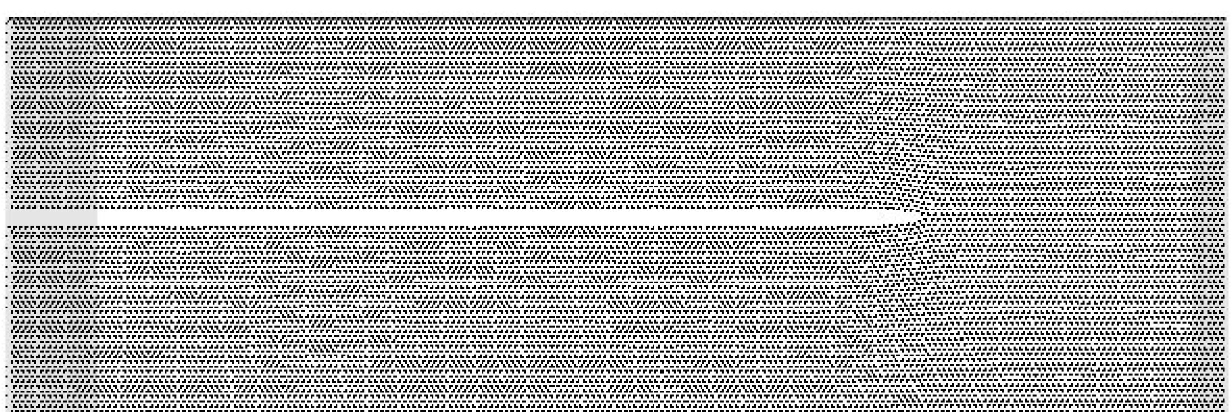
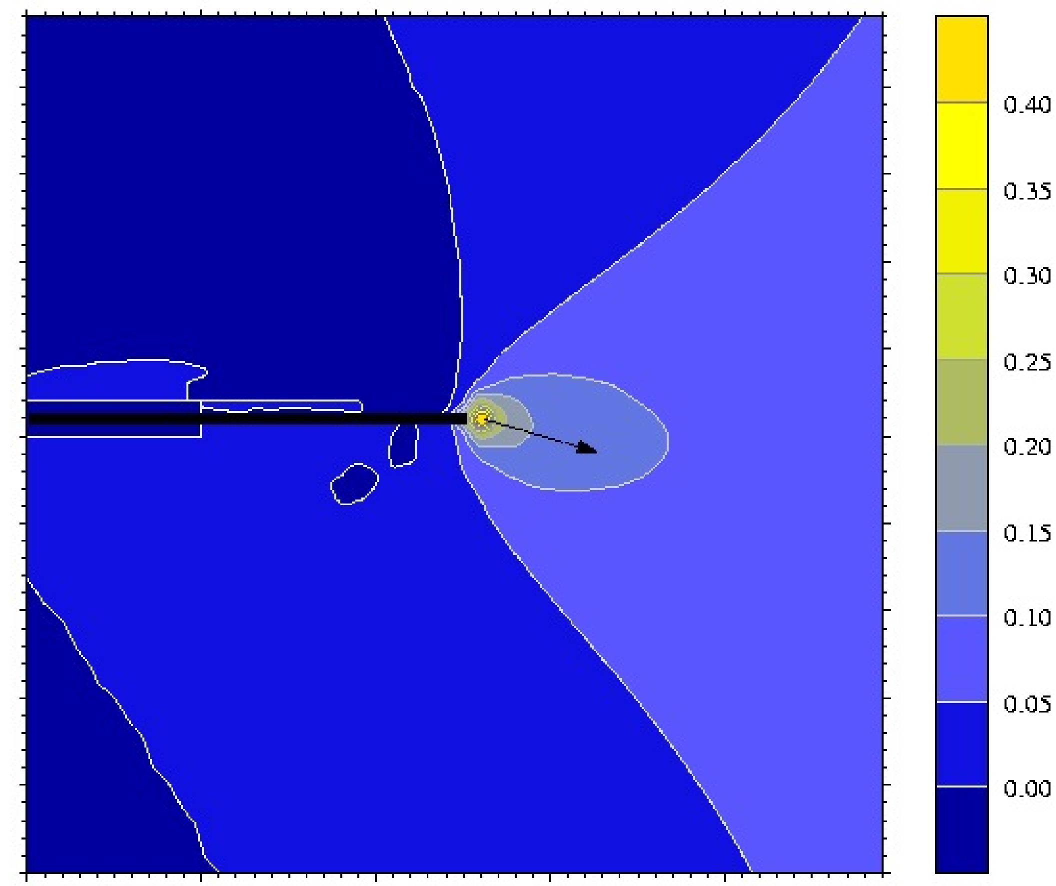
# Michael Marder

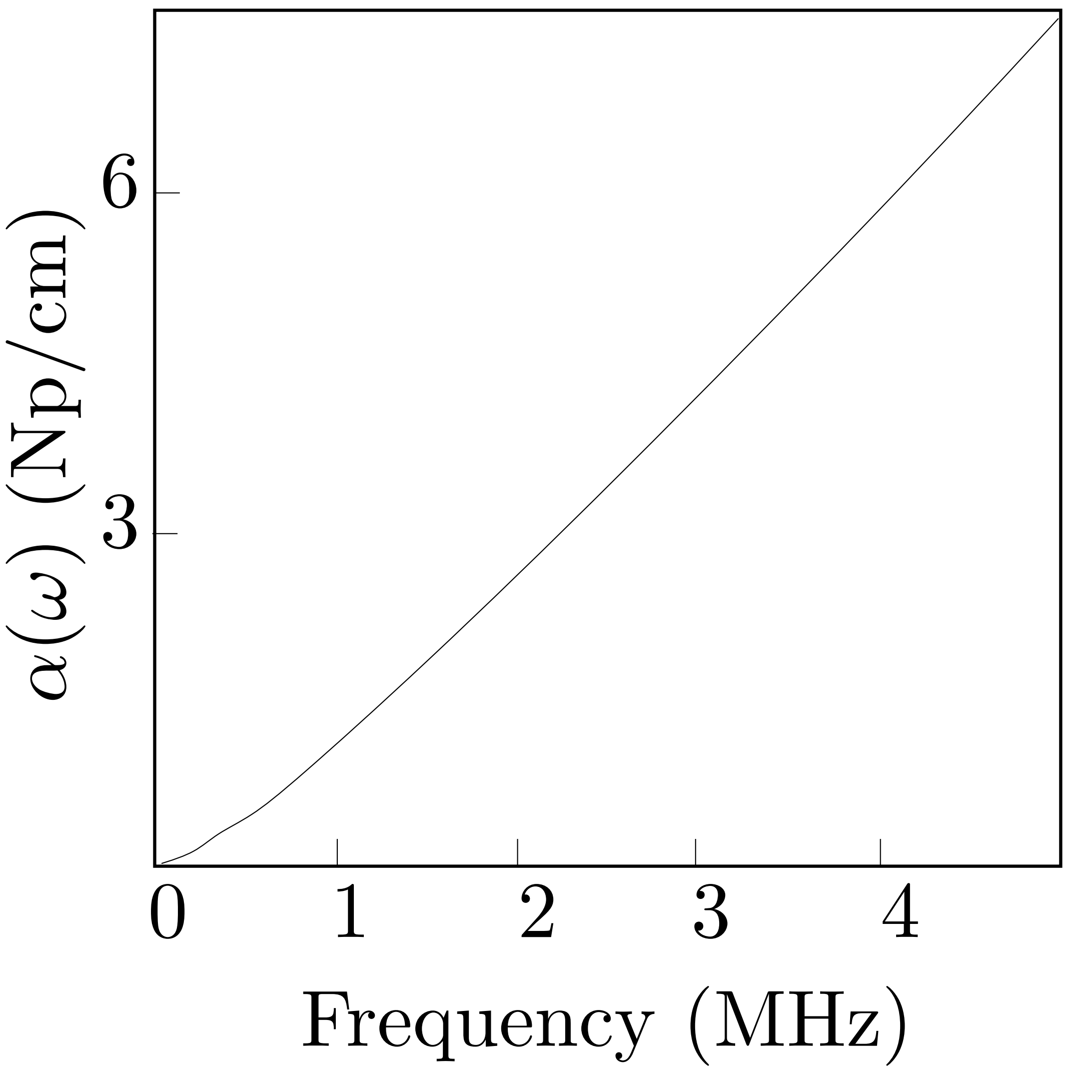
Center for Nonlinear Dynamics
and Department of Physics
The University of Texas at Austin

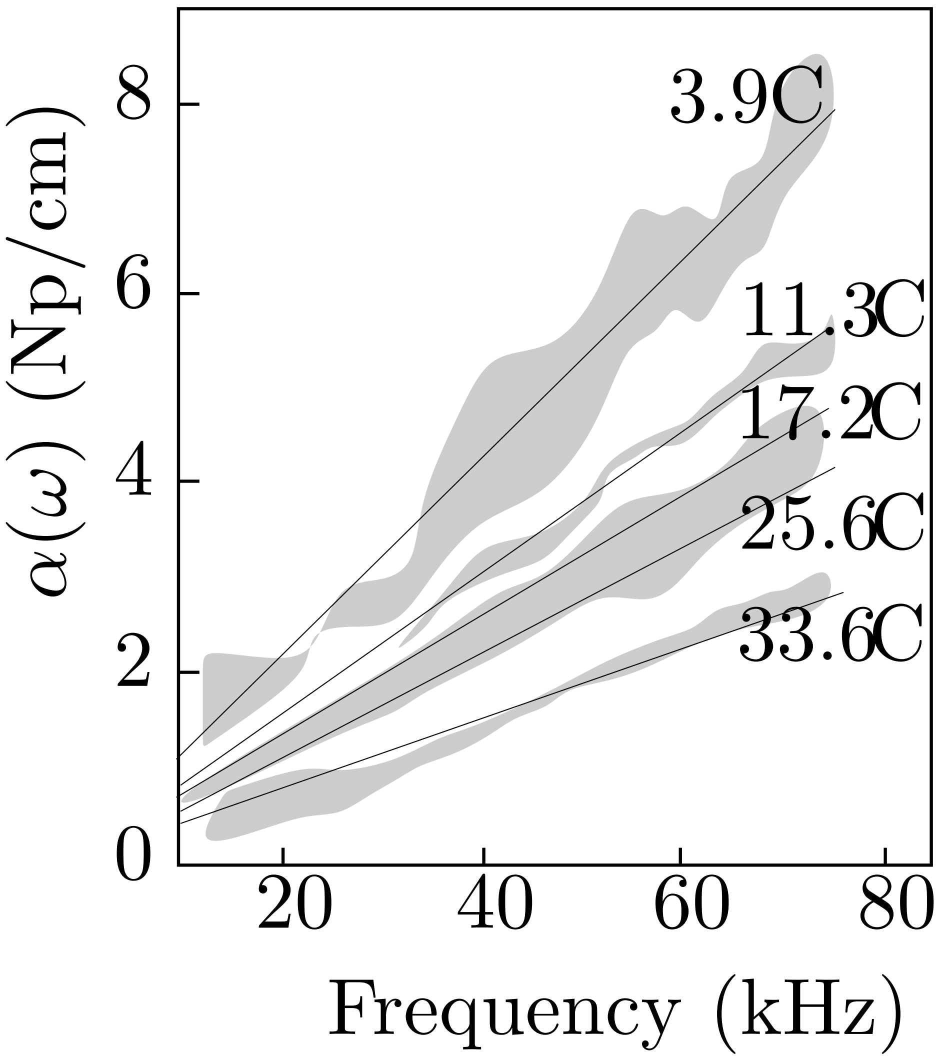




Hey, it's a workshop,
so let's go off topic

# Brief Interlude on Dissipation

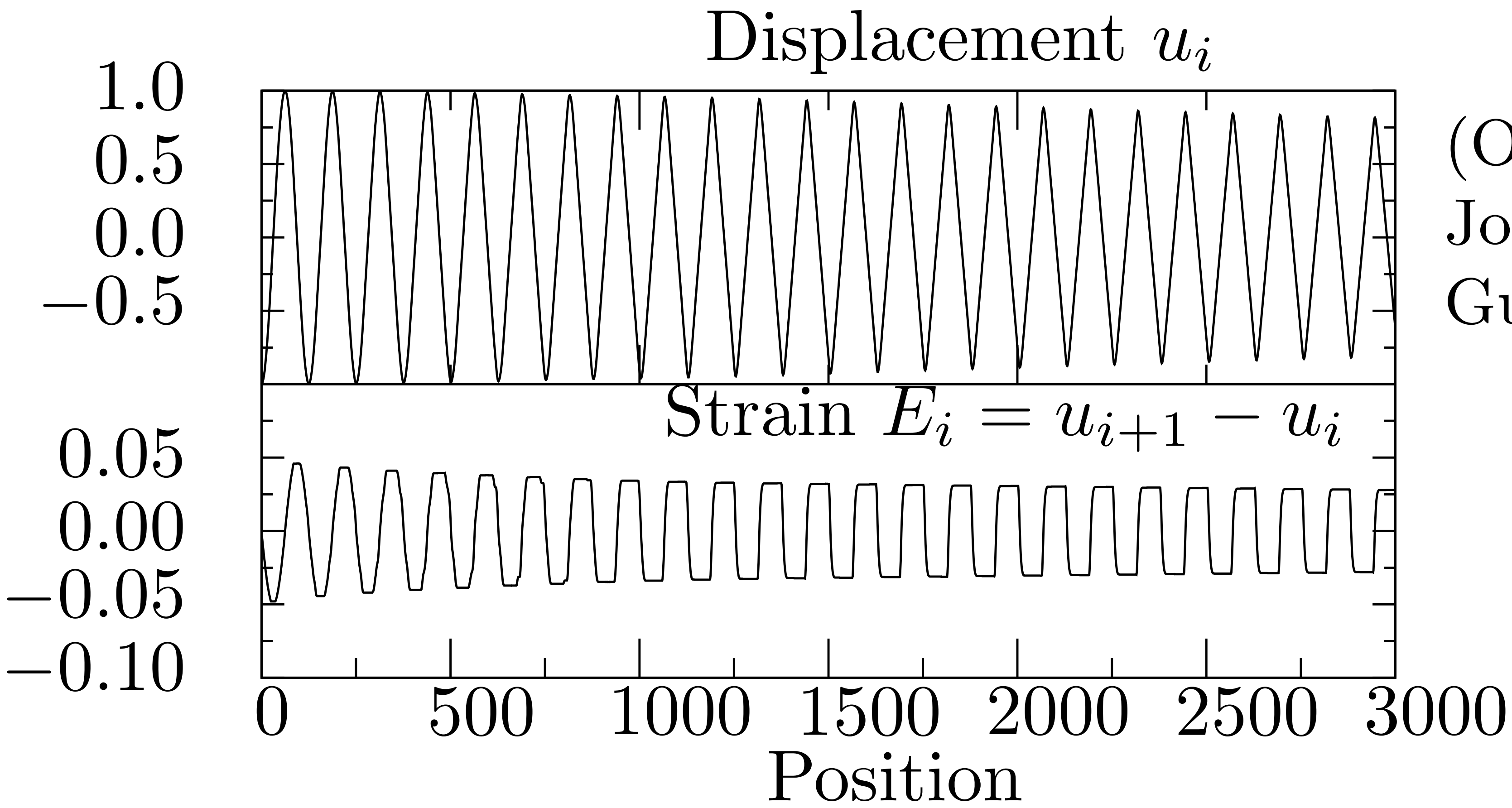



*The principal result of reviewing the experimental data is that for many solids...the specific dissipation function is independent of frequency– a generalization well known to engineers but largely neglected in physical theories of attenuation,* Knopoff and MacDonald, 1958

# Two Possible Scenarios for Dissipation

Hysteresis




(Ostrovsky, Johnson, Guyer)

Broad spectrum of dampers

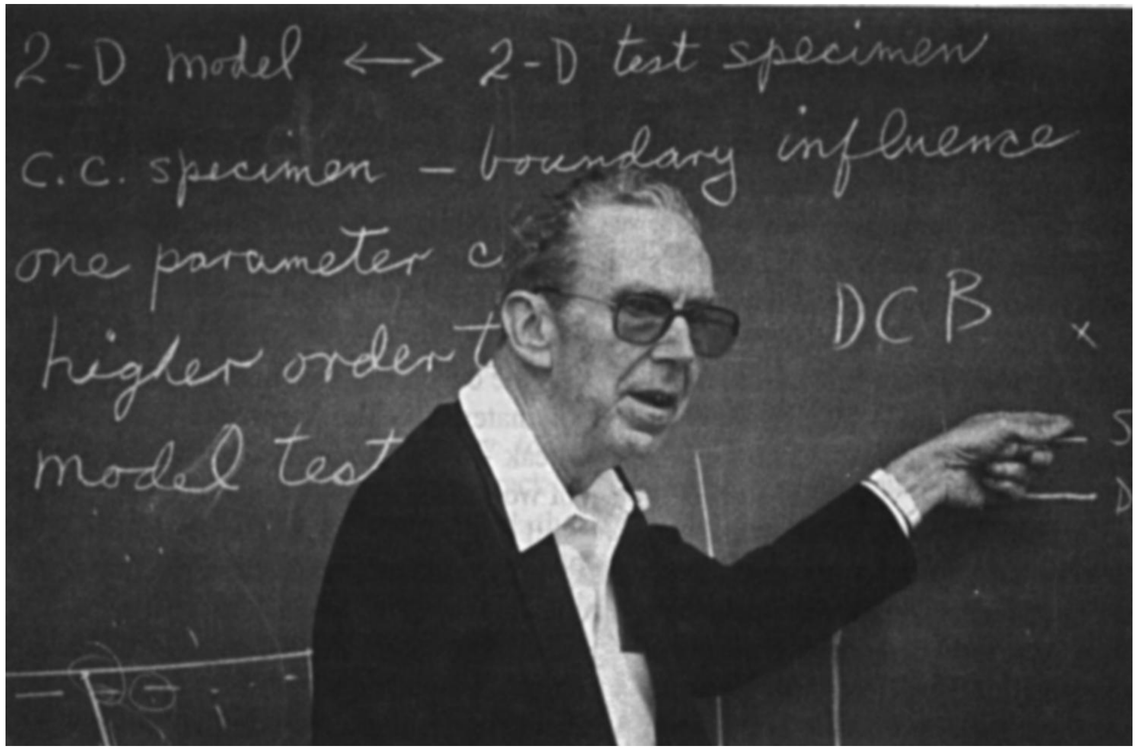
(Jackle, 1972)

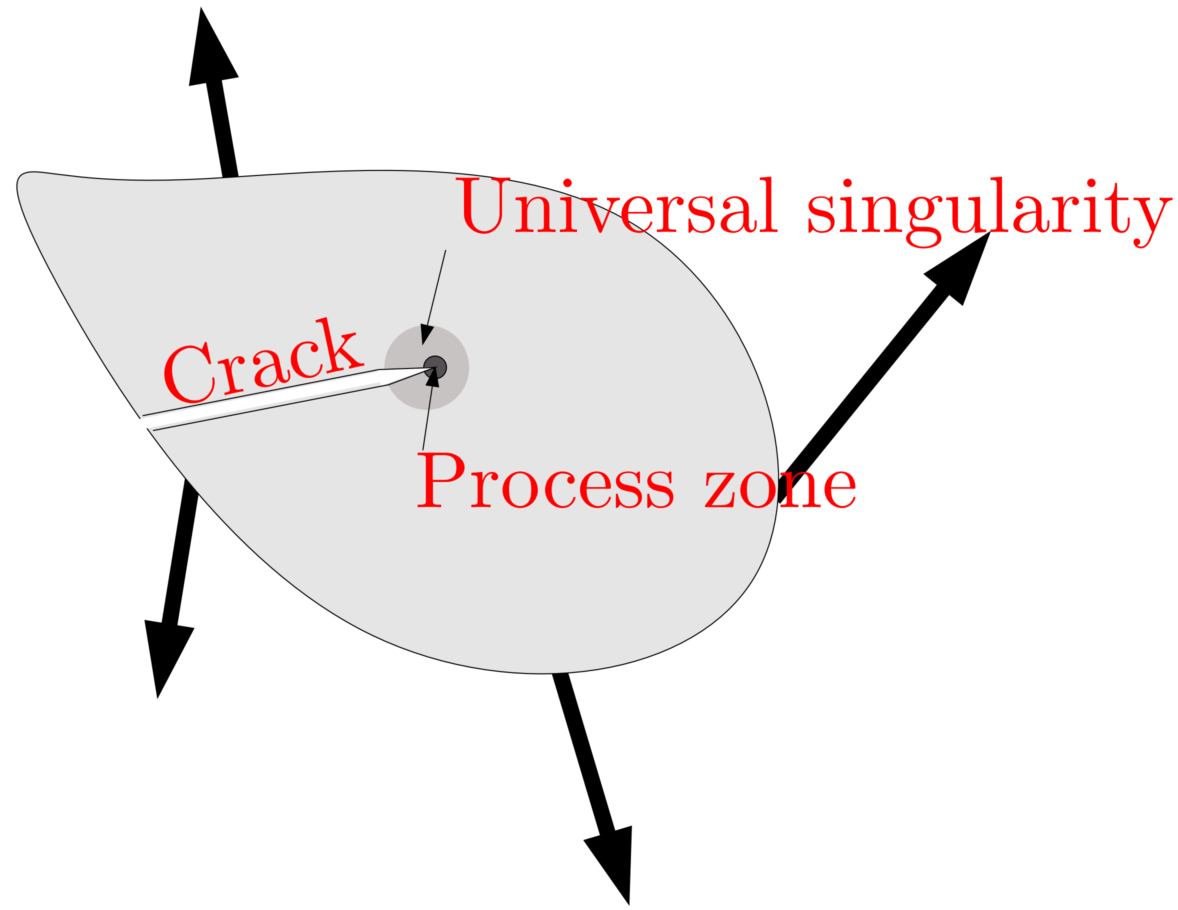
$$\alpha = g\pi\omega/4c$$

$$v = 1 - (g/2)\ln[(\omega^2 + /b^2_{max})/(\omega^2 + b^2_{min})]$$

And now back to what I was asked to speak about....

