From nano to macro: Introduction to atomistic modeling techniques

IAP 2006

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

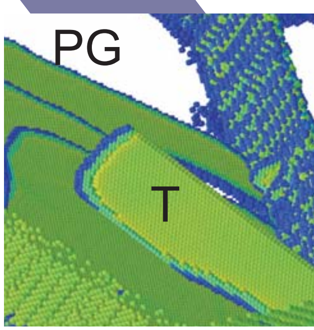
(Buehler *et al*., *Nature*, 2003, Buehler and Gao, Nature 2006)

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

(Buehler *et al*., *CMAME*, 2004)

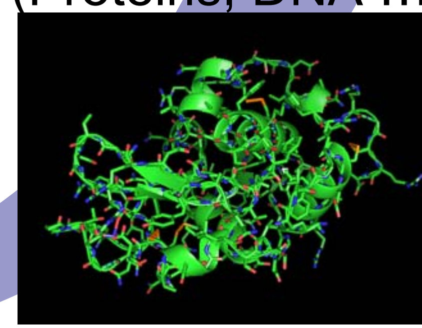
How to use large-scale computing in multi-scale modeling in order to develop fundamental understanding

"geometric confinement"
Nanostructured materials, carbon nanotubes



(Buehler *et al*., *JMPS*, 2002)

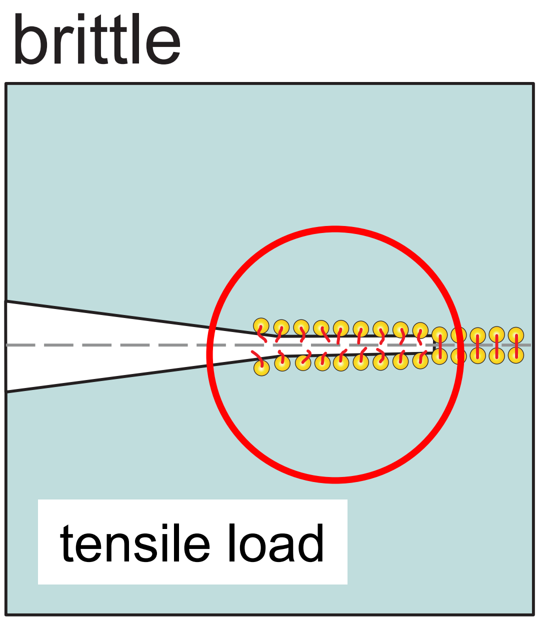
"biological materials"
(Proteins, DNA …)

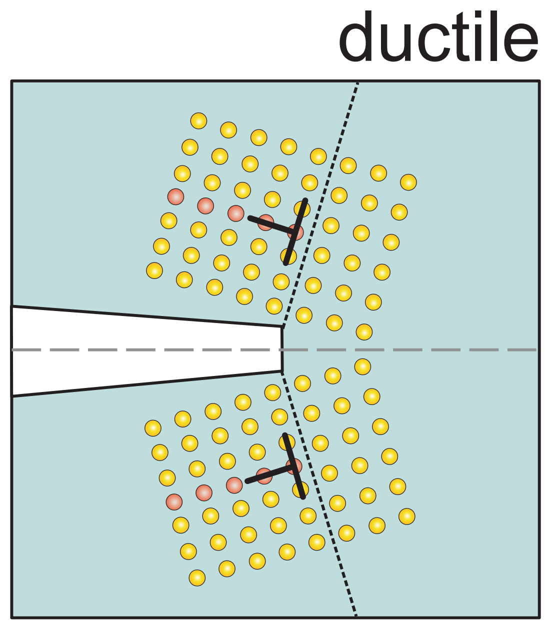


(Buehler *et al*., *MRS Proceedings*, 2004)

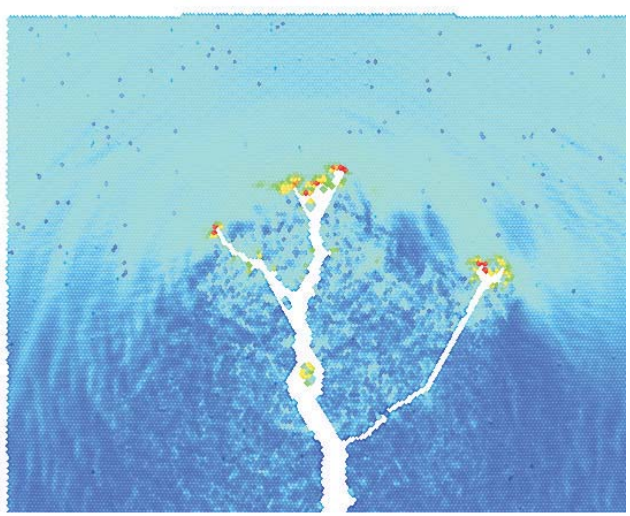
Ductile versus brittle materials

Glass,
Polymers,
Ice…

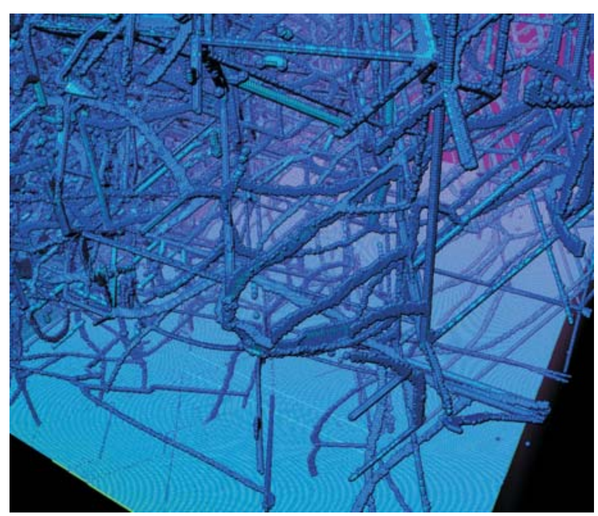




Copper,
Gold,
…

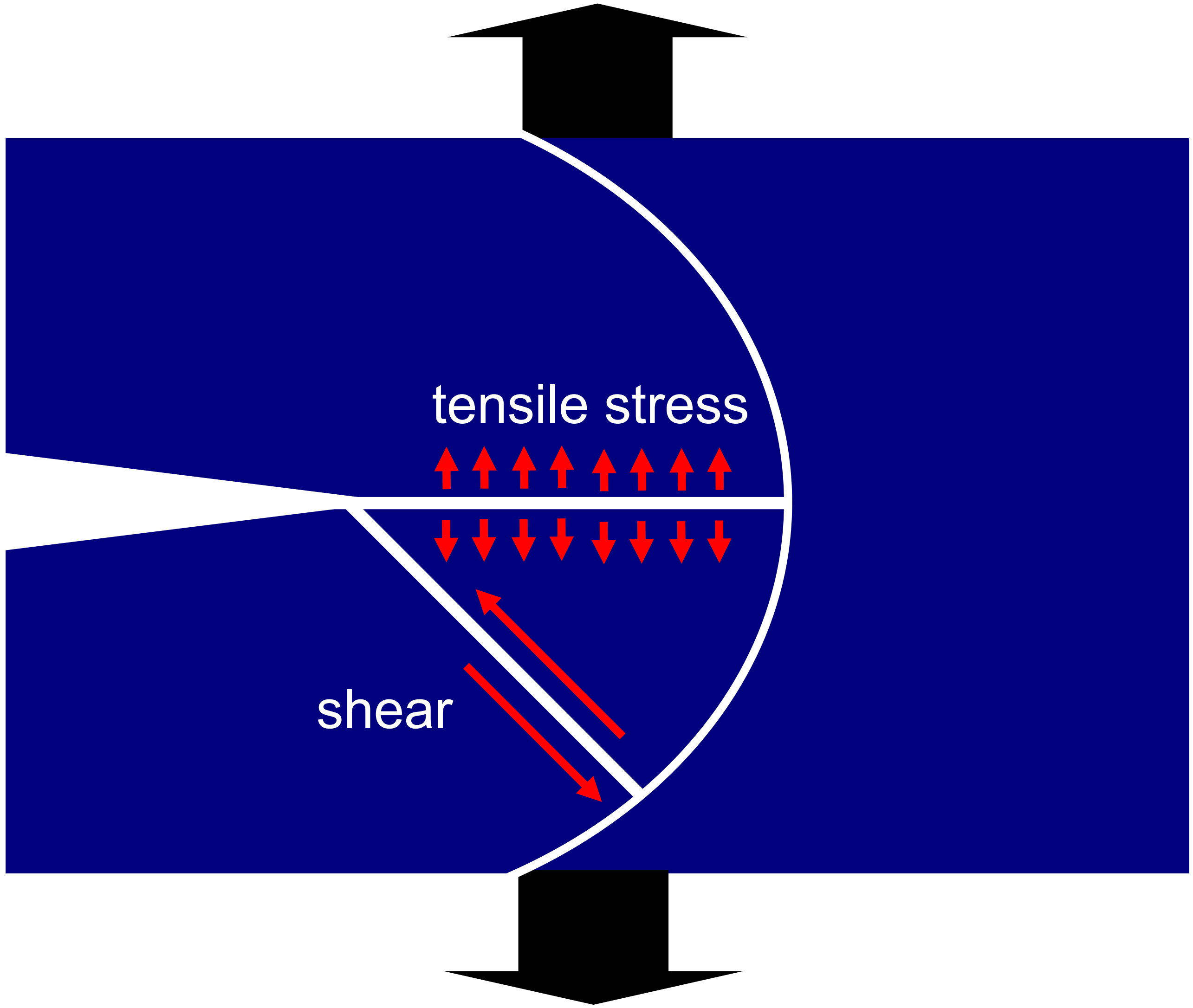


(a)



(b)

Schematic of stress field around a single (static) crack

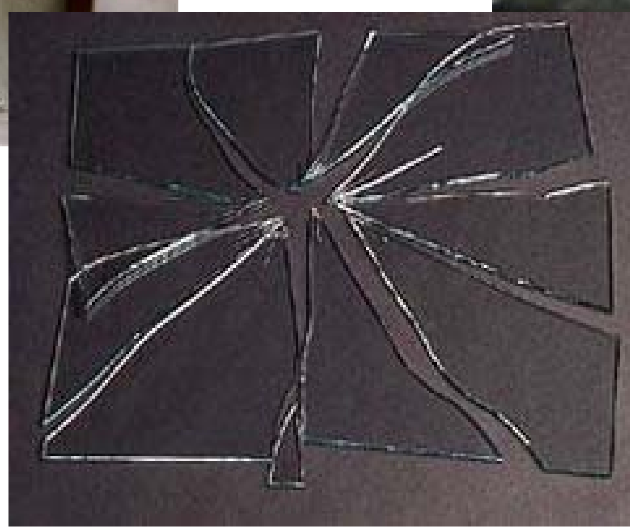


➢ The stress field around a crack is complex, with regions of dominating tensile stress (crack opening) and shear stress (dislocation nucleation)

Examples

http://simscience.org/cracks/advanced/image/cracked_concrete.jpg

http://www.wolispace.com/html/documents/pictures/glass/fracture.jpg



http://www.pilkington.com/resources/ord_glass.jpg

Dynamic fracture: Deals with cracks approaching the sound speed (km/sec)

Review: Brittle Fracture

Discrepancies theory-experiment-simulation

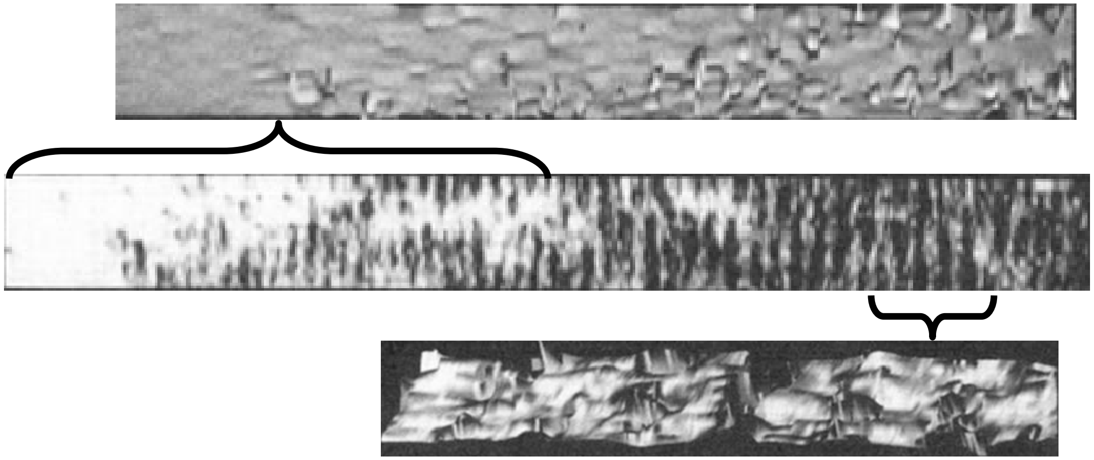
- Significantly reduced maximum crack speed in some experiments and simulation compared to theory prediction (Freund, 1990)

- 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.



Open questions in dynamic fracture

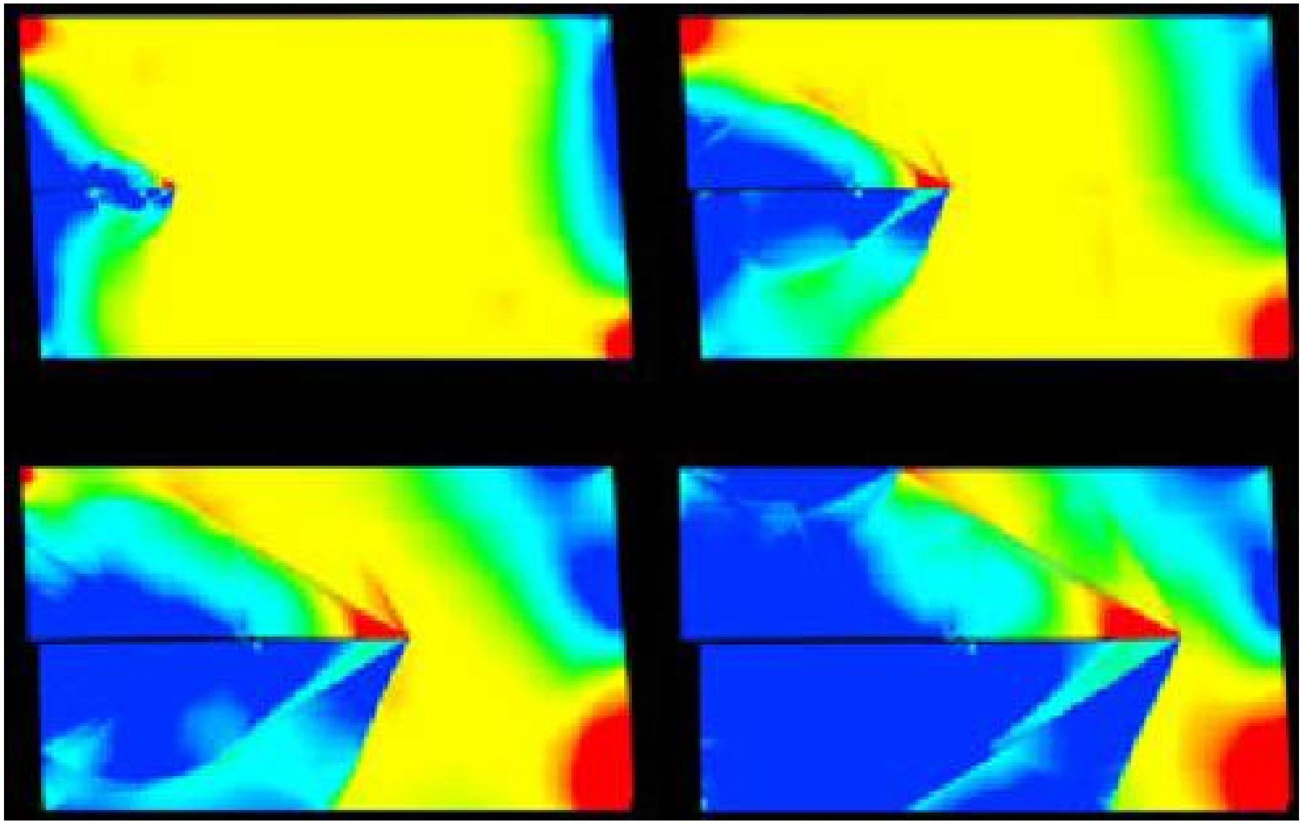
(1) How fast can cracks propagate?

(2) Mechanisms and physics of dynamic crack tip instabilities?

(3) Dynamics of cracks at materials interfaces

- Here: Use joint continuum-atomistic approach to address these questions

(4) Challenge: Concepts in coupling continuum theory-atomistic simulation



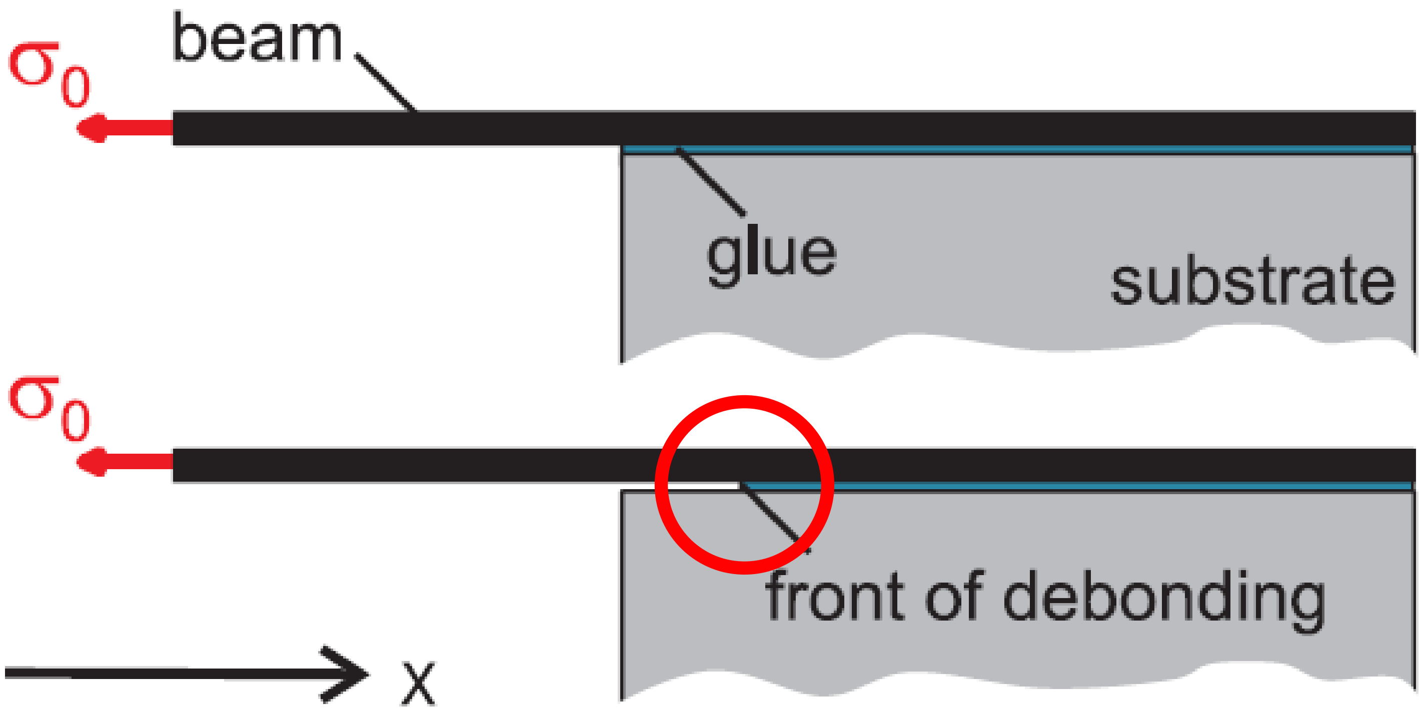
Section A:

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.

