Dynamic Fracture of Brittle Materials
Lecture 3

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Behavior of different “kinds” of materials

“brittle”: Materials that experience little, if any, plastic deformation before the onset of fracture

“ductile”: Materials that experience significant plastic deformation before the onset of fracture

“geometric confinement”
Nanostructured materials, carbon nanotubes

“How to use large-scale computing in multi-scale modeling in order to develop fundamental understanding

“biological materials”
(Proteins, DNA …)

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Ductile versus brittle materials

Glass, Polymers, Ice…

Copper, Gold,…

tensile load

(a) (b)

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The stress field around a crack is complex, with regions of dominating tensile stress (crack opening) and shear stress (dislocation nucleation).
Dynamic fracture: Deals with cracks approaching the sound speed (km/sec)
Discrepancies theory-experiment-simulation

- Significantly reduced maximum crack speed in some experiments and simulation compared to theory prediction (Freund, 1990)

- Onset of crack tip instability at reduced speed in experiment and simulation compared to prediction by theory (Fineberg, 1992, Abraham, 1994, Gao, 1996, 1997)

Example: Fineberg et al. (1992, 1993)

- Reduced crack speed, instability at ~ 30% $c_R$ (instead at 73% $c_R$)

- Microbranches with speeds and angles not consistent with Yoffe’s or Eshelby’s theories.

“mirror-mist-hackle”
Open questions in dynamic fracture

1. How fast can cracks propagate?

2. Mechanisms and physics of dynamic crack tip instabilities?

3. Dynamics of cracks at materials interfaces

- Use joint continuum-atomistic approach to address these questions

Section A:
How fast can cracks propagate?
Motivation: A 1D model of fracture

- Most of the theoretical modeling and most computer simulations have been carried out in 2D or 3D.

- Finding analytical solutions for dynamic fracture in nonlinear materials seems extremely difficult, if not impossible in many cases.

- In order to investigate the nonlinear dynamics of fracture at a simple level, we propose a one-dimensional (1D) model of dynamic fracture, as originally reported by Hellan (1984) for linear elastic material behavior.

- One-dimensional model is chosen as the simplest possible model for fracture.
Theoretical model of 1D fracture

- 1D model represents a beam glued to a substrate
- Under axial loading the beam detaches and a crack-like front of debonding propagates leading to failure

Crack motion in the 1D model

Rubber band

Substrate

Crack or debonding
Using Hooke’s law:

\[ \sigma = E \varepsilon = E \frac{\partial u}{\partial x} \]

\[ c_0^2 \frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 u}{\partial t^2} \]

\[ u(x,t): \text{Displacements} \]

This represents a PDE to be solved for \( u(x,t) \)

\( c_0 \) wave speed

Solutions for this equation:

\[ u = f(x \mp c_0 t) = f(\xi) \]

Signals traveling through the material with constant speed and profile

\[ \sigma = E \frac{\partial f}{\partial \xi} = E H(\xi) = E \ H(x \mp c_0 t) \]

\[ \dot{u} = \mp c_0 \frac{\partial f}{\partial \xi} = \mp c_0 H(x \mp c_0 t) = \mp \frac{c_0}{E} c \]
Continuum mechanical model (ii)

\[ \dot{u} = -\varepsilon_t \dot{a} = -\frac{\dot{a}}{E} \sigma_t \]  \quad (1)

\[ \sigma_t = \sigma_0 + \sigma_e \]  \quad (2)

\[ \dot{u} = \frac{c_0}{E} \sigma_e \]  \quad (3)

Combine (1), (2) and (3):

\[ \sigma_e = -\frac{\alpha}{1 + \alpha} \sigma_0 \]  \quad \sigma_t = \frac{1}{1 + \alpha} \sigma_t

\[ \dot{u} = -\frac{\dot{a}}{1 + \alpha} \frac{\sigma_0}{E} \]  

\[ \varepsilon_t = \frac{1}{1 + \alpha} \frac{\sigma_0}{E} \]

\[ \frac{\varepsilon_t}{\varepsilon_0} = \frac{1}{1 + \alpha} \]

\[ \alpha = \frac{\dot{a}}{c_0} \]  \quad Crack speed: Unknown

Particle velocity as a function of crack speed

Strain field left behind of moving crack

\[ \dot{u}=0, \sigma_0, \varepsilon_0 \quad \text{du}=-\varepsilon_t \text{da} \]
Crack speed remains unknown
Use energy balance:

\[ G = W - \frac{dT}{da} - \frac{d\phi}{da} = R(\alpha) \]