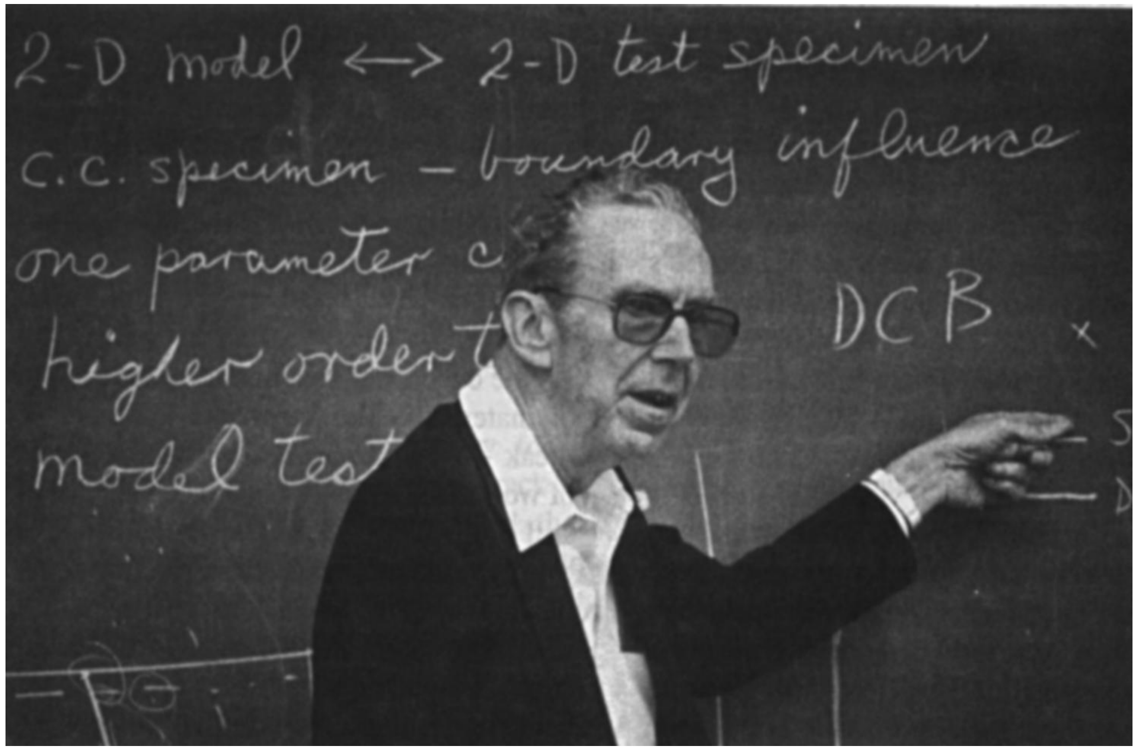
# Continuum Fracture Mechanics




- Initiation of fracture depends upon energy (Griffith)
- Energy and (singular) stress criteria are identical (Irwin)
- Structure of stress near crack tips is universal (Irwin and Rice)

# Continuum Fracture Mechanics




- Microscopic unknowns bundled into one number — toughness – that can be tabulated from tests on standard specimens.

- Crack driving forces computed through continuum mechanics and finite elements in arbitrary geometries

# Dynamic Fracture Mechanics

- Rough equations of motion (Mott 1948, Dulaney and Brace, 1960)
- Dynamic calculation of stress fields (Yoffe 1951)
- Limiting speed 60% of shear wave speed (Schardin, 1955)
- Rayleigh wave speed should be limit (Stroh, 1957)
- Exact equation of motion: crack tip has no inertia (Kostrov, 1966 Eshelby, 1969)
- Extension of exact results to Mode I (Freund, Kostrov, 1974)

Net results:

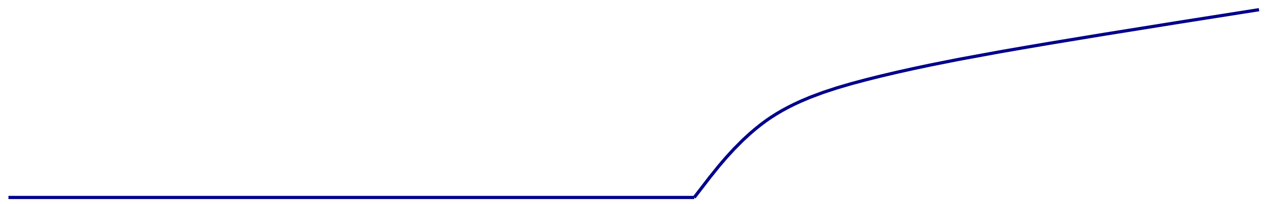
- For semi-infinite crack in infinite plate, can compute energy flowing to tip of straight crack moving with velocity $v(t)$ for arbitrary time-dependent loading on crack faces.
- Crack velocity and path are given.
- Assumption plate is infinite is not mere technicality.
- Energy cost function $\Gamma(v)$ closes theory.
- Many felt $\Gamma(v)$ had to be largely independent of velocity, but nothing in structure of theory demanded this

# Crack Paths

Gol'dstein and Salganik, 1974

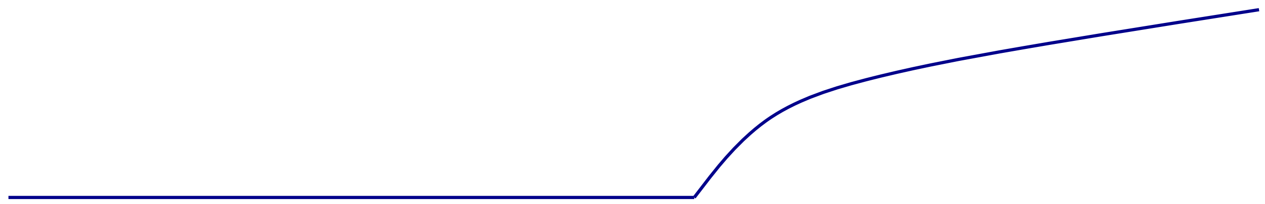
- Crack moves along a path such that $K_{II}$ vanishes
- Energy consumption maximized in this direction

Seed cracks placed in mixed mode loading kink in expected direction



# Crack Paths

- Equation of motion for small deviations from straightness (Rice and Cotterell, 1980)
- Upper cutoff on curvature and extension to three dimensions (Sethna and Hodgdon, 1993)
- Generalization to dynamic fractures (Adda-Beddia, Ben-Amar, and Lund 1999; Oleaga, 2001)



# Continuum Summary

- Industrial applications rely mainly on simple strength of materials analysis, or in critical applications on continuum fracture mechanics
- Continuum analysis handles complex geometries and loading better than any other framework.
- Hence beliefs widely held though rarely stated:

Real materials are not made of atoms!

or

In fracture atoms matter, for materials that don't!

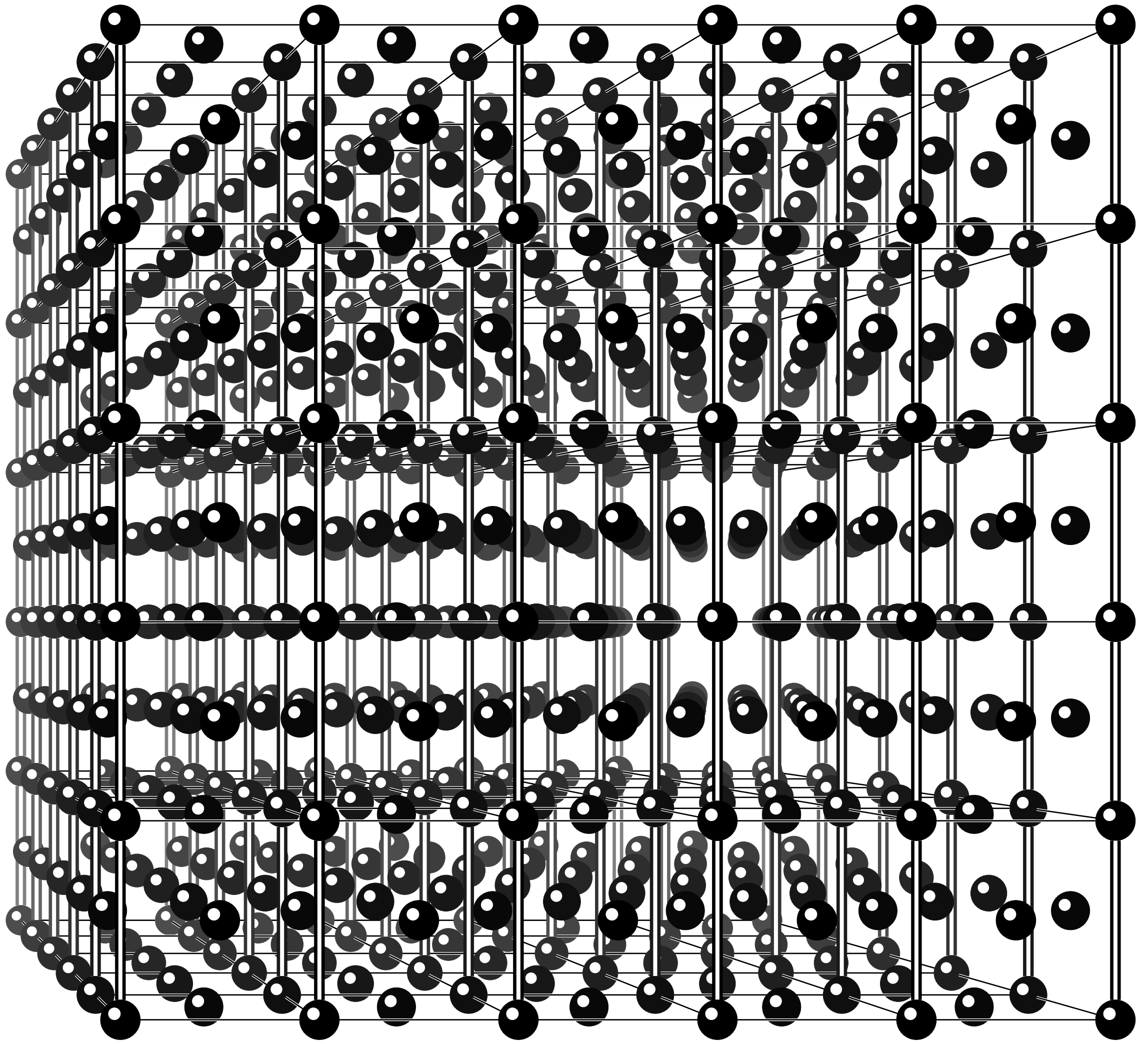
# Lacking from Continuum

- Static Cracks: Compute criterion for initiation (usually one number)
- Dynamic Cracks: Compute speed from driving force (usually a function of one variable)
- ... and probably for both Static and Dynamic: Compute crack path (functions of several variables)

A physically based theory of brittle fracture cannot be created entirely within a continuum description.

A physically based theory of brittle fracture cannot be created entirely within a continuum description.

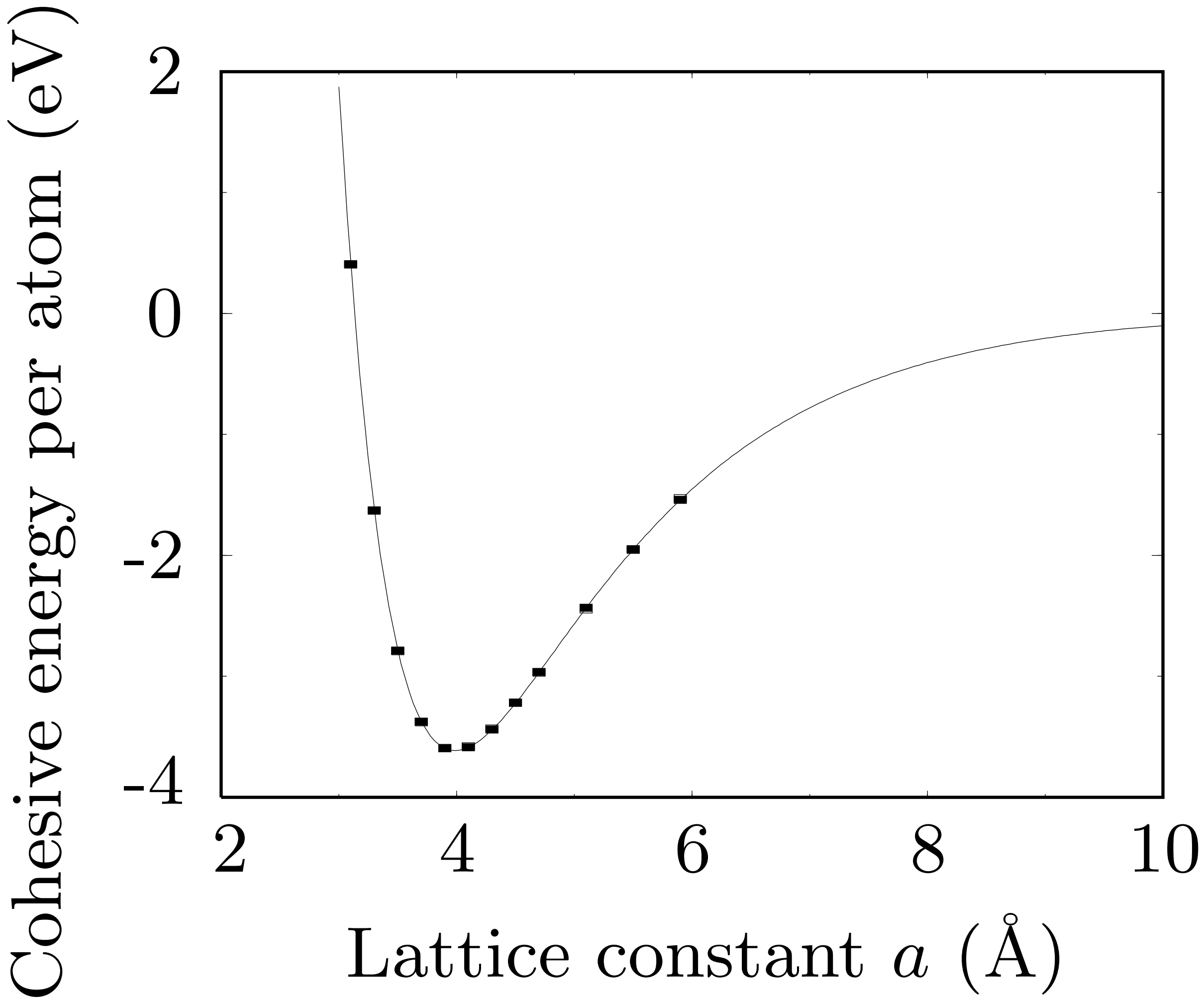
The cohesive forces between atoms rise and fall on the scale of atomic separations.



# Physics of fracture

A physically based theory of brittle fracture cannot be created entirely within a continuum description.

The cohesive forces between atoms rise and fall on the scale of atomic separations.



# Physics of fracture

A physically based theory of brittle fracture cannot be created entirely within a continuum description.

The cohesive forces between atoms rise and fall on the scale of atomic separations.

Modeling should not be grid-independent; nature has established a grid at the atomic scale and fracture depends upon it.

# Physics of fracture

A physically based theory of brittle fracture cannot be created entirely within a continuum description.

The cohesive forces between atoms rise and fall on the scale of atomic separations.

Modeling should not be grid-independent; nature has established a grid at the atomic scale and fracture depends upon it.

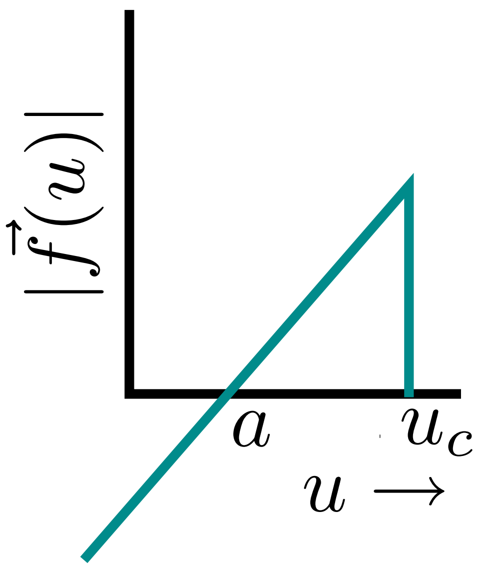
Analytical and numerical techniques allow one to move well beyond continuum analysis.

# Ideal Brittle Crystal

Acceleration    Snapping Bonds    Kelvin Dissipation

Mass

$$m\ddot{\vec{u}}_i = \sum_j \left[\vec{f}(\vec{u}_{ji}) + \vec{g}(\dot{\vec{u}}_{ji}, \vec{u}_{ji})\right]$$




$$\vec{g}(\dot{\vec{u}}_{ji}, \vec{u}_{ji}) = \dot{\vec{u}}_{ji}\, \theta(u_c - u_{ji})$$

MPM, *International Journal of Fracture* **130** 517-555 (2004)

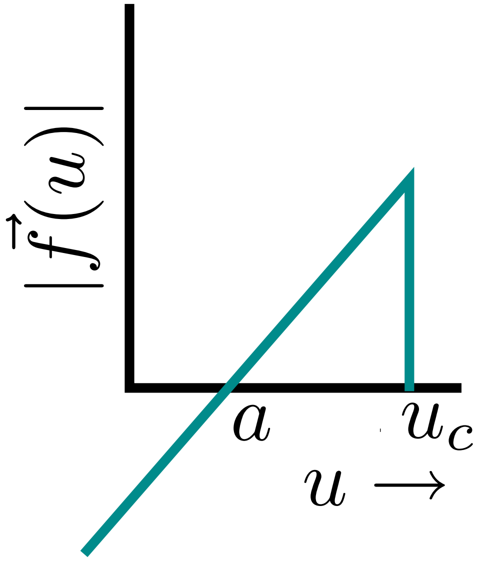
# Ideal Brittle Crystal

This model can be solved *exactly* when $u_c - a \ll a$ (Slepyan, 1980... MPM, 1995...Kessler and Levine...)

