Capturing the Singular Sets of Solids

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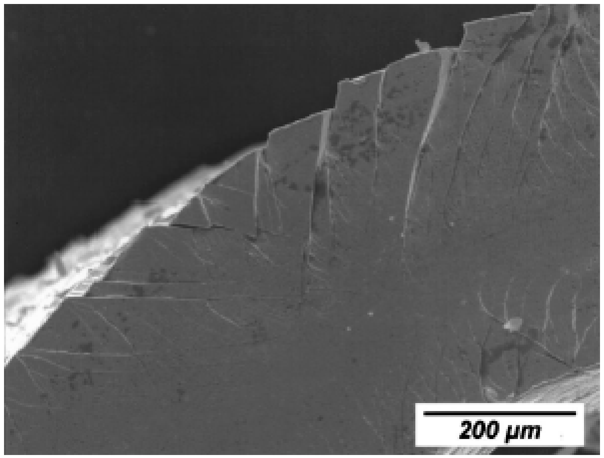
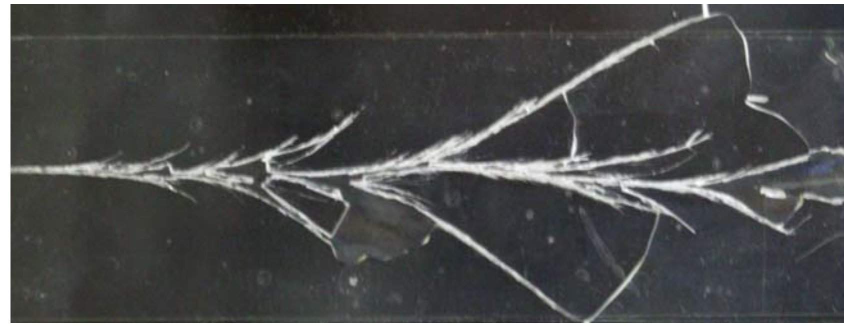
Stanford, April 21, 2004

Singular sets in solids



BMG bending experiments
(Conner et al., 2003)



Dynamic crack brancking
(Fineberg and Sharon, 1992)

Detonation-driven Al-tube fracture
(Shepherd et al., 2003)

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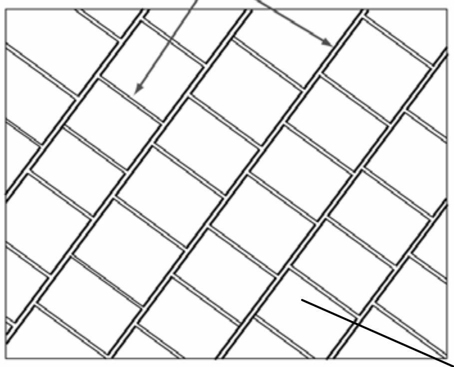
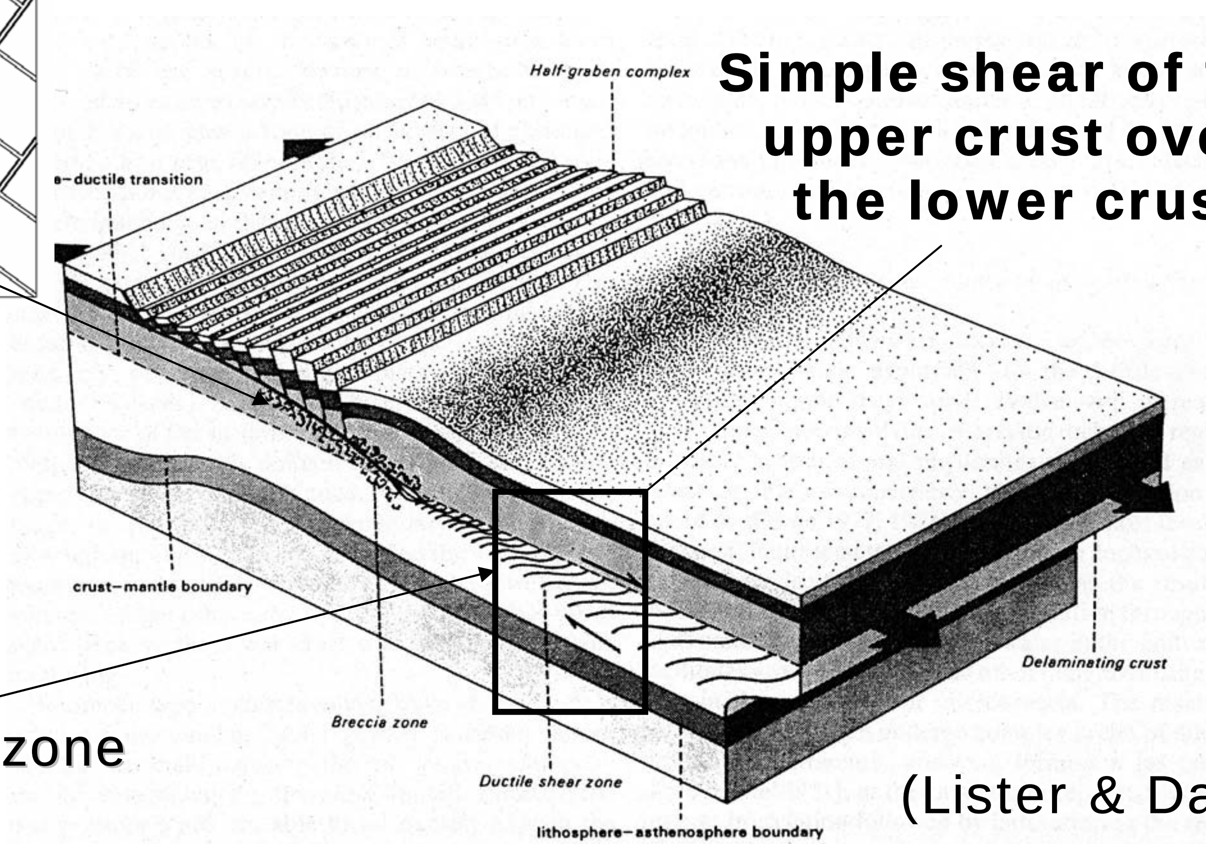
Singular sets in solids

cohesive faults





Simple shear of the upper crust over the lower crust

Ductile shear zone

(Lister & Davis, 89)

Crustal shear zone at the bd transition

Free-discontinuity problems

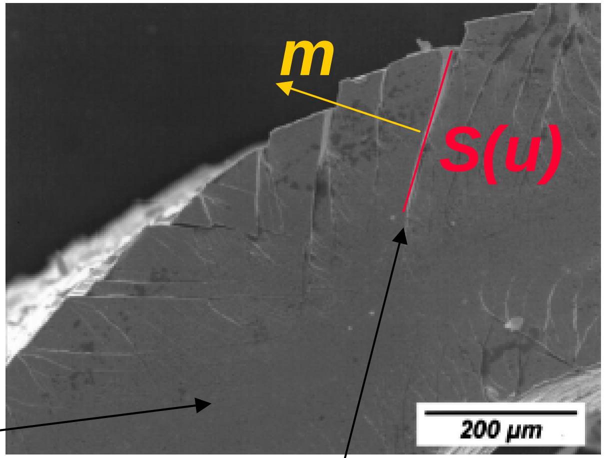
- Field gradient has the structure:

$$Du = \nabla u + [\![u]\!] \otimes m \delta_S$$

where:

i) ∇u absolutely continuous

ii) $S = S(u) \equiv$ *singular set*, $m \equiv$ unit normal.



- The energy has the form

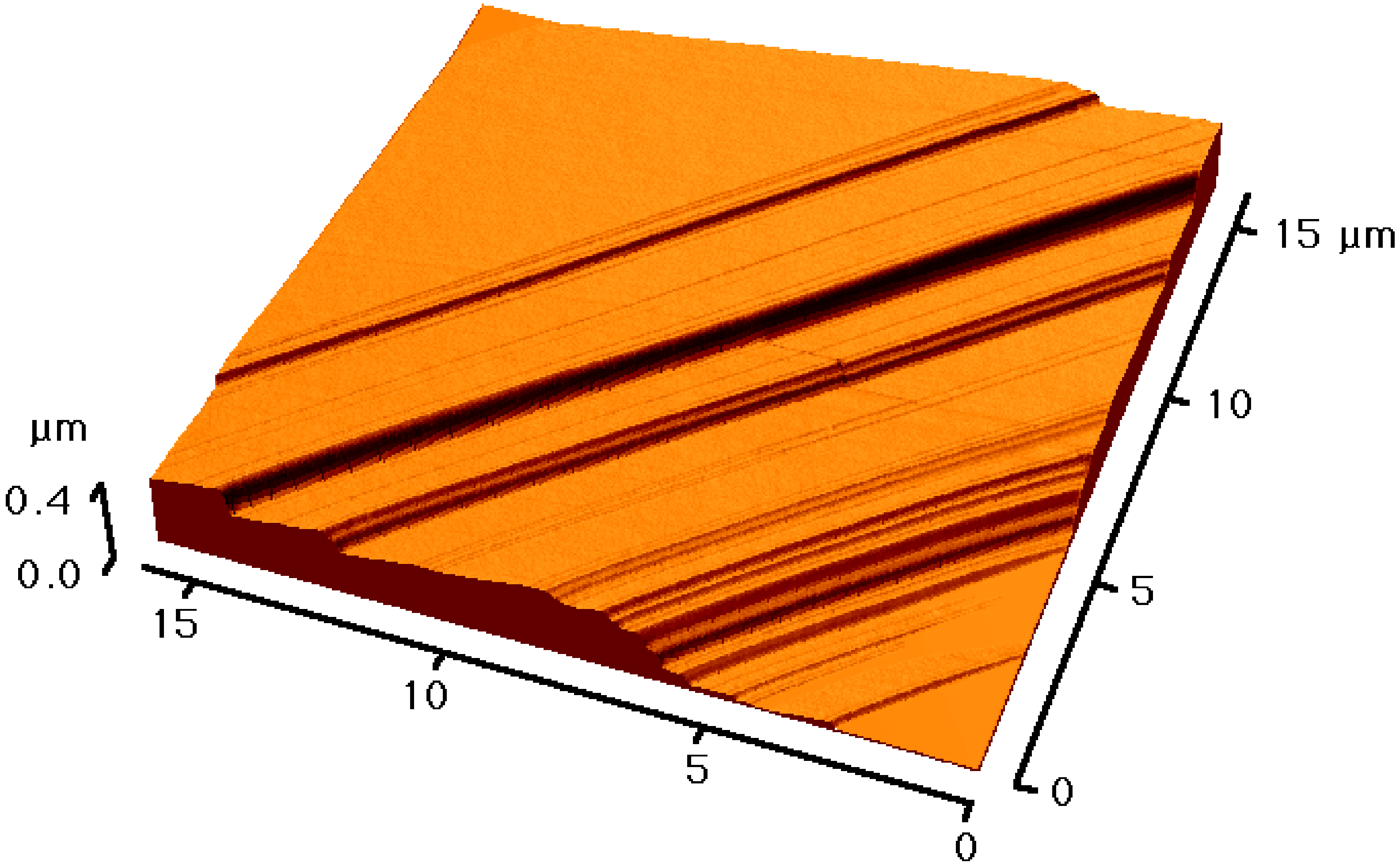
$$E(u) = \int W(\nabla u)dx + \int_S \phi([\![u]\!], m)dS$$