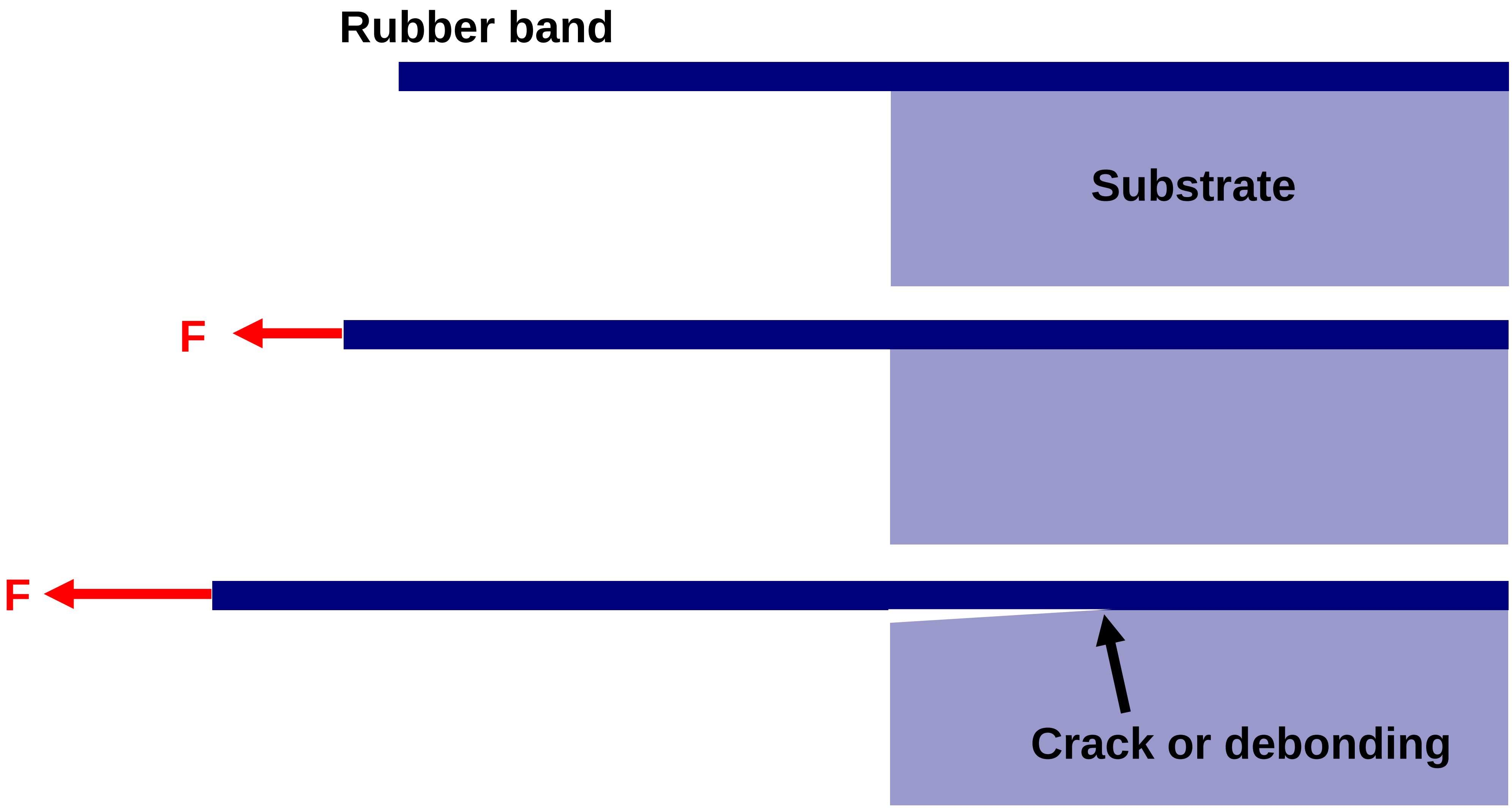
Theoretical model of 1D fracture



- 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

K. Hellan, Introduction to Fracture Mechanics, McGraw Hill Book Co., New York

Crack motion in the 1D model

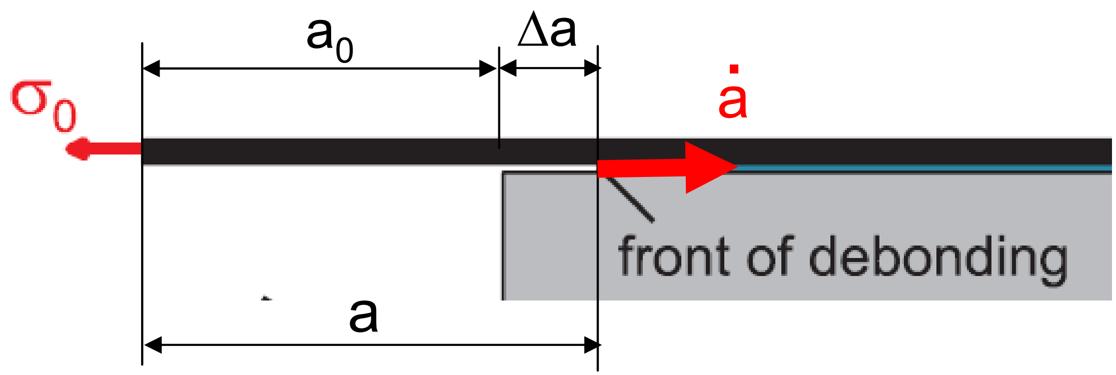


Continuum mechanical model (i)

$$\frac{\partial \sigma}{\partial x} = \rho \frac{\partial^2 u}{\partial t^2}$$

Equation of motion

(*F=ma*)



Using Hooke's law:

$$\sigma = E\varepsilon = E\frac{\partial u}{\partial x}$$

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

u(*x*,*t*): Displacements

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

c_0 wave speed

Solutions for this equation:

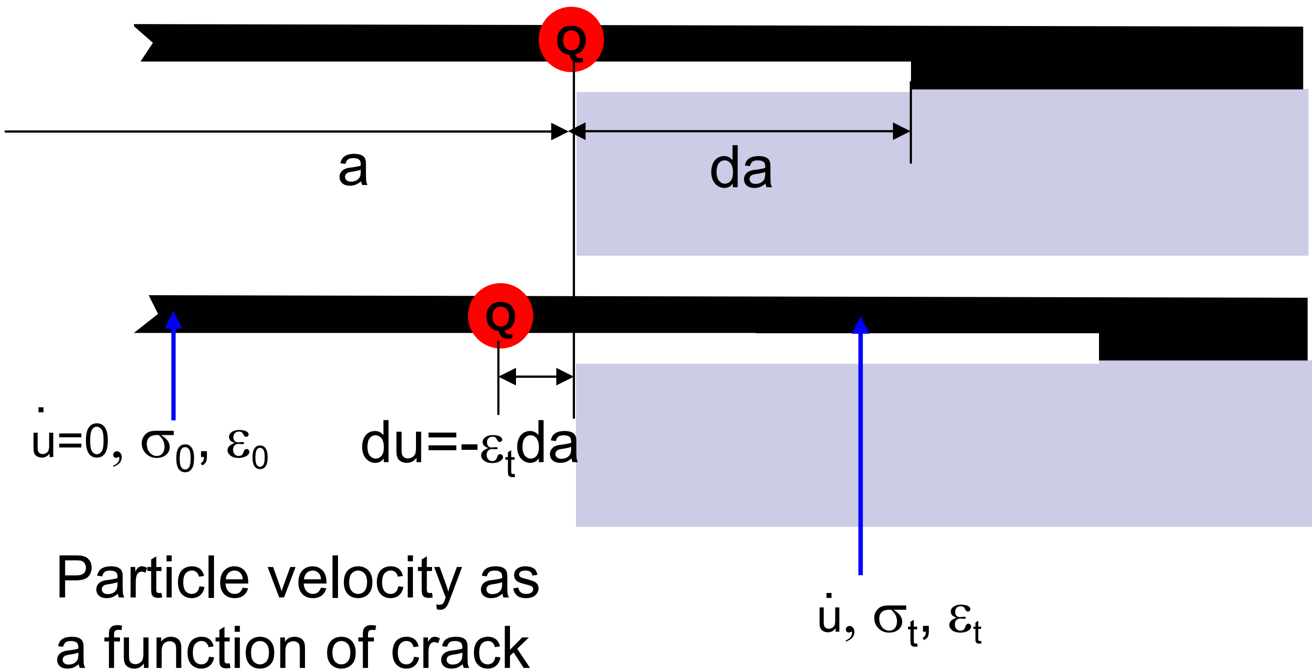
$$u = f(x \mp c_0 t) = f(\xi)$$

Signals traveling through the material with constant speed and profile

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

$$\dot{u} = \mp c_0 \frac{\partial f}{\partial \xi} = \mp c_0 H(x \mp c_0 t) = \mp \frac{c_0}{E}\sigma$$

Continuum mechanical model (ii)



$$\dot{u} = -\varepsilon_t \dot{a} = -\frac{\dot{a}}{E}\sigma_t \qquad (1)$$

$$\sigma_t = \sigma_0 + \sigma_e \qquad (2)$$

$$\dot{u} = \frac{c_0}{E}\sigma_e \qquad (3)$$

Particle velocity as a function of crack speed

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

$$\sigma_e = -\frac{\alpha}{1+\alpha}\sigma_0 \qquad \sigma_t = \frac{1}{1+\alpha}\sigma_0$$

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

$$\varepsilon_t = \frac{1}{1+\alpha}\frac{\sigma_0}{E}$$

$$\varepsilon_t/\varepsilon_0 = \frac{1}{1+\alpha}$$

Strain field left behind of moving crack

$$\alpha = \dot{a}/c_0$$

Crack speed: Unknown

Continuum mechanical model (iii)

Crack speed remains unknown

Use energy balance:

External work (≈0)

Change in potential energy per unit crack extension

$$G = W - \frac{\mathrm{d}T}{\mathrm{d}a} - \frac{\mathrm{d}\phi}{\mathrm{d}a} = R(\alpha)$$

Change in kinetic energy per unit crack extension

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

with

$$G_0 = \frac{\sigma_0^2}{2E}$$

$$g(\alpha) = \frac{1-\alpha}{1+\alpha} \qquad \frac{\sigma_0^2}{2E} = R_0 \qquad R(\alpha) = \frac{\sigma_0^2}{2E}\frac{1-\alpha}{1+\alpha}$$

R=fracture surface energy
R(α) 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)

$$G_0 g(\alpha) = R(\alpha)$$ with $$G_0 = \frac{\sigma_0^2}{2E}$$ $$g(\alpha) = \frac{1-\alpha}{1+\alpha}$$

>0 (fracture surface energy)

For

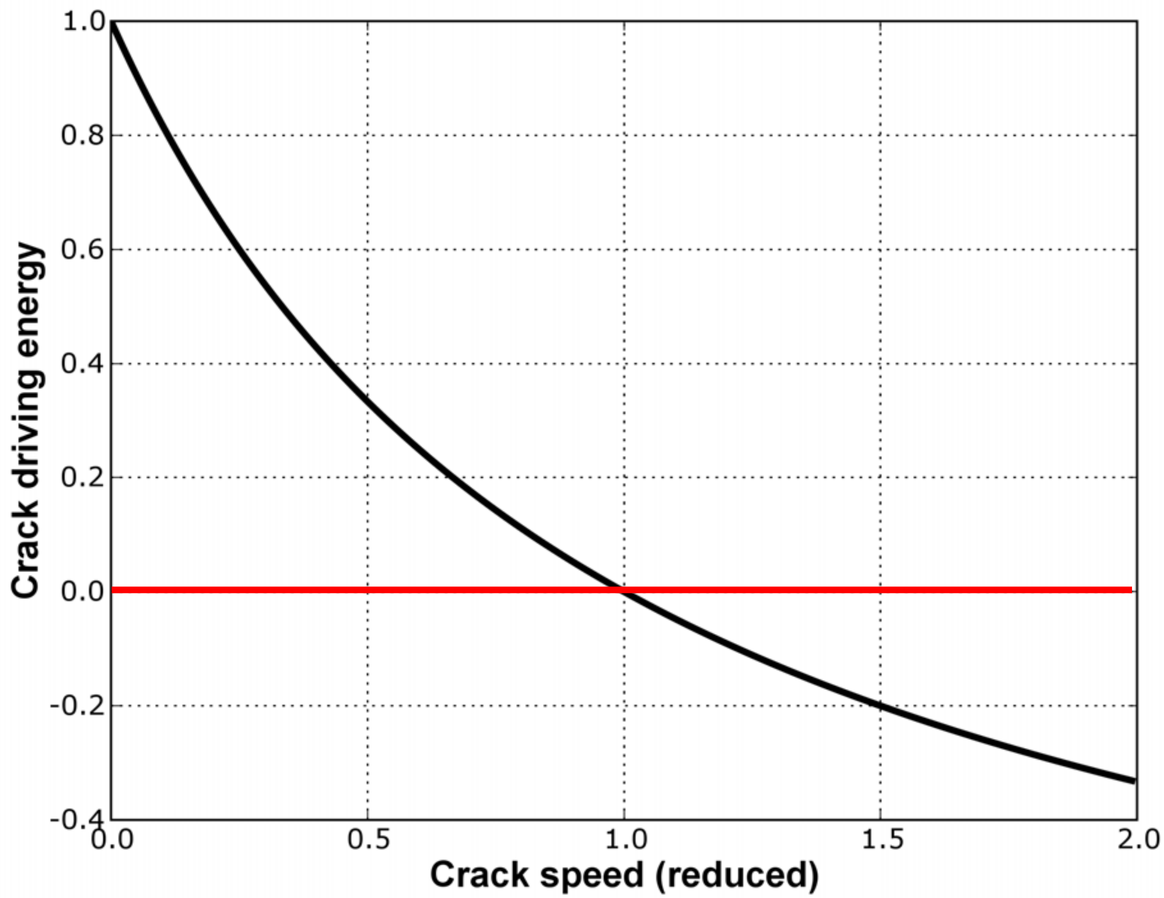
$$\alpha \to 1$$

the stress

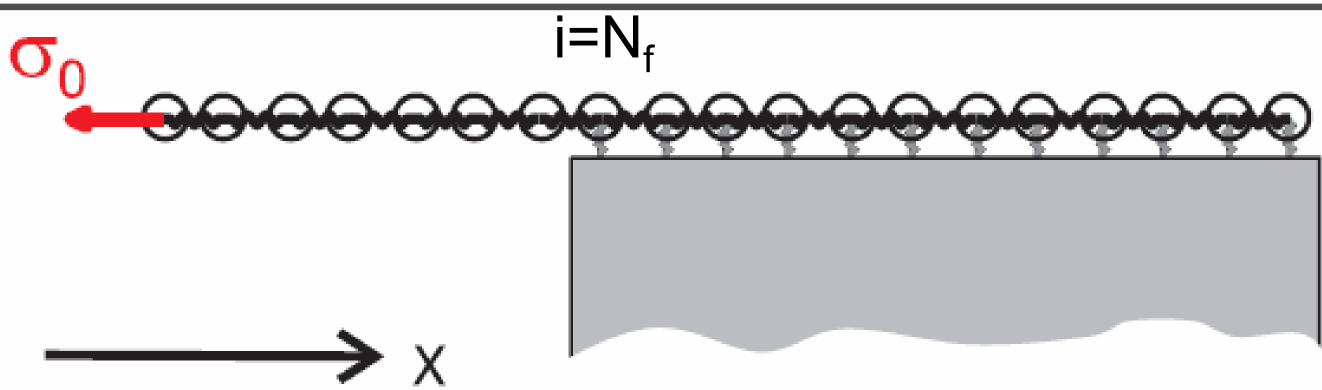
$$\sigma_0 \to \infty$$

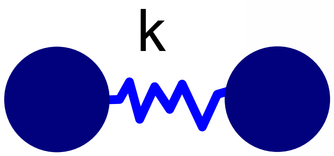
The wave speed c_0 is an upper limit for the crack speed

$$\alpha = \dot{a} / c_0$$



Atomistic model





weak atomic bonds

strong atomic bonds

Ca. 1,000 atoms
~ µm dimension

$$U = \sum_{i,j} \left(\frac{1}{2} k (r_{ij} - a_0)^2 \right) + \sum_i \left(\frac{1}{2} H(i - N_f) k_p \hat{r}_i^2 \right) \qquad \hat{r}_i = | x_{0,i} - x_i |$$

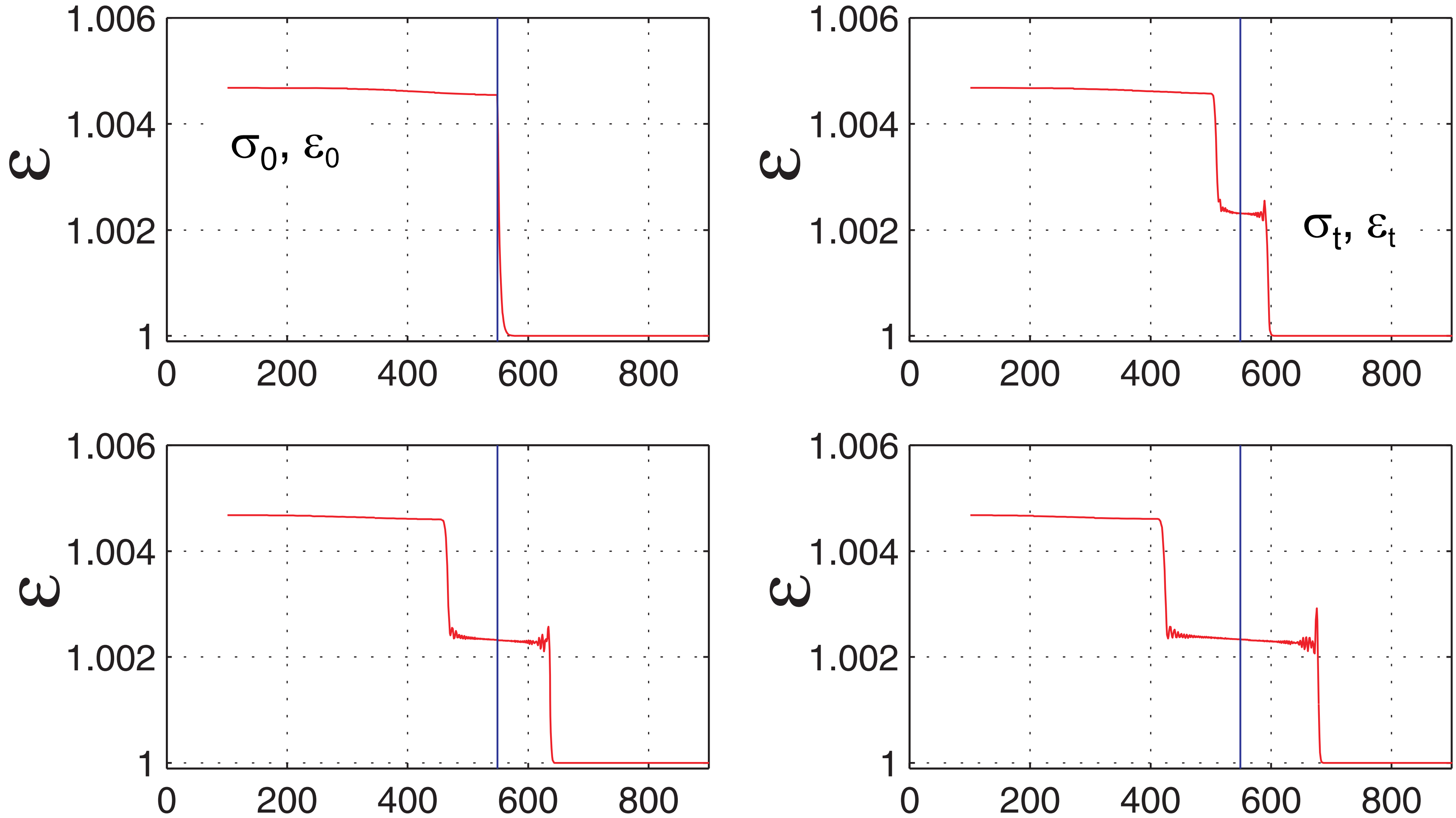
$$U = \sum_{i,j} \left(\frac{1}{2} k (r_{ij} - a_0)^2 \right) + \sum_i \left(\frac{1}{2} H(i - N_f) H(r_{\text{break}} - \hat{r}_i) k_p \hat{r}_i^2 \right)$$

$$R_0 = \frac{1}{2} \frac{k_p \hat{r}^2}{a_0} \qquad E = k\, a_0 \qquad c_0 = \sqrt{\frac{E}{\rho}} \qquad \varepsilon_i = \frac{x_{i-1} - x_{i+1}}{2\, a_0}$$