Acceleration  Snapping Bonds  Kelvin Dissipation

Mass

$$m\ddot{\vec{u}}_i = \sum_j \left[\vec{f}(\vec{u}_{ji}) + \vec{g}(\dot{\vec{u}}_{ji}, \vec{u}_{ji})\right]$$




$$\vec{g}(\dot{\vec{u}}_{ji}, \vec{u}_{ji}) = \dot{\vec{u}}_{ji}\,\theta(u_c - u_{ji})$$

MPM, *International Journal of Fracture* **130** 517-555 (2004)

# Ideal Brittle Crystal

Example: for triangular lattice in Mode III

$$\ddot{u}_i^y = \frac{2c^2}{3a^2} \sum_{j \in n(i)} \left( u_{ij}^y + \beta \dot{u}_{ij}^y \right) \theta(\lambda_f - u_{ij}). \tag{1}$$

complete solution reads

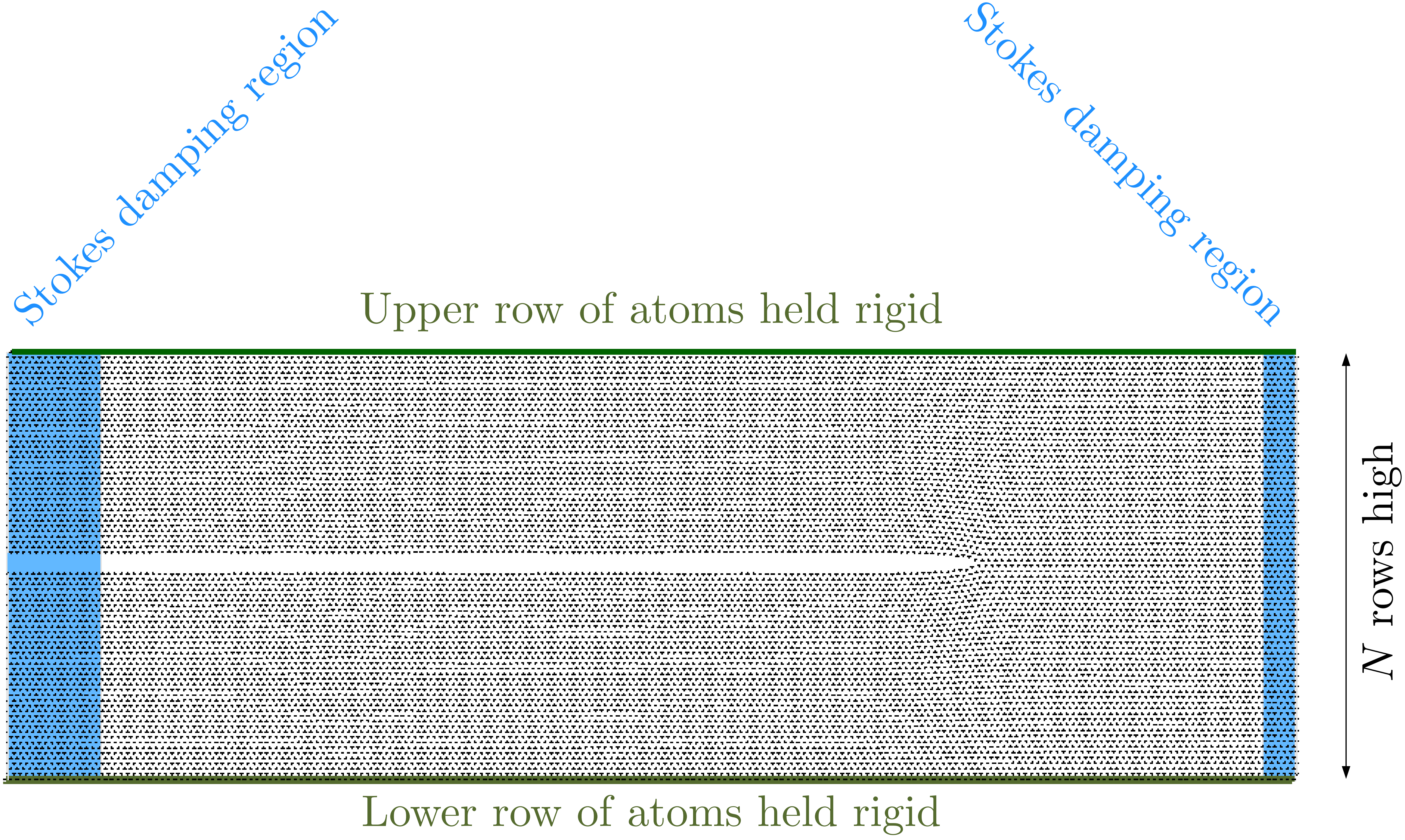
$$\tilde{v} = v/c, \;\; \tilde{\beta} = \beta c/a; \, z = \frac{3 - \cos(\omega/\tilde{v}) - 3\omega^2/[4(1 - i\tilde{\beta}\omega)]}{2\cos(\omega/2\tilde{v})} \tag{2}$$

$$y = z + \sqrt{z^2 - 1}\text{with} \quad \text{abs}(y) > 1, ; F(\omega) = \left\{ \frac{y^{[N-1]} - y^{-[N-1]}}{y^N - y^{-N}} - 2z \right\} \cos(\omega/2\tilde{v}) + 1 \tag{3}$$

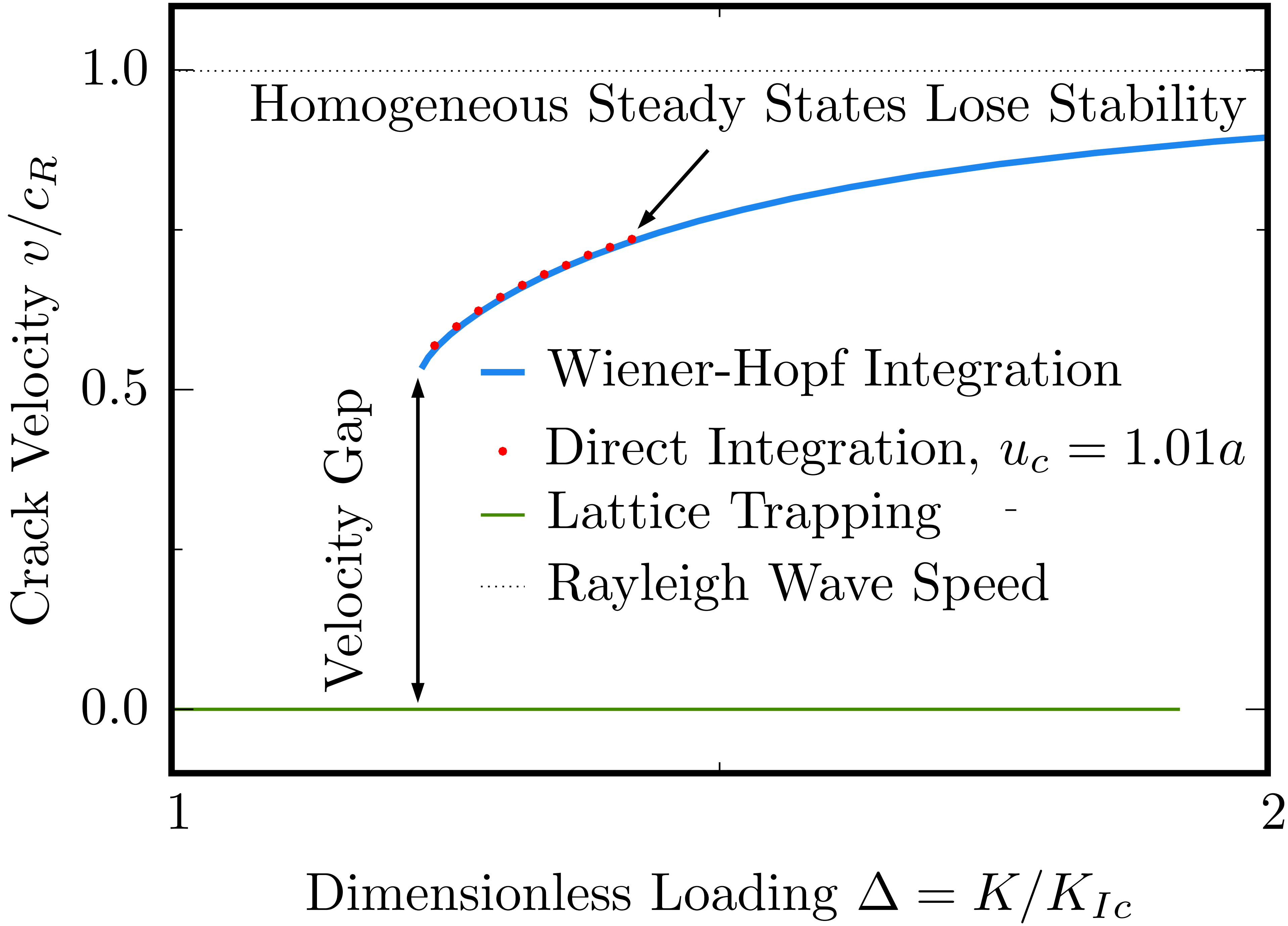
$$Q(\omega) = \frac{F}{F - 1 - \cos(\omega/2\tilde{v})}; \tilde{\lambda}_y = \lambda_y / \sqrt{(4\lambda_f^2 - \lambda_x^2)/3} \tag{4}$$

$$\tilde{\lambda}_y \quad = \quad \frac{1}{\sqrt{2N+1}} \exp\left[ - \int \frac{d\omega'}{4\pi} \left\{ \frac{1}{i\omega'(1 + \tilde{\beta}^2\omega'^2)} \left[ \ln Q(\omega') - \overline{\ln Q(\omega')} \right] + \frac{\tilde{\beta} \ln |Q(\omega')|^2}{1 + \tilde{\beta}^2 \omega'^2} \right\} \right].$$