(+ forcing) (+ kinetics) (+ inertia) (+ nonlocal)

Free-discontinuity problems

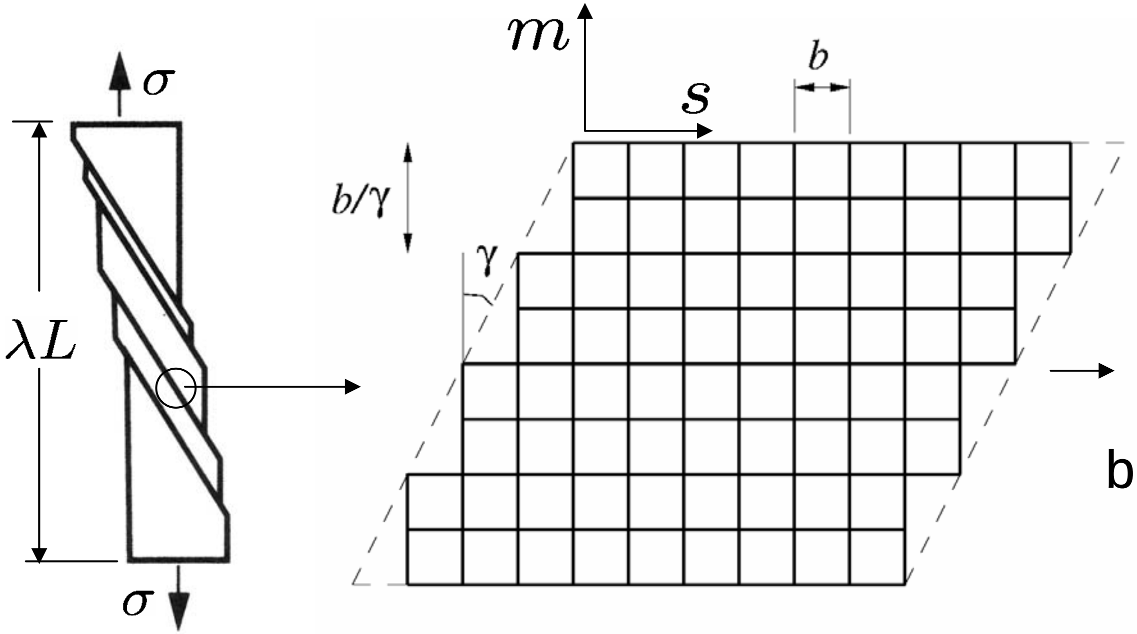
- `Free-discontinuity' problems arise in a number of areas of application:
  - *Solids:*
    - *Crystallographic slip*
    - *Fracture and fragmentation*
    - *Strain/damage localization*
    - *Fault systems in earth's crust*
  - Image reconstruction (Mumford-Shah model)
- Questions:
  - *How can the physics be modeled?*
  - *How can the models be solved?*
  - *What does one learn from the solutions?*

Crystallographic slip



Slip traces on crystal surface
(Atomic force microscopy, C. Coupeau)

Slip as a free-discontinuity problem



Irreversible accommodation of shear deformation by crystallographic slip

- Estimate of peak stress: $\tau_{\mathrm{max}} \sim \mu/30$, much higher than experimentally observed.
- Alternative mechanism: dislocation nucleation and transport (Orowan, Taylor, Polanyi, 1934).

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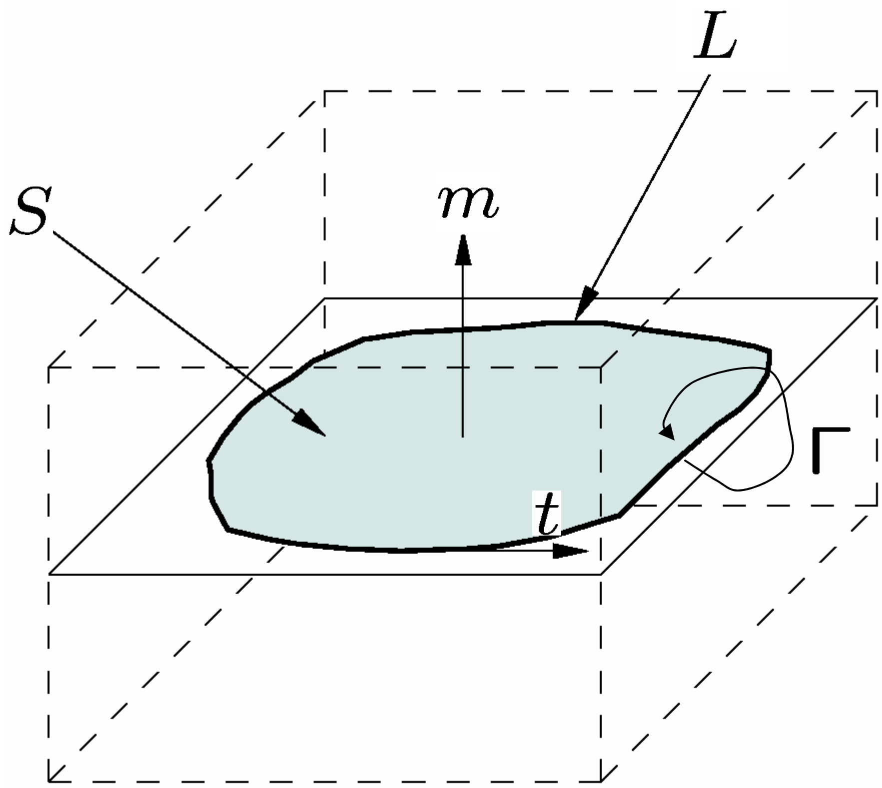
Slip as a free-discontinuity problem



- Volterra dislocation:

$$\text{div} C\nabla u = 0, \quad \text{in } \mathbb{R}^3$$
$$[\![u]\!] = b, \quad \text{on } S$$
$$[\![C\nabla u]\!] \cdot m = 0, \quad \text{on } S$$

- Burgers circuit:

$$b = \oint_{\Gamma \setminus S} \nabla u dr$$

- Dislocation dipole: $\frac{E}{L} \sim \frac{\mu b^2}{4\pi(1-\nu^2)} \log \frac{R}{r_0} \to \infty$
- Need to model dislocation core!

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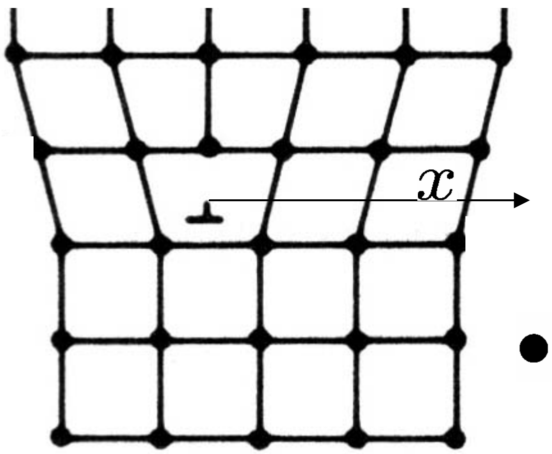
Slip as a free-discontinuity problem

- Peierls theory of the dislocation core (Peierls '47):
Let $\delta(x) = [\![u_x]\!](x)$, $\phi(\delta)$ periodic of period b,



$$E(\delta) = \int_{-\infty}^{\infty} \phi(\delta(x))dx + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{B}{2} \log \frac{R}{|x-y|} \delta'(x)\delta'(y)dxdy$$

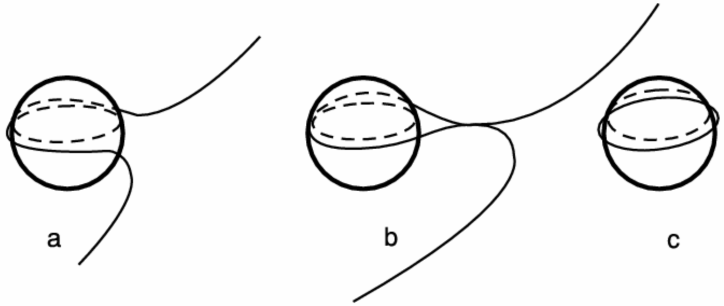
- Nabarro's potential (Nabarro '47):

$$\phi(u) = A\left(1 - \cos\frac{2\pi\delta}{b}\right)$$

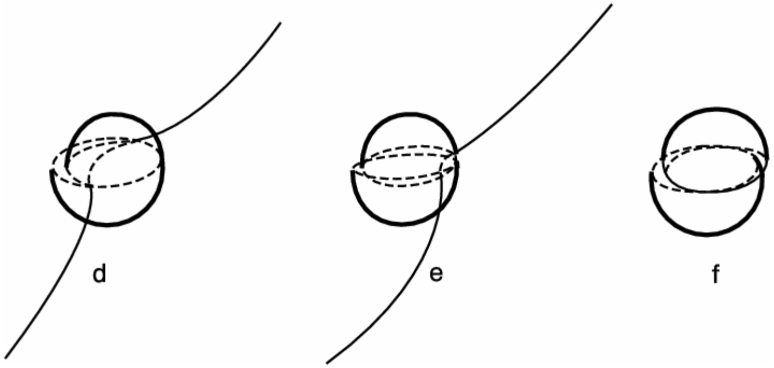
- Nabarro's solution: $\delta(x) = \frac{b}{2}\left(1 - \frac{2}{\pi}\arctan\frac{x}{c}\right)$
- Logarithmic singularity is eliminated!