Atomic strain

Solved using standard MD methods

Compare: Strain field close to crack
Atomistic-continuum

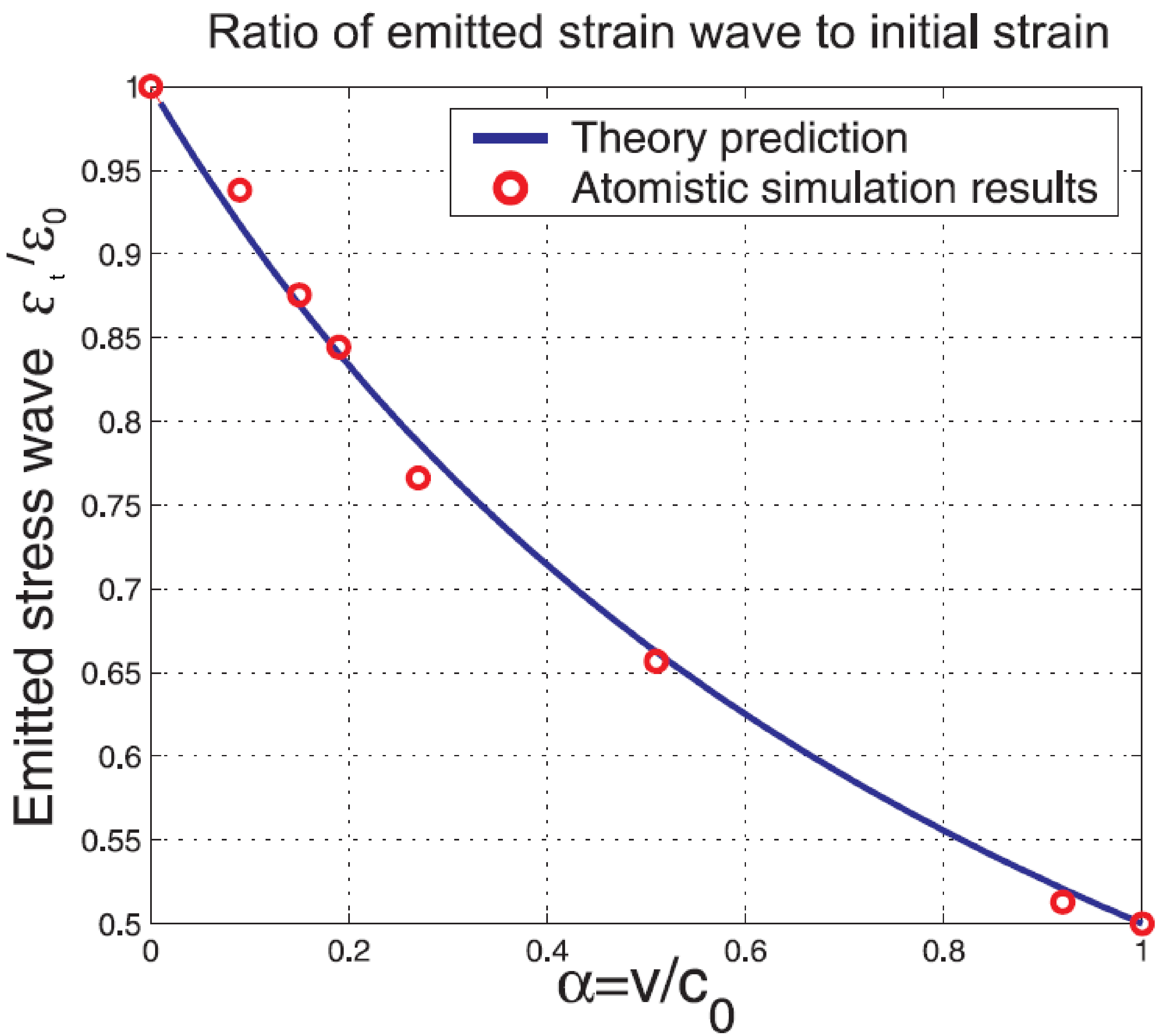


$$\sigma_t = \sigma_0 + \sigma_e$$

Compare: Strain field close to crack Atomistic-continuum

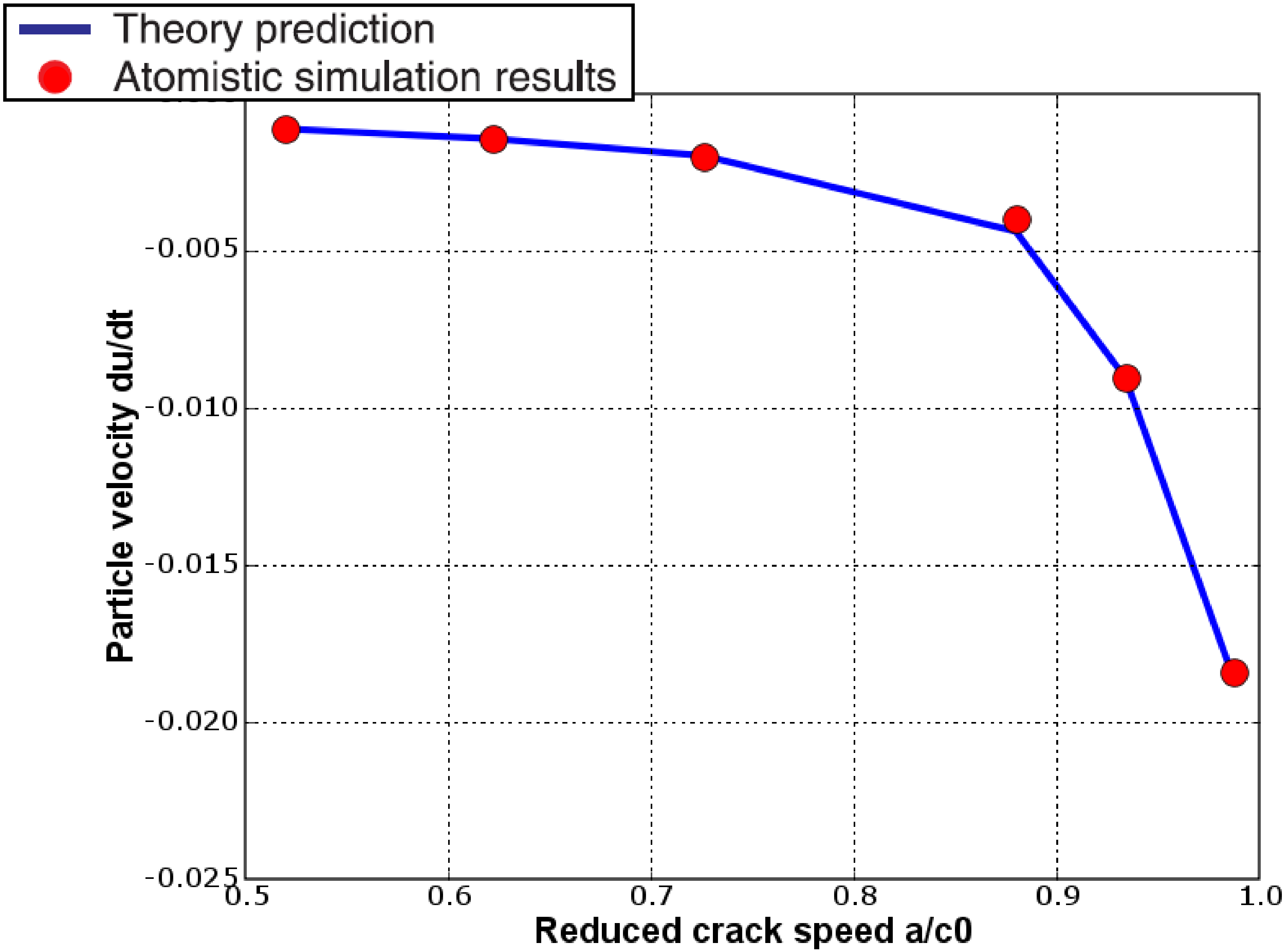
Prediction continuum model:

$$\varepsilon_t / \varepsilon_0 = \frac{1}{1+\alpha}$$

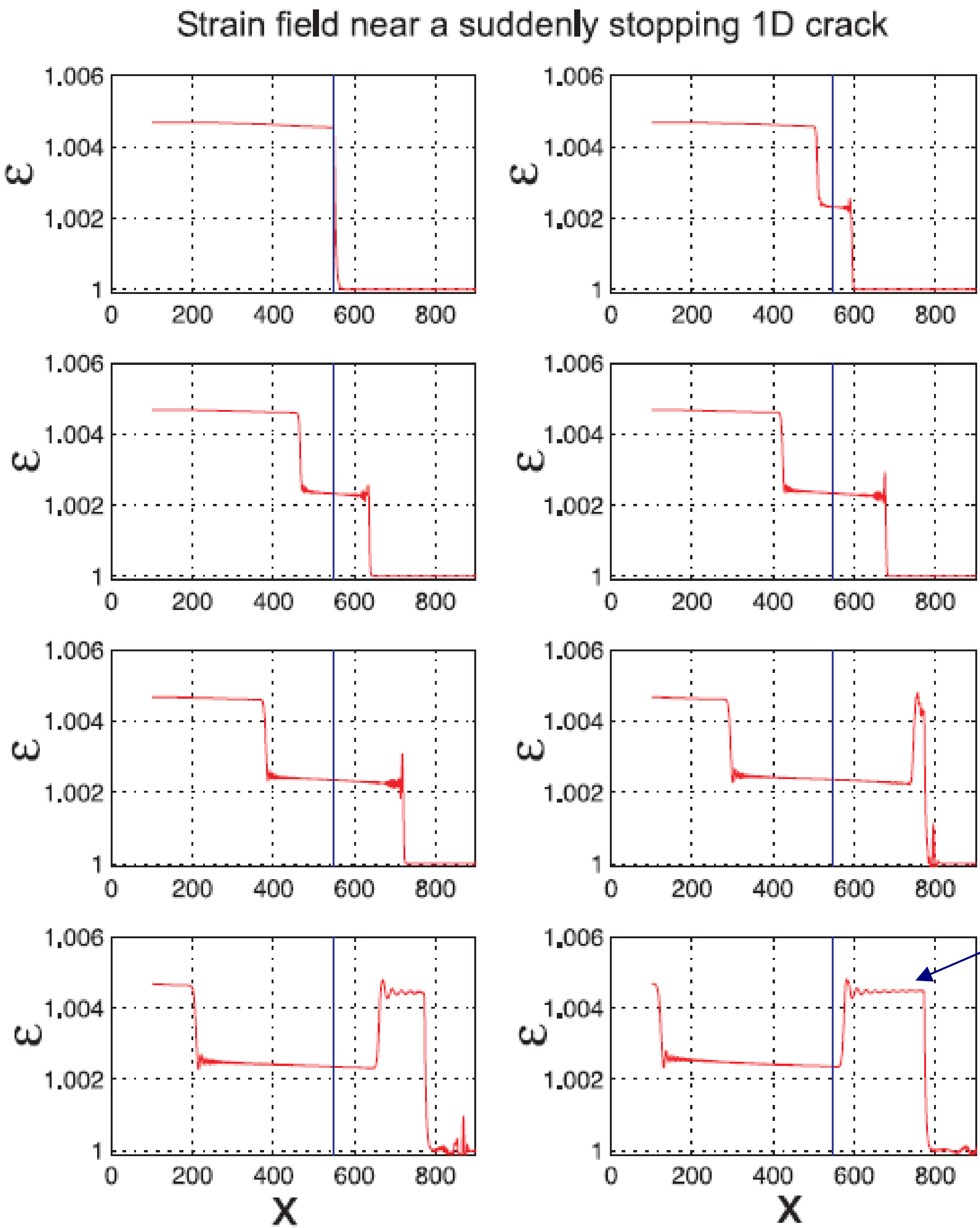


Compare: Particle velocity

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



Suddenly stopping 1D crack

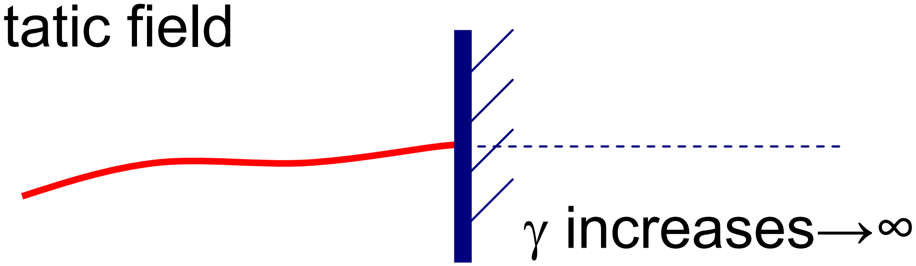


- Calculate strain field near a suddenly stopping 1D crack
- LEFM: Cracks do not have any inertia
(see also Buehler *et al*., 2003)

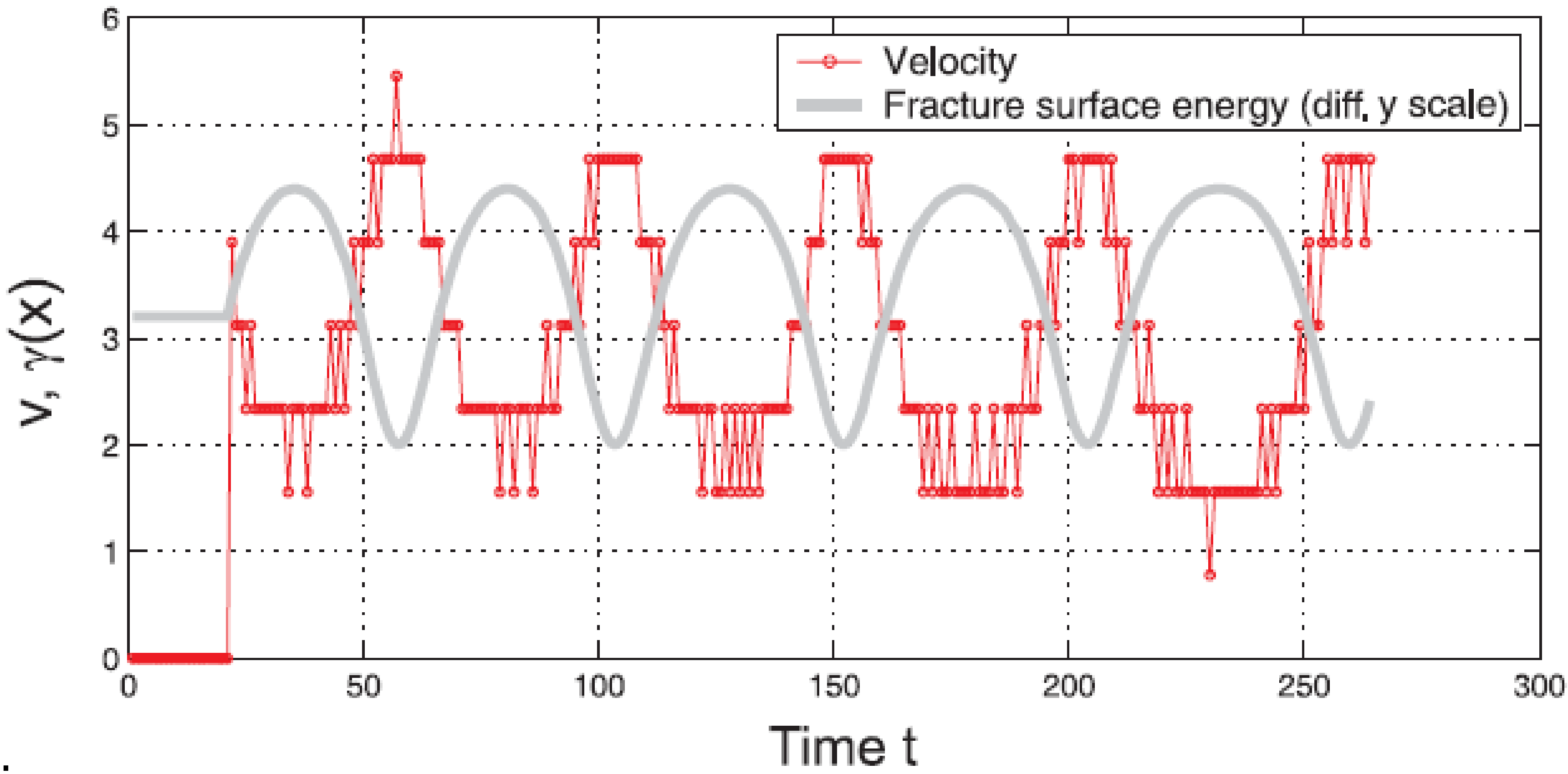
Result:

- Static stress field ($\varepsilon=\varepsilon_0$) spreads out as soon as crack stops