# Numerical Methodology

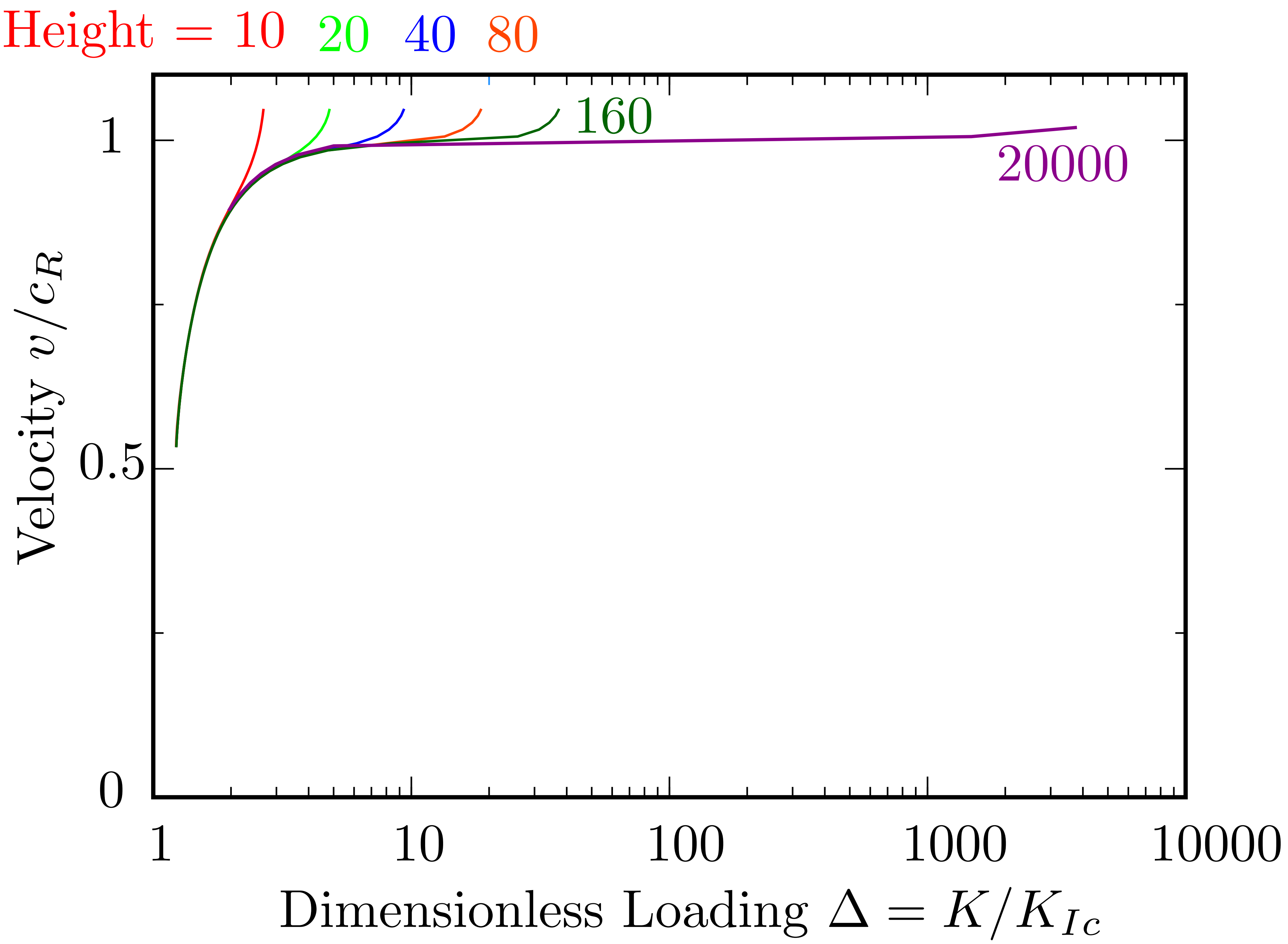


# Exact Solution when $u_c - a \ll a$

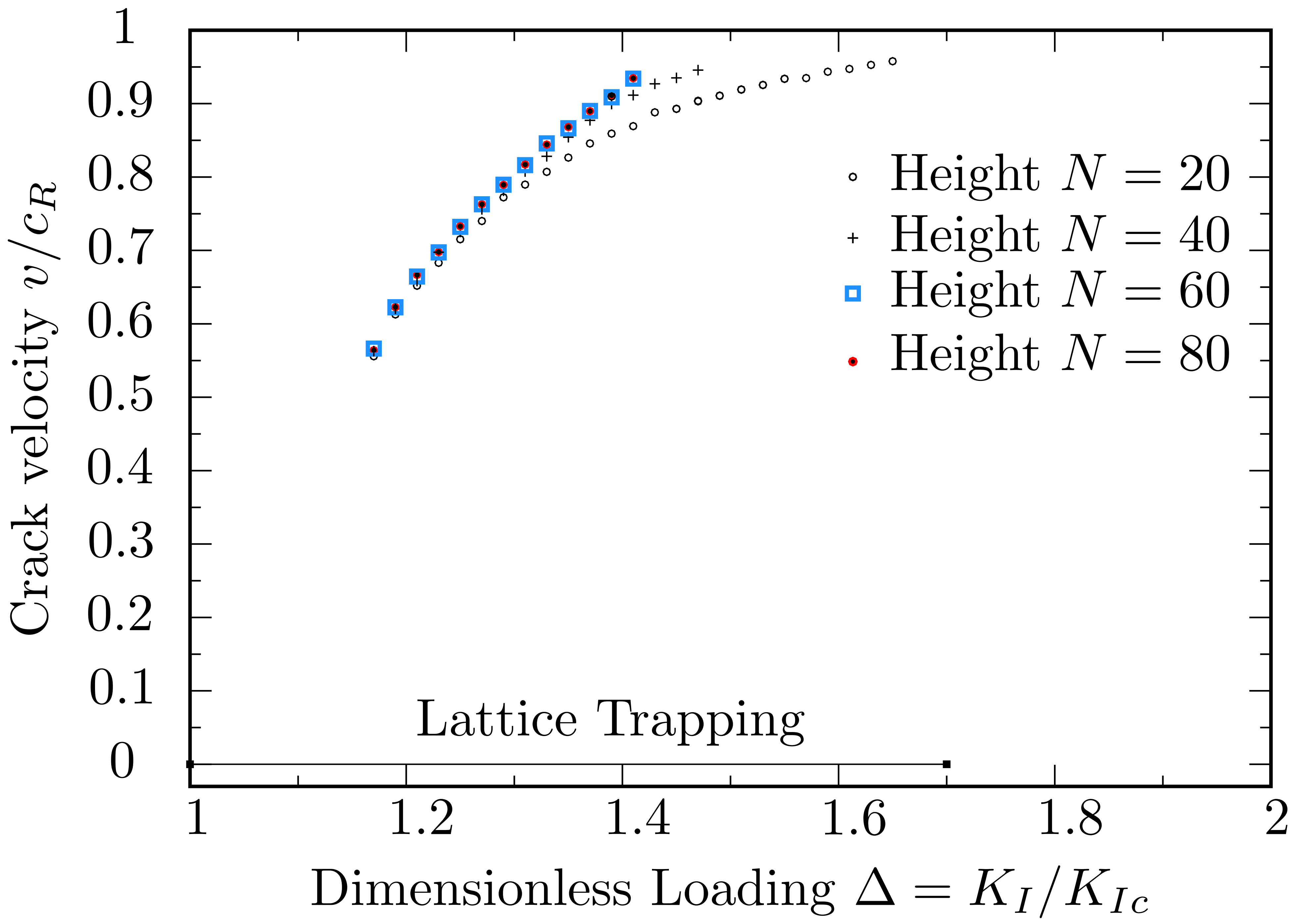


# Scaling of Steady States

Wiener-Hopf techniques allow 800,000,000 atom MD... on a laptop in 30 minutes

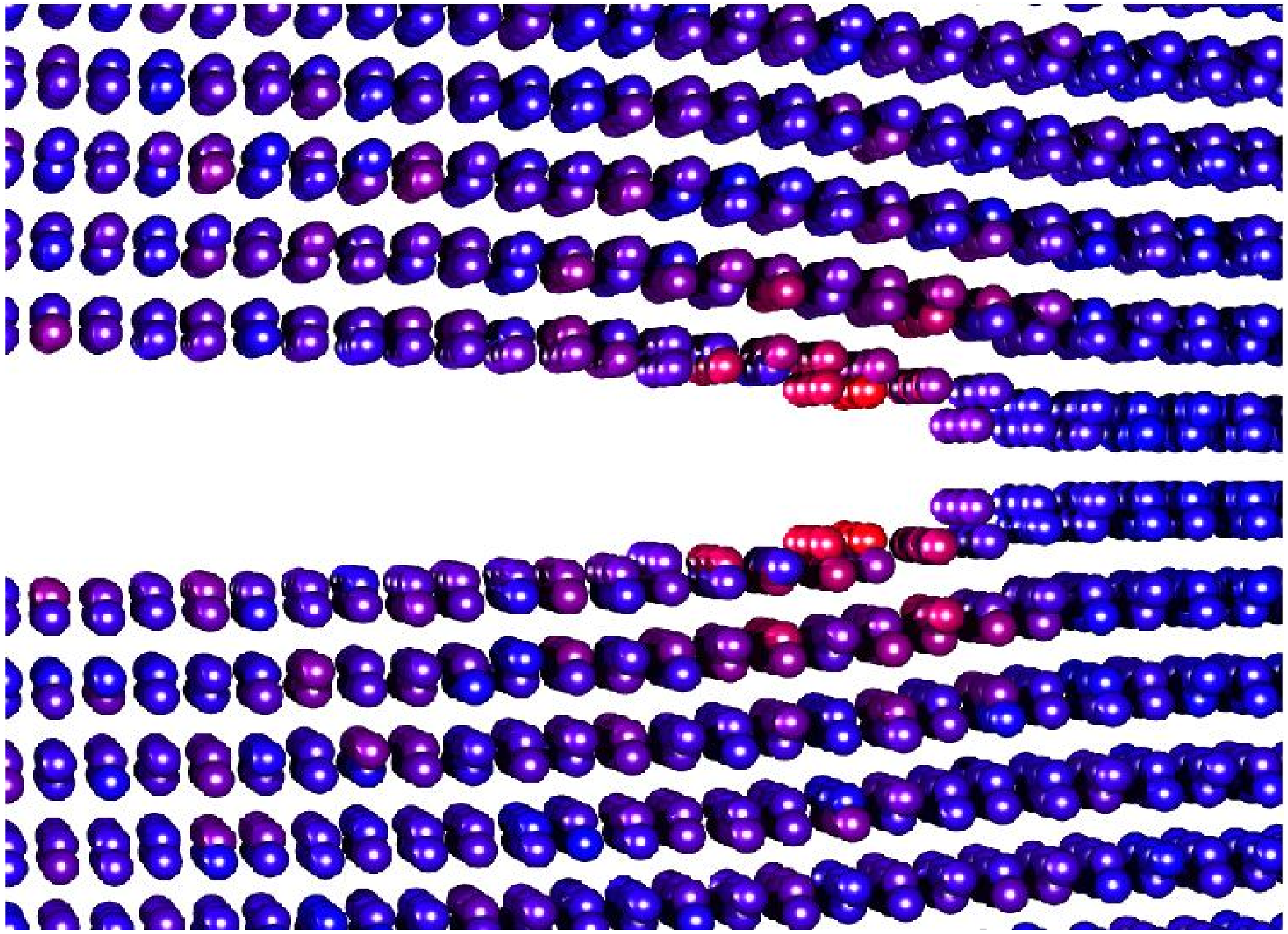


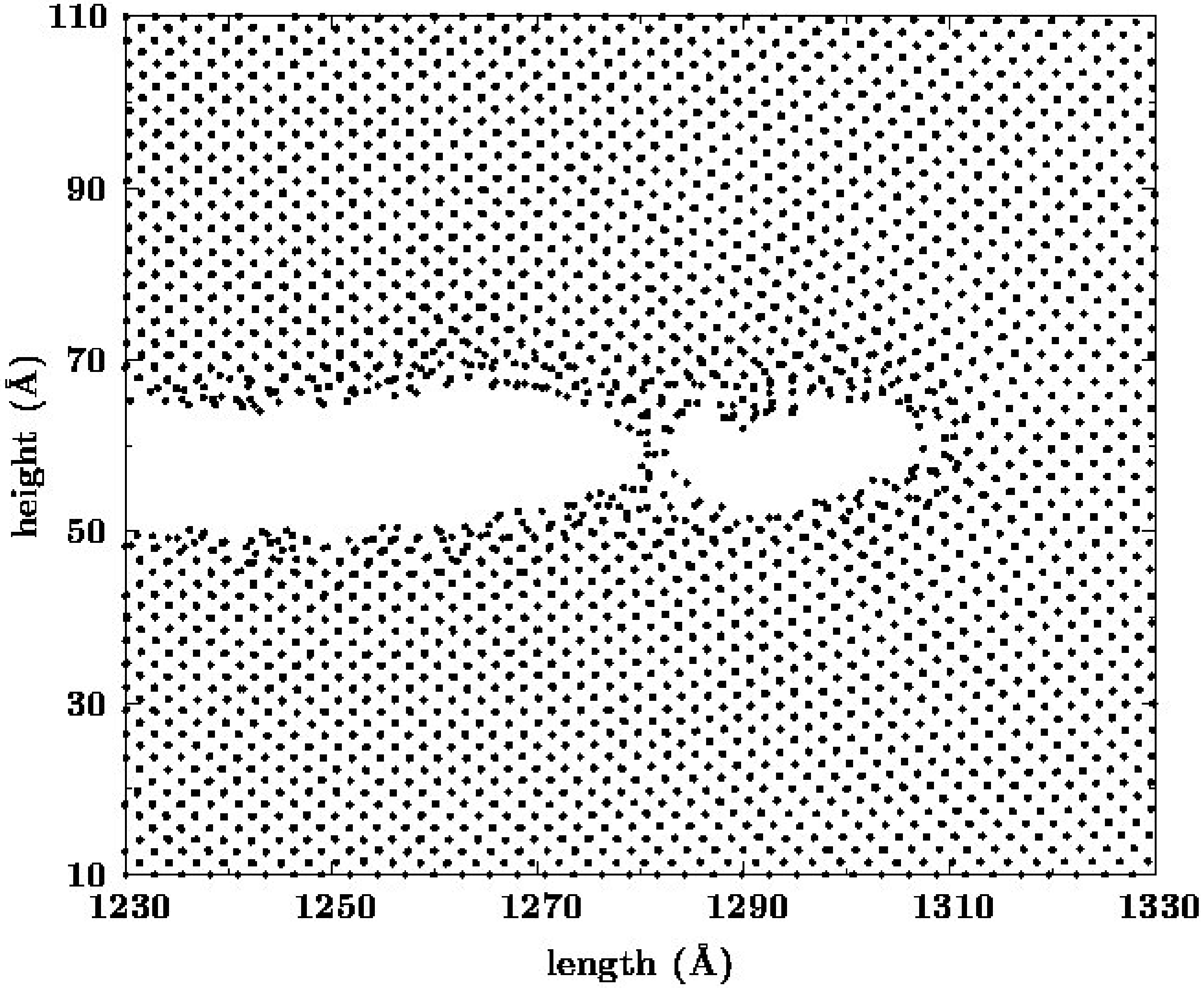
# Scaling of Steady States



Silicon is "well known" to cleave cleanly along the (111) and (110) planes, but not at all along (100)

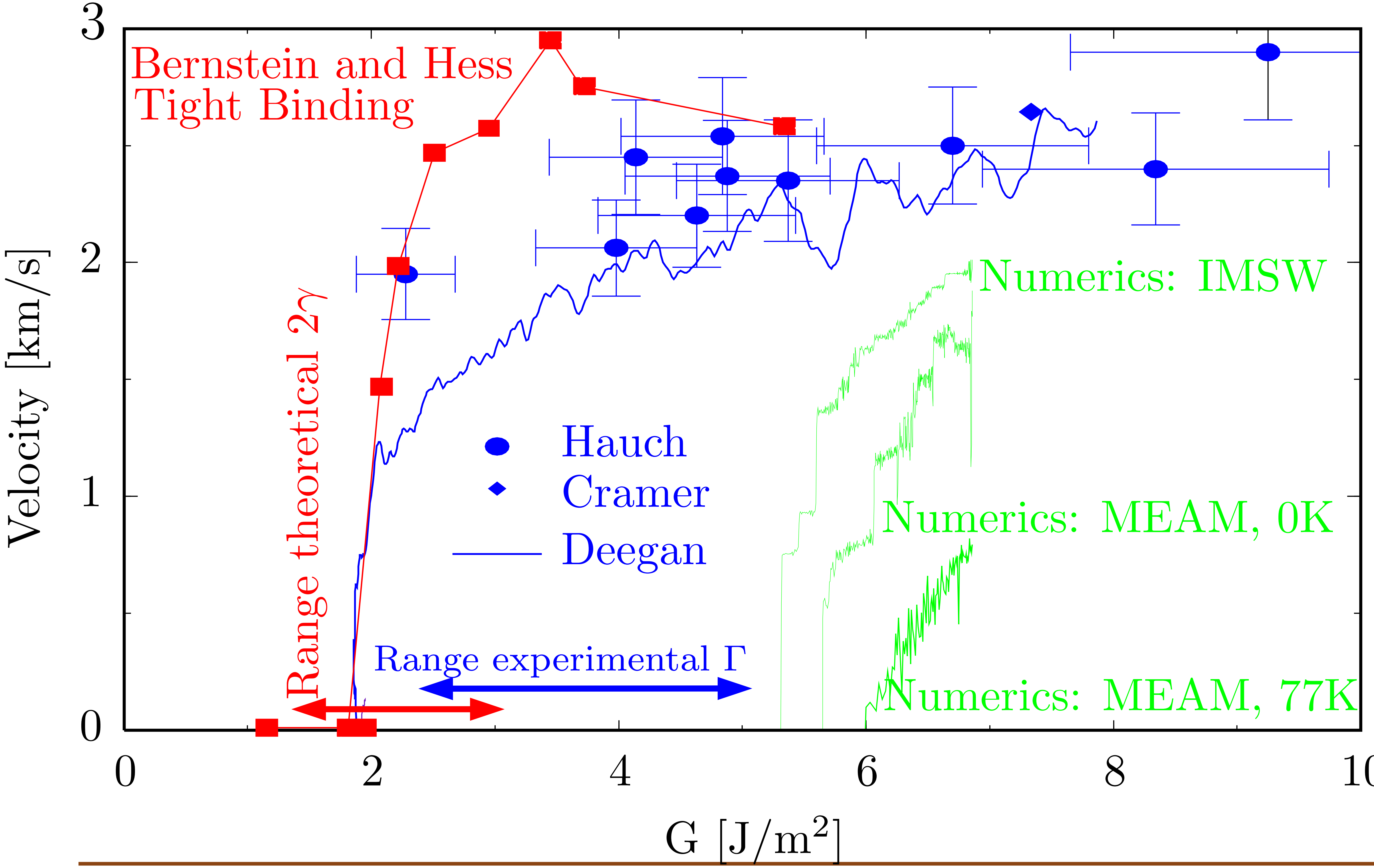
Clean failure along (110) | Rough failure along 100





# Application I: single-crystal silicon

Theory and experiment for single crystal silicon may finally agree... but it seems to take quantum mechanics!