Slip as a free-discontinuity problem

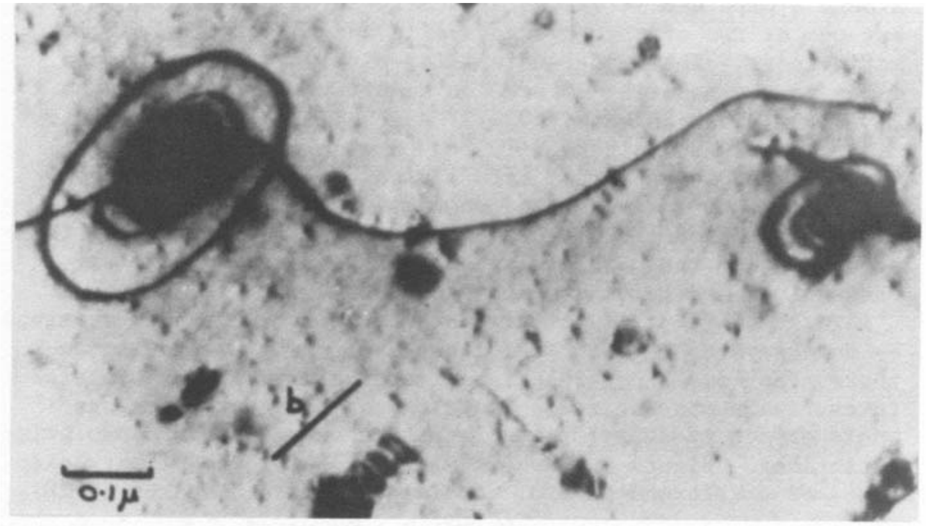
- Example: Precipitation hardening.



Impenetrable obstacles



Obstacles of finite strength



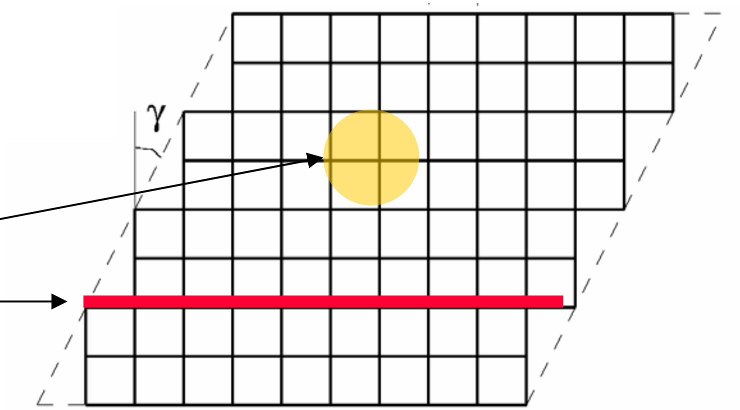
(Humphreys and Hirsch '70)

Slip as a free-discontinuity problem

- Assumption: *Singular set* $S \equiv$ set of all slip planes,

$$\nabla u = \beta^e + \beta^p$$

$$\begin{cases} \beta^e \text{ absolutely continuous} \\ \beta^p = [\![u]\!] \otimes m \delta_S \end{cases}$$



- Assumption: The energy is of the form

$$E(u) = \underbrace{\int \frac{1}{2} c_{ijkl} \beta^e_{ij} \beta^e_{kl} dx}_{\text{Elastic energy}} + \underbrace{\int_S \phi([\![u]\!]) dS}_{\text{Core energy}}$$

$\phi \equiv$ periodic *Peierls potential.*

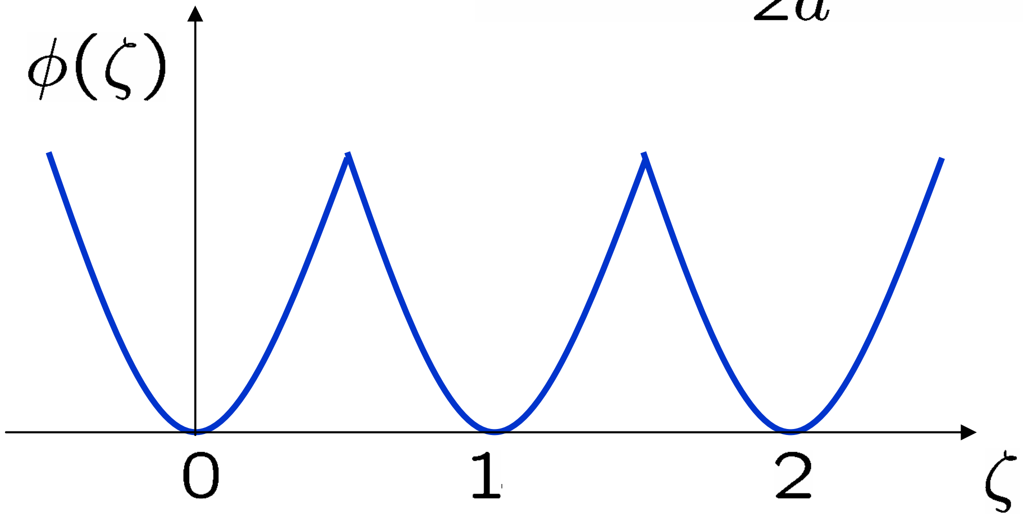
Slip as a free-discontinuity problem

- Special case (Koslowski, Cuitiño and Ortiz '02):

  i) Activity on single slip system, single slip plane.

  iii) Constrained slip assumption (Rice and Beltz '92):
  $[\![u]\!](x) = b\zeta(x)s, \quad \zeta : \mathbb{R}^2 \to \mathbb{R}$ ('slip field')

  iv) Peierls potential: $\phi(\zeta) = \frac{\mu b^2}{2d}\text{dist}^2(\zeta, \mathbb{Z})$



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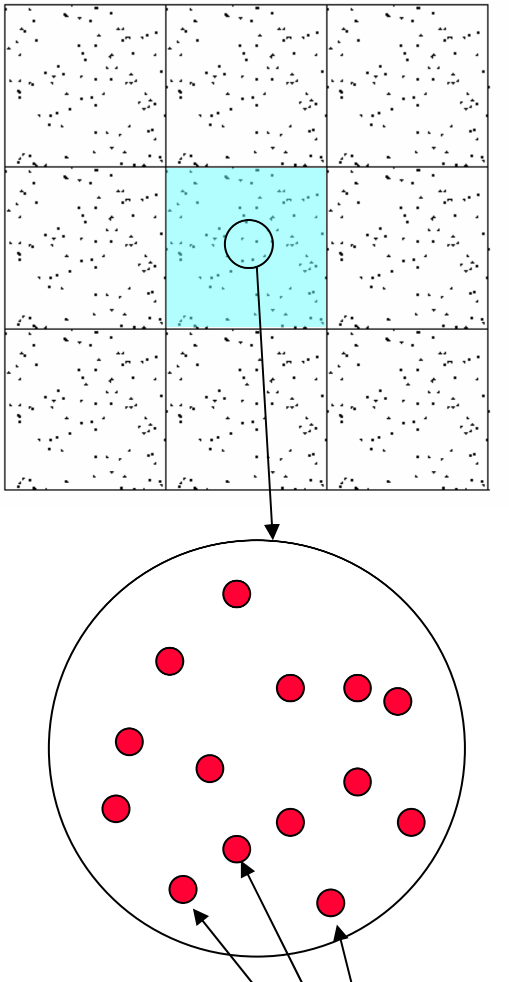
Slip as a free-discontinuity problem



obstacles

- Normalized total energy:

$$E_\epsilon(\zeta) = \frac{1}{2\epsilon}\int_{T^2} \text{dist}^2(\zeta, \mathbb{Z})dx$$
$$+ \int_{T^2\times T^2} K_\nu(x-y)|\zeta(x)-\zeta(y)|^2 dx dy$$
$$+ \sum_{\text{obstacles}} f|\zeta| + \text{applied loading}$$

where $K_\nu(x) \sim |x|^{-3}, \quad \epsilon = d/L$

- Problem: Minimize energy

$$\inf_{\zeta\in H^{1/2}(T^2)} E_\epsilon(\zeta)$$

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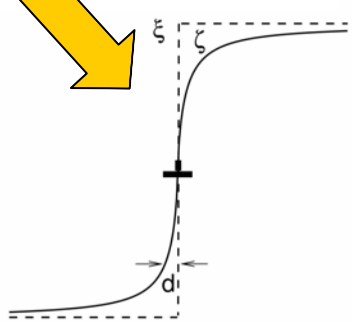
Slip in crystals – Solution strategy

i) Unconstrained problem: $\eta(x) = \sum_{i=1}^{N} G(x - x_i) f_i$

ii) Projection: $\xi =$ closest integer-valued function to η

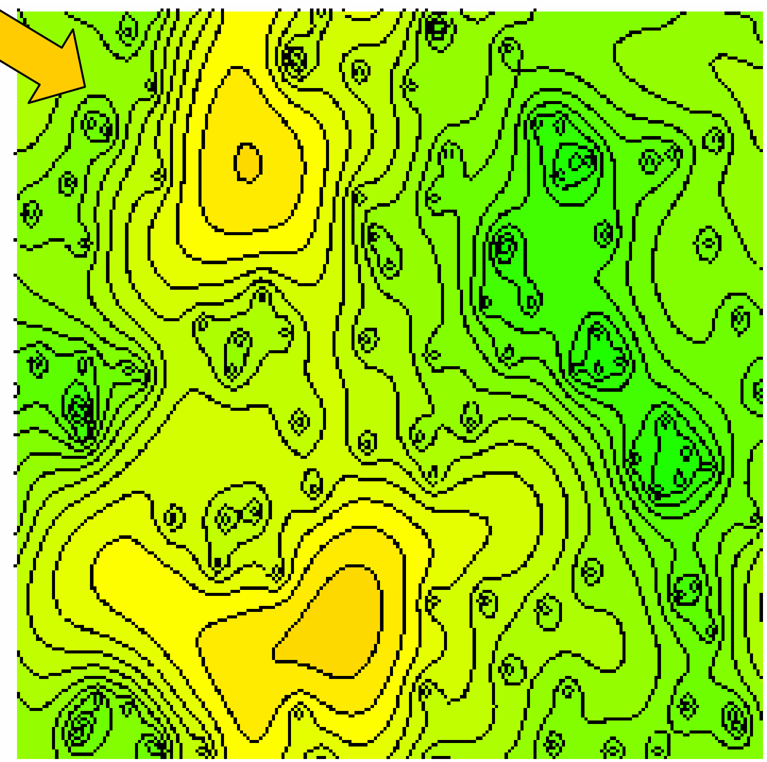
iii) Mollification: $\zeta = \phi_\epsilon * \xi$

iv) On obstacles:

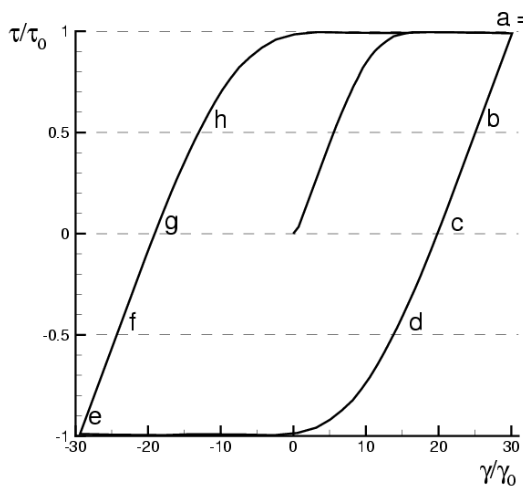


$$\begin{cases} |f_i| \leq f \\ \zeta_i \geq 0 \\ (|f_i| - f)\zeta_i = 0 \end{cases}$$

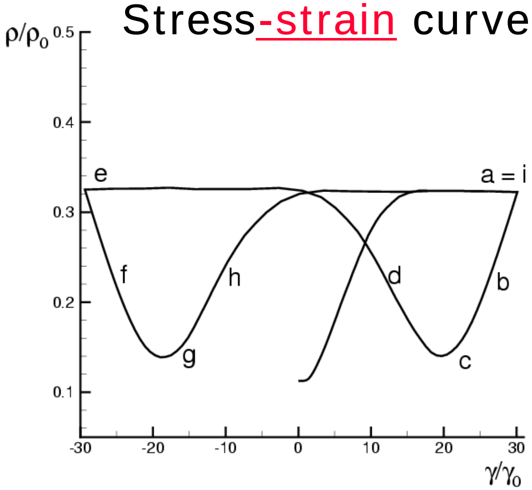
(Kuhn-Tucker conditions)



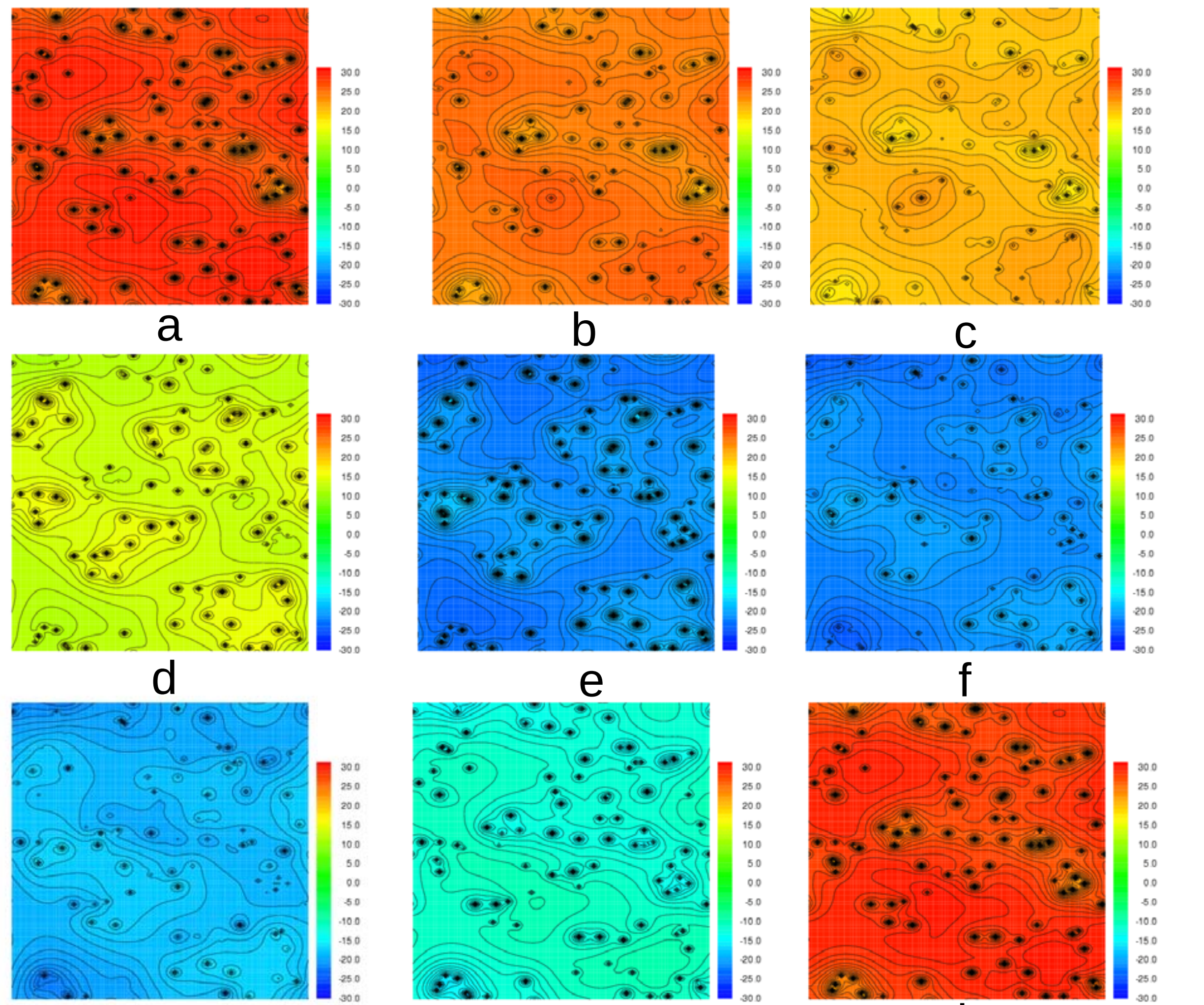
Slip in crystals – Strain hardening



Stress-strain curve



Dislocation density



(Movie)

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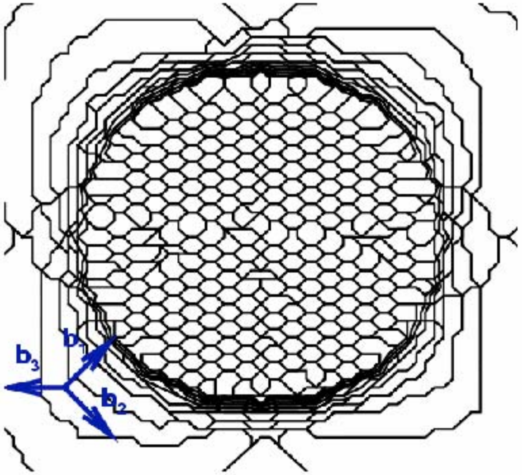
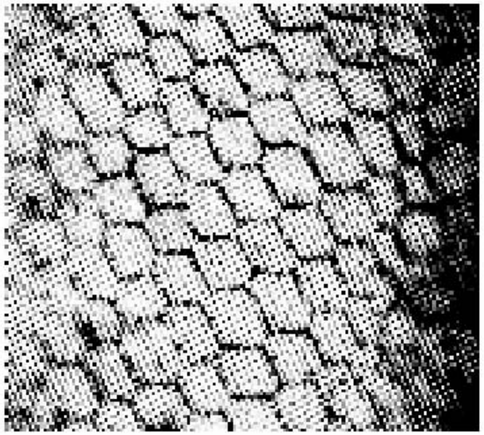
Slip in crystals – Twist boundaries

When the rotation axis is the [111] the grain boundary is a hexagonal grid of screw dislocations with Burgers vectors:

$$b_1 = \tfrac{1}{2}[1,1,0] \quad b_2 = \tfrac{1}{2}[1,0,1]$$

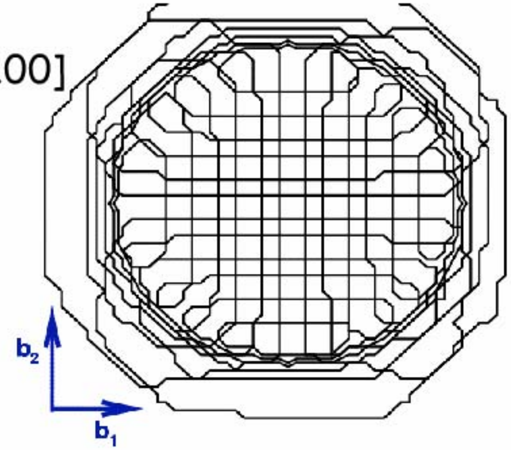
$$b_3 = \tfrac{1}{2}[0,1,1]$$

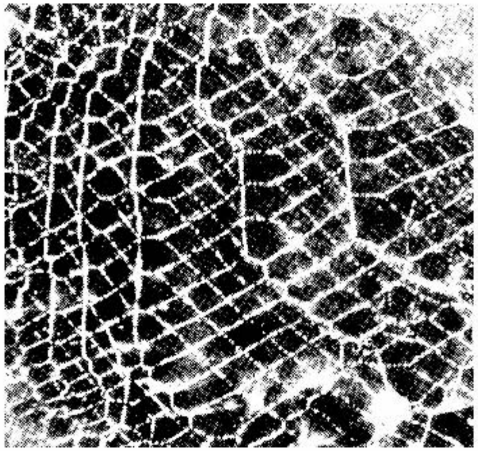




A twist boundary having a [100] rotation axis consists of a square grid of screw dislocations with Burgers vectors: $b_1 = \tfrac{1}{2}[0,1,1]$

$$b_2 = \tfrac{1}{2}[0,1,-1]$$

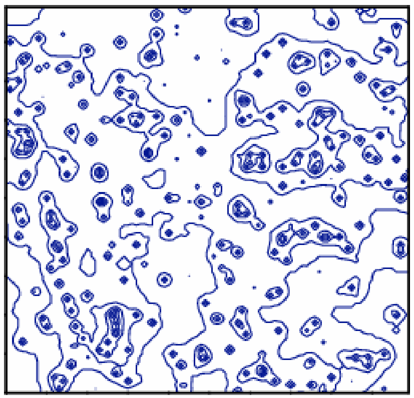




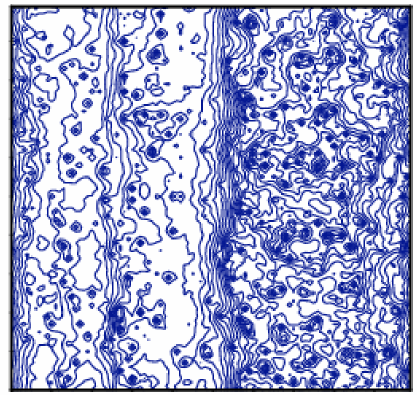
S. Amelinckx, 1958

(Koslowski and Ortiz '04)