Static field



Periodically varying fracture surface energy

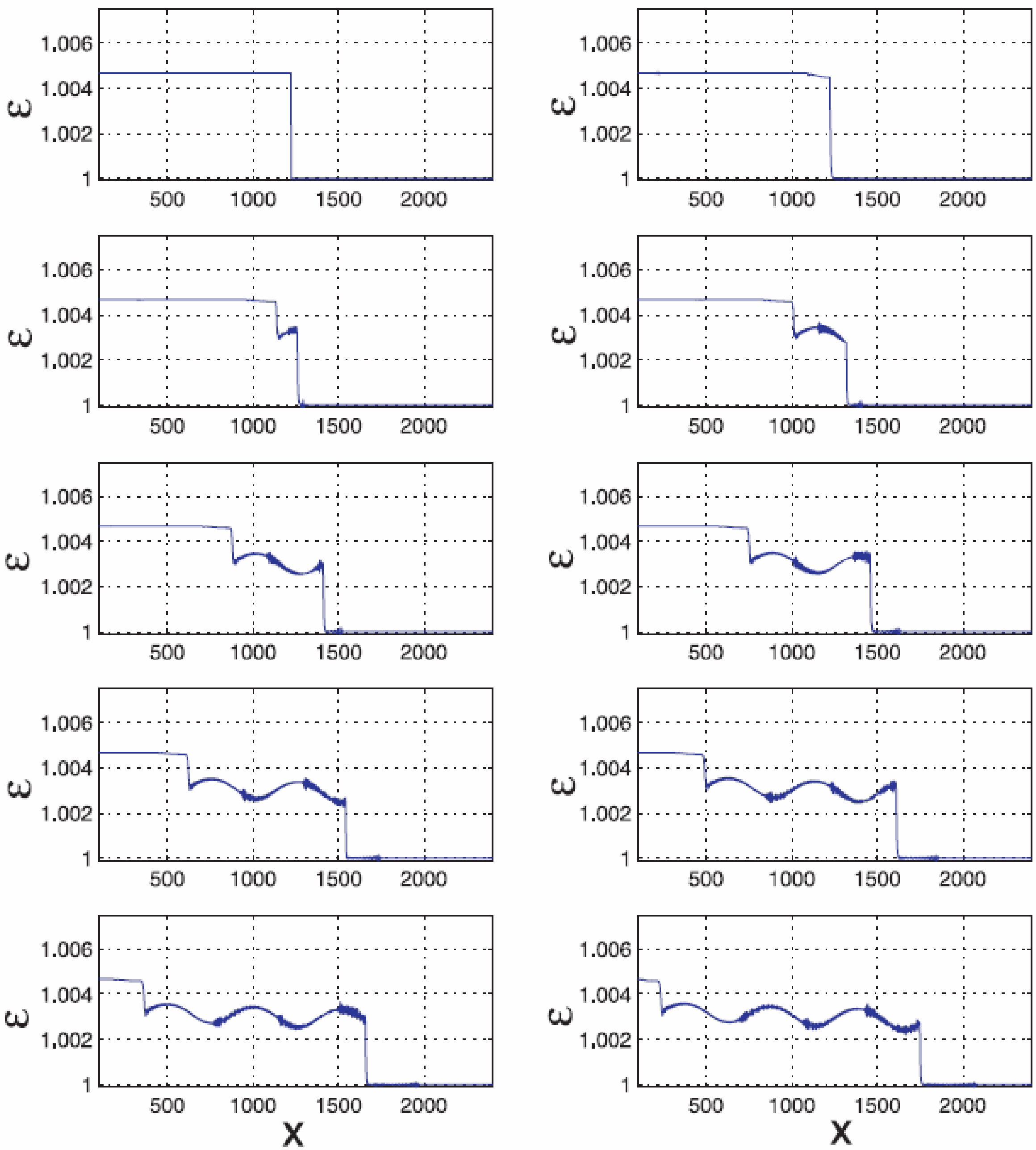


Predictions

$$\hat{r} = \hat{r}_0 + \Delta\hat{r}\,\sin(x/p)$$

$$v = \hat{v}_0 + \Delta v\,\sin(x/p)$$

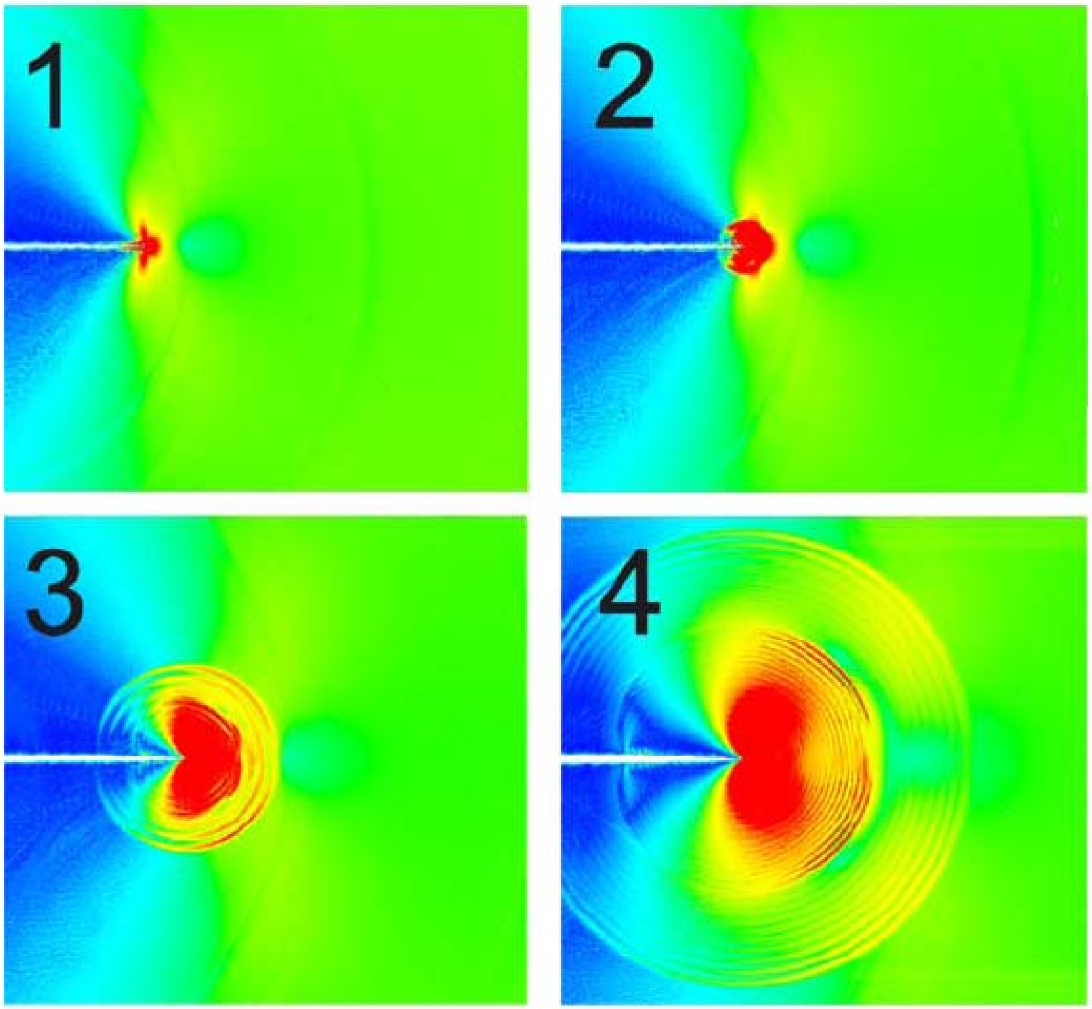
Strain field during oscillatory fracture energy



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

- In agreement with prediction, the emitted strain wave changes periodically

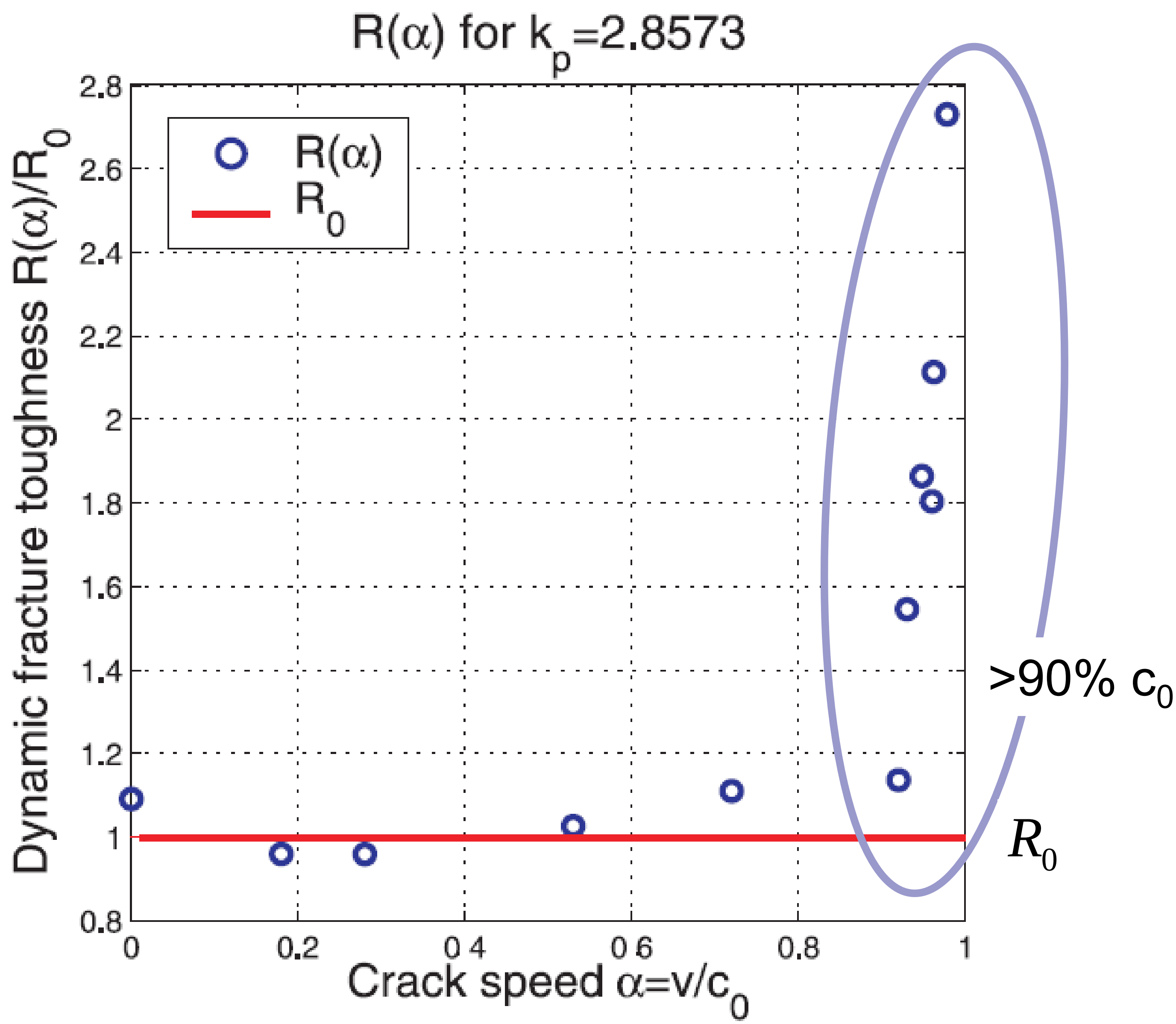
Suddenly stopping 2D crack



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



<u>Assume</u>: Constant dynamic fracture toughness

$$R_0 g(\alpha) = R(\alpha)$$

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

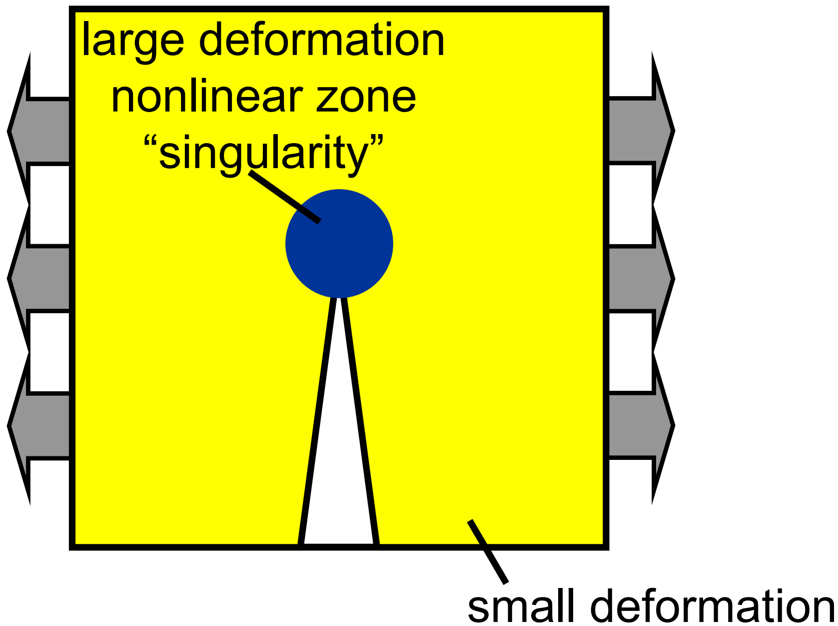
- Introduced nonlinear elastic behavior and showed importance of this for the dynamics of cracks: Hyperelasticity can govern dynamical fracture and may lead to supersonic fracture

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

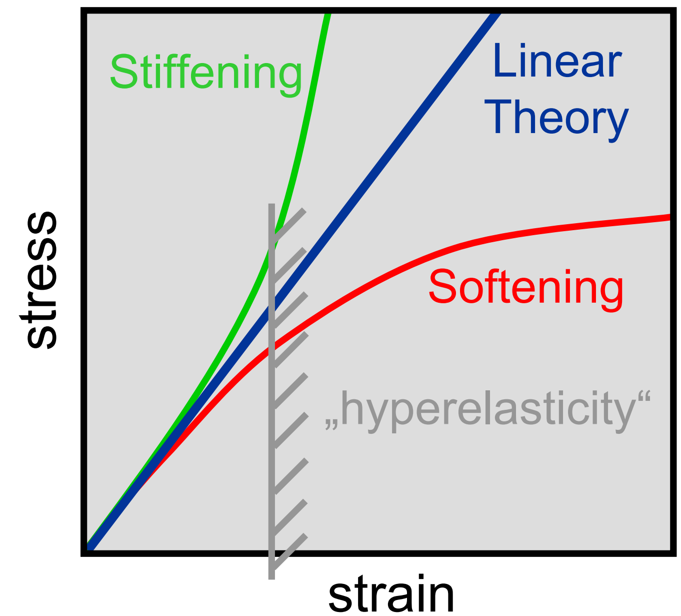
- Theory clearly predicts supersonic fracture

Brittle fracture in “real” materials

Deformation field near a moving crack



Elastic properties of
a piece of defect-free material



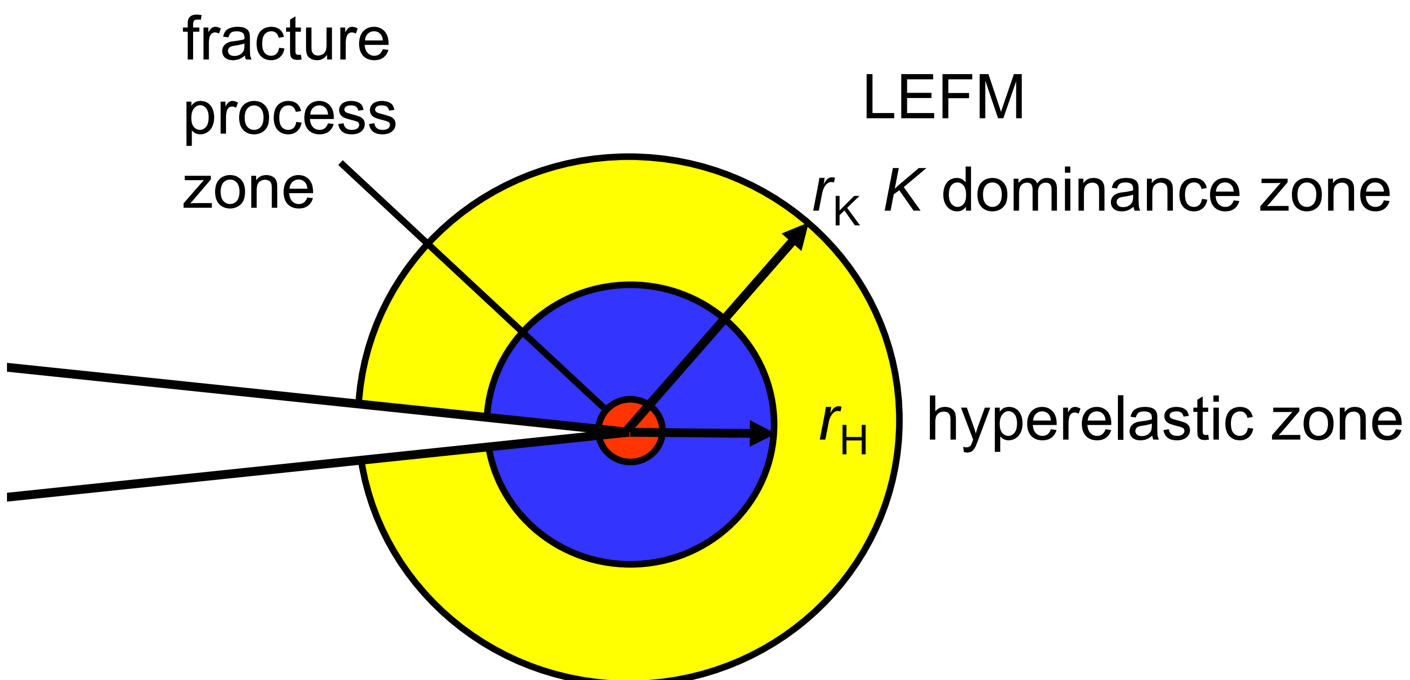
„local Young‘s modulus“
Therefore: „local wave speed“

Classical theory: Assume linear elastic material law

Poor approximation for “real” materials …

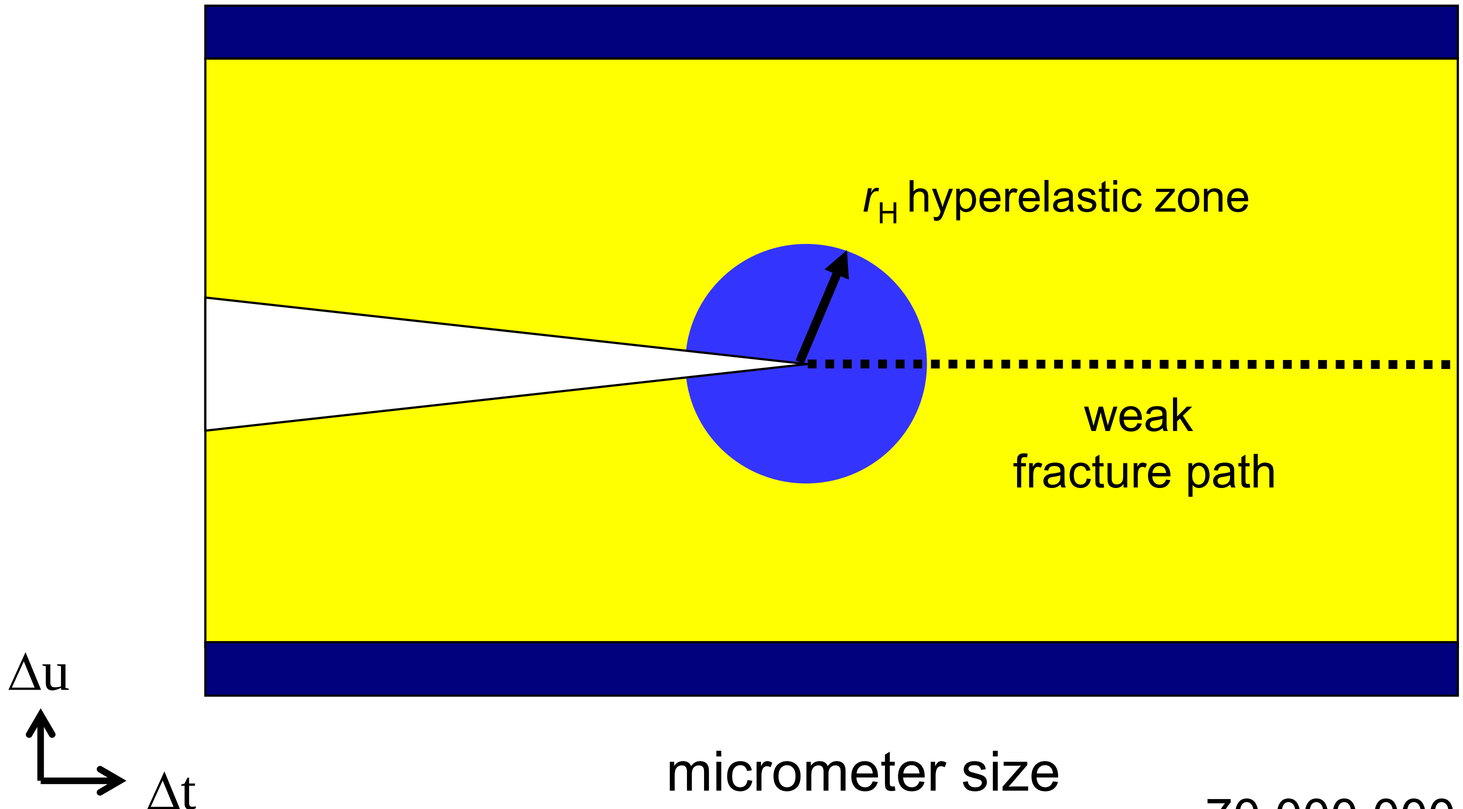
Hypotheses

- 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



micrometer size simulations

70,000,000 atoms

Strategy of Investigation

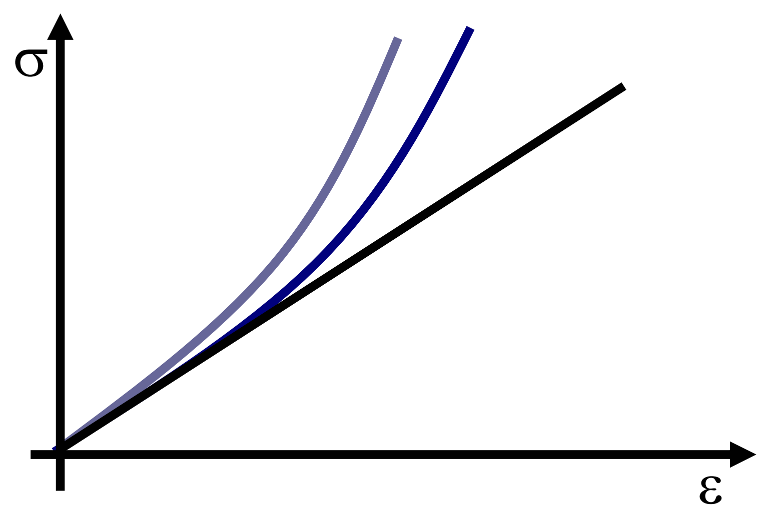
- Use LEFM theory as reference:

