EFFECT OF HYPERELASTICITY ON DYNAMICAL CRACK TIP INSTABILITIES

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ABSTRACT

The relation between stress and strain in real solids can be strongly nonlinear at large deformation near a crack tip. Many existing theories of fracture neglect such hyperelasticity behavior and instead assume a linear elastic stress-strain law. We have previously investigated the role of hyperelasticity in intersonic mode I and supersonic mode II crack motion (Buehler *et al*., Nature, 2003). In the present study, we focus on the effect of hyperelasticity on dynamical crack tip instabilities. Using a series of large-scale atomistic simulations involving millions of atoms, we show that hyperelasticity can also play a governing role in dynamical crack tip instability. The classical linear elastic theories can not describe crack dynamics in real materials which often show a softening hyperelastic effect. Our numerical experiments reveal that hyperelastic material properties have a significant influence on instability dynamics. We illustrate that the hyperelastic effects can be understood with an energy-flow induced instability (Gao *et al*., 1996) that competes with Yoffe's classical deformation field controlled mechanism (Yoffe, 1951). Which phenomenon dominates depends on the strength of the softening effect and could be directly linked to interatomic potential parameters that describe the amount of softening near the moving crack. If the hyperelastic softening is small, energy flow plays a minor role and the instability dynamics is largely deformation field controlled. If, on the other hand, the hyperelastic softening region is large, energy flux controls the instability dynamics. In this paper we attempt, for the first time, a unified treatment of the instability problem with a transition from energy flow controlled mechanism (Gao model) to deformation field controlled mechanism (Yoffe model).

1. INTRODUCTION

The dynamics of cracking is a fundamental problem in the field of materials failure under extreme conditions [1-4]. How do cracks evolve, and what is the underlying atomic mechanism? How does the shape of the interatomic potential affect the dynamics of cracking [4-6]? These are some of the questions we address in the present study. It was observed that the crack face morphology changes as the crack speed increases, a phenomenon also referred to as dynamical instability of cracks [2-4]. Up to a critical speed, the crack surface is atomically flat (mirror). At higher speeds the crack starts to roughen (mist) and eventually becomes very rough (hackle). The dynamical crack tip instability has received significant attention in the past 50 years. Yoffe reported in 1951 the solution of a steadily translating mode I crack [1]. The Yoffe solution suggested that the crack should branch at a critical speed of about 73 % of the Rayleigh wave speed, as the circumferential hoop stress exhibits a maximum at an inclined cleavage plane for high crack speeds. However, experiments have shown that the critical instability speed is much lower in real materials. In 1992, Fineberg *et al*. [2] observed an instability speed at about 1/3 of Rayleigh wave speed, which significantly deviates from Yoffe's theory! Similar instability dynamics with a mirror-mist-hackle transition at about 1/3 of the Rayleigh-wave speed was observed in the large-scale MD simulations of Abraham and coworkers [4].

Gao [5] attempted to explain the discrepancy between theory, experiment and simulation based on the concept of hyperelasticity where the main argument for reduced instability speed was that the atomic bonding in real materials softens with increasing strain. A nonlinear continuum mechanics analysis suggests that the softening leads to reduced instability speed. Figure 1 illustrates the concept of hyperelasticity in contrast to linear elastic behaviour.

The hyperelastic effects can significantly modify the classical Yoffe picture: In the linear elastic Yoffe model [1], a purely deformation field approach is taken in that changes in stress distribution close to the crack tip determines the critical conditions for the onset of instability. On the other hand, Gao's model [5] is focused on the change of local wave speed close to a crack tip. Because of the large deformation induced softening near the crack tip, both the local stress and the energy flow field are altered. The reduction in energy flow can be understood based on the lower local wave velocities. If the crack speed moves faster than the speed of local energy flow, the crack motion could become unstable!

More recently, hyperelasticity has also been discussed in association with intersonic and supersonic fracture along a weak layer in an elastically stiffening solid [6]. Simulations have shown intersonic mode I and supersonic mode II cracking [6]; the former has also been verified in experiment [7].

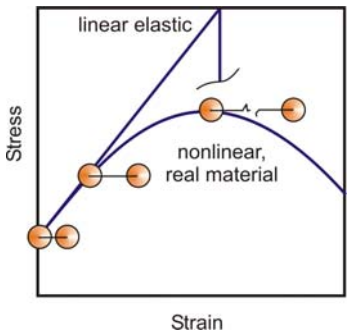

Figure 1: Schematic comparison of linear elastic stress-strain behavior with hyperelastic softening. Despite most real materials show a significant hyperelastic effect, this is completely neglected in most existing theories of fracture. This paper addresses the question if failure to include this concept into modeling could explain the discrepancies of theory, experiment and simulation.