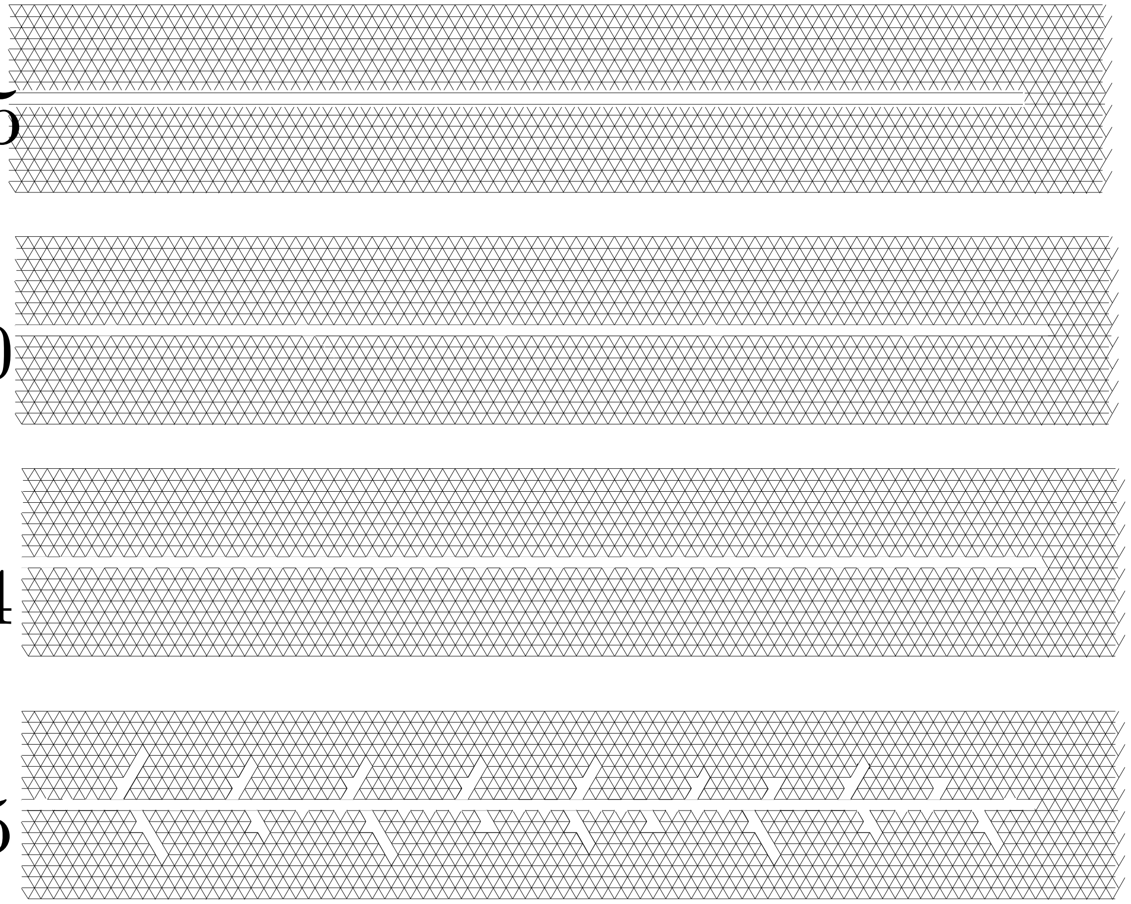
# Application II: Crack-tip instability

$\Delta = 1.147$
$v/c = 0.645$

$\Delta = 1.165$
$v/c = 0.630$

$\Delta = 1.376$
$v/c = 0.624$

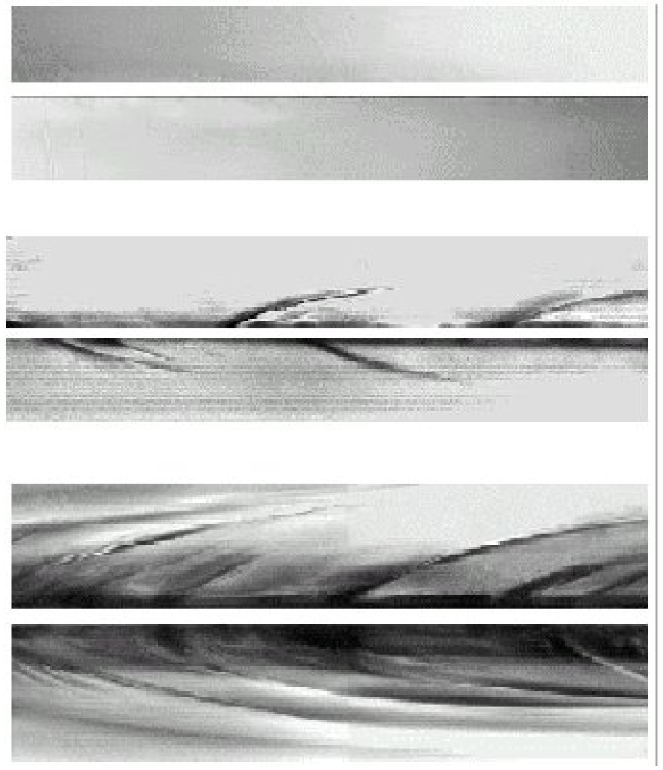
$\Delta = 1.835$
$v/c = 0.775$



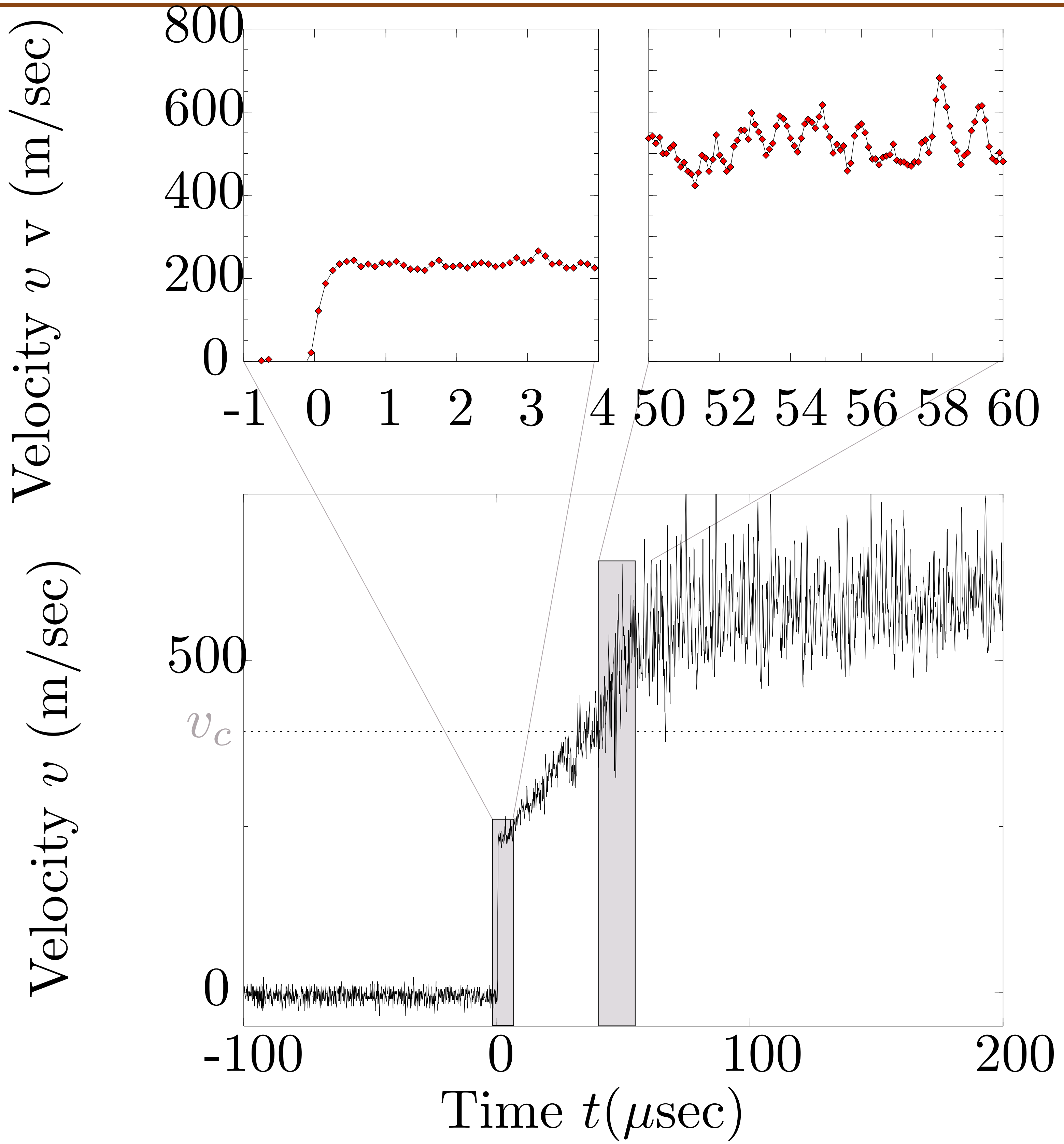
$v < v_c$

$v \approx v_c$

$v > v_c$

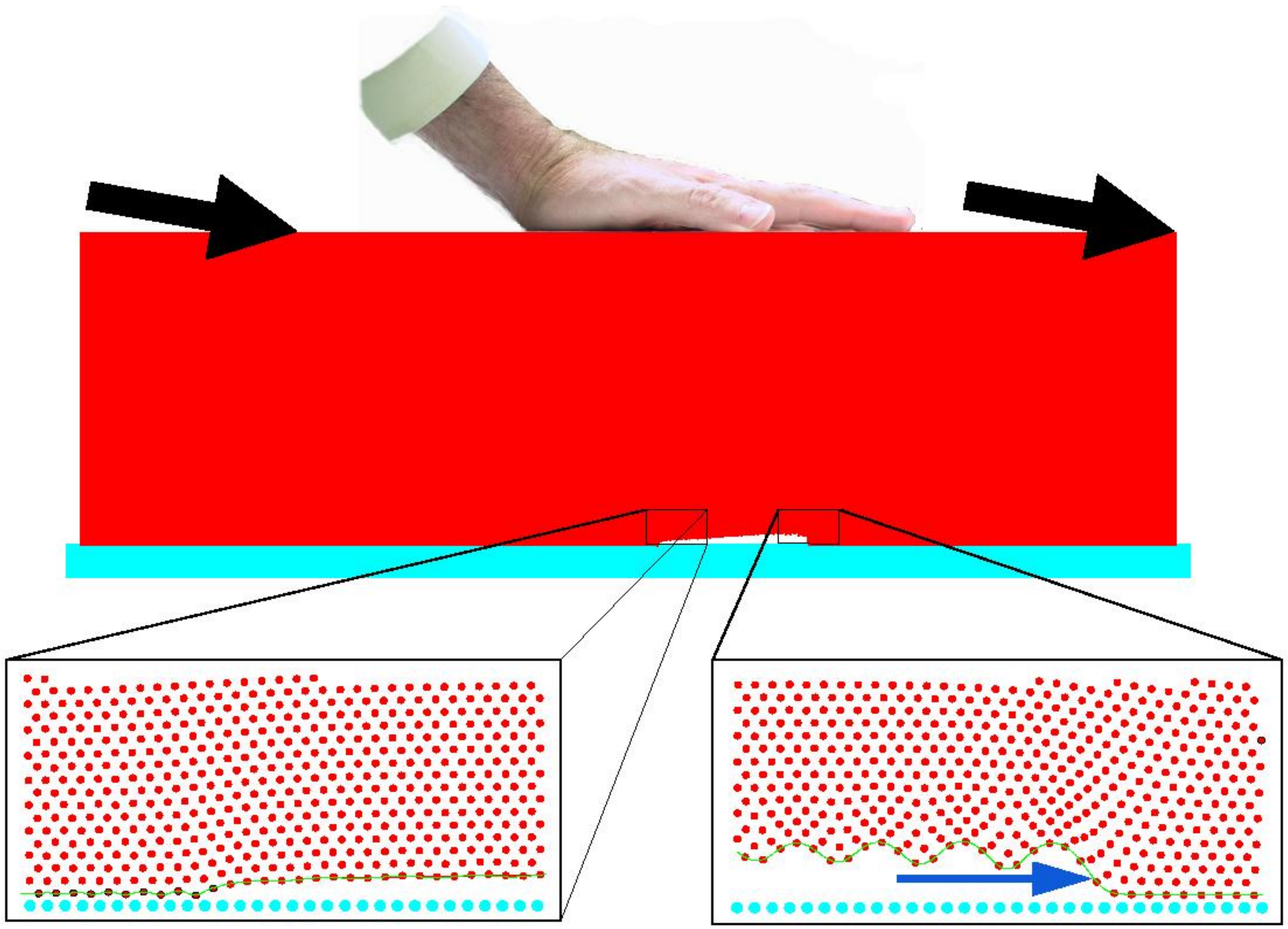


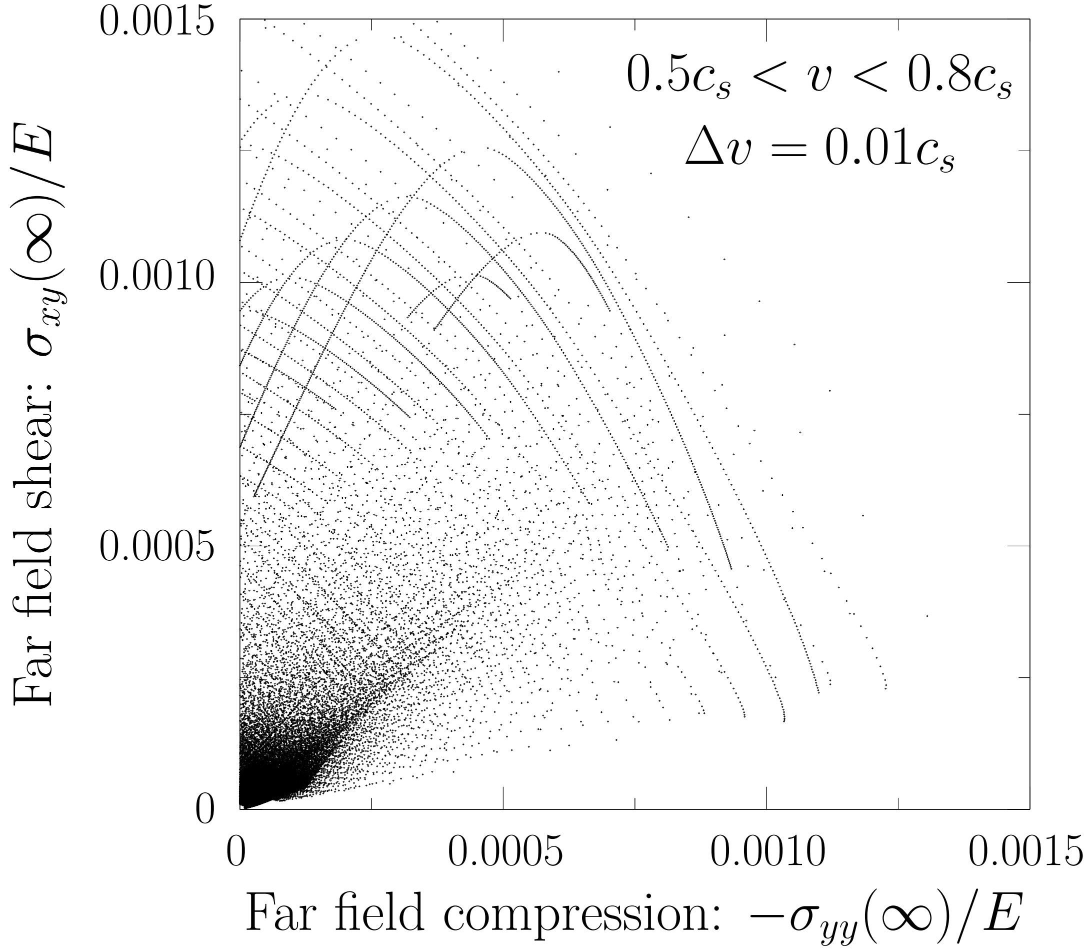
# Application II: Crack-tip instability



# Application III: Self-healing pulses

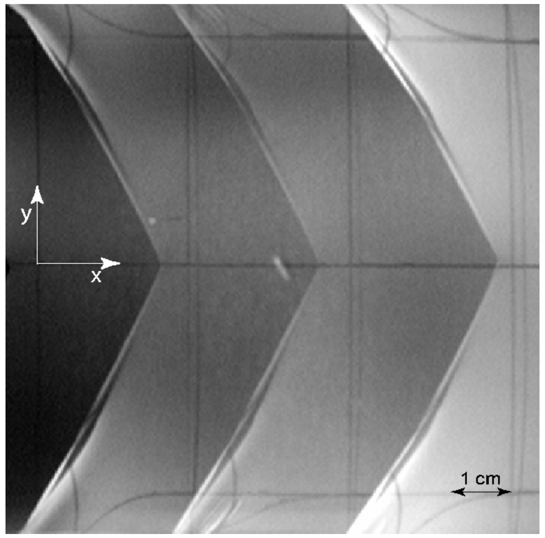
$\mu \approx .2$






Gerde and Marder, *Nature* 2001

# Application IV: Rupture of Rubber

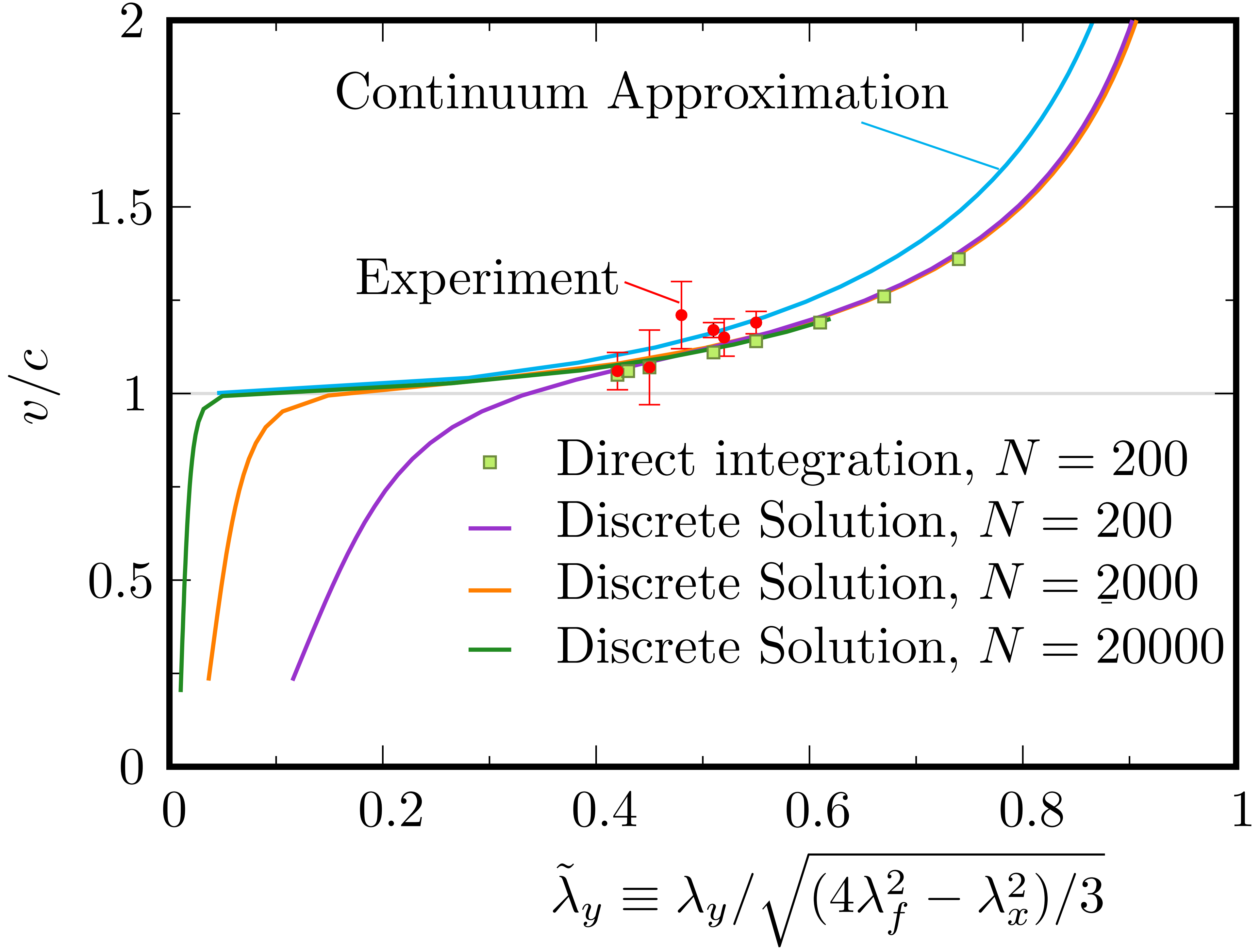




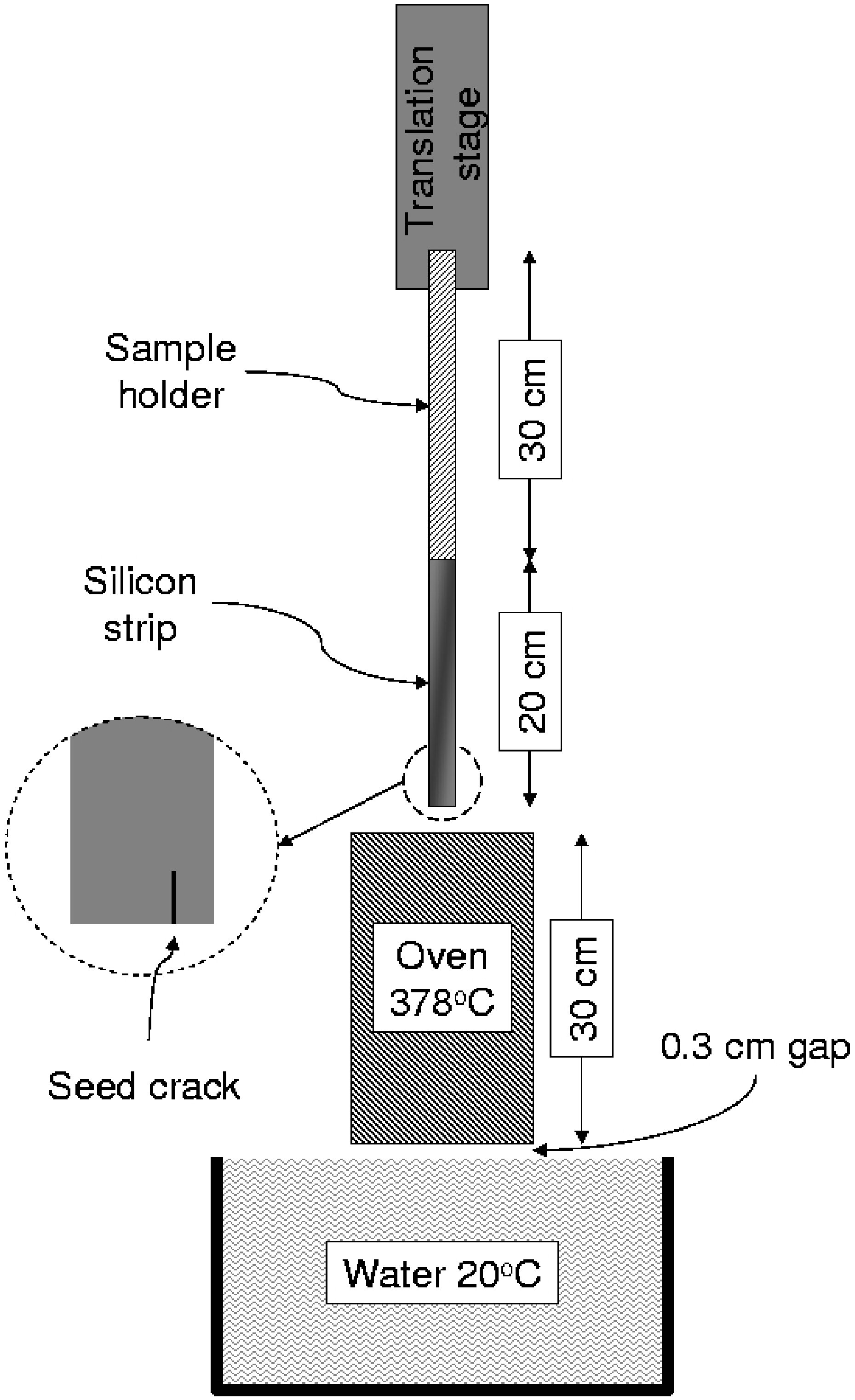

*PRL* **94** 048001 (2005)