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

for mode I
< 0 for v > c_R

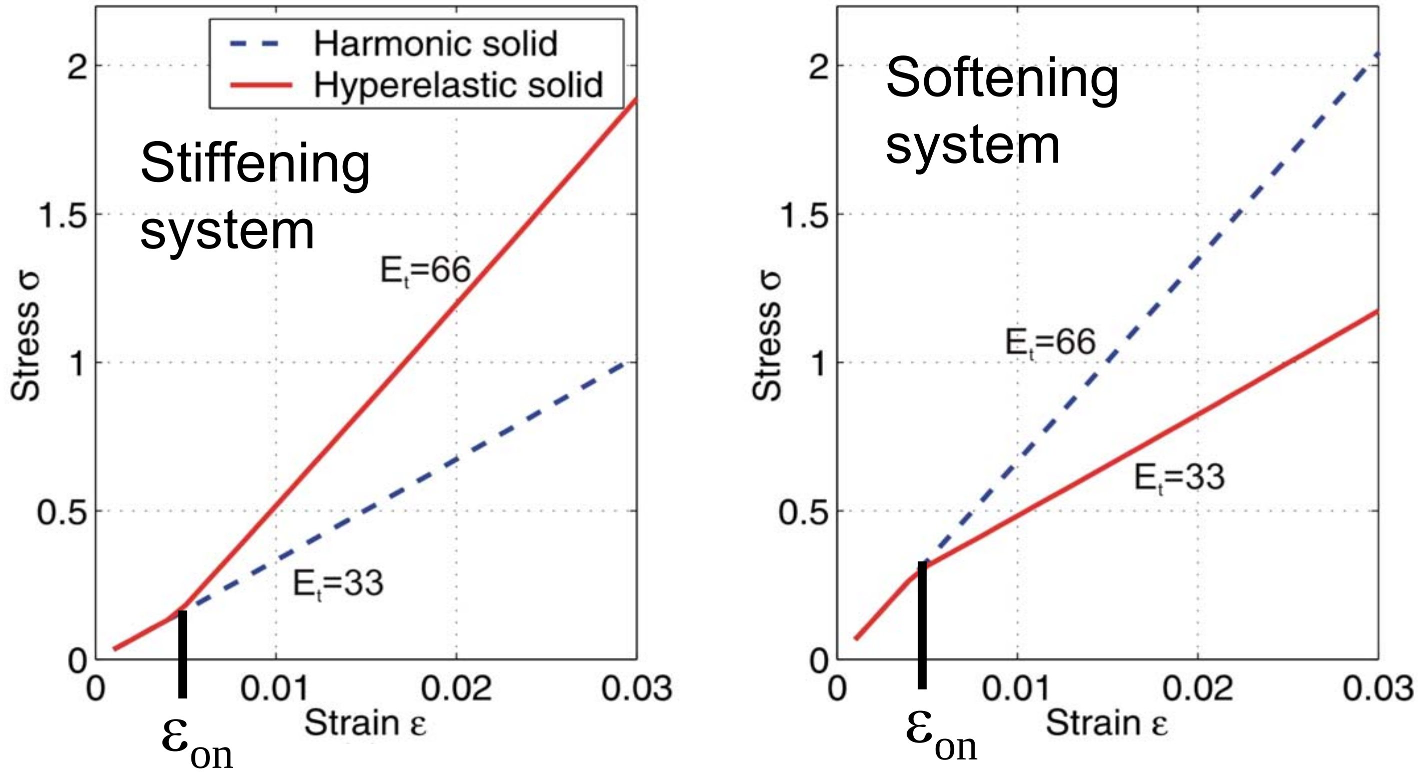
universal function

- Start with harmonic systems and show agreement with LEFM
- Then introduce (stronger) nonlinearities and observe difference



Simplistic bilinear "model material" for hyperelasticity

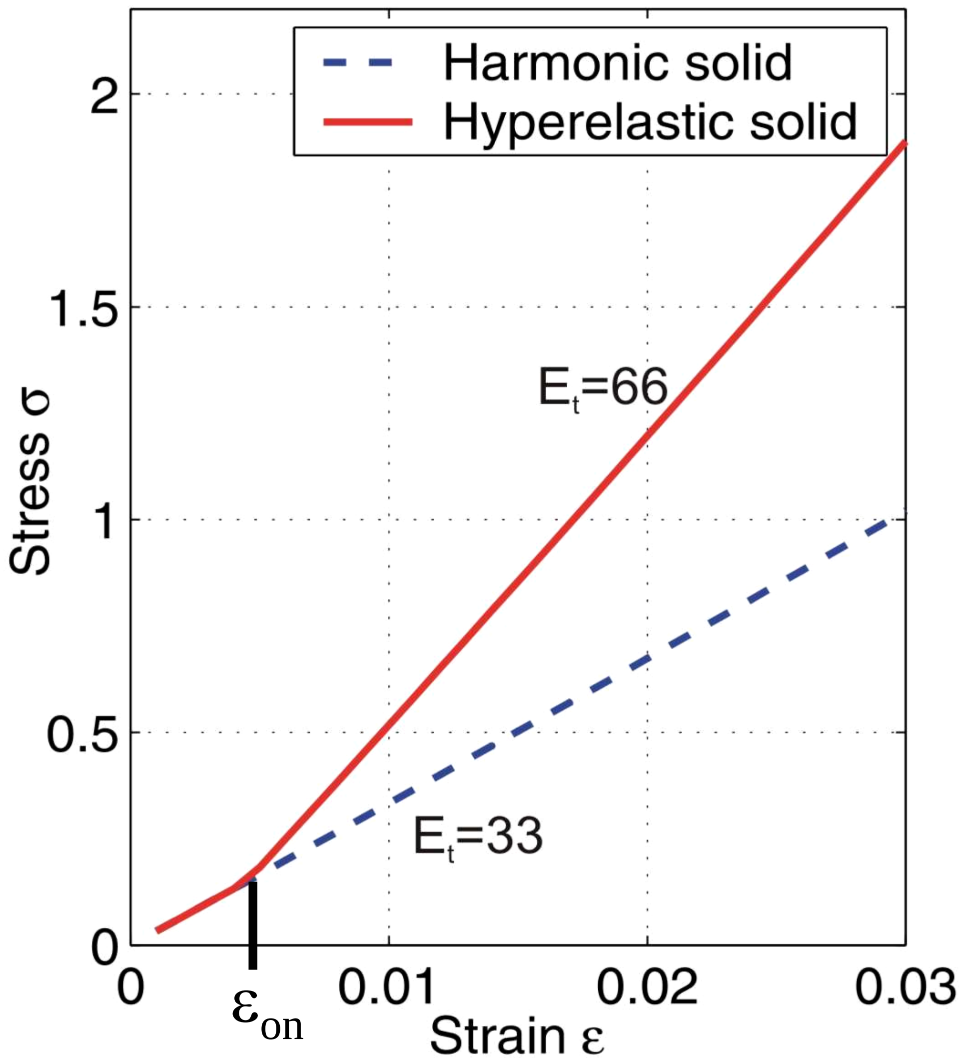
Objective:
Develop new potential that yields material properties common to a large class of real materials

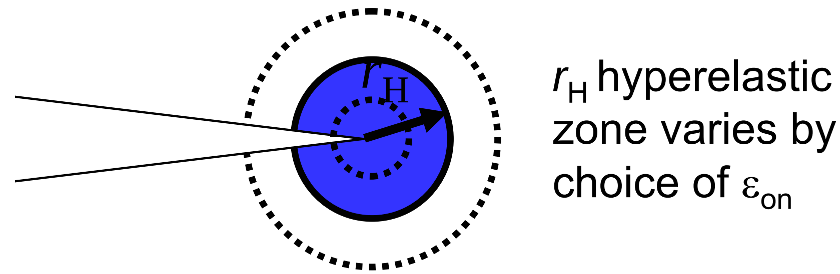


- Many accurate interatomic potentials for a variety of different brittle materials exist, many of which are derived form first principles
- However: Difficult to identify generic relationships between macroscopic potential parameters and macroscopic observables
- We deliberately avoid these complexities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

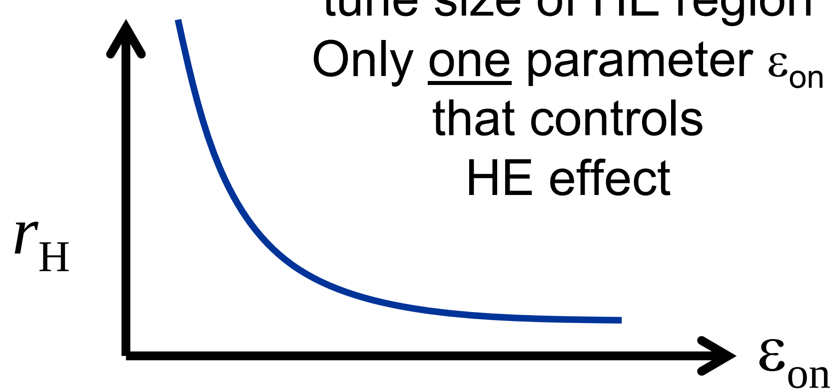
(Buehler *et al.*, Nature, 2003)

Simplistic bilinear "model material" for hyperelasticity





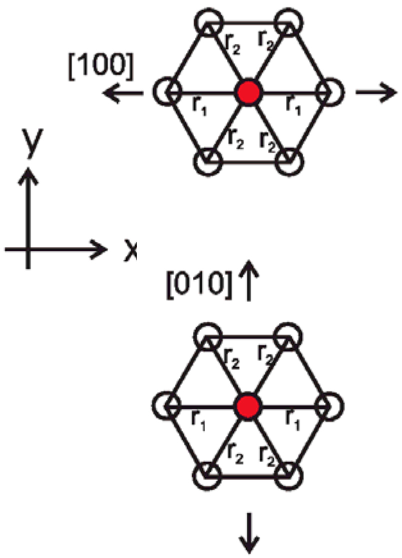
Biharmonic potential yields bilinear elastic behavior

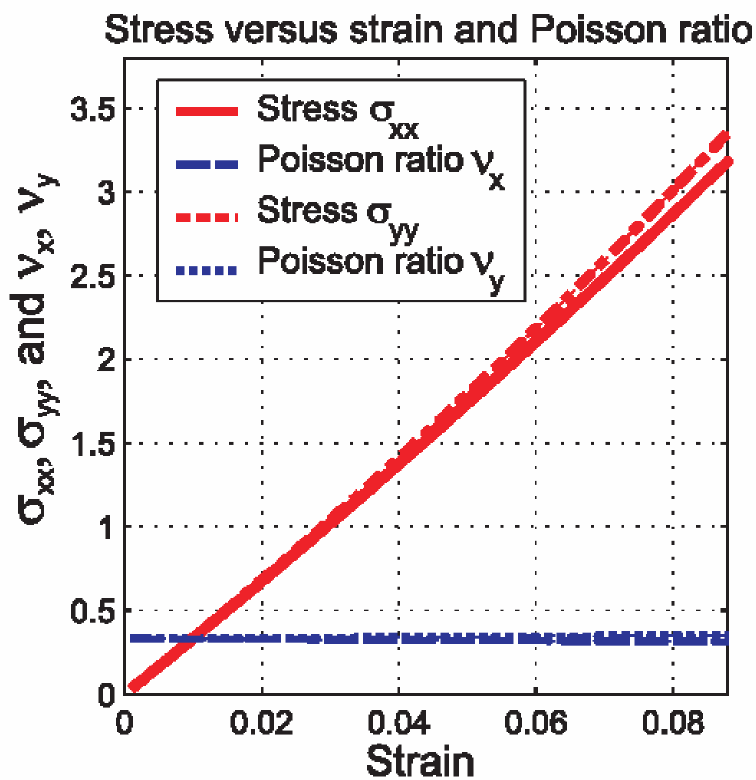


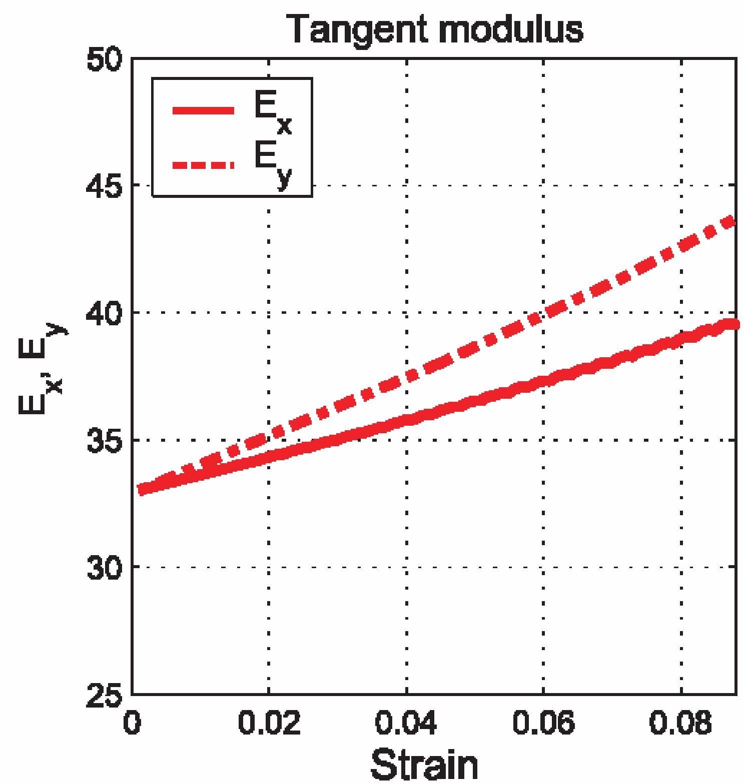
"tune size of HE region"
Only <u>one</u> parameter ε_{on} that controls HE effect

(Buehler *et al.*, Nature, 2003)

Atomistic model: Elasticity of harmonic systems







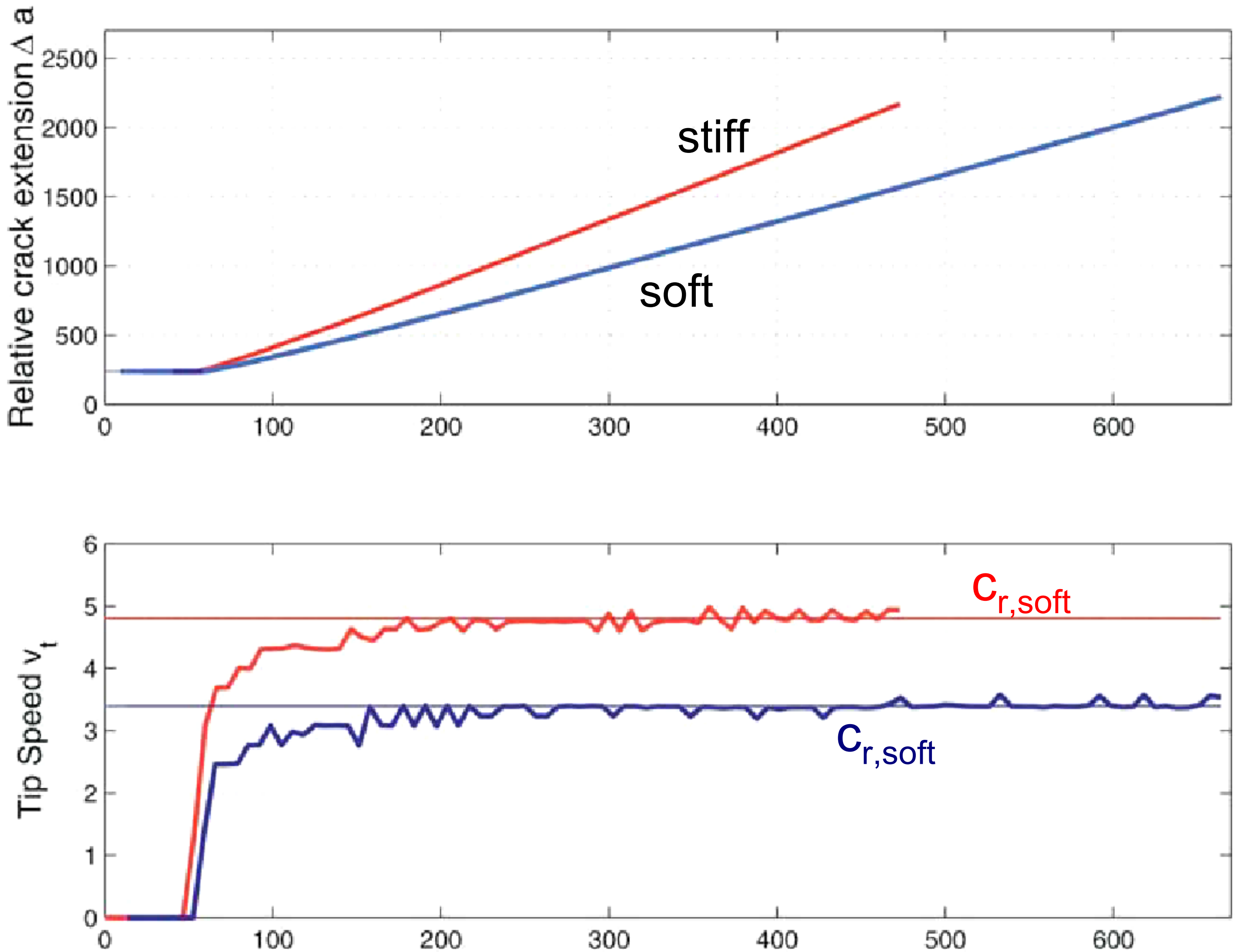
$$\phi_{ij}(r_{ij}) = a_0 + \frac{1}{2}k(r_{ij} - r_0)^2 \qquad E = \frac{2}{\sqrt{3}}k, \quad \mu = \frac{\sqrt{3}}{4}k$$

	k	E	μ	ν	c_l	c_s	c_r
Soft	$36\sqrt[3]{2} \approx 28.57$	33	12.4	0.33	6.36	3.67	3.39
Stiff	$72\sqrt[3]{2} \approx 57.14$	66	24.8	0.33	9	5.2	4.8