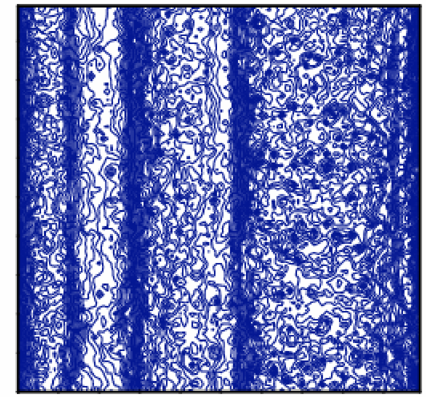
Slip in crystals – Dislocation structures



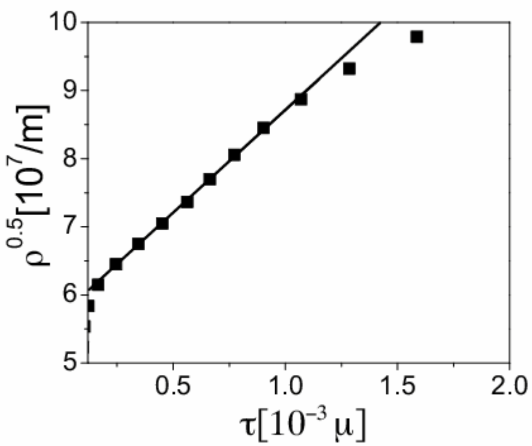
Stage I

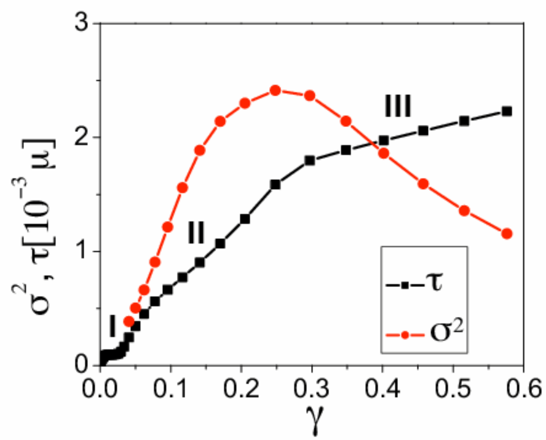


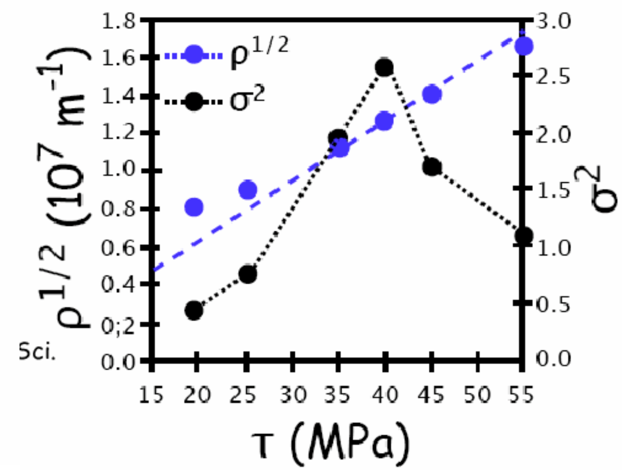
Stage II



Stage III







Koslowski *et al.* '04

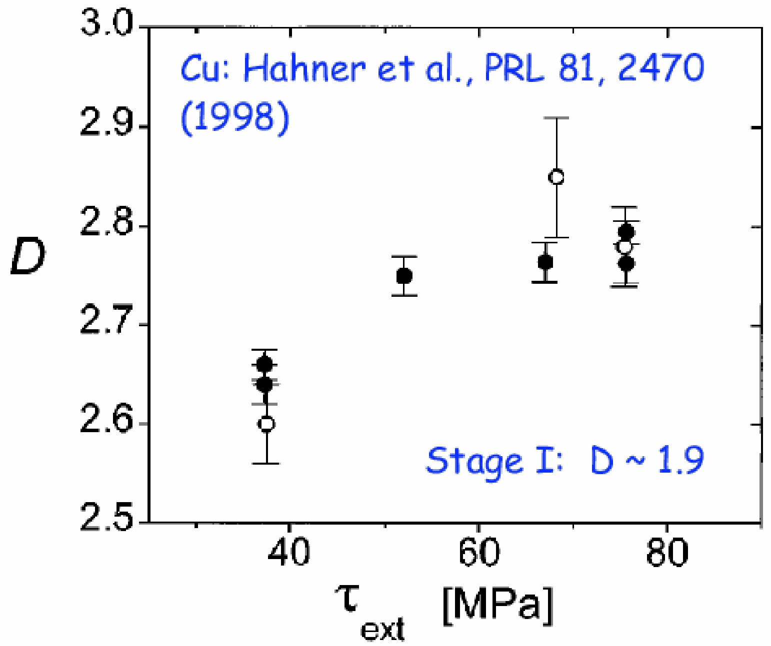
$$\sigma^2 = \frac{\langle \rho^2 \rangle - \langle \rho \rangle^2}{\langle \rho \rangle^2}$$

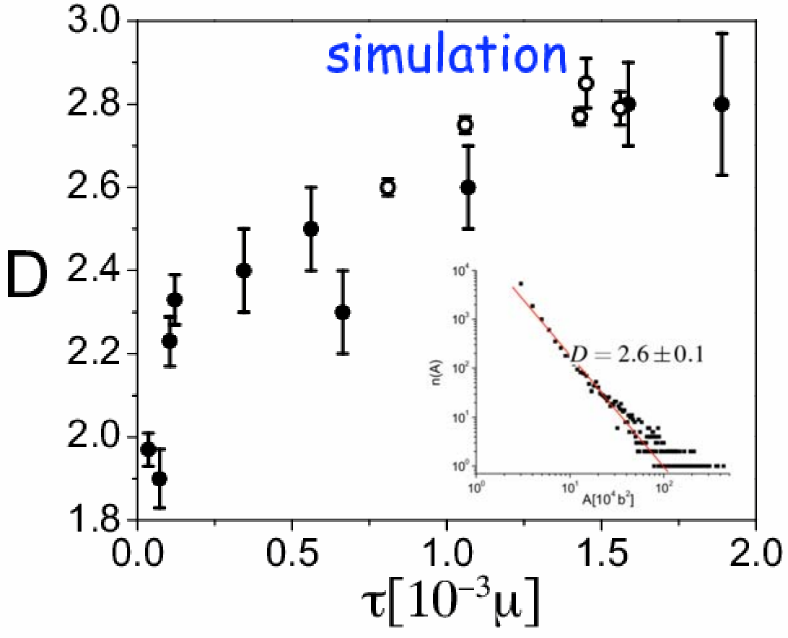
Szekely, Groma, Lendvai, Mat. Sci. Engin. A **324**, 179 (2002)

Crystals – Self-similar structures

Dislocation patterning is **fractal**

- first discussed by Gil Sevillano and shown in Cu by Hahner
- probability of cells of size A $n(A) \sim A^{-D}$
  - D is the fractal dimension.





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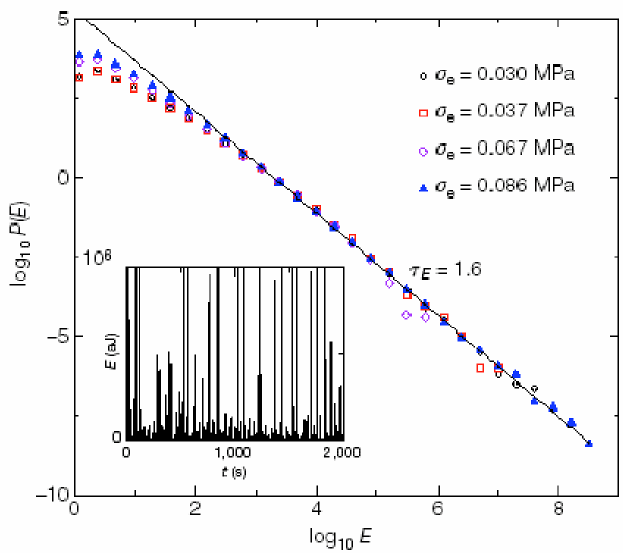
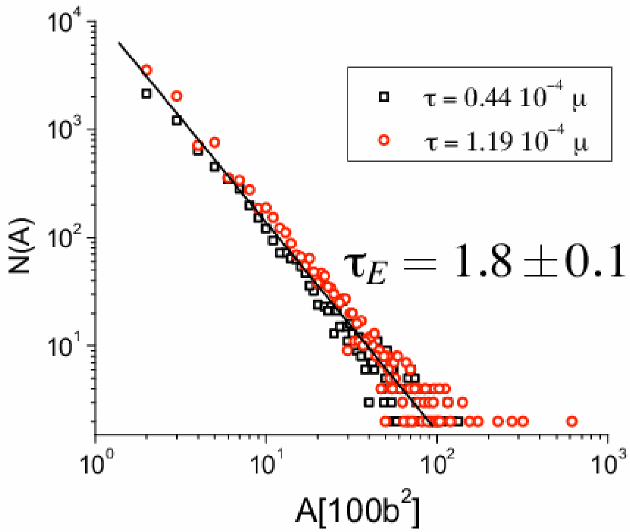
Slip in crystals – Dislocation avalanches

- Recently, acoustic emission experiments on single crystals of ice showed an intermittent and heterogeneous plastic flow.
- The probability density function of the energy, follows a power law distribution

$$P(E) \sim E^{-\tau_E}$$



Statistical properties of acoustic energy bursts under constant stress (Miguel, 2001)



Simulated acoustic energy bursts under constant stress.