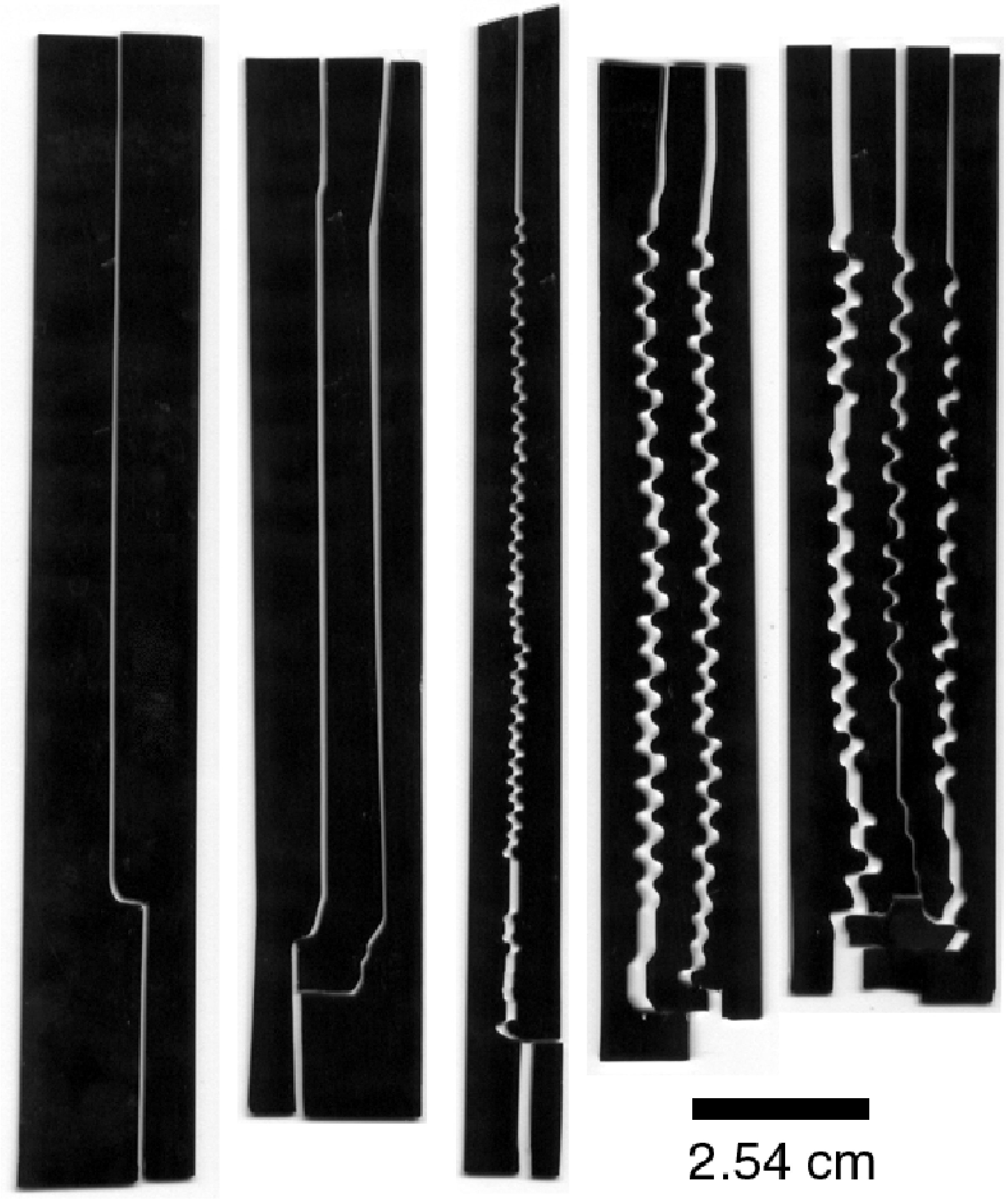
cond-mat/0504613

# Application IV: Rupture of Rubber

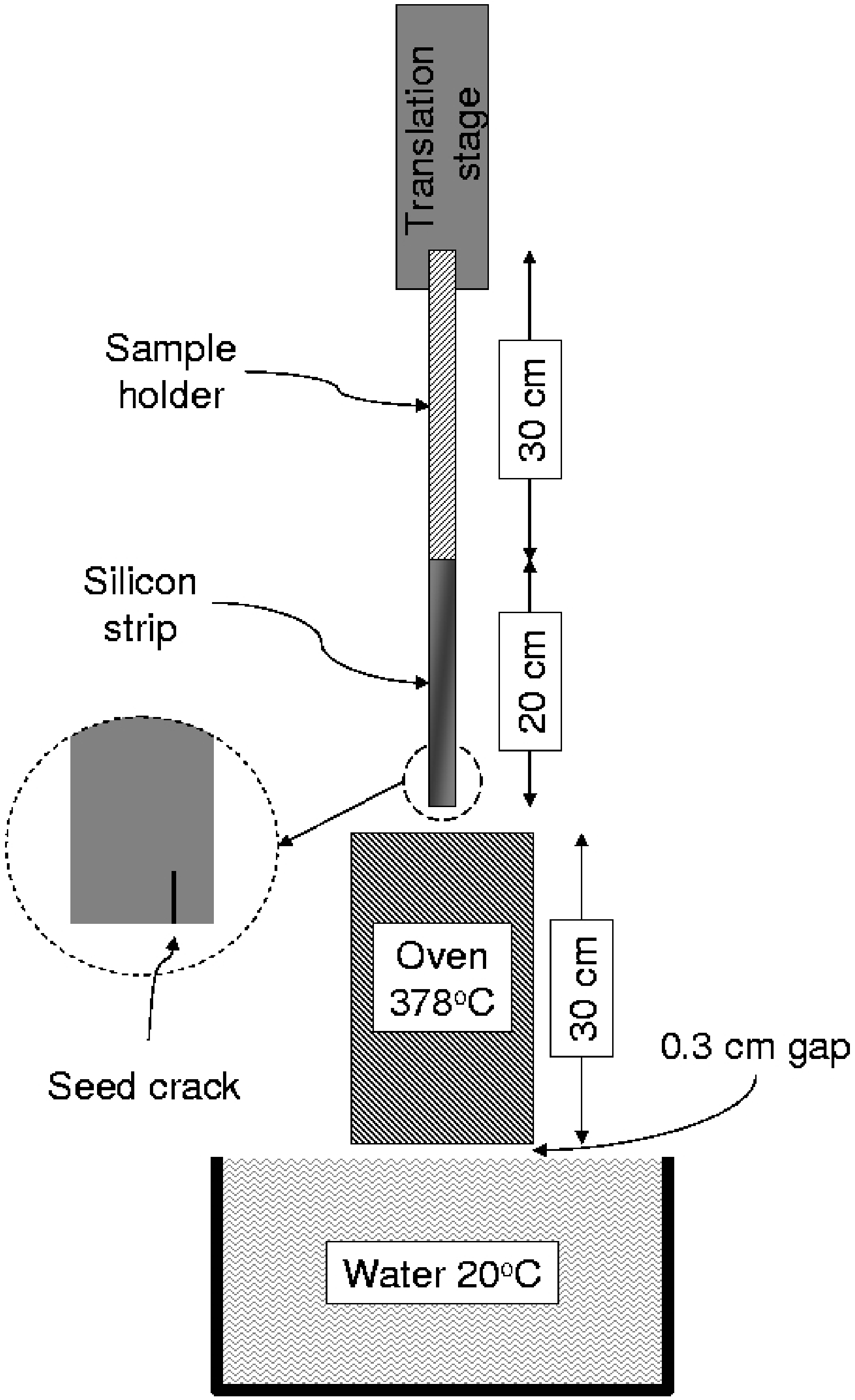


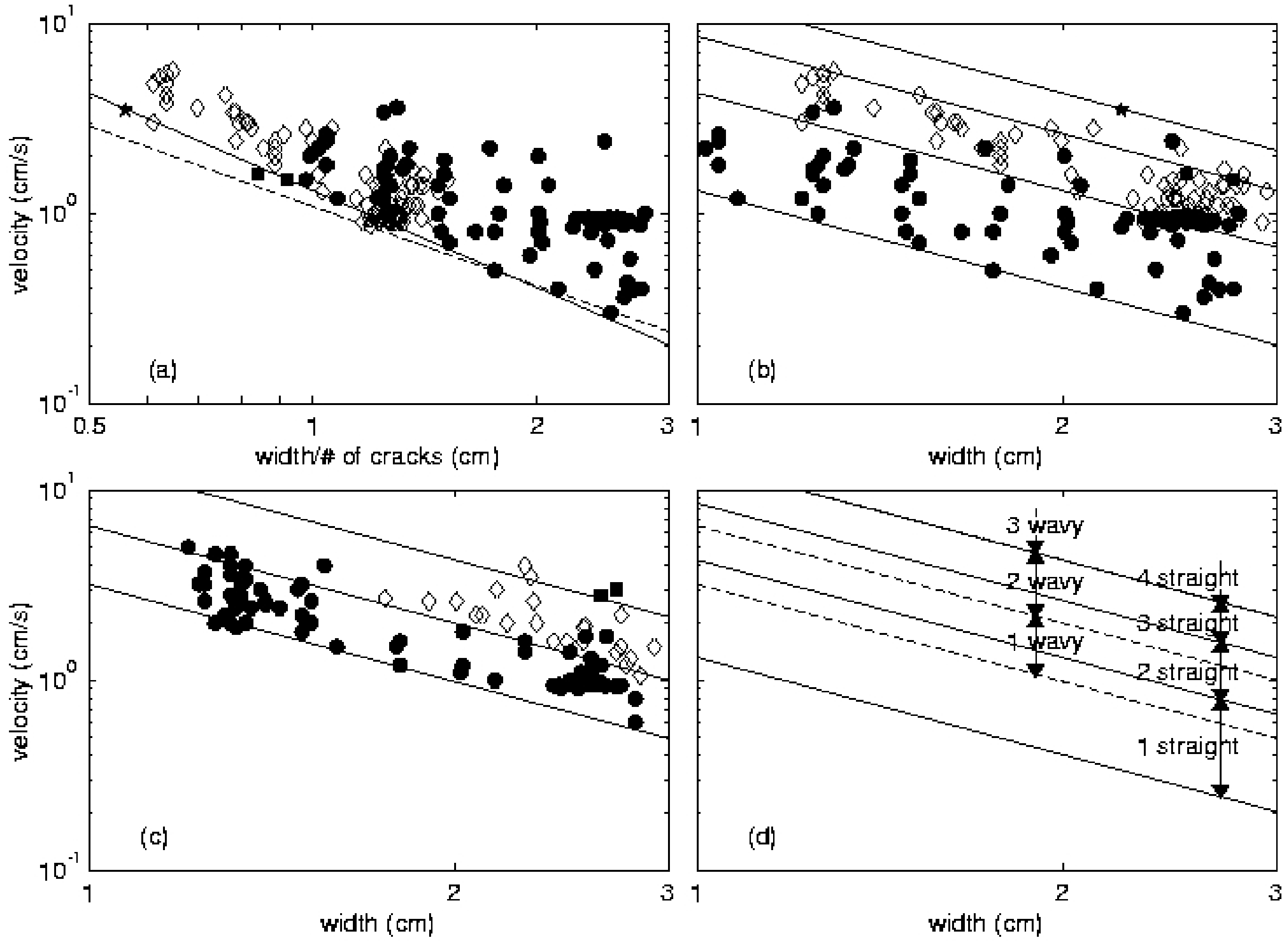
# Application V: Crack paths in crystal



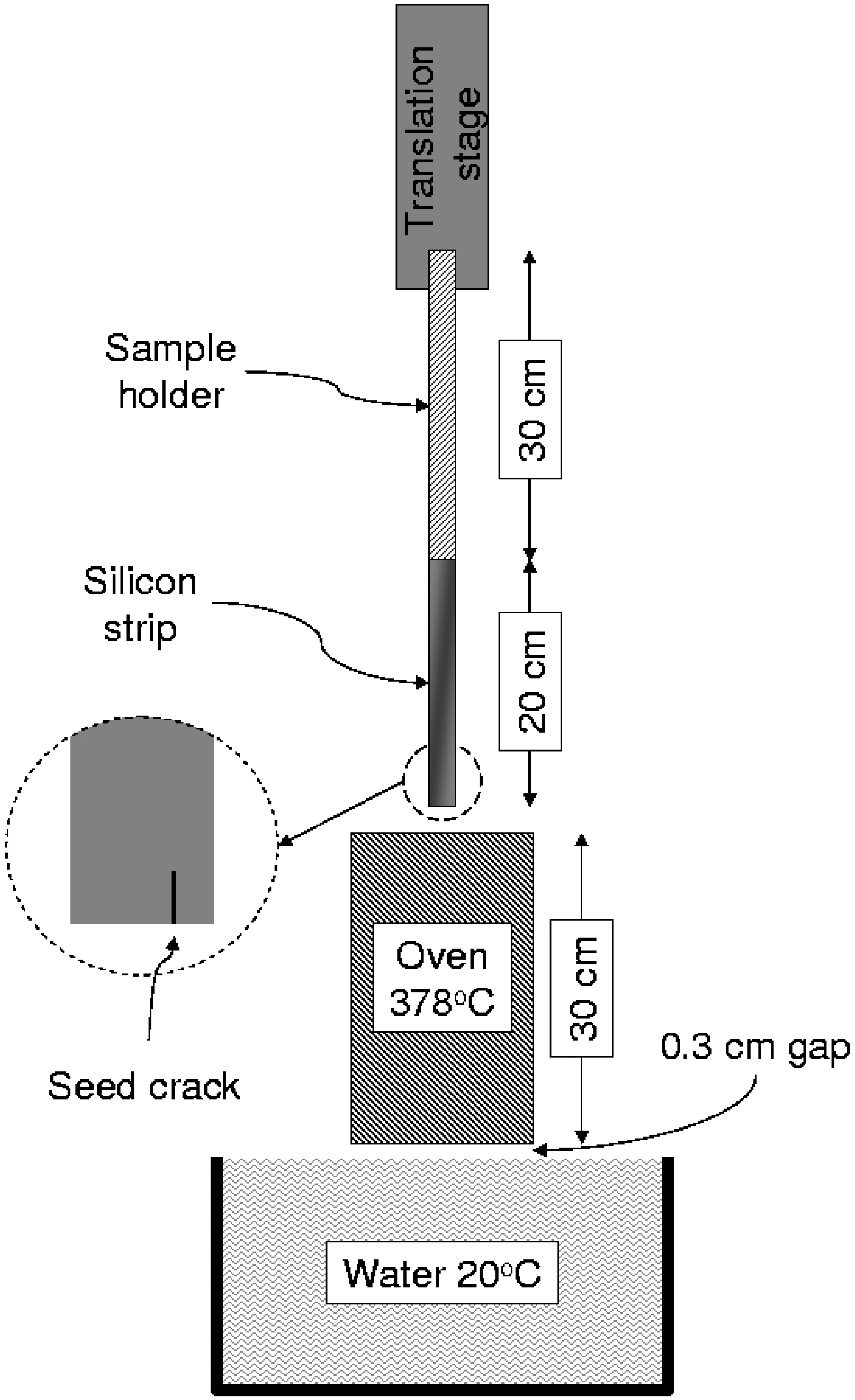



# Application V: Crack paths in crystal

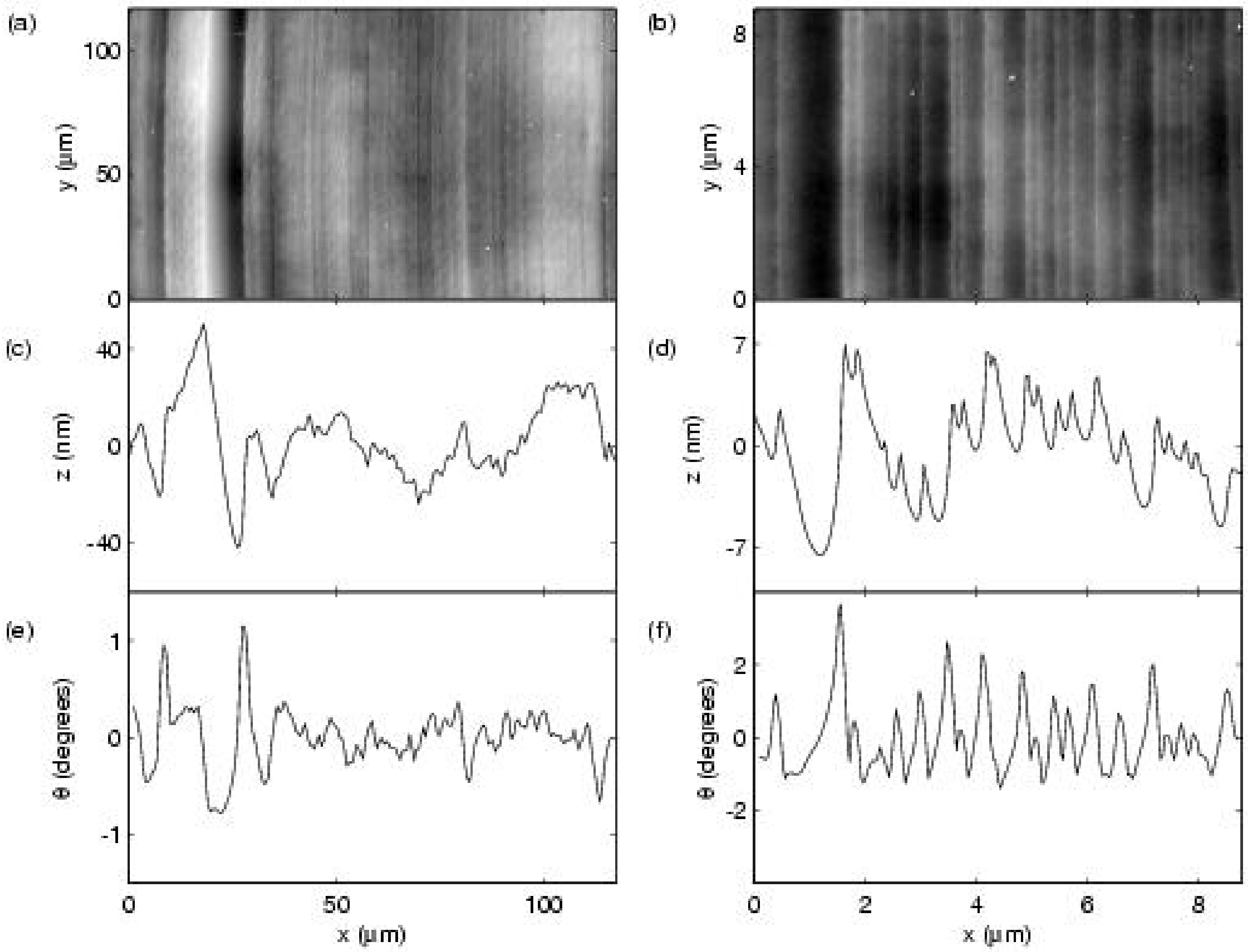


# Application V: Crack paths in crystal




Expecting to find faceting that traced out continuous curves, we instead found a self-affine fractal along direction of crack motion



# Application V: Crack paths in crystal

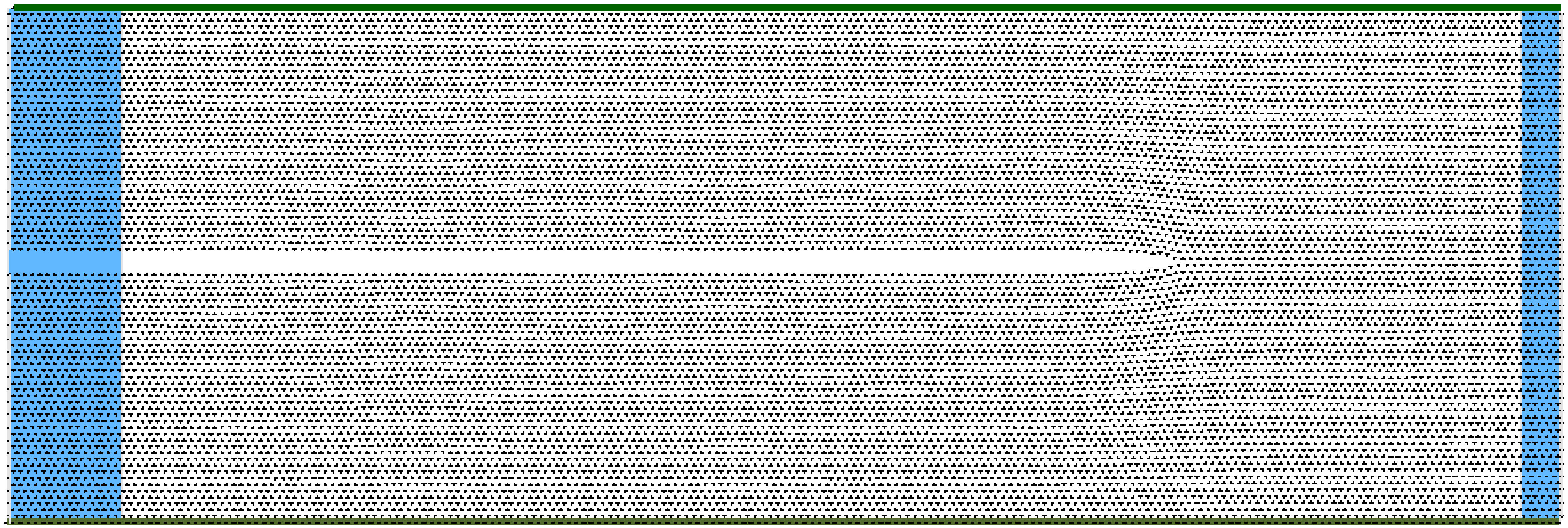
Is principle of local symmetry always correct?

In a material that is isotropic and homogeneous at the macroscopic level, do cracks always travel in the direction it predicts?