(Buehler, Doctoral Thesis, 2004)

Crack limiting speed: Harmonic systems

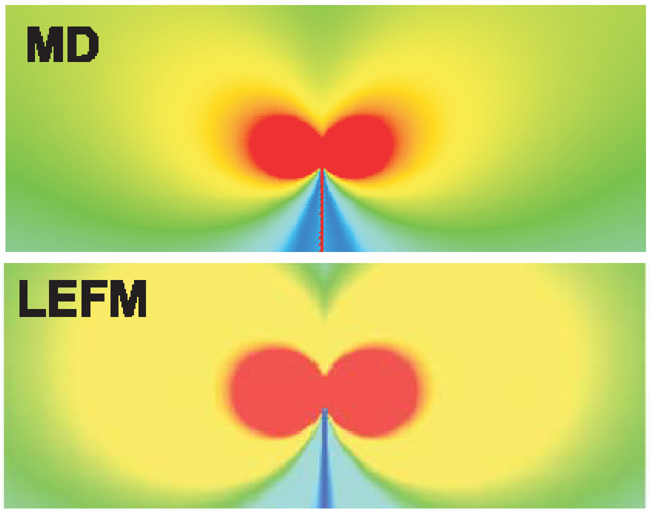
- The limiting speed of **mode I cracks** in soft and stiff reference systems is the Rayleigh-wave speed, in accordance with predictions



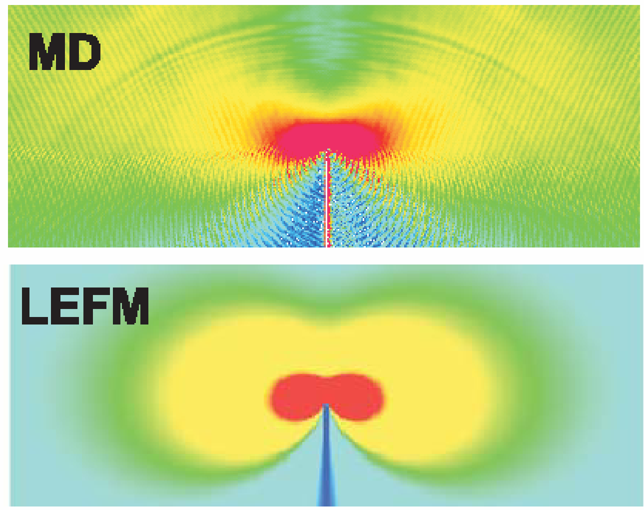
(Buehler, Gao, Huang, Theor. Appl. Fracture Mechanics, 2004)

Principal strain field at various crack velocities

$v/c_r=0$



$v/c_r=0.5$

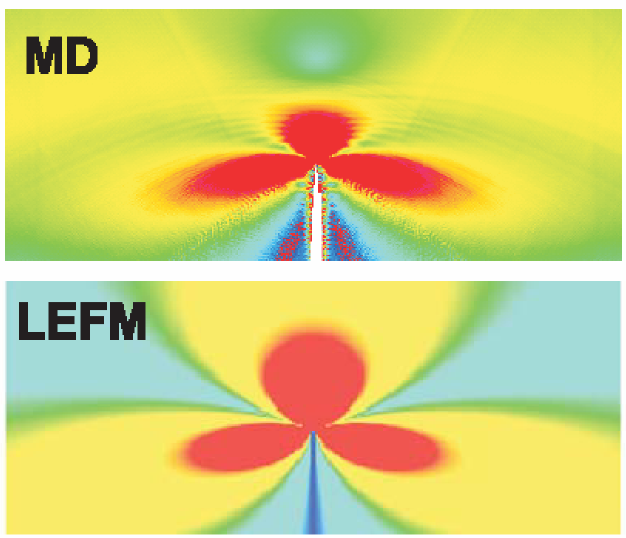


Atomic virial strain

$$q_{ij}^{l} = \frac{1}{N}\sum_{k=1}^{N}\left(\frac{\Delta x_i^{kl}\Delta x_j^{kl}}{r_0^2}\right)$$

$$b_{ij}^{l} = \frac{N}{\lambda}q_{ij}^{l} = \frac{1}{\lambda}\sum_{k=1}^{N}\left(\frac{\Delta x_i^{kl}\Delta x_j^{kl}}{r_0^2}\right)$$

$v/c_r=1$



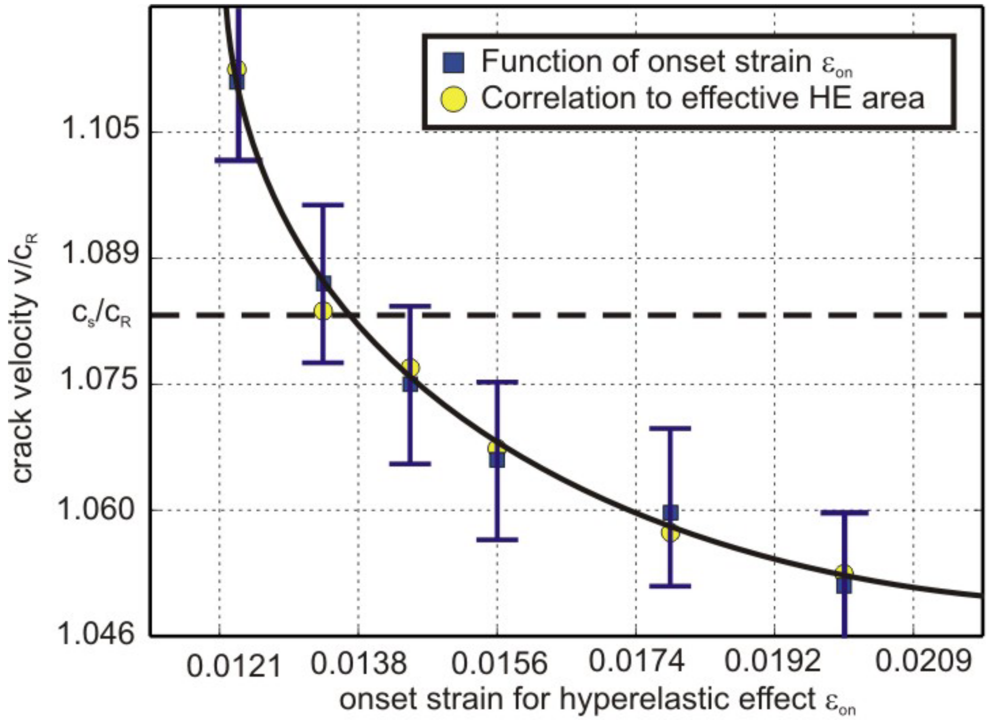
$$\sigma_{ij}(\Theta, v) = \frac{K_I(t,v)}{\sqrt{2\pi r}}\Sigma_{ij}(\Theta, v) + \sigma_{ij}^{(1)} + O(1)$$

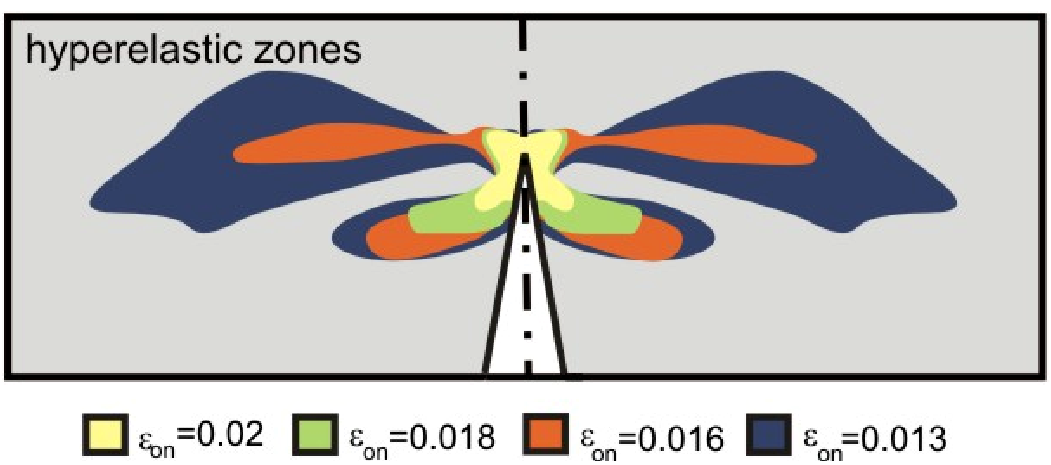
(e.g. Freund, 1990)

Result: Reasonable agreement

(Buehler, Gao, Huang; Theor. Appl. Fracture Mechanics, 2004)

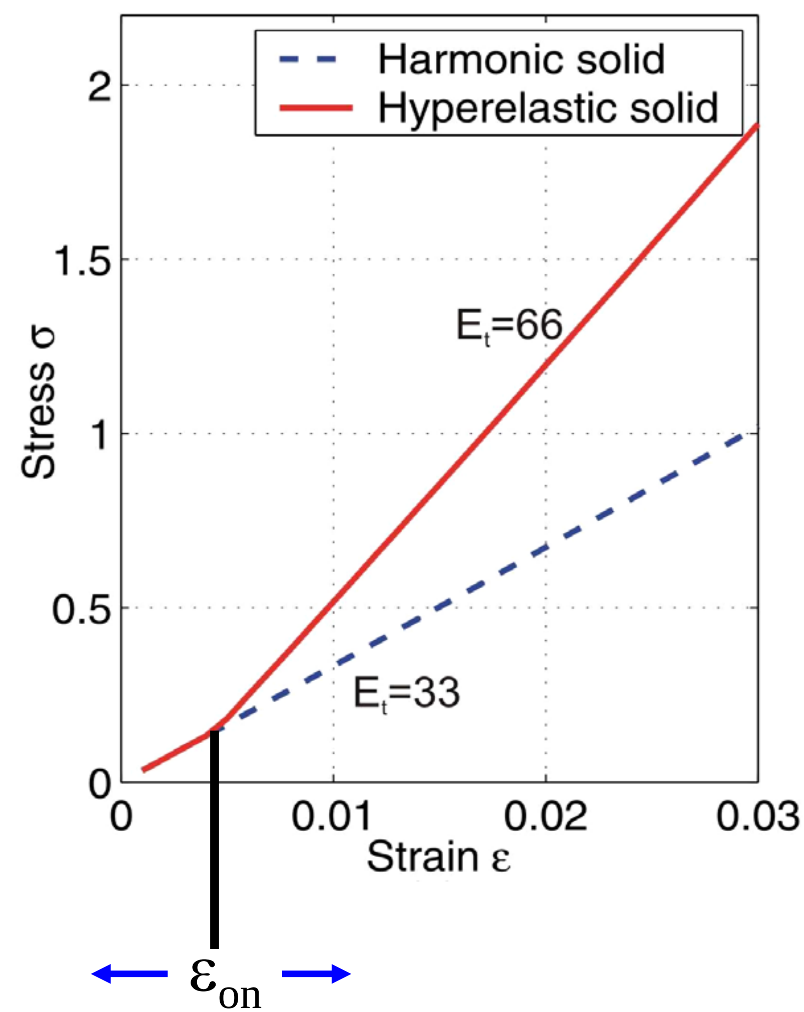
Hyperelasticity can change the crack speed





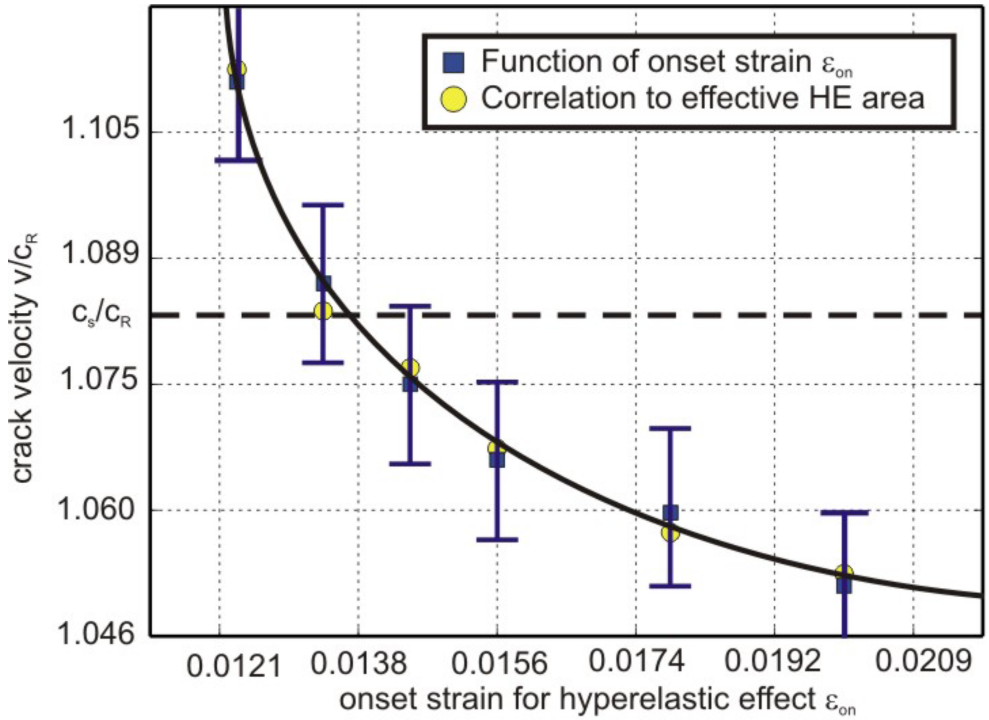
(Buehler *et al*., Nature, 2003)

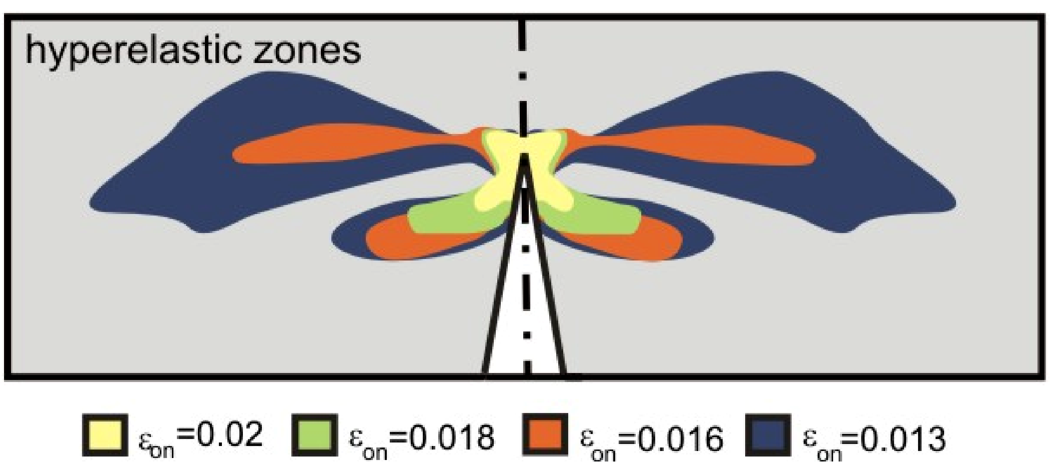
Breaking strain: 0.043



vary critical onset strain

Hyperelasticity can change the crack speed





(Buehler *et al*., Nature, 2003)

- ➢ 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

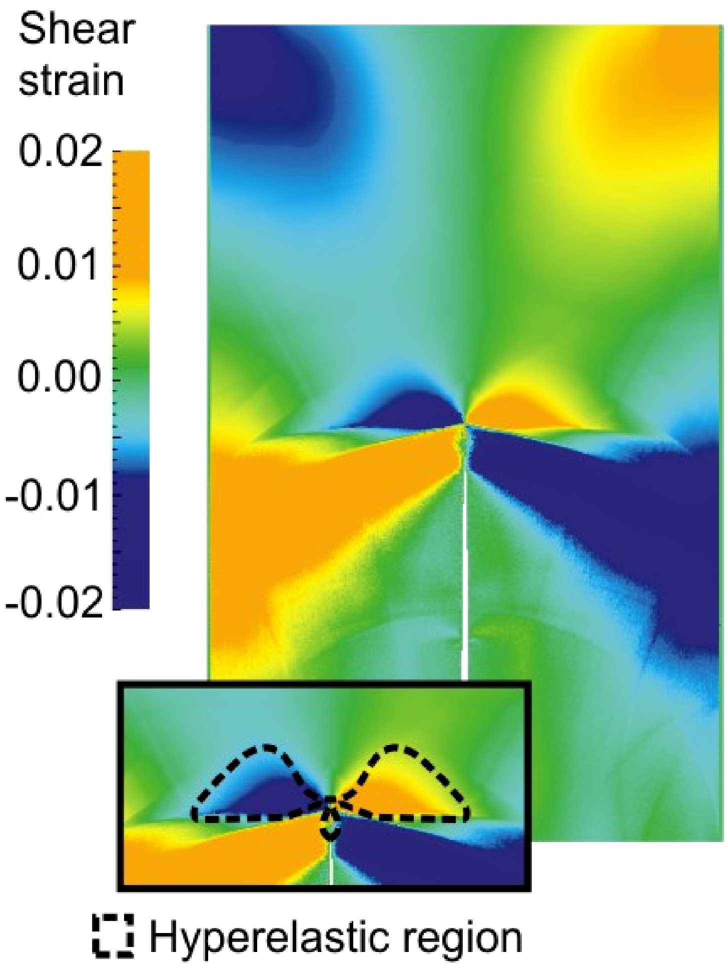
$$(1-\frac{v}{c_R})G_0 = 2\gamma$$

This suggests:

➢ The universal function $A(v/c_R)$ is incorrect !!

How fast can cracks propagate?

Mode I intersonic crack



• Mode I cracks faster than the shear wave speed

(Buehler *et al*., Nature, 2003)

Mode II supersonic crack

➢ Energy release rate is not zero even for supersonic cracking!! Universal function $A(v)$ of classical theories of fracture incorrrect!