Change in kinetic energy per unit crack extension

Change in potential energy per unit crack extension

External work \((\approx 0)\)

\[ G_0 g(\alpha) = R(\dot{a}) \]

with

\[ G_0 = \frac{\sigma_0^2}{2E} \]

\( R = \text{fracture surface energy} \) \( R(\alpha) \) typically not known (resistance to crack growth as a function of increasing crack speed)

Assume: Constant dynamic fracture toughness (generally valid for low crack speeds):

\[ R_0 g(\alpha) = R(\dot{a}) \]

Used to determine crack speed for given loading
Continuum mechanical model (iv)

\[ G_0 g(\alpha) = R(\alpha) \quad \text{with} \quad G_0 = \frac{\sigma_0^2}{2E} \]
\[ g(\alpha) = \frac{1 - \alpha}{1 + \alpha} > 0 \quad \text{(fracture surface energy)} \]

For
\[ \alpha \to 1 \]
the stress
\[ \sigma_0 \to \infty \]

The wave speed \( c_0 \) is an upper limit for the crack speed
\[ \alpha = \dot{\alpha} / c_0 \]
Atomistic model

\[ U = \sum_{i,j} \left( \frac{1}{2} k (r_{ij} - a_0)^2 \right) + \sum_i \left( \frac{1}{2} H(i - N_f) k_p \hat{r}_i^2 \right) \]

\[ \hat{r}_i = | x_{0,i} - x_i | \]

\[ U = \sum_{i,j} \left( \frac{1}{2} k (r_{ij} - a_0)^2 \right) + \sum_i \left( \frac{1}{2} H(i - N_f) H(r_{\text{break}} - \hat{r}_i) k_p \hat{r}_i^2 \right) \]

\[ R_0 = \frac{1}{2} \frac{k_p \hat{r}_i^2}{a_0} \quad E = k a_0 \quad c_0 = \sqrt{\frac{E}{\rho}} \quad \varepsilon_i = \frac{x_{i-1} - x_{i+1}}{2 a_0} \]

Atomic strain

Solved using standard MD methods
Compare: Strain field close to crack
Atomistic-continuum

\[
\sigma_t = \sigma_0 + \sigma_e
\]
Compare: Strain field close to crack
Atomistic-continuum

Prediction continuum model:

\[ \varepsilon_t / \varepsilon_0 = \frac{1}{1 + \alpha} \]

Ratio of emitted strain wave to initial strain

- Theory prediction
- Atomistic simulation results
\[ \dot{u} = -\frac{\dot{a}}{1 + \alpha} \frac{\sigma_0}{E} \]

**Compare:** Particle velocity

- **Theory prediction**
- **Atomistic simulation results**

**Graph:**
- X-axis: Reduced crack speed $a/c_0$
- Y-axis: Particle velocity $\dot{u}$

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Suddenly stopping 1D crack

• Calculate strain field near a suddenly stopping 1D crack

• LEFM: Cracks do not have any inertia (see also Buehler et al., 2003)

Result:

• Static stress field ($\varepsilon = \varepsilon_0$) spreads out as soon as crack stops
Periodically varying fracture surface energy

Predictions

\[ \hat{r} = \hat{r}_0 + \Delta \hat{r} \sin(x/p) \]
\[ v = \hat{v}_0 + \Delta v \sin(x/p) \]
Strain field during oscillatory fracture energy

- Strain field of a crack traveling in a material with periodically varying fracture toughness.

- In agreement with prediction, the emitted strain wave changes periodically.
Suddenly stopping 2D crack

Results of 2D MD studies by Buehler, Gao, Huang (CMS, 2003)

Also show inertia-less crack
Dynamic fracture toughness as a function of crack speed

Assume: Constant dynamic fracture toughness

\[ R_0 g(\alpha) = R(\alpha) \]

\[ R(\alpha) \text{ for } k_p = 2.8573 \]
Summary and conclusion

- Developed 1D model of fracture: Simultaneous continuum-atomistic studies
- Such a model is the simplest possible approach of dynamical fracture
- Enables analytical model to understand the importance of local elasticity at the crack tip (=debonding front)

- Extended Hellan’s linear model to the bilinear case

- Introduced nonlinear elastic behavior and showed importance of this for the dynamics of cracks: Hyperelasticity can govern dynamical fracture and may lead to supersonic fracture

- New theoretical model predicts stress and strain field reasonably well, including the nonlinear, supersonic case

- Theory clearly predicts supersonic fracture
Brittle fracture in “real” materials

Classical theory: Assume linear elastic material law

Poor approximation for “real” materials …
Hypotheses

- We believe that hyperelasticity, the elasticity of large strains, is crucial for dynamic fracture.