Answer: no. For example, cracks can follow crystal planes that are completely invisible to continuum elasticity

# Application V: Crack paths in crystal

Displace upper boundary by $(\delta_x, \delta_y)$

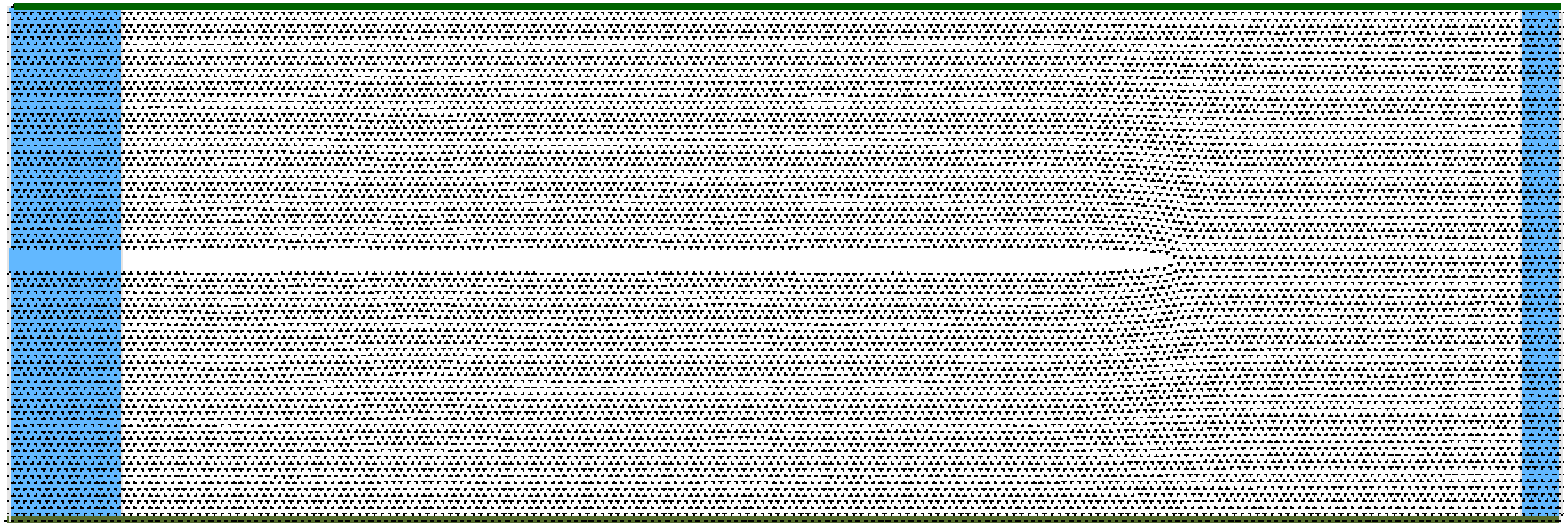


Hold lower boundary rigid

In each case, compute shear stress versus angle, find where $K_{II}$ vanishes

# Application V: Crack paths in crystal

Displace upper boundary by $(\delta_x, \delta_y)$

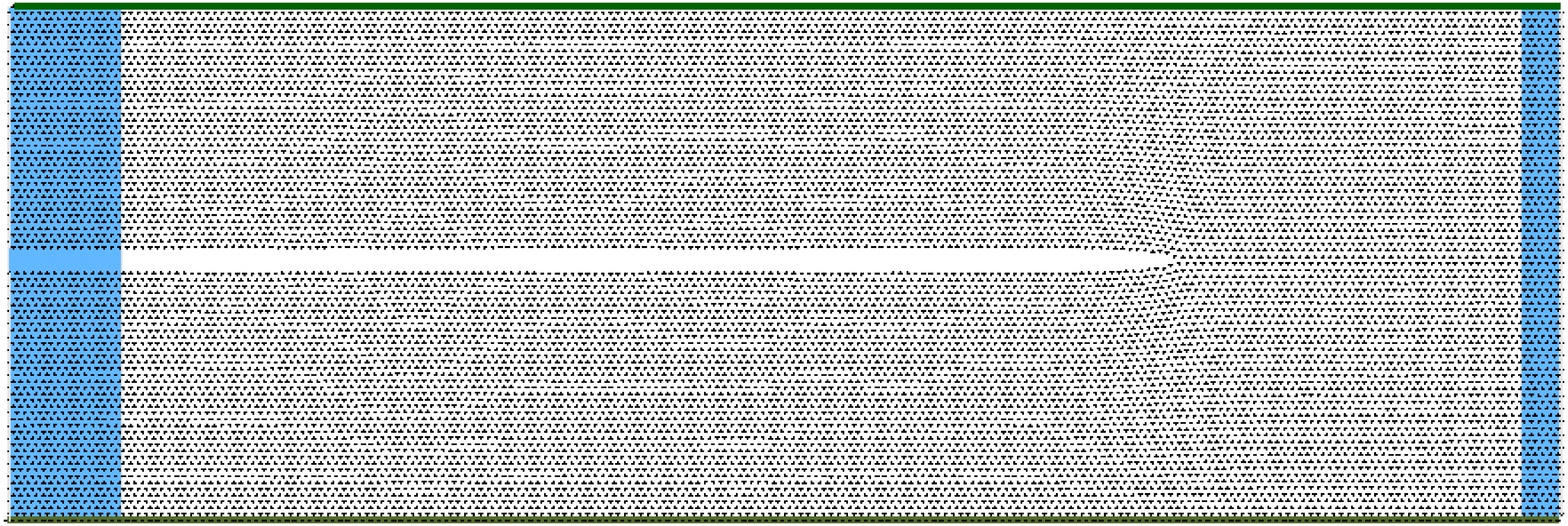


Hold lower boundary rigid

By varying Kelvin dissipation, for fixed loading conditions, one can obtain different steady velocity solutions.

# Application V: Crack paths in crystal

Displace upper boundary by $(\delta_x, \delta_y)$

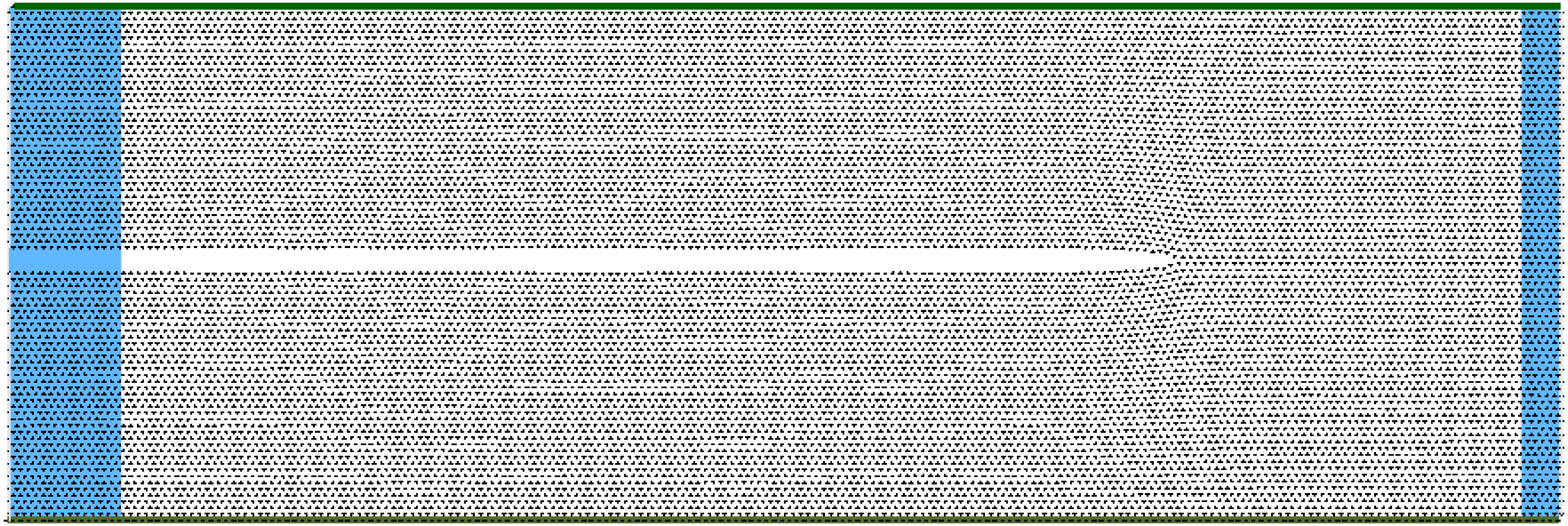


Hold lower boundary rigid

Take height $N = 200$, $u_c = 1.2$, displace top by $\delta_y = 20$, and $\delta_x = .23\delta_y$. Set Kelvin dissipation to $\beta = 2$ and then to $\beta = .02$.

# Application V: Crack paths in crystal

Displace upper boundary by $(\delta_x, \delta_y)$

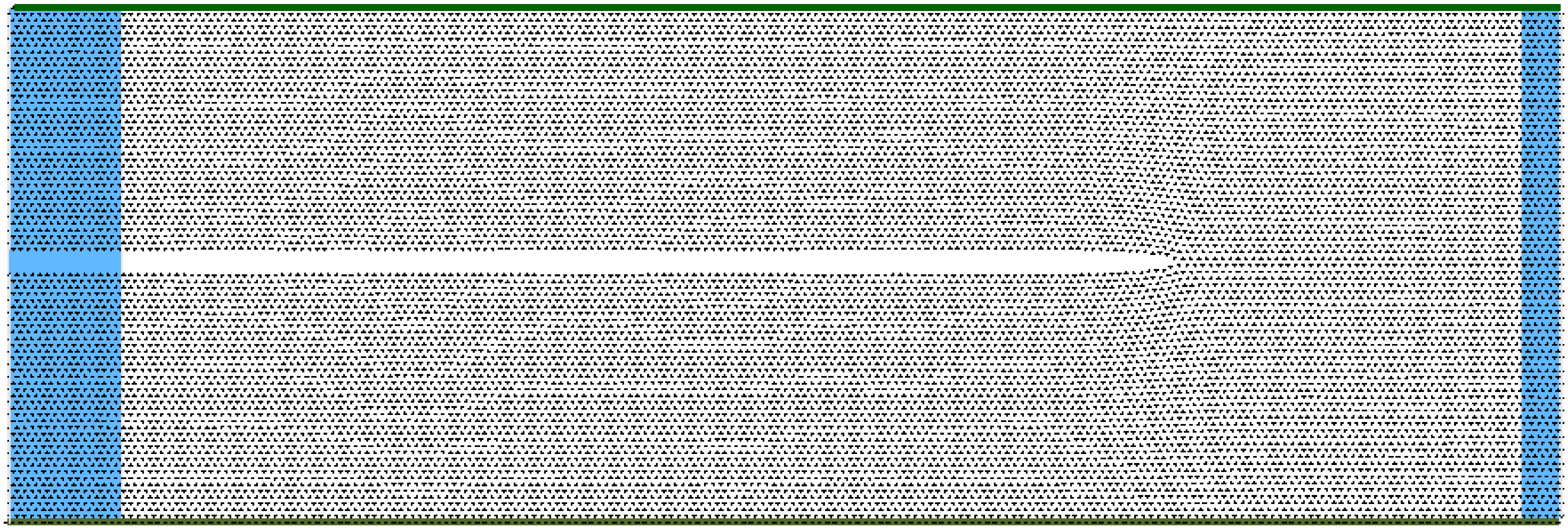


Hold lower boundary rigid

Obtain cracks moving at $v/c_R = .01$ and $v/c_R = .83$.