Koslowski *et al.* '04

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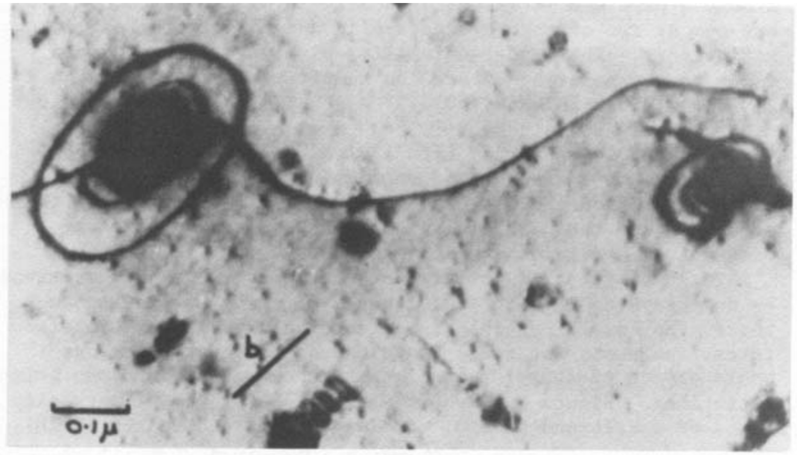
Slip in crystals – Rigorous results

- Energy scaling (Garroni and Müller '04):
  - Continuum limit: $\epsilon \equiv b/L \to 0$.
  - Γ-convergence in L^2.
  - Limiting energy:

$$E_\epsilon(\zeta) \to \frac{N\epsilon}{\log(1/\epsilon)} F(\zeta)$$

where (for large integer ζ)

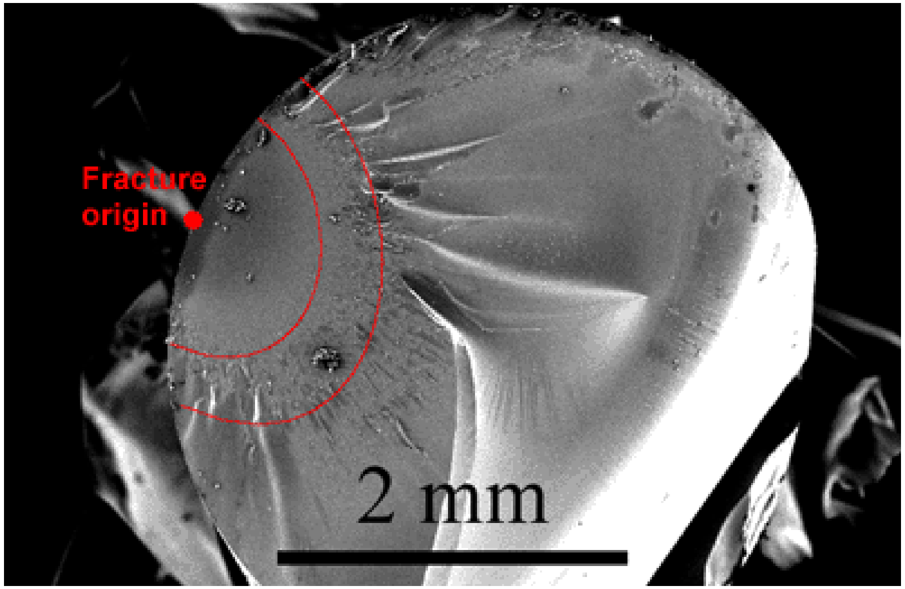
$$F(\zeta) \sim \int_{T^2} \gamma |\nabla \zeta| dx + \int_{T^2} \tau_0 |\zeta| dx$$

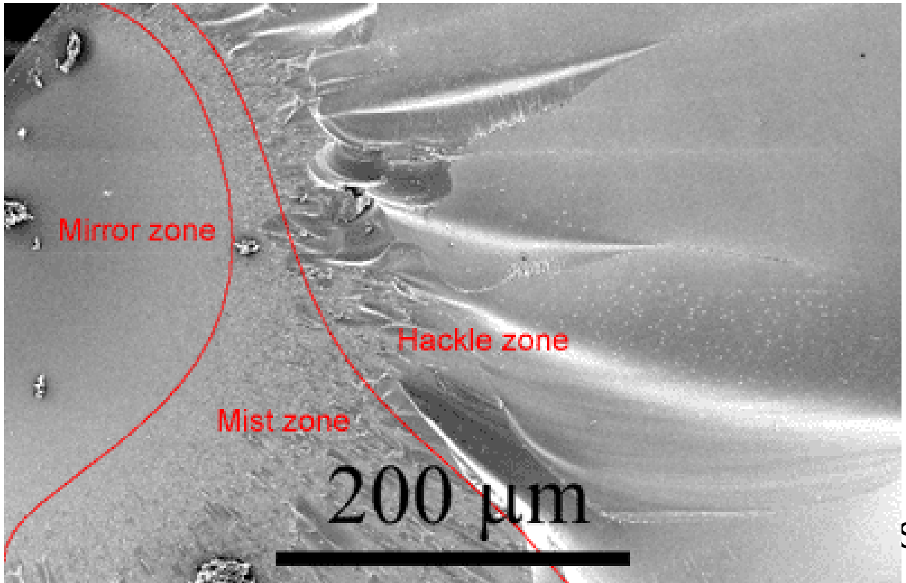


(Humphreys and Hirsch '70)

Line-tension 'approximation' is exact!

Fracture





Fracture of soda-lime glass rod

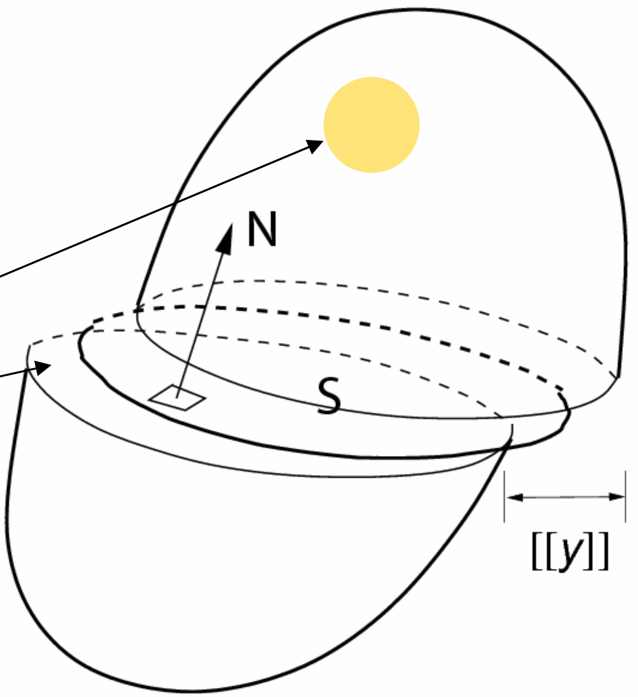
Dept. Materials Science and Metallurgy, University of Cambridge

Fracture as a free-discontinuity problem

- Deformation gradient:

$$\nabla y = F + [\![y]\!] \otimes N \delta_S$$

$$\begin{cases} F \text{ absolutely continuous} \\ S \equiv \text{cohesive surface} \end{cases}$$

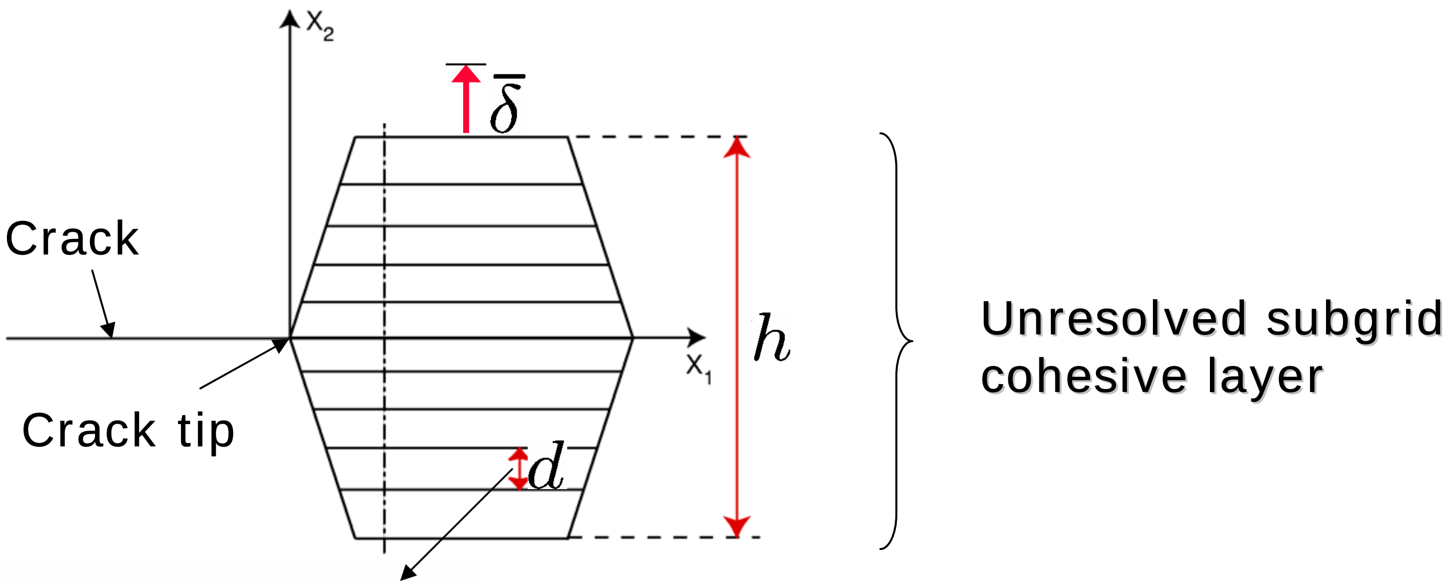


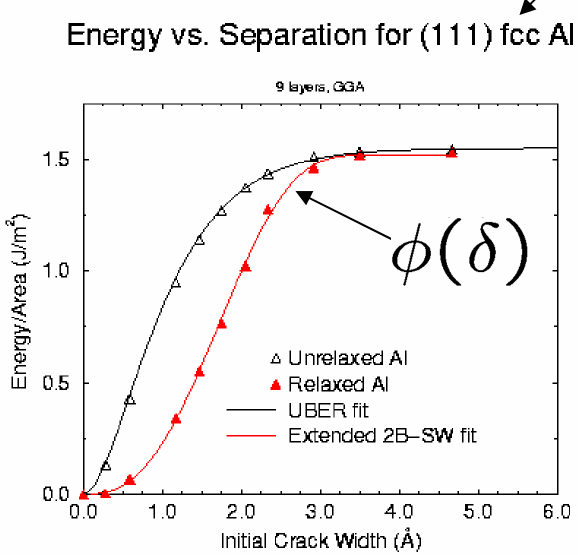
- Energy (possibly incremental):

$$E(y) = \underbrace{\int W(F) dx}_{\text{Bulk energy}} + \underbrace{\int_S \phi([\![y]\!], N) dS}_{\text{Cohesive energy}}$$