Despite important progress in the past, the existing literature does not provide a satisfactory explanation of the role of hyperelastic effects in the instability dynamics of fracture. There is still a lack of understanding on the transition from the linear elastic Yoffe model [1] to Gao's hyperelastic model [5]. In most computational work, the analysis was performed only for a single potential, such as done for a LJ potential by Abraham *et al.* [4]. There have been no systematic numerical studies based on continuously varying potential parameters that would focus on the prediction of Gao's model versus that of the Yoffe model.

In the present work, we conduct a systematic parameter study via large-scale molecular dynamics simulations. An interatomic potential that allows a systematic transition from linear elastic to strongly nonlinear materials behavior is adopted to bridge different existing theories and determine the conditions of their validity.

The outline of this paper is as follows. By systematically changing the large-strain elastic properties while keeping the small-strain elastic properties constant, and thus tuning the strength of the hyperelastic effect, we will determine the conditions when the elasticity of large strains governs the instability dynamics of cracks. Linear elastic materials serve as reference systems for our studies, where we find that the instability speed agrees well with the predicted value from Yoffe's linear analysis [1]. Our results suggest that changing the strength of hyperelastic effect allows tuning the instability speed. If the hyperelastic softening region is very small, energy flow plays a minor role and the instability dynamics is largely deformation field controlled. If, on the other hand, the hyperelastic softening region is large, energy flux controls the instability dynamics. In this paper, we achieve, for the first time, a unified treatment of the instability problem. A simple analytical model provides quantitative estimates on the instability speed in our model system and explains the transition from Gao's to Yoffe's model.

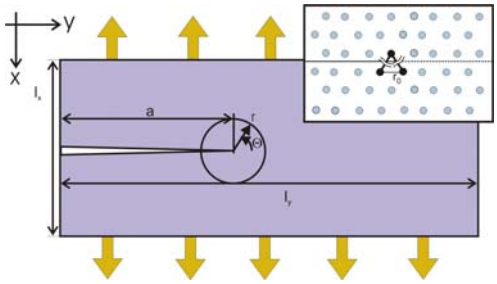

Figure 2: Slab geometry used for the numerical studies of instability dynamics of cracks. The crack is oriented such that it propagates along the direction of low fracture surface energy.

2. SIMULATION METHOD AND ATOMISTIC MODEL

We consider a crack in a two-dimensional geometry with slab width l_x. The crack propagates in a triangular hexagonal lattice along the direction of lowest surface energy (for details see [6]). We adopt a harmonic interatomic potential with spring constant k_0 in combination with a smooth cutoff of the force based on the Fermi-Dirac (F-D) distribution function to describe bond breaking. The force versus atomic separation is then given by

$$\frac{d\phi}{dr}(r) = k_0(r - r_0)\left[\exp\left(r\frac{\Xi}{r_{\text{break}}} - \Xi\right) + 1\right]^{-1} . \qquad (1)$$

The parameter $r_0 \approx 1.12246$ refers to the nearest neighbor spacing of atoms. Assuming that the spring constant k_0 is fixed, the potential has two parameters, r_{break} and Ξ. The parameter r_{break} (corresponding to the Fermi energy in the F-D-function) denotes the critical separation for breaking of the atomic bonds and allows tuning the breaking strain as well as the cohesive stress at breaking of bonds ($\sigma_{coh} \propto d\phi/dr$). The parameter Ξ (corresponding to the temperature in the F-D-function) describes the amount of smoothing at the breaking. For small values of Ξ (around 50), the softening effect is quite large. For large values of Ξ, the region of softening becomes very small, and the solid behaves like one with snapping bonds (as used in [6]). Figure 3 depicts the interatomic potential used for the calculations (showing force versus atomic separation given by eqn. (1)). This model serves as a simplistic model of hyperelasticity common to a large class of real materials, as it allows a systematic variation of the cohesive stress and the amount of softening at bond breaking [6]. Further details of the potential will be published elsewhere.

3. HYPERELASTICITY GOVERNS CRACK TIP INSTABILITIES

We have carried out a series of numerical experiments by systematically varying the potential parameters r_{break} and Ξ. In this short paper, we may only summarize the main findings of our work. The first important result is that cracks in homogeneous materials with linear elastic properties (harmonic potential, achieved by setting Ξ to infinity) show a critical instability speed of about 73 % c_R, independent of the choice of r_{break}. This is in agreement with the prediction by linear elastic theory [1]. We also find that the occurrence of the instability can be correlated with the development of a bimodal hoop stress as proposed by Yoffe [1].

