain elastic properties. This result is important since is strong indication that the large-strain elastic properties govern the instability dynamics! It is interesting to note that in the stiffening systems, cracks can move straight up to speeds close to the Rayleigh-wave speed according to our predictions. Further results will be presented in forthcoming publications [16].

5. DISCUSSION AND CONCLUSIONS

Our studies suggest that hyperelasticity plays a dominating role in the dynamics of cracks. The effect of nonlinearities close to the crack tip is two-fold: Firstly, it has strong impact on energy flow, and secondly, it governs the instability dynamics. 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.

6. ACKNOWLEDGMENTS

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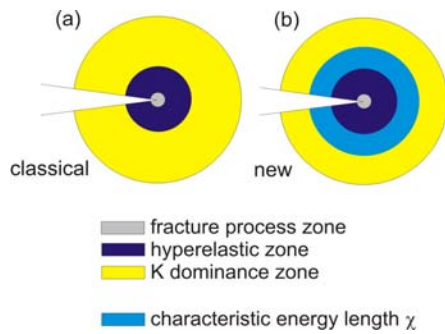


Figure 6: The characteristic energy length scale in dynamic fracture, in comparison with classical length scales. In the classical picture, there exist only the fracture process zone, the K dominance zone and the zone of large deformation (hyperelastic zone). With the new concept of the characteristic 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.

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