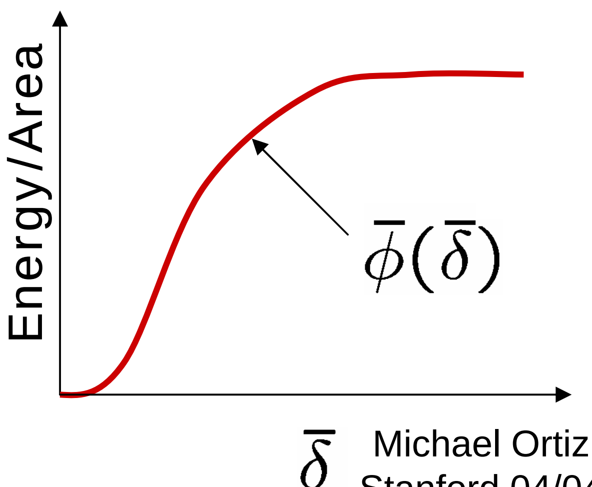
$\phi \equiv$ Cohesive (binding) energy density.

Fracture – Effective cohesive law





$$N = h/d \gg 1$$



Fracture – Rigorous results

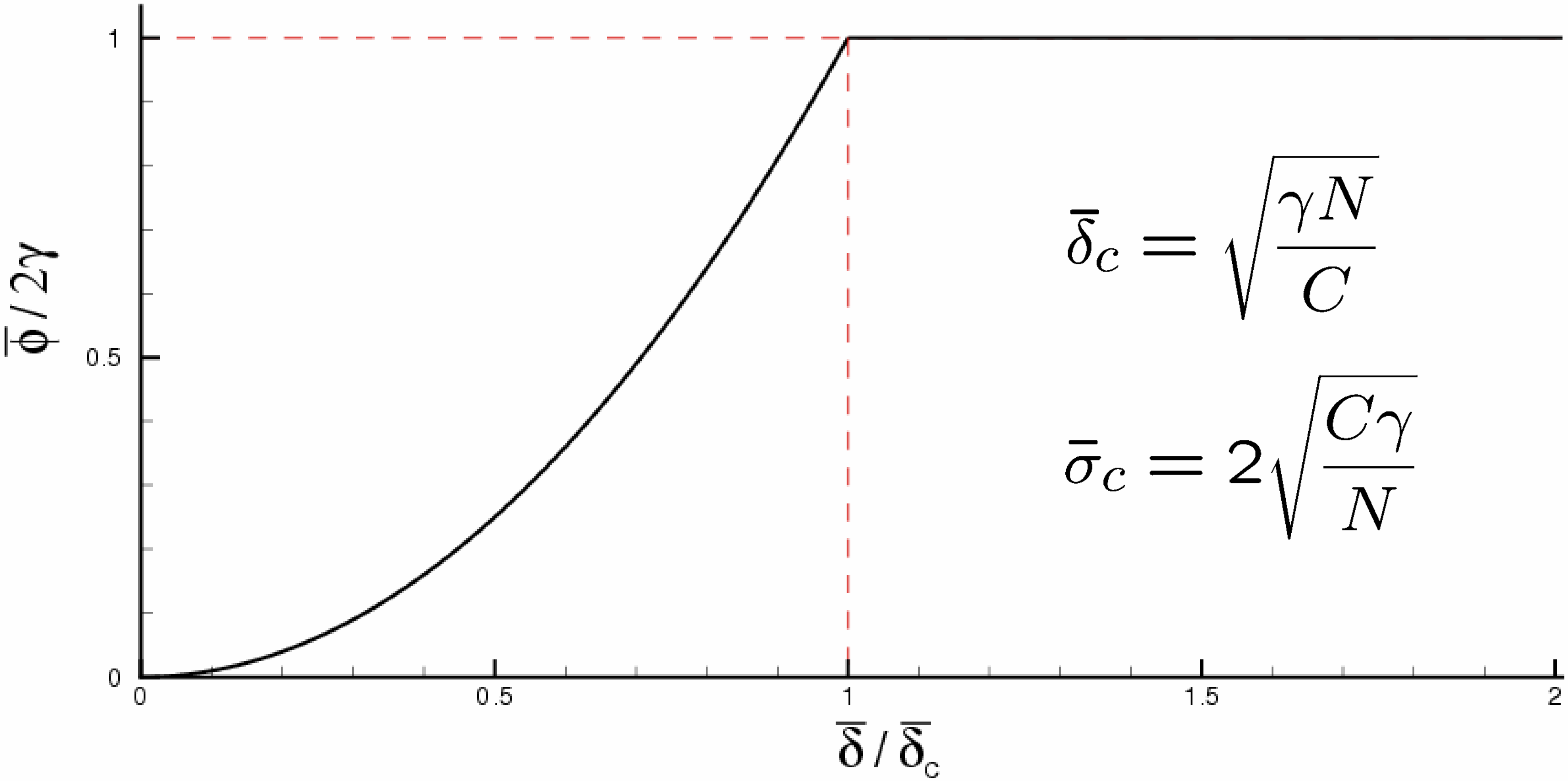
Theorem (*Braides, Lew and Ortiz '04*) *There exist constants* α *and* β *such that the functionals* E_N Γ-*converge to the functional* E_0 *defined on piecewise-*H^1_{loc} *functions such that* $u - \delta x$ *is* 1-*periodic by*

$$E_0(u) = \alpha \int_0^1 |u'|^2 dx + \beta \#(S(u) \cap (0,1])$$

with $u^+ > u^-$ *on* $S(u)$. *Moreover, if* $\delta > 0$ *the minimum values above converge to the minimum value*

$$\min E_0 = \min\{\alpha\delta^2, \beta\}.$$

Fracture – Universal cohesive law



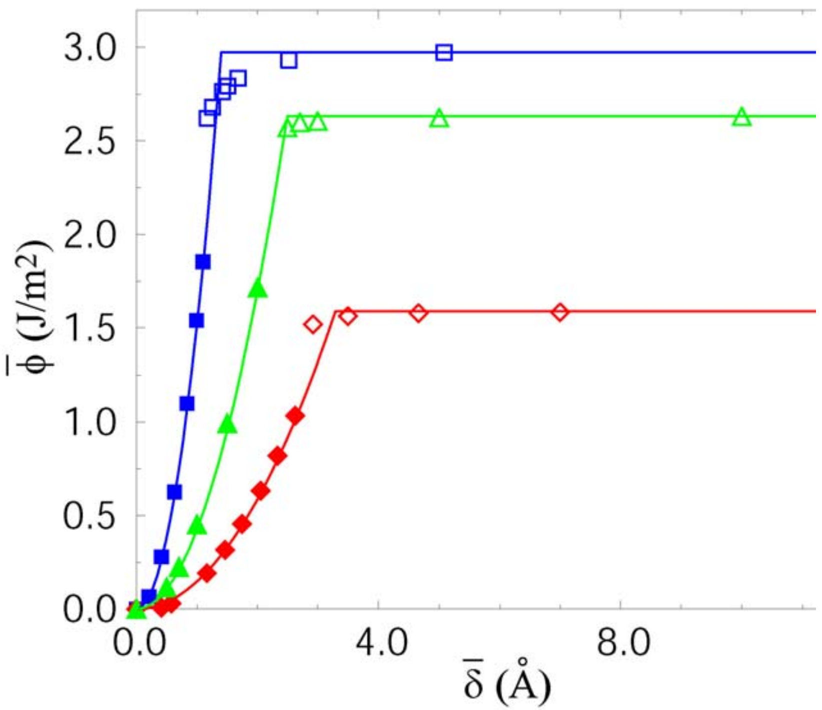
$$\bar{\delta}_c = \sqrt{\frac{\gamma N}{C}}$$

$$\bar{\sigma}_c = 2\sqrt{\frac{C\gamma}{N}}$$

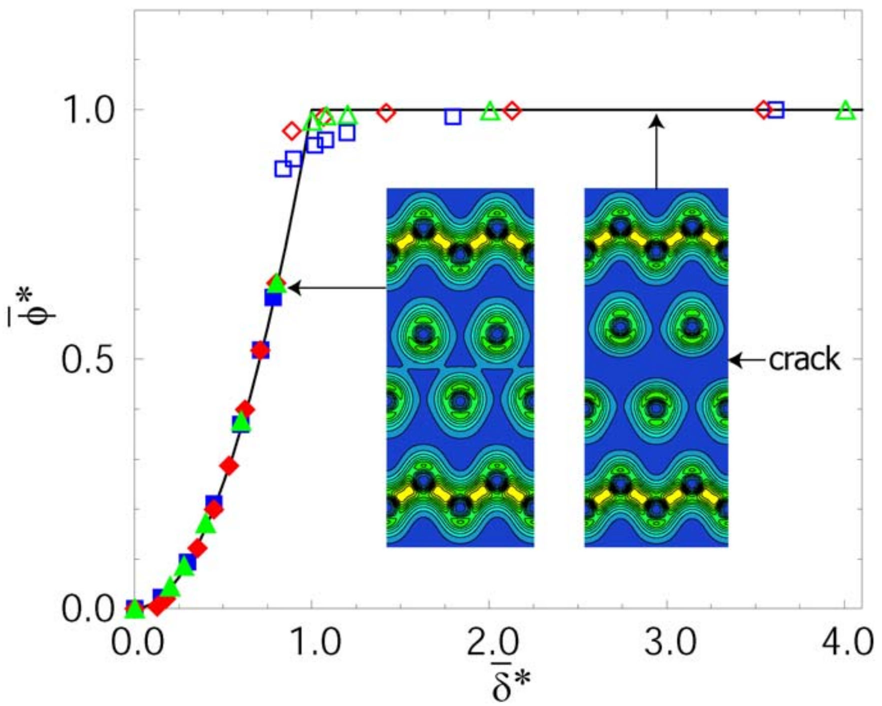
Limiting form of cohesive law for all materials!