- Failure to fully understand its significance has created the apparent discrepancies or controversies in the literature!
Strategy of Investigation

- Large scale MD simulation with well defined localized HE zone
- Confine crack propagation to a weak path to eliminate instability

\[ \Delta u \quad \Delta t \]

$r_H$ hyperelastic zone

weak fracture path

micrometer size simulations 70,000,000 atoms
**Strategy of Investigation**

- Use LEFM theory as reference:

\[ A(v/c_R)G_0 = 2\gamma \quad G_0 = \frac{(\Delta u)^2 E^*}{2l_x} \quad A(v/c_R) = 1 - \frac{v}{c_R} \]

for mode I

\(< 0 \text{ for } v > c_R \]

- Start with harmonic systems and show agreement with LEFM

- Then introduce (stronger) nonlinearities and observe difference
Objective: Develop new potential that yields material properties common to a large class of real materials

- Many accurate interatomic potentials for a variety of different brittle materials exist, many of which are derived from first principles
- However: Difficult to identify generic relationships between macroscopic potential parameters and macroscopic observables
- We deliberately avoid these complexities associated, and instead suggest to adopt a simple pair potential based on a harmonic interatomic potential

(Buehler et al., Nature, 2003)
Simplistic bilinear “model material” for hyperelasticity

$r_H$ hyperelastic zone varies by choice of $\varepsilon_{on}$

Biharmonic potential yields bilinear elastic behavior

“tune size of HE region”

Only one parameter $\varepsilon_{on}$ that controls HE effect

(Buehler et al., Nature, 2003)
Atomistic model: Elasticity of harmonic systems

\[ \phi_{ij}(r_{ij}) = a_0 + \frac{1}{2}k(r_{ij} - r_0)^2 \]

\[ E = \frac{2}{\sqrt{3}}k, \quad \mu = \frac{\sqrt{3}}{4}k \]

<table>
<thead>
<tr>
<th></th>
<th>$k$</th>
<th>$E$</th>
<th>$\mu$</th>
<th>$\nu$</th>
<th>$c_l$</th>
<th>$c_s$</th>
<th>$c_r$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soft</td>
<td>$36\sqrt{2} \approx 28.57$</td>
<td>33</td>
<td>12.4</td>
<td>0.33</td>
<td>6.36</td>
<td>3.67</td>
<td>3.39</td>
</tr>
<tr>
<td>Stiff</td>
<td>$72\sqrt{2} \approx 57.14$</td>
<td>66</td>
<td>24.8</td>
<td>0.33</td>
<td>9</td>
<td>5.2</td>
<td>4.8</td>
</tr>
</tbody>
</table>
Crack limiting speed: Harmonic systems

- The limiting speed of mode I cracks in soft and stiff reference systems is the Rayleigh-wave speed, in accordance with predictions (Buehler, Gao, Huang, Theor. Appl. Fracture Mechanics, 2004).
Principal strain field at various crack velocities

Atomic virial strain

\[ q_{ij}^{l} = \frac{1}{N} \sum_{k=1}^{N} \left( \frac{\Delta x_{ij}^{kl} \Delta x_{ij}^{kl}}{r_0^2} \right) \]

\[ b_{ij}^{l} = \frac{N}{\lambda} q_{ij}^{l} = \frac{1}{\lambda} \sum_{k=1}^{N} \left( \frac{\Delta x_{ij}^{kl} \Delta x_{ij}^{kl}}{r_0^2} \right) \]

\[ \sigma_{ij}(\Theta, v) = \frac{K_I(t, v)}{\sqrt{2\pi r}} \sum_{ij} \sigma_{ij}^{(1)}(\Theta, v) + O(1) \]

(e.g. Freund, 1990)

Result: Reasonable agreement

Hyperelasticity can change the crack speed

(Buehler et al., Nature, 2003)
Hyperelasticity can change the crack speed

- Mode I cracks can move faster than the Rayleigh wave speed!
- Speed increases with increase of hyperelastic (HE) area, characterized by $r_H$

- Super-Rayleigh crack motion is possible due to local hyperelastic stiffening region

- Energy release rate does not vanish for mode I cracks in excess of Rayleigh speed

This suggests:
- The universal function $A(v/c_R)$ is incorrect!!

(Buehler et al., Nature, 2003)
How fast can cracks propagate?