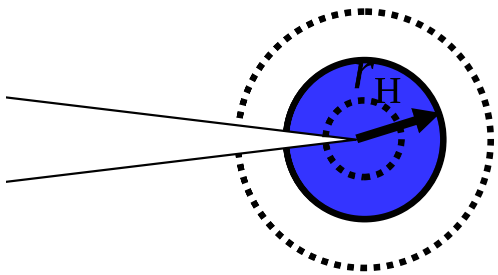
New concept: Energy characteristic scale

Dimensional analysis suggests that

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

c_1 und c_2 are wave speeds of linear elasticity and hyperelasticity
E_2 hyperelastic properties (large-strain elasticity); r_H size of HE region

Dynamic energy balance



$$G = 2\gamma$$

The crack velocity v can therefore be expressed as

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

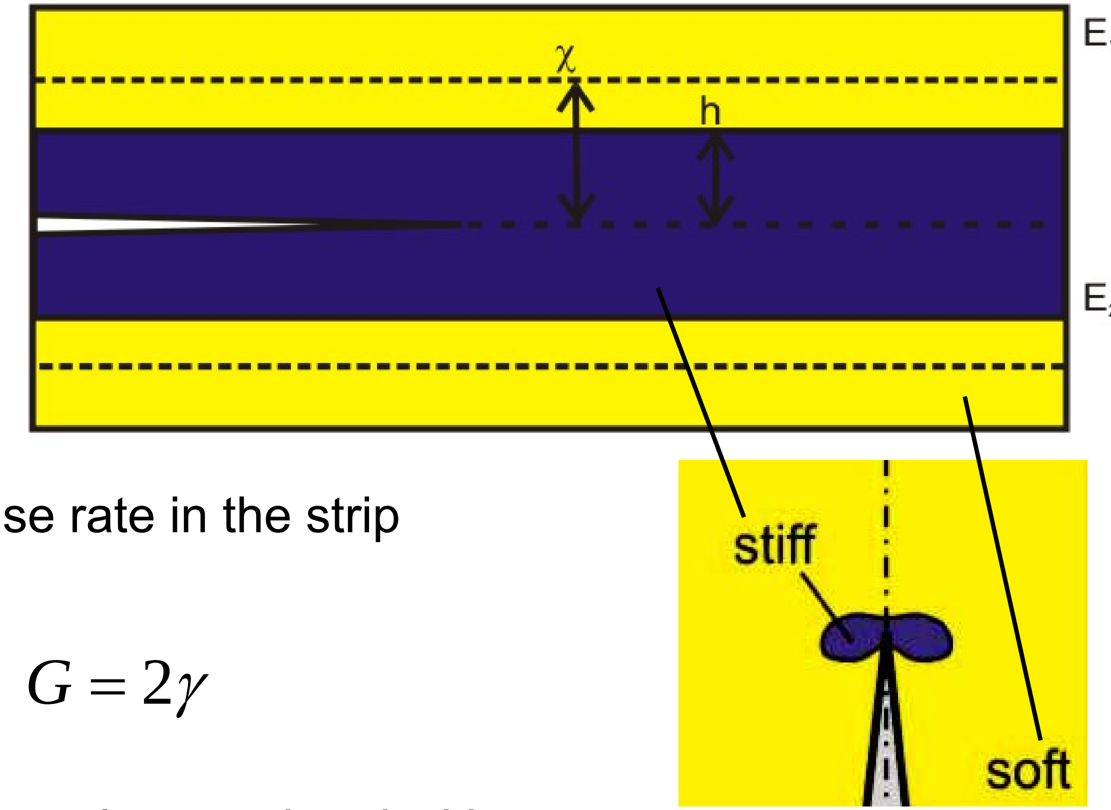
define $\chi \propto \gamma E / \sigma^2$ Has unit of length

This indicates that crack propagation velocity is a function of the ratio r_H / χ

Obtaining *f* for the hyperelastic case is very difficult…

New concept: Energy characteristic scale

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 $G = 2\gamma$

$$\chi \propto \gamma E / \sigma^2$$ Characteristic length scale associated with energy flux to the crack tip

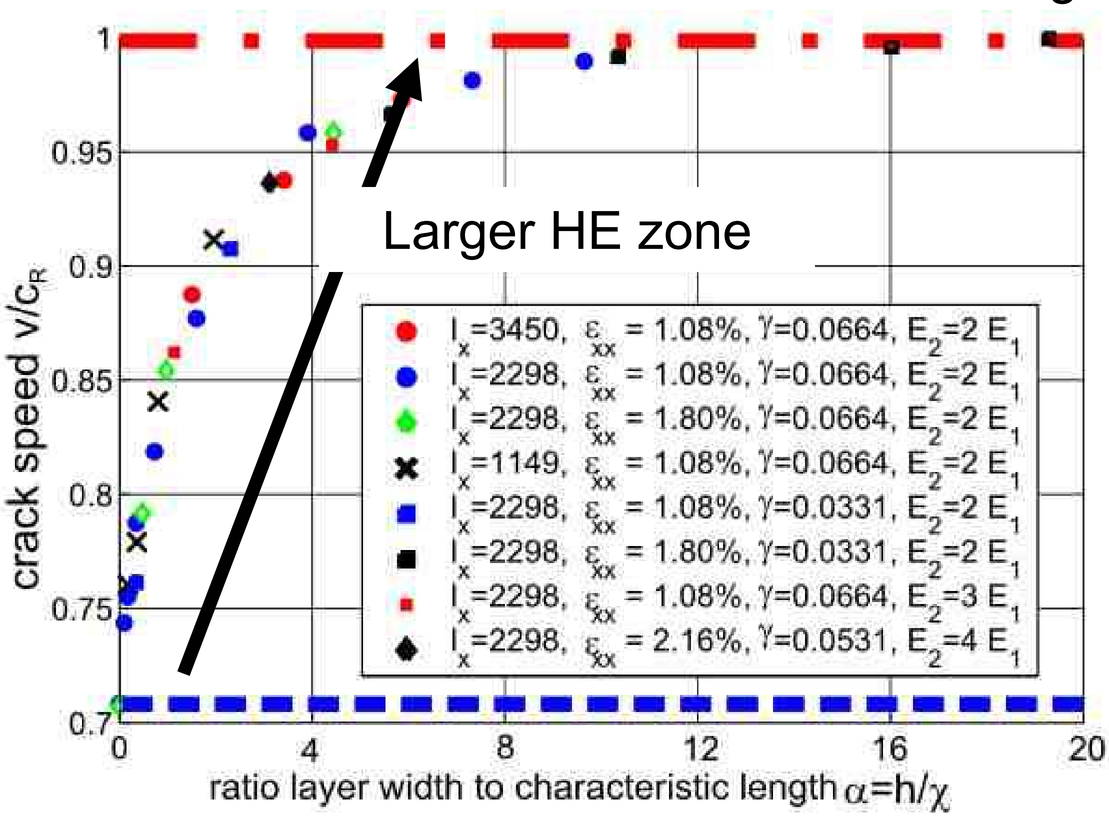
$$\chi = \beta \frac{\gamma E}{\sigma^2}$$ Energy characteristic length scale

Confirmation of characteristic energy length scale: Mode I Broberg problem

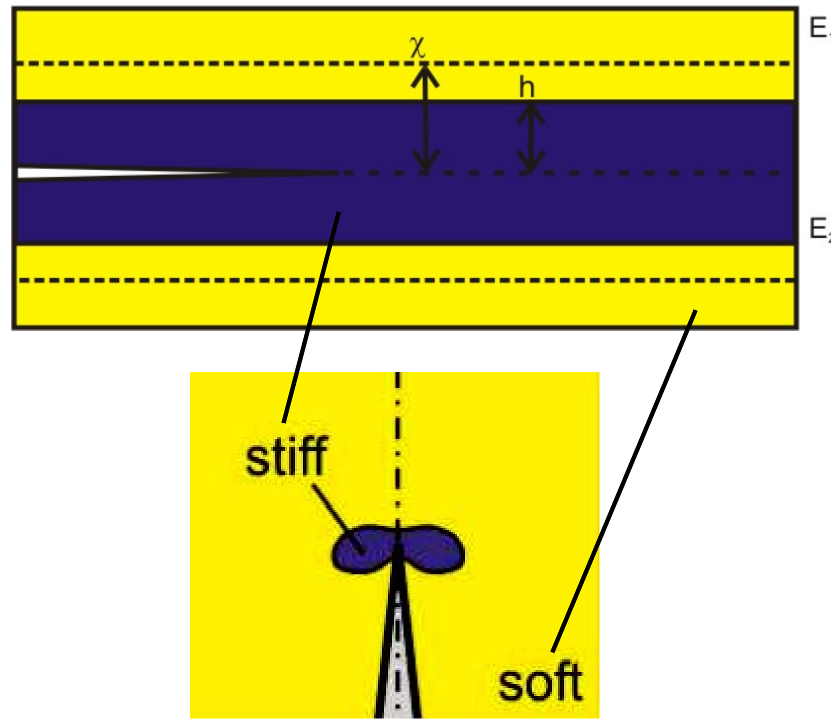
- Independently varying σ, *E* and γ
- Measuring the crack speed

$r_H / \chi >> 1$

"**local** HE limiting speed"



$\chi \propto \gamma E / \sigma^2$



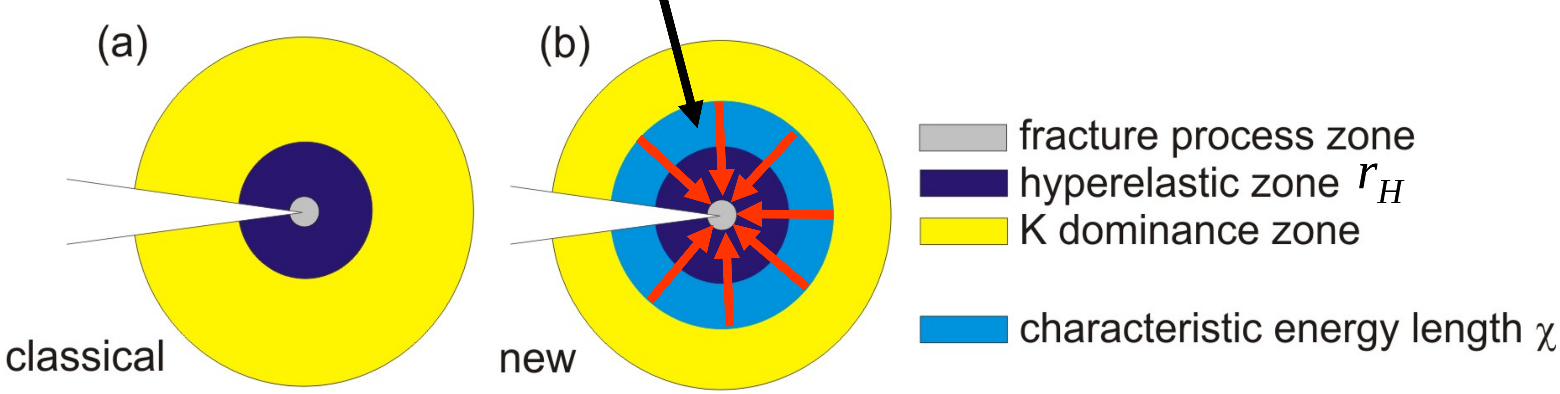
"small-strain limiting speed" $r_H / \chi \approx 0$

✓ Concept & scaling law numerically verified

Characteristic energy length scale

Characteristic energy length scale χ describes region of energy transport to crack tip

$$\chi \propto \gamma E / \sigma^2$$



HE governs:

$$r_H / \chi \approx 1$$

$\chi \approx O(mm)$ for 0.1% shear strain in PMMA

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)

Experimental verification of intersonic cracking

- 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

Cracks in Rubber Propagate Faster than the Speed of Sound

Since the classical work by Griffith, Inglis, and Irwin on the physics of cracking, one of the most fundamental questions associated with crack dynamics is the maximum speed that cracks can propagate. Depending on the type of loading (e.g., tensile, shear, or antiplane shear), there is a unique maximum speed cracks can achieve. For tensile-loaded cracks, theory predicts that this limiting speed is the Rayleigh wave speed, the speed of elastic waves on a surface. Recent theoretical work, including atomistic simulations, has challenged this classical view. Now, P.J. Petersan and co-workers from the University of Texas at Austin have shown experimentally that tensile-loaded cracks in rubber can actually propagate faster than the Rayleigh wave speed and even break the sound barrier.

As reported in the July issue of *Physical Review Letters* (105504), Petersan and colleagues identified the intersonic crack speed by the observation of shock fronts near the crack tip by high-speed photogra-

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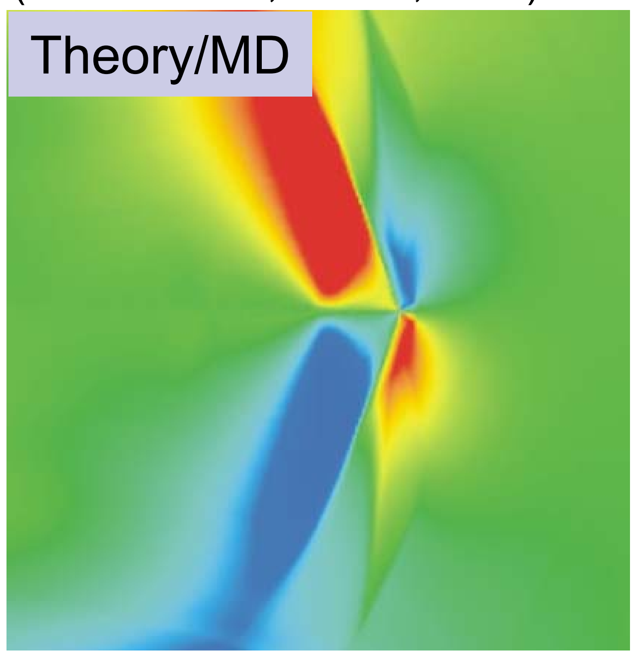
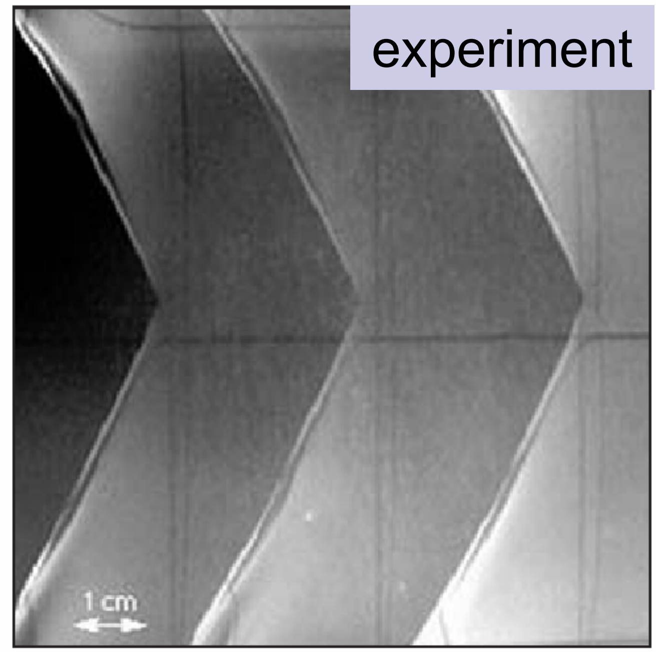
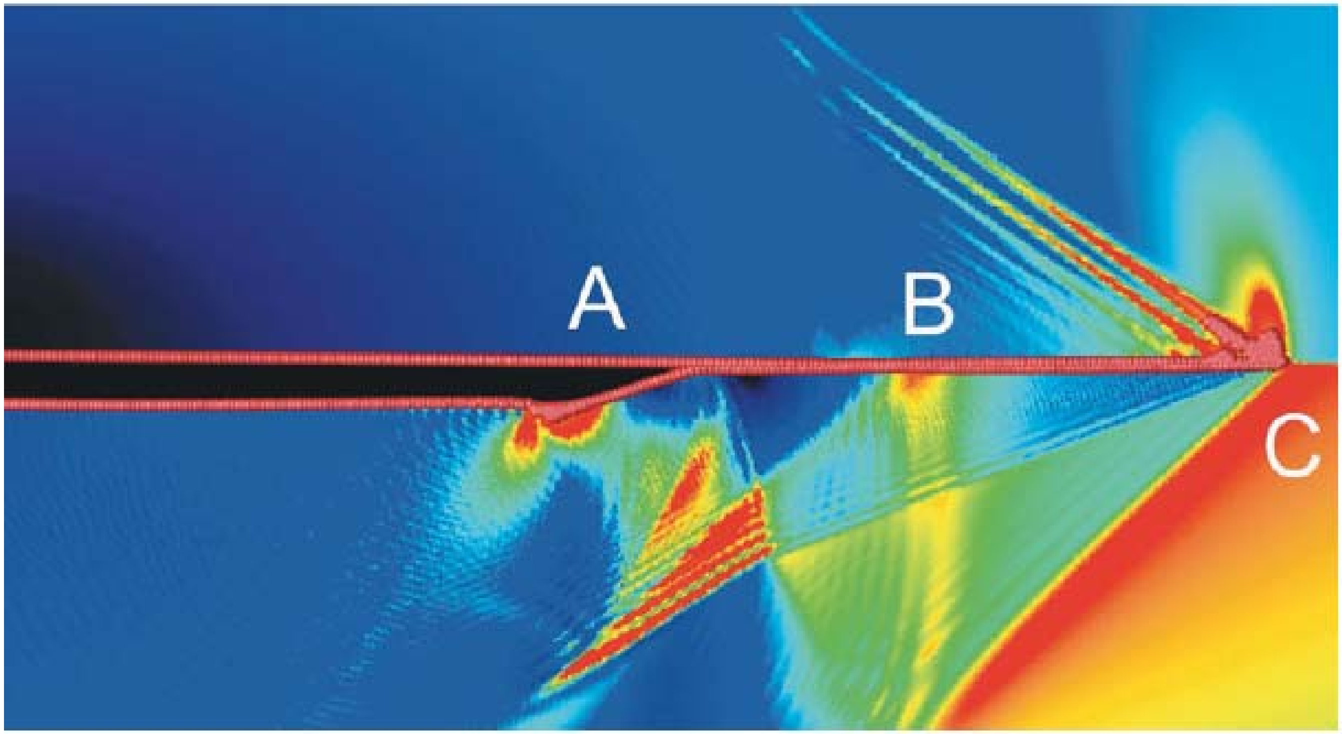
(Buehler *et al*., Nature, 2003)



(Petersan *et al*., PRL, 2004)



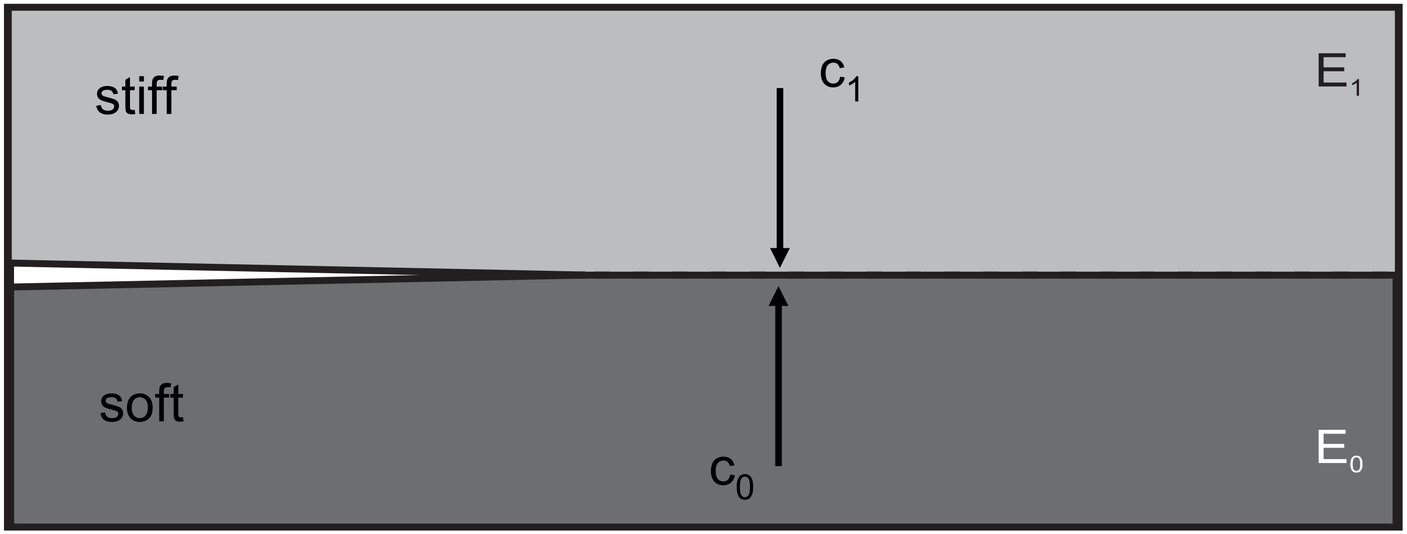
Multiple-exposure photograph of a crack propagating in a rubber sample (λ_x = 1.2, λ_y = 2.4); speed of the crack, ~56 m/s (Petersan *et al*.).