# Application V: Crack paths in crystal

Displace upper boundary by $(\delta_x, \delta_y)$

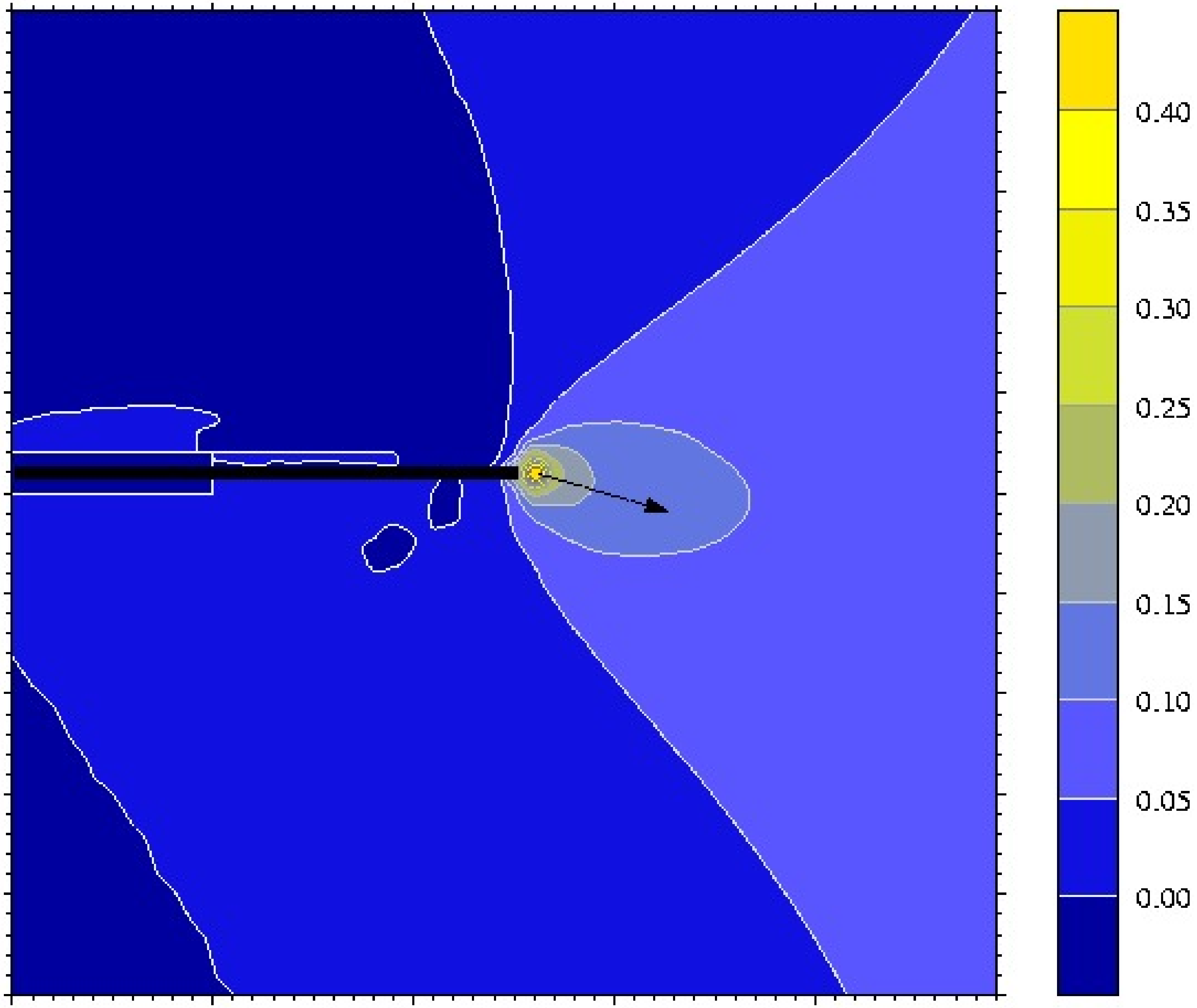


Hold lower boundary rigid

In each case, compute shear stress versus angle, find where $K_{II}$ vanishes

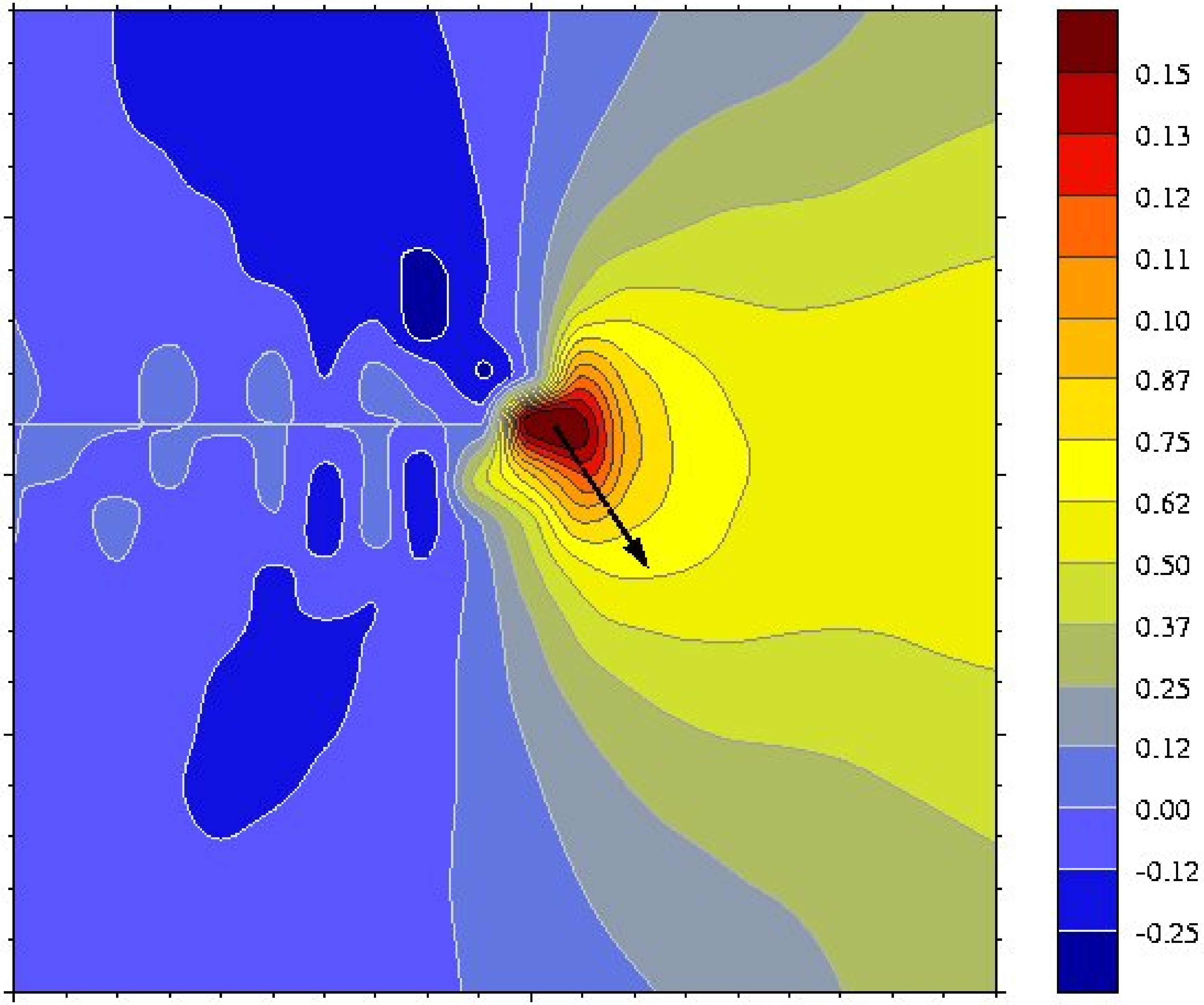
# Application V: Crack paths in crystal

Crack with $v = .01 c_R$, should kink at $-16°$



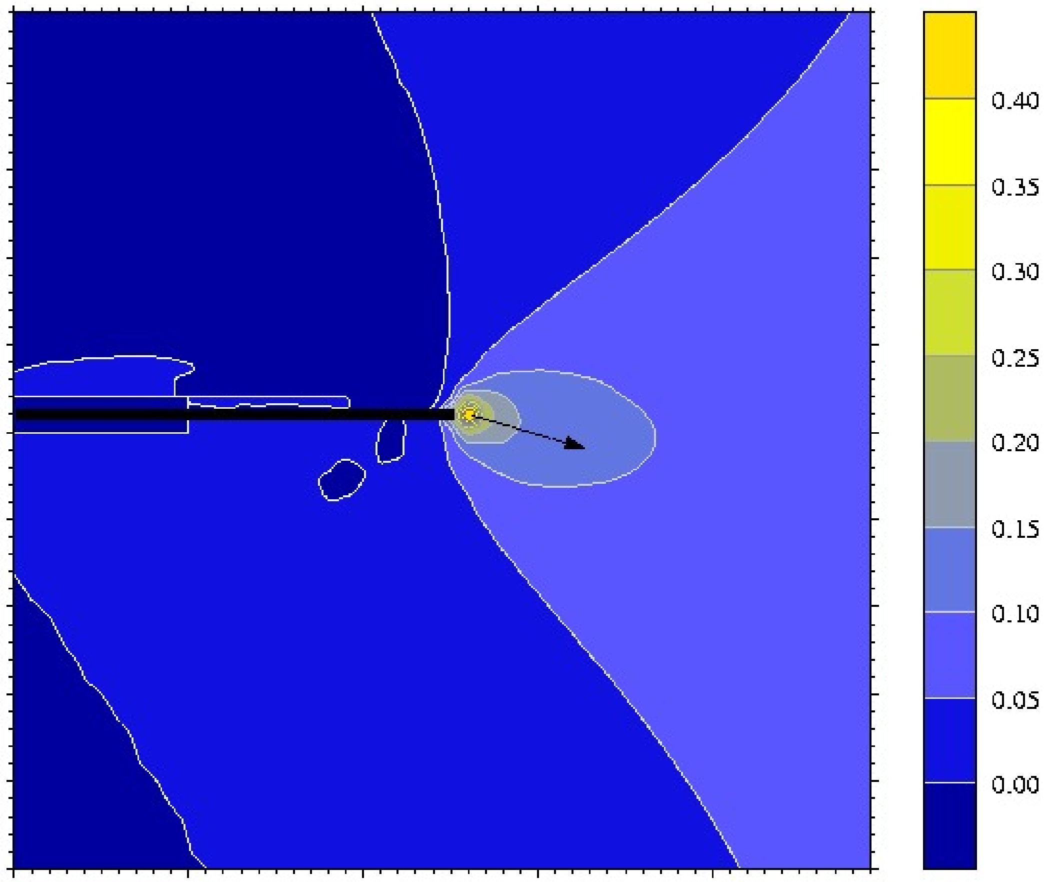
# Application V: Crack paths in crystal

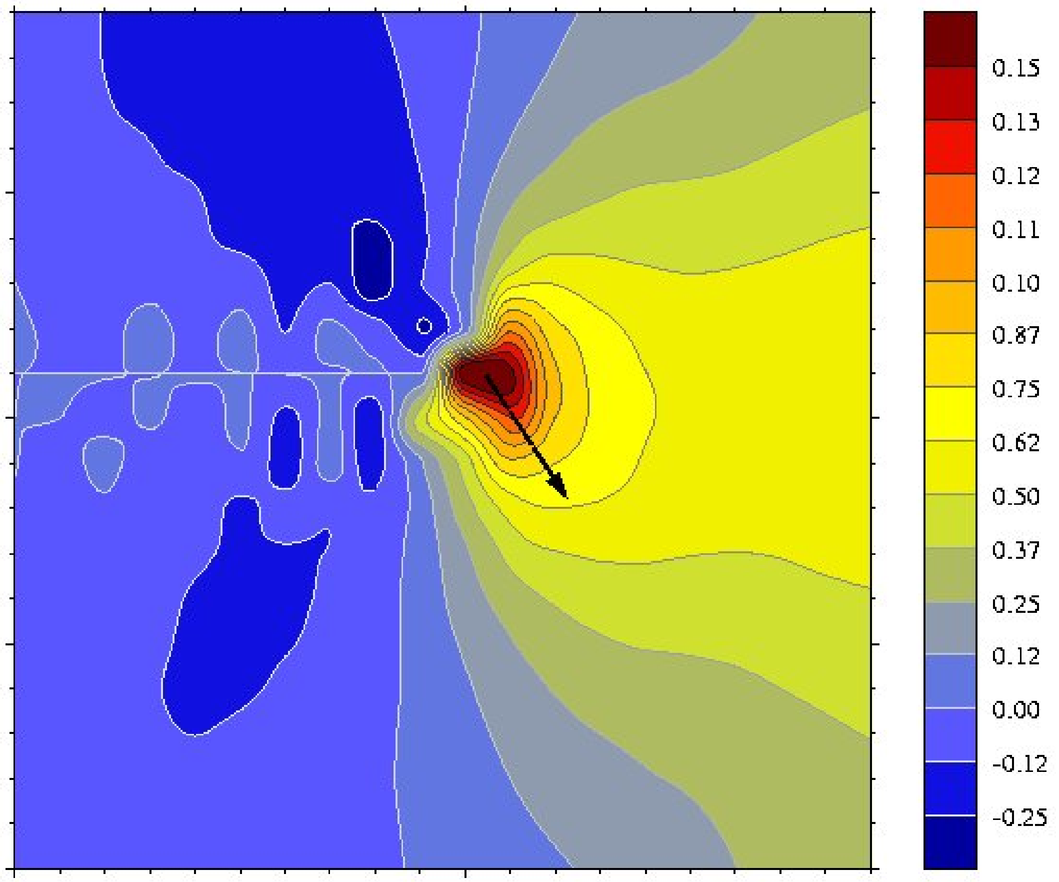
Crack with $v = .83c_R$, should kink at $-57°$



# Application V: Crack paths in crystal

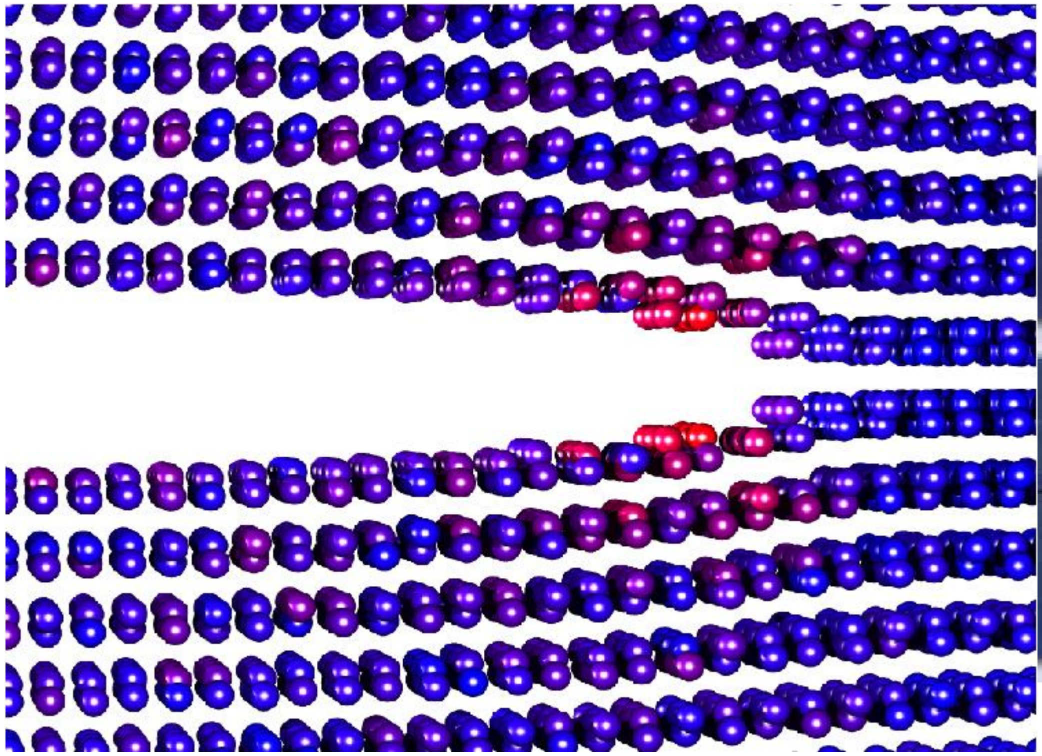
However, both cracks travel straight along horizontal axis forever

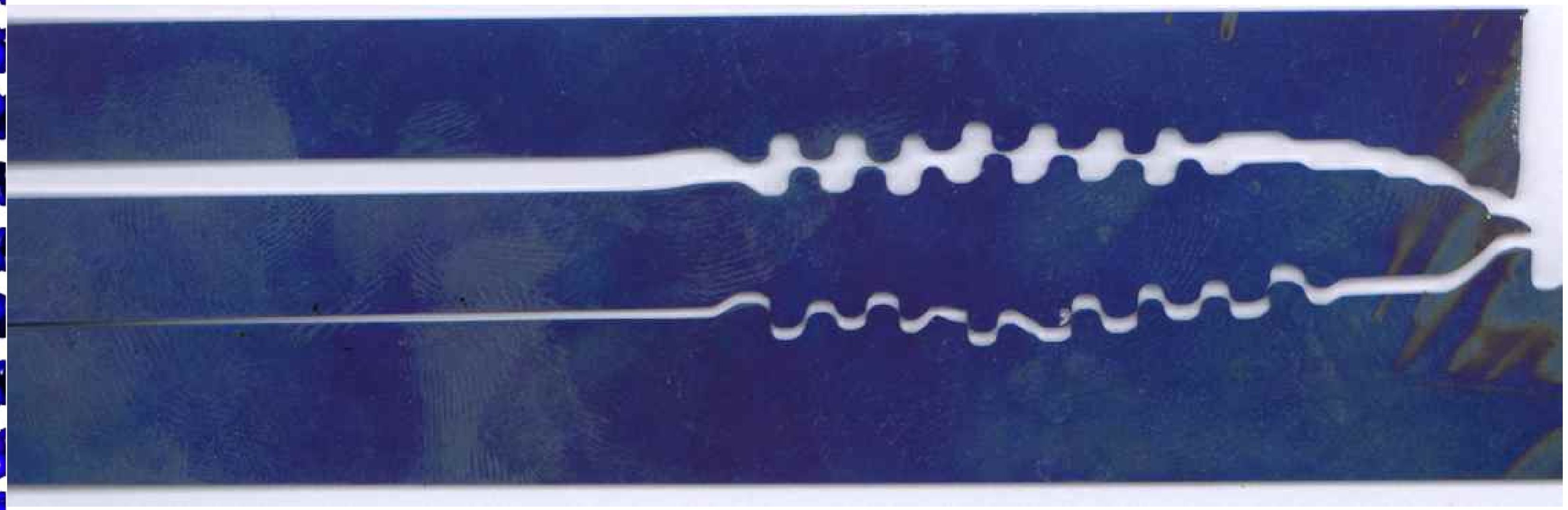


# Atoms matter for fracture

Range of cohesive forces and atomic spacings are the same...this causes trouble for continuum theories of brittle crack tips.

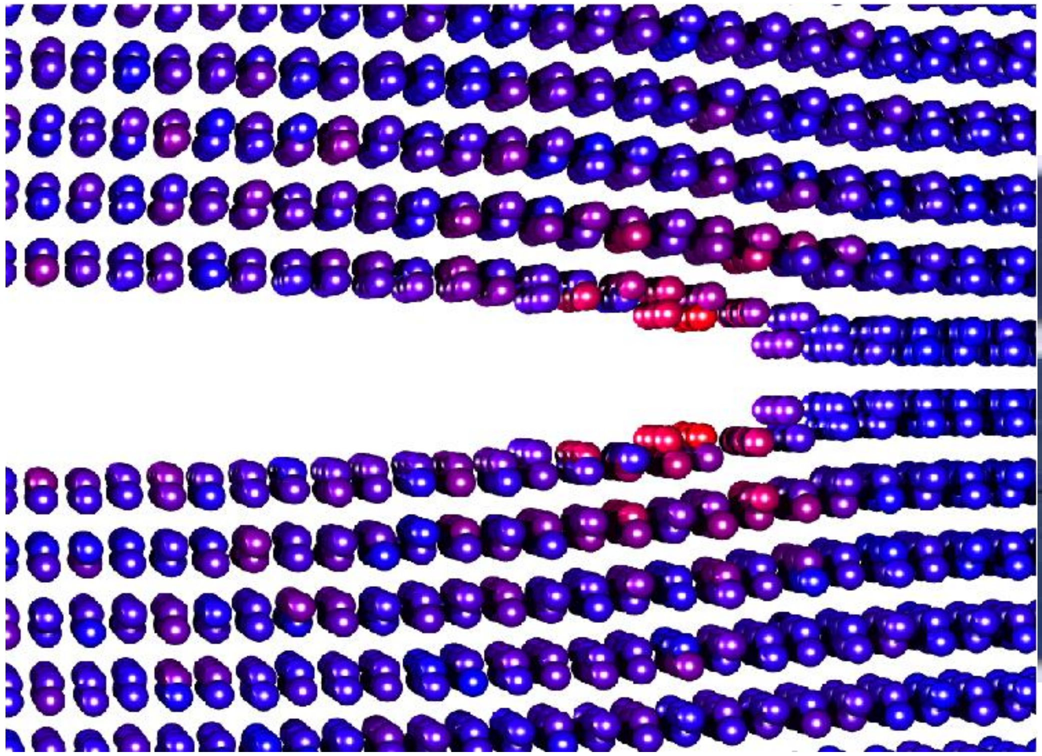


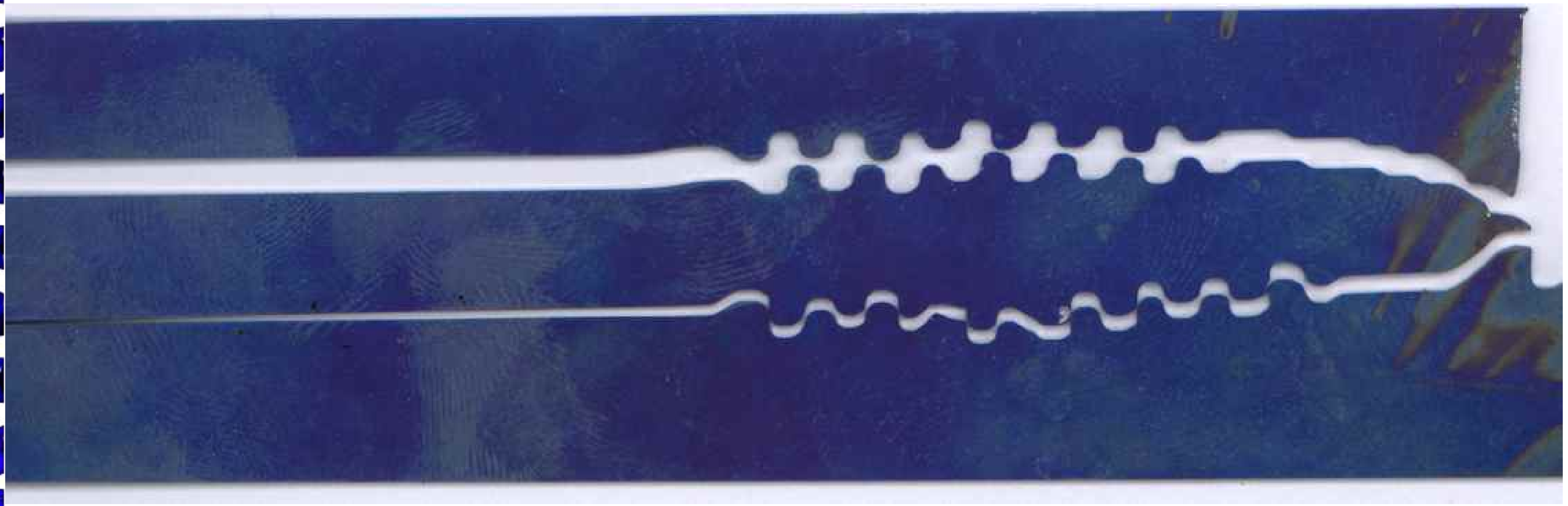


# Atoms matter for fracture

Range of cohesive forces and atomic spacings are the same...this causes trouble for continuum theories of brittle crack tips.

Experiments and computations in crystals clearly show macroscopic consequences of microscopic arrangement



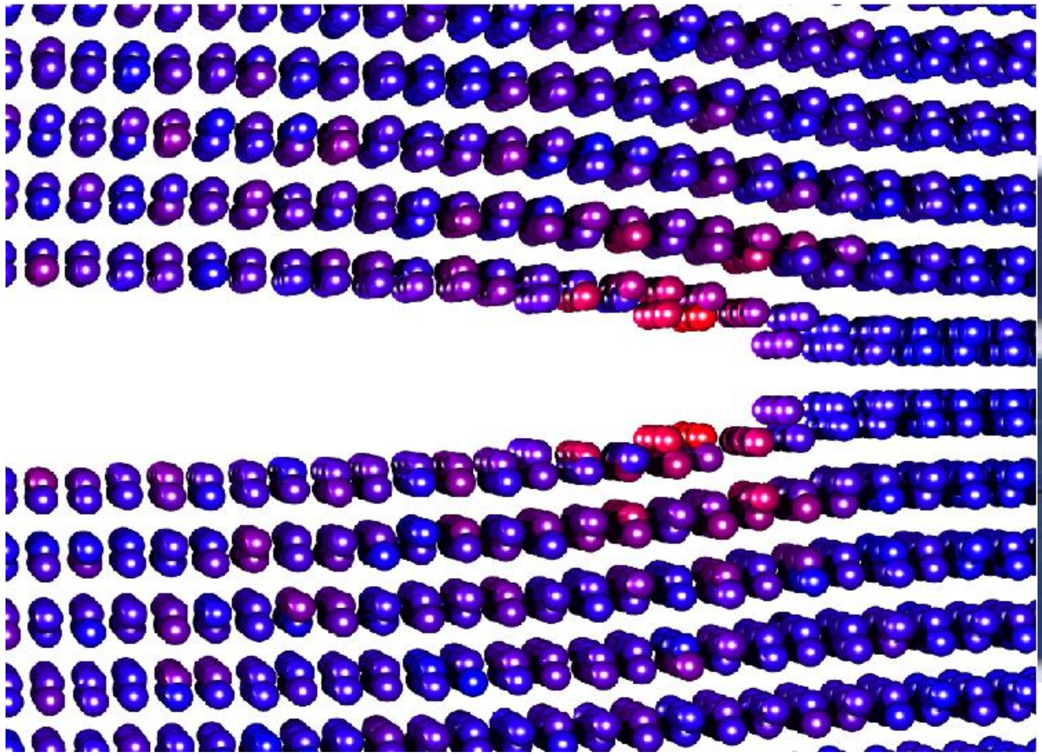


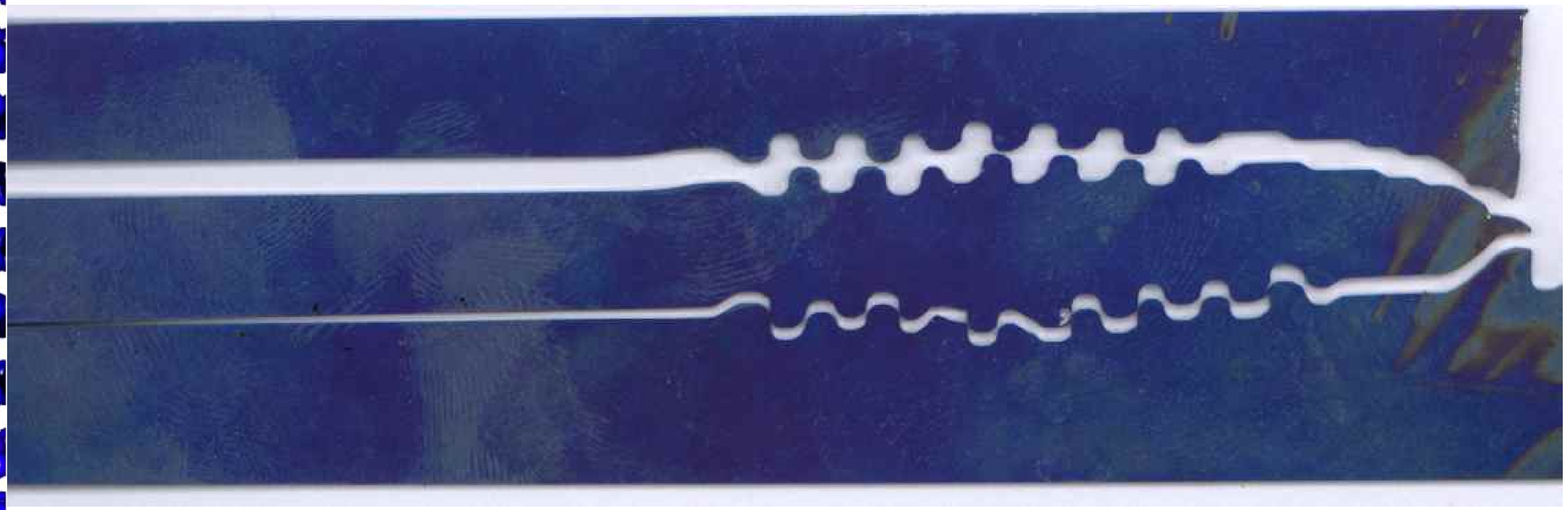
# Atoms matter for fracture

Range of cohesive forces and atomic spacings are the same...this causes trouble for continuum theories of brittle crack tips.

Experiments and computations in crystals clearly show macroscopic consequences of microscopic arrangement

Elimination of crack singularities by discreteness continues to be important even in polymeric materials, where separating units are much larger than atoms.





# Atoms matter for fracture

Atomic-scale studies answer questions about crack initiation, speed, and direction to complement continuum studies involving complex geometries and loading.