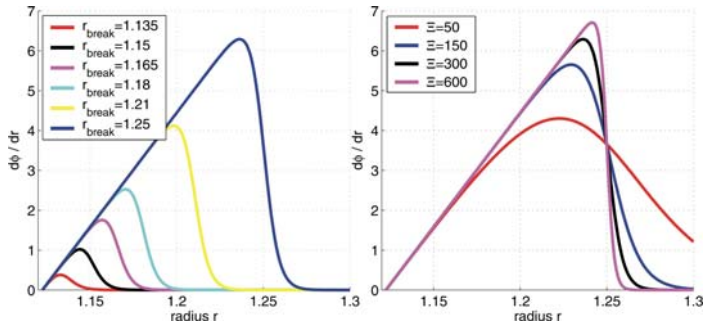

Figure 3: The interatomic potential (showing force versus atomic separation) used for the calculations. The potential has two parameters, r_{break} and Ξ. The parameter r_{break} denotes the critical separation for breaking of the atomic bonds. The parameter Ξ gives the amount of smoothing at the breaking. The parameter r_{break} is used to adjust the breaking stress, whereas the parameter Ξ is used to control the softening behavior near the crack tip. For small values of Ξ, the soft region is rather large, and the potential approaches the shape of a LJ-type interatomic potential. For large values of Ξ, the region of softening is very small, and the solid behaves much like one with snapping bonds. Note that $\sigma_{coh} \propto d\phi / dr$.

How does crack dynamics change once significant softening at the crack tip is introduced? To assess the dependence of crack instability dynamics on the large-strain properties of the interatomic potential, we systematically vary the parameters r_{break} and Ξ, and compare the instability speed with the predictions by Gao's model and Yoffe's model. We observe that the instability speed is in between the prediction by Gao's model and the prediction by Yoffe's model. How much it deviates from the different models depends on the choice of r_{break} and Ξ. We find that the deviation from Gao's model vanishes for smaller values of Ξ, and the results approach Yoffe's model for large values of Ξ. For small value of Ξ, we further find that the instability speed depends on the cohesive stress, which is an important feature of Gao's model. In fact, we observe that the first derivative of the instability speed with respect to the cohesive stress agrees reasonably well in Gao's model and our MD simulations. This suggests that for small values of Ξ, the two results differ only by a constant parameter.

Therefore, we introduce an additional parameter, the shift velocity $v_{shift}(\Xi)$, to obtain quantitative predictions of the instability speed. In terms of physical interpretation, the shift parameter accounts for the strength of hyperelastic softening. Gao's model corresponds to the *limiting case* when the softening region size is large, and it therefore constitutes a *lower limit* for the instability speed [5]. For very strong softening, that is, $\Xi \to 0$, v_{shift} vanishes. In contrast, it assumes larger values when the softening effect vanishes, that is $\Xi \to \infty$. With the new parameter v_{shift}, the instability speed is given by

$$v_{inst} = v_{shift}(\Xi) + \sqrt{\frac{\sigma_{coh}}{\rho}}, \qquad (2)$$

which we refer to as the *modified Gao model*. Note that σ_{coh} is the cohesive stress, and ρ is the

density as in [5]. Without describing the details, the physical significance of this parameter can also be understood from within the perspective of the characteristic energy length scale χ proposed earlier [6]. We determined the function $v_{shift}(\Xi)$ by a series of MD simulations. The results are shown in Figure 4.

Now we focus on the dependence of the instability speed on the parameter r_{break} for fixed $\Xi = 150$ (Fig. 5). We have studied the dynamics for several choices of Ξ, but we only discuss the results for $\Xi = 150$. Whereas the observed limiting speeds agree well with the predictions by the modified Gao model (eqn. (2)) for $r_{\text{break}} < 1.22$, the results deviate for larger values of $r_{\text{break}} > 1.22$. In this case, we observe that the instability speeds are very close to Yoffe's prediction of 73 % of Rayleigh-wave speed, and virtually independent of r_{break}. This suggests that the instability speed is governed by a deformation field mechanism. For $r_{\text{break}} > 1.22$, the predictions by Gao's model are higher than the Yoffe speed (see Fig. 5). This is a significant result, as it suggests a change in the dynamical mechanism of the instability from cohesive-stress and thus energy flow controlled, to a deformation field controlled Yoffe mechanism. Note that we observe the same phenomenon for different choices of Ξ ranging from about 50 to 1,500.