Brief summary

Cracks at interfaces
Mother-daughter granddaughter cracks

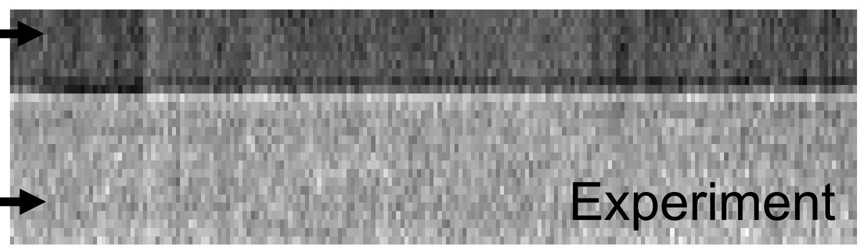
Focus: Cracks at interfaces



Here: Crack propagation constrained to interface

SiC mono-filamentary fiber

Ti-6Al- 4V matrix

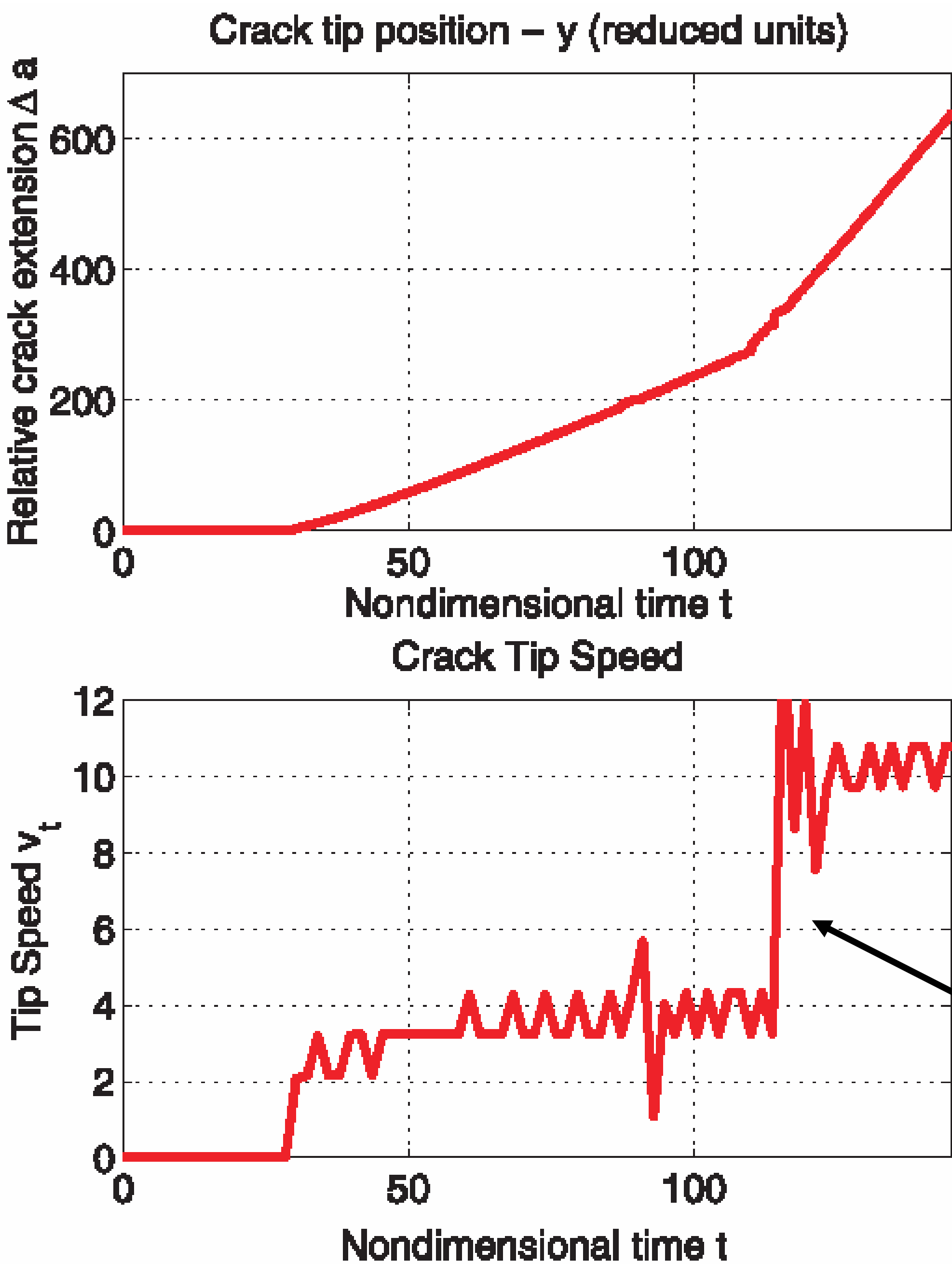


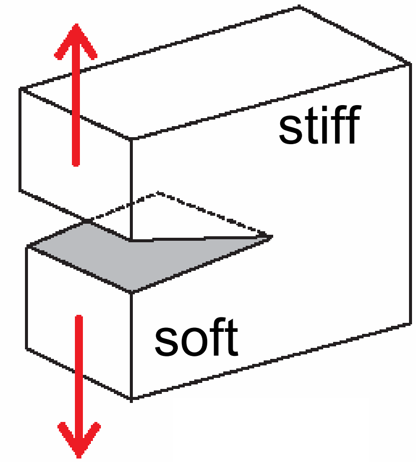
E.g.: Metal Matrix / fiber interface in composite material (e.g. Preuss *et al.*, 2002)

- 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)

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

Crack speed history





Mismatch: Ξ=10 (similar dynamics also observed for values 2..10)

Main result: Mother-daughter mechanism of mode I cracks: supersonic cracking along interface!

Sudden jump in crack speed

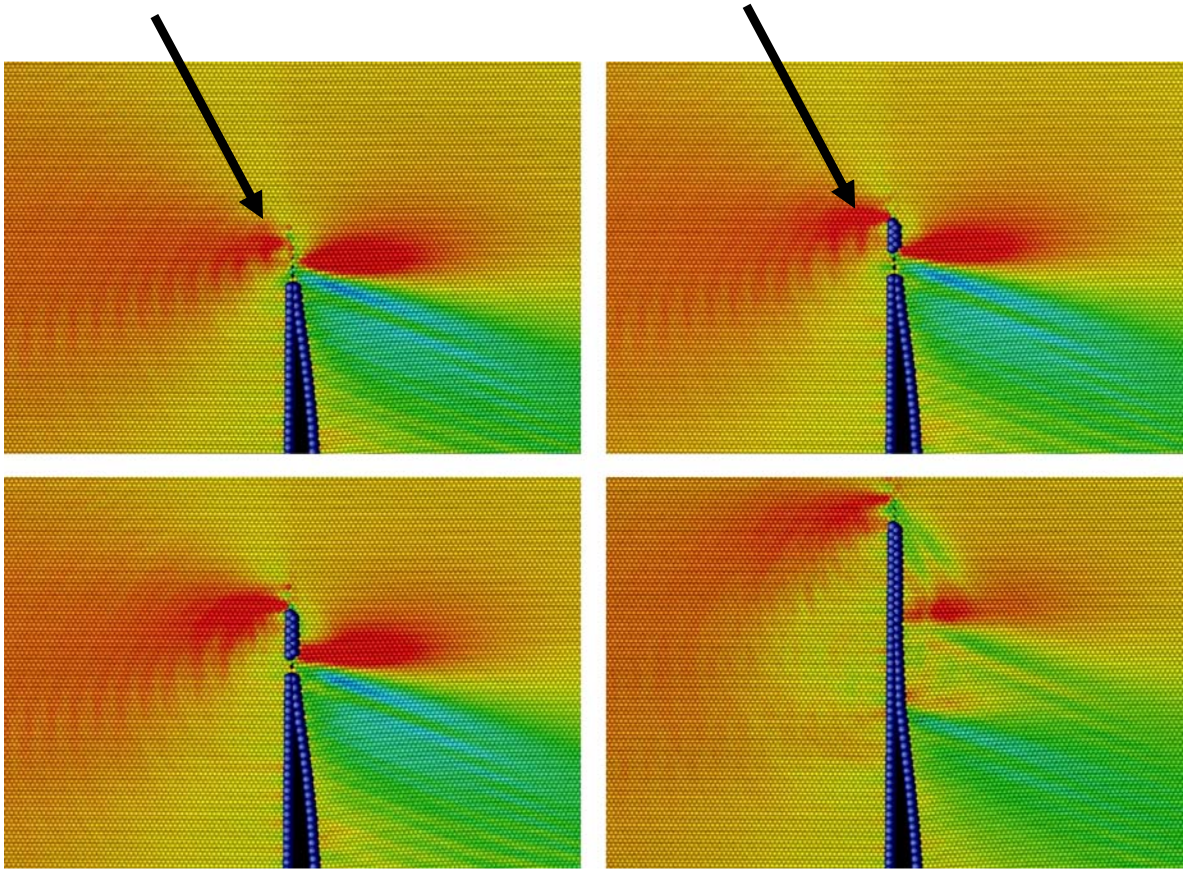
(Buehler *et al.*, to appear)

Mechanism: Nucleation of daughter crack

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

Ongoing theoretical analysis

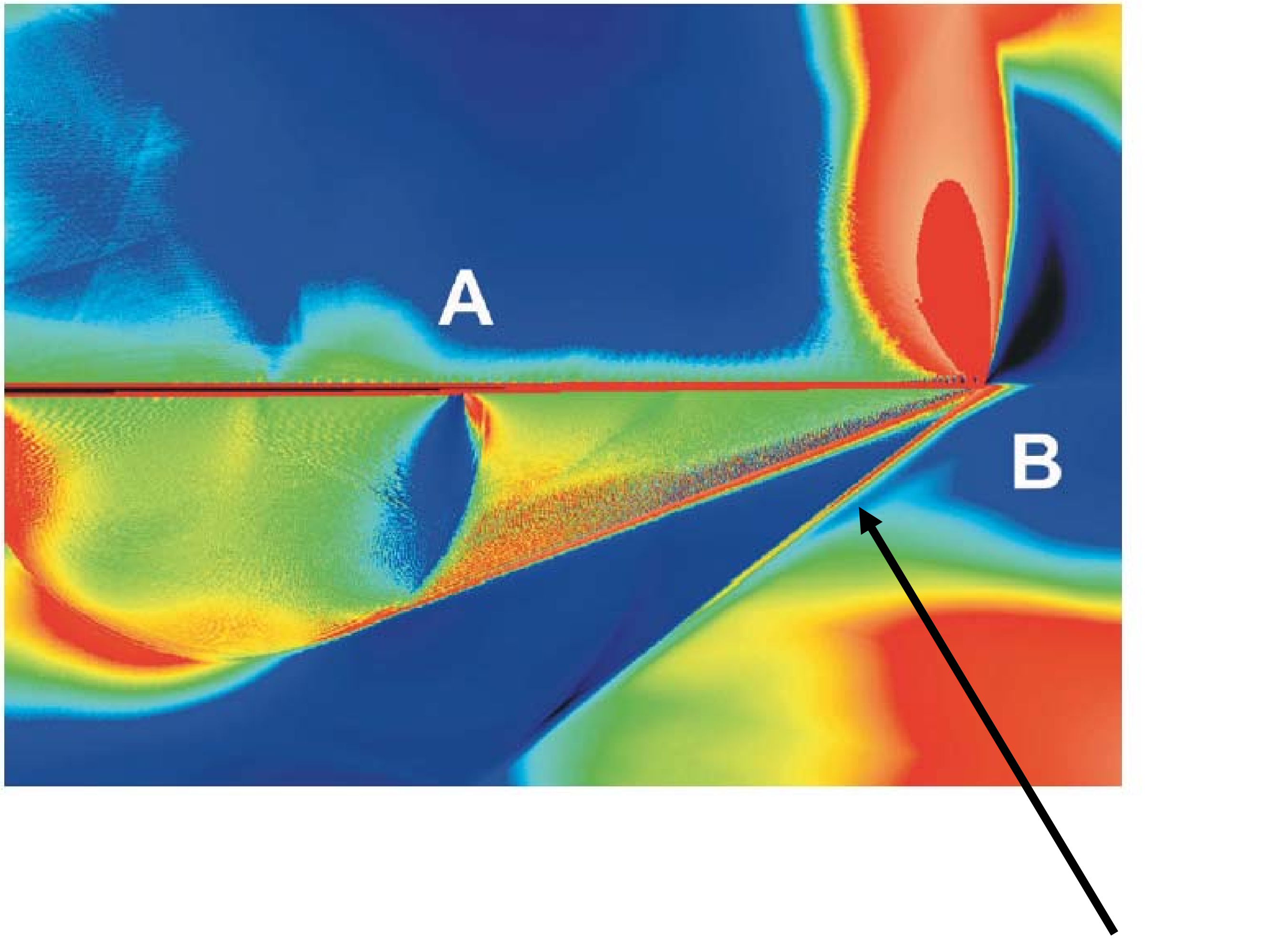
σ_{xy}



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

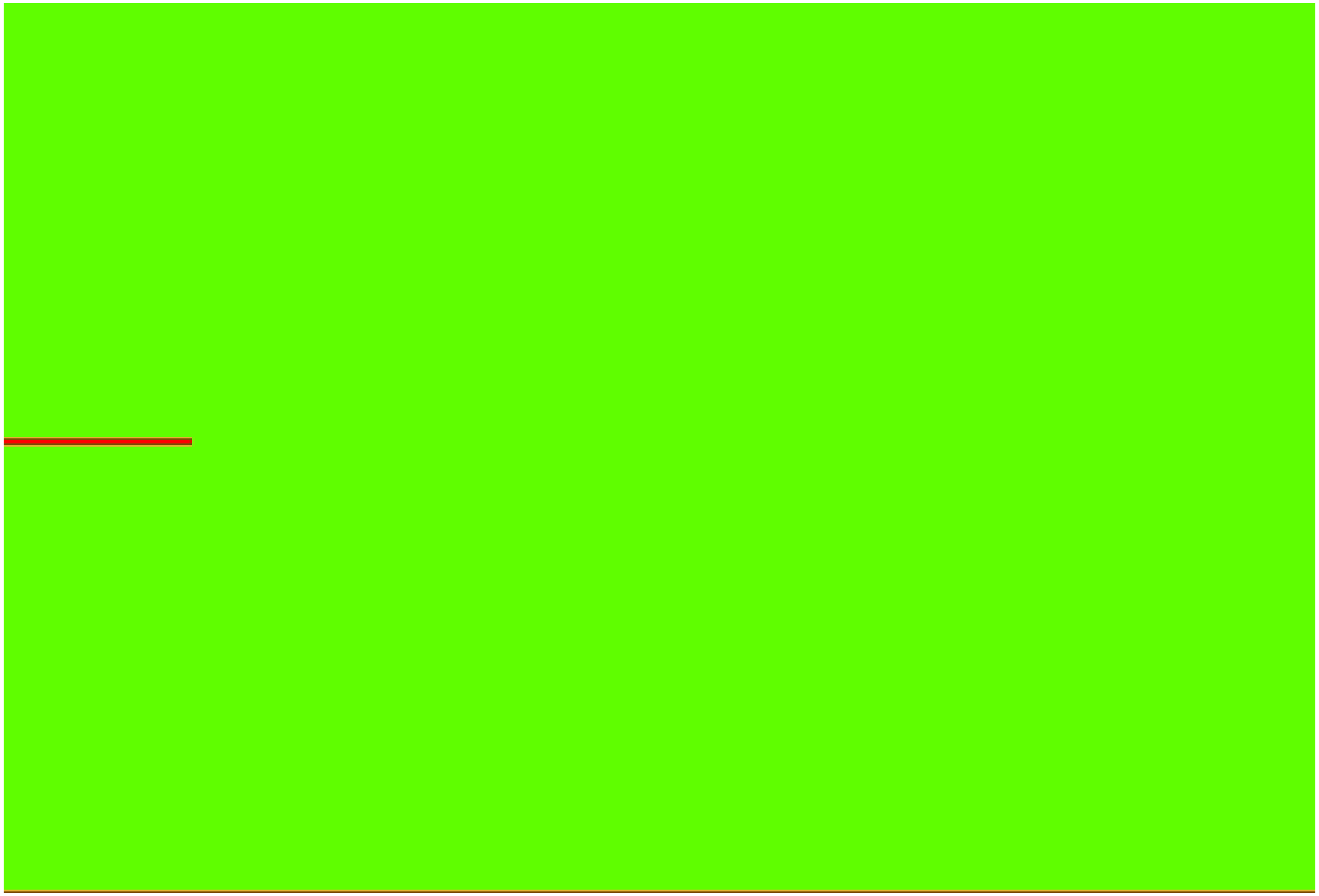


A: Mother crack

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

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

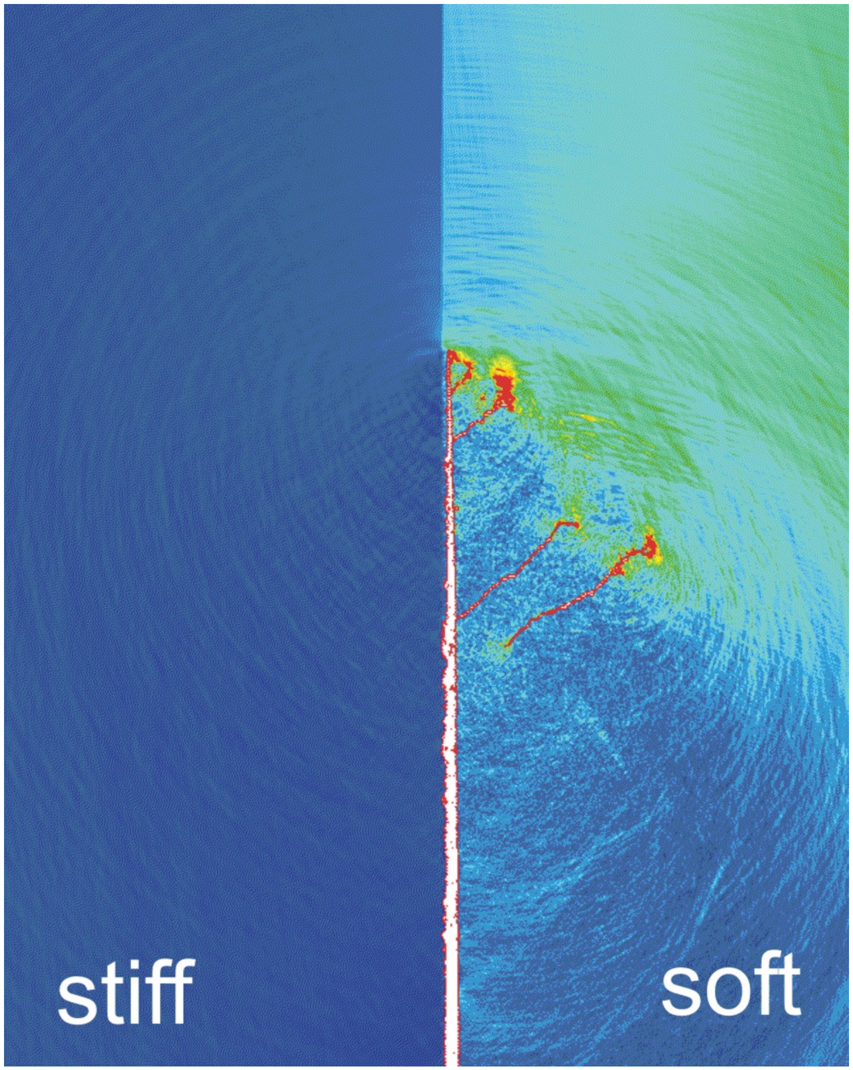
Movie



- 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 χ helped to form a quantitative understanding on the relative importance of hyperelasticity in dynamical fracture
- The characteristic energy length scale χ is found in 1D, 2D and 3D, and also plays a critical role in the instability problem