- **Mode I** intersonic crack
  - Energy release rate is not zero even for supersonic cracking!! Universal function $A(v)$ of classical theories of fracture incorrect!
  - Mode I cracks faster than the shear wave speed

(Buehler et al., Nature, 2003)
New concept: Energy characteristic scale

Dimensional analysis suggests that

\[ G = \frac{\sigma^2 r_H}{E_2} f(v, c_1, c_2) \]

Dynamic energy balance

\[ G = 2\gamma \]

The crack velocity \( v \) can therefore be expressed as

\[ v = f^{-1}\left(\frac{r_H}{\gamma E / \sigma^2}\right) \]

define \( \chi \propto \gamma E / \sigma^2 \) Has unit of length

This indicates that crack propagation velocity is a function of the ratio \( r_H / \chi \)

Obtaining \( f \) for the hyperelastic case is very difficult…
Broberg’s problem of a crack in a thin strip is somewhat analogous (Broberg, *IJSS*, 1995)

Broberg showed that

\[
G = \frac{\sigma^2 h}{E_2} f(v, c_1, c_2)
\]

energy release rate in the strip

Dynamic energy balance requires that \( G = 2\gamma \)

\[
\chi \propto \frac{\gamma E}{\sigma^2}
\]

Characteristic length scale associated with energy flux to the crack tip

\[
\chi = \beta \frac{\gamma E}{\sigma^2}
\]

Energy characteristic length scale
Confirmation of characteristic energy length scale: Mode I Broberg problem

- Independently varying $\sigma$, $E$ and $\gamma$
- Measuring the crack speed

\[ r_H / \chi \gg 1 \]

"Local HE limiting speed"

\[ \chi \propto \gamma E / \sigma^2 \]

"Small-strain limiting speed" \[ r_H / \chi \approx 0 \]

\checkmark Concept & scaling law numerically verified
Characteristic energy length scale $\chi$ describes region of energy transport to crack tip

\[ \chi \propto \frac{\gamma E}{\sigma^2} \]

**Important:**

- In order to sustain steady state crack motion, cracks need to draw energy **only** from a local region: There is no need for long distance energy transport

**Consequence:** Supersonic crack motion predicted & explained

(Buehler et al., Nature, 2003)
Mike Marder’s group at Univ. of Texas verified the phenomenon of intersonic cracking in a hyperelastic stiffening material (PRL, 2004)

Agreement and confirmation of our theoretical predictions

Multiple-exposure photograph of a crack propagating in a rubber sample ($\lambda_x = 1.2$, $\lambda_y = 2.4$); speed of the crack, $\sim 56$ m/s (Petersan et al.).
Brief summary

Cracks at interfaces
Mother-daughter granddaughter cracks
Focus: Cracks at interfaces

Cracks at interfaces are critical to understand properties of numerous engineering structures, e.g. in composite materials.

Crack dynamics is more complicated than in homogeneous materials (e.g., limiting speed is not well-defined any more).

- Ti-6Al-4V matrix
- SiC monofilamentary fiber

E.g.: Metal Matrix / fiber interface in composite material (e.g. Preuss et al., 2002)
Main result: Mother-daughter mechanism of mode I cracks: supersonic cracking along interface!

Mismatch: $\Xi=10$ (similar dynamics also observed for values 2..10)
Mechanism: Nucleation of daughter crack

Peak in shear stress ahead of the crack causes nucleation of secondary daughter crack

Ongoing theoretical analysis

Main result: There exists a mother-daughter mechanism also for mode I cracks, and the crack speed can be supersonic w.r.t. the soft material layer

(Buehler et al., to appear in: Int. J. STRENGTH, FRACTURE & COMPLEXITY)
Overview: Different cracks

A: Mother crack
B: Daughter crack (supersonic with respect to soft material)

(Buehler et al., to appear in: Int. J. STRENGTH, FRACTURE & COMPLEXITY)
Movie

- Pure mode I loading
- Bimaterial interface (upper part: stiff, lower part: soft)

(Buehler et al., to appear)
Branching behavior

- Fracture strength in stiff and soft part is equal
- Observe tendency to branch into the soft region
- In agreement with Needleman’s continuum/cohesive element studies

(Buehler et al., to appear)
Summary

- Large-scale MD modeling is a useful tool to investigate the dynamics of rapidly moving cracks in brittle materials.

- Length-and time scales associated with dynamic fracture of brittle materials are particularly suitable.

- We have shown that hyperelasticity has a significant effect on crack dynamics, and can control the dynamics of cracks completely.

- The discovery of the characteristic energy length scale $\chi$ helped to form a quantitative understanding on the relative importance of hyperelasticity in dynamical fracture.

- The characteristic energy length scale $\chi$ is found in 1D, 2D and 3D, and also plays a critical role in the instability problem.