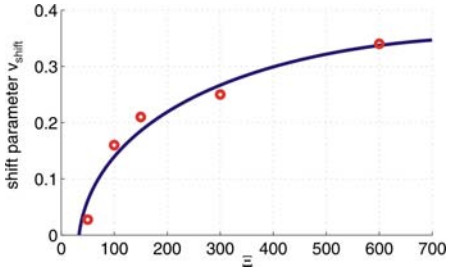

Figure 4: Change of shift parameter v_{shift} as a function of the smoothing parameter. The physical interpretation of the shift parameter is that it is a measure for how strong is the effect of energy flow reduction close to the crack tip. The main result is that the stronger the smoothing close to the crack tip, the smaller the value of the shift parameter v_{shift} (eqn. (4). When the shift parameter vanishes, the instability dynamics is completely governed by energy flow (as in Gao's model [5]). For large values of the shift parameter, energy flow becomes negligible and the instability dynamics is largely controlled by the deformation field [1].

4. DISCUSSION AND MAIN CONCLUSIONS

The studies confirmed that the large-deformation potential properties play a critical role in the instability dynamics of cracks. It remains an open question, how can the hyperelastic model [5] and the Yoffe model [1] be combined? Based on the results of our numerical experiments, we propose that this can be achieved by taking the minimum of the Yoffe speed and the prediction by the modified Gao model. The critical crack tip instability speed is then given by

$$v_{inst}^{MOD} = \min\left(v_{YOFFE}, v_{shift}(\Xi) + \sqrt{\frac{\sigma_{coh}}{\rho}} \right). \qquad (3)$$

Note that $v_{YOFFE} \approx 0.73 \times c_R$ is a constant. We reiterate that the physical interpretation of v_{shift} is related to the size of the hyperelastic softening region and the importance of energy flow on the instability dynamics. The shift parameter vanishes if energy flux completely governs the instability

dynamics, corresponding to very small values of Ξ. It increases to larger values as $\Xi \to \infty$, when the hyperelastic region is very small and the effect of softening on the instability is negligible—therefore, the Yoffe theory dominates the instability and Gao's model is no longer valid. We find that a square-root dependence of v_{shift} on Ξ provides a good fit to the MD results:

$$v_{shift}(\Xi) = \alpha\sqrt{\Xi}\,. \tag{4}$$

Note that $\alpha = 0.0138$ is determined from the numerical calculation results (the fit is plotted in Fig. 4).

This set of equations and numerical parameters, to the best of our knowledge for the first time allow quantitative predictions about the onset of the instability in the system at hand. Most importantly, eqns. (3) and (4) provide a direct link between Yoffe's and Gao's model of instability dynamics, which should at least *qualitatively* be generally valid in "real" solids.

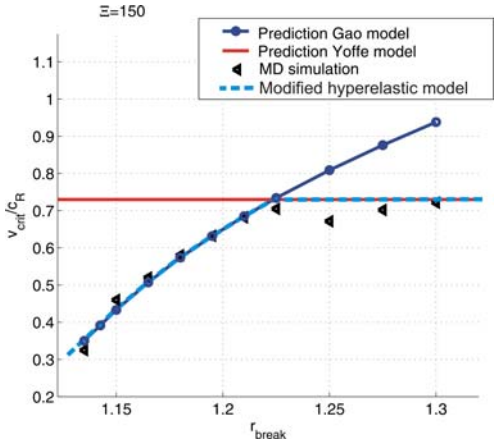

Figure 5: Instability speed as a function of the parameter r_{break}, for $\Xi = 150$. The results show that the instability speed varies with r_{break} and thus with the cohesive stress, but the Yoffe speed [1] provides an upper limit for the instability speed. This suggests a change in dynamical mechanism from cohesive-stress controlled, or energy flow controlled, to deformation field controlled. The plot also depicts the prediction by the *modified hyperelastic model* given in eqn. (3) and (4).

5. ACKNOWLEDGMENTS

We acknowledge discussions with Dr. Farid Abraham (IBM Almaden Research Center) on atomistic modeling of dynamic fracture.

6. 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. 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).
5. Gao, H. A Theory of Local Limiting Speed in Dynamic Fracture. Mech. Phys. Solids **44**, 1453-1474 (1996).
6. Buehler, M.J., Abraham, F.F., Gao, H. Hyperelasticity Governs Dynamic Fracture at a Critical Length Scale. Nature **426**, 141-146 (2003)
7. Petersan, P.J., Deegan, R.D., Marder, M., Swinney, H.L. Cracks in Rubber under Tension Break the Shear Wave Speed Limit. Phys. Rev. Lett. **93**, 015504 (2004).