(Nguyen and Ortiz '02; Braides, Lew and Ortiz '04)

Fracture – Universal cohesive law



First-principles binding relations for aluminum, alumina and silicon



Normalized binding relations exhibit universality!

(Hayes, Carter and Ortiz '04)

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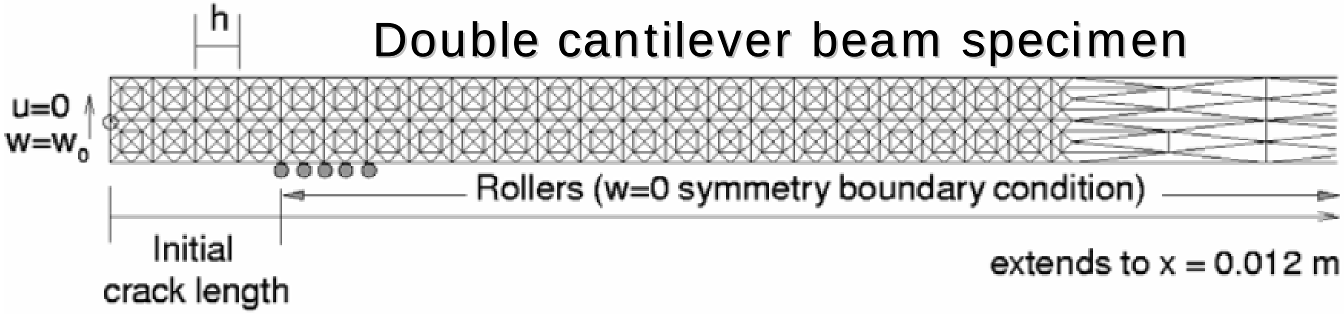
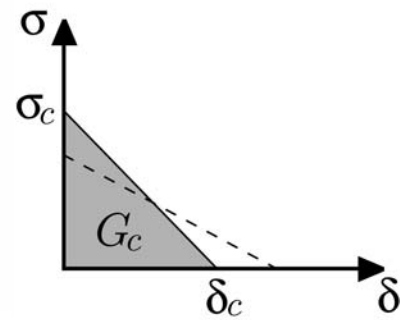
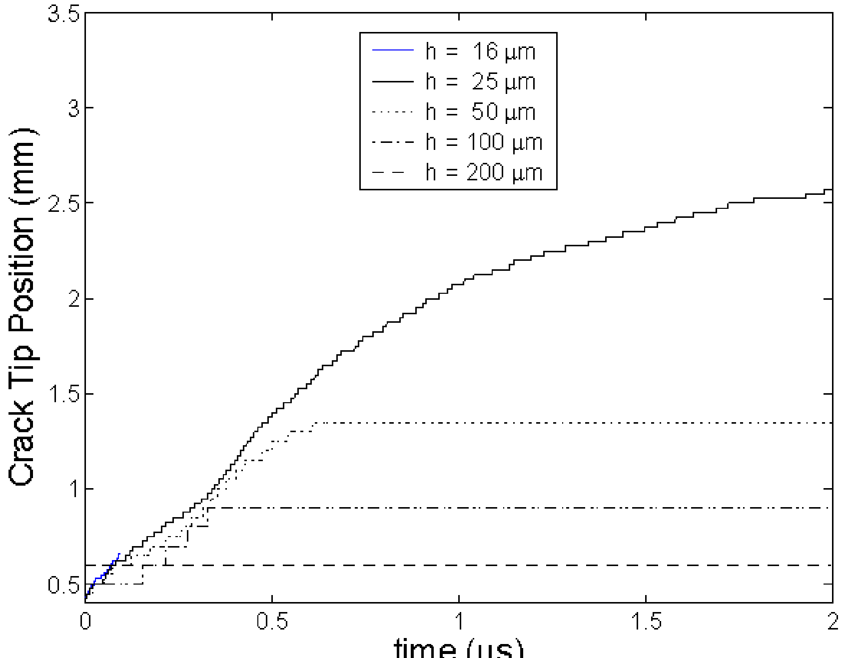
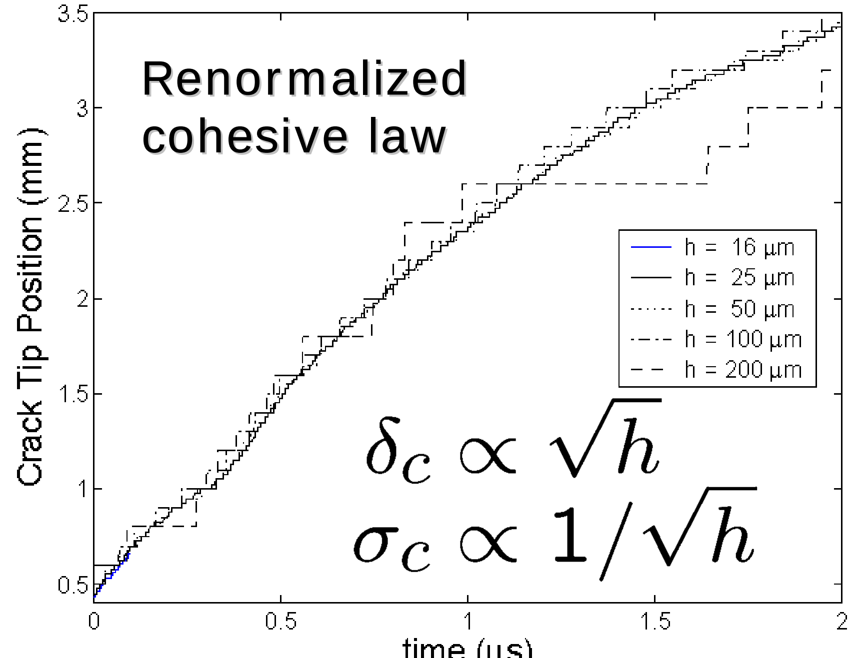
Renormalized Cohesive Laws









$$\delta_c \propto \sqrt{h}$$
$$\sigma_c \propto 1/\sqrt{h}$$

Crack-tip trajectory as a function of mesh size (h)

(Arias, Knap and Ortiz '04)

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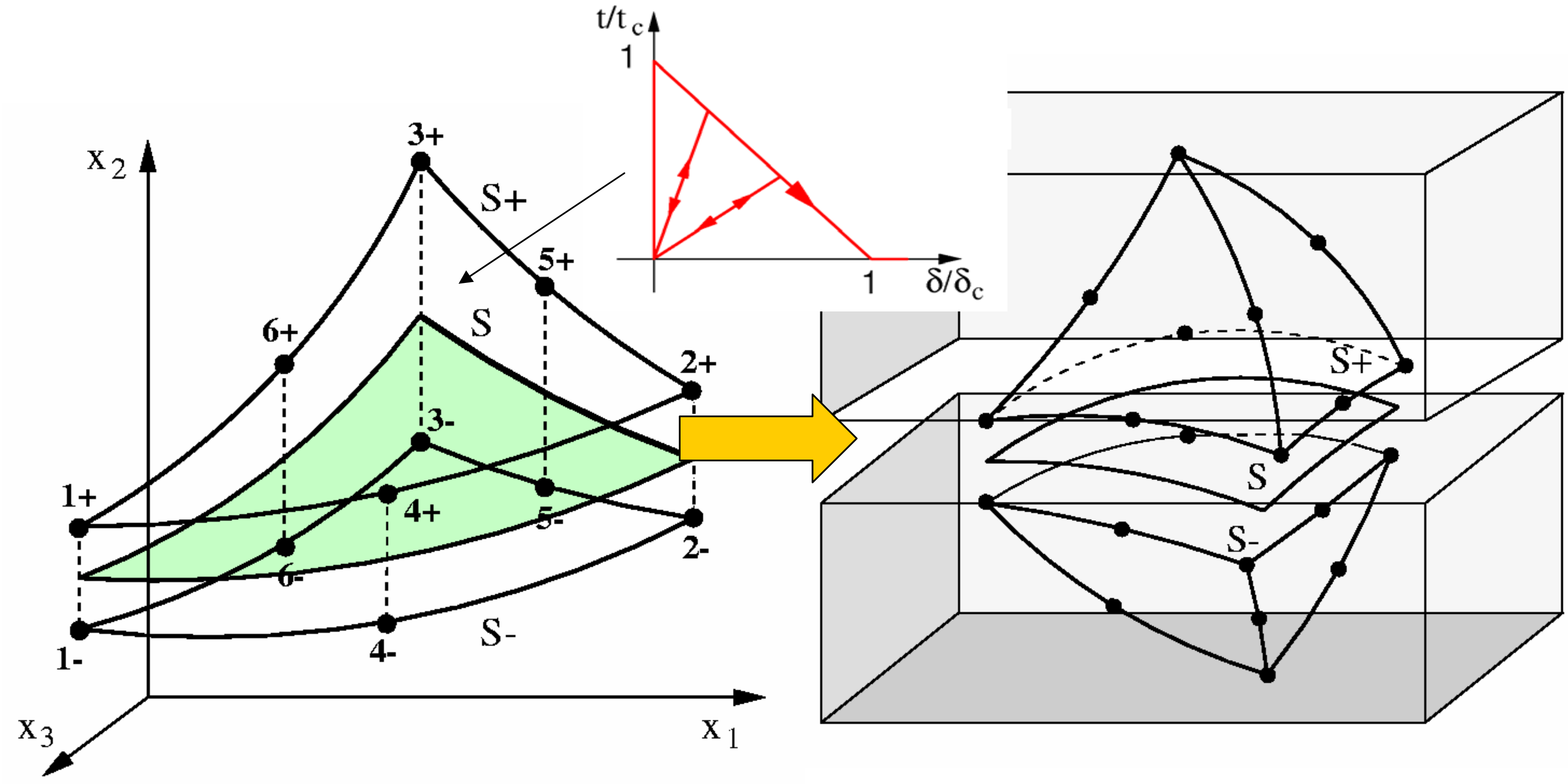
Fracture - Cohesive elements



12-node quadratic cohesive elements

Insertion of cohesive element between two volume elements

(Ortiz and Pandolfi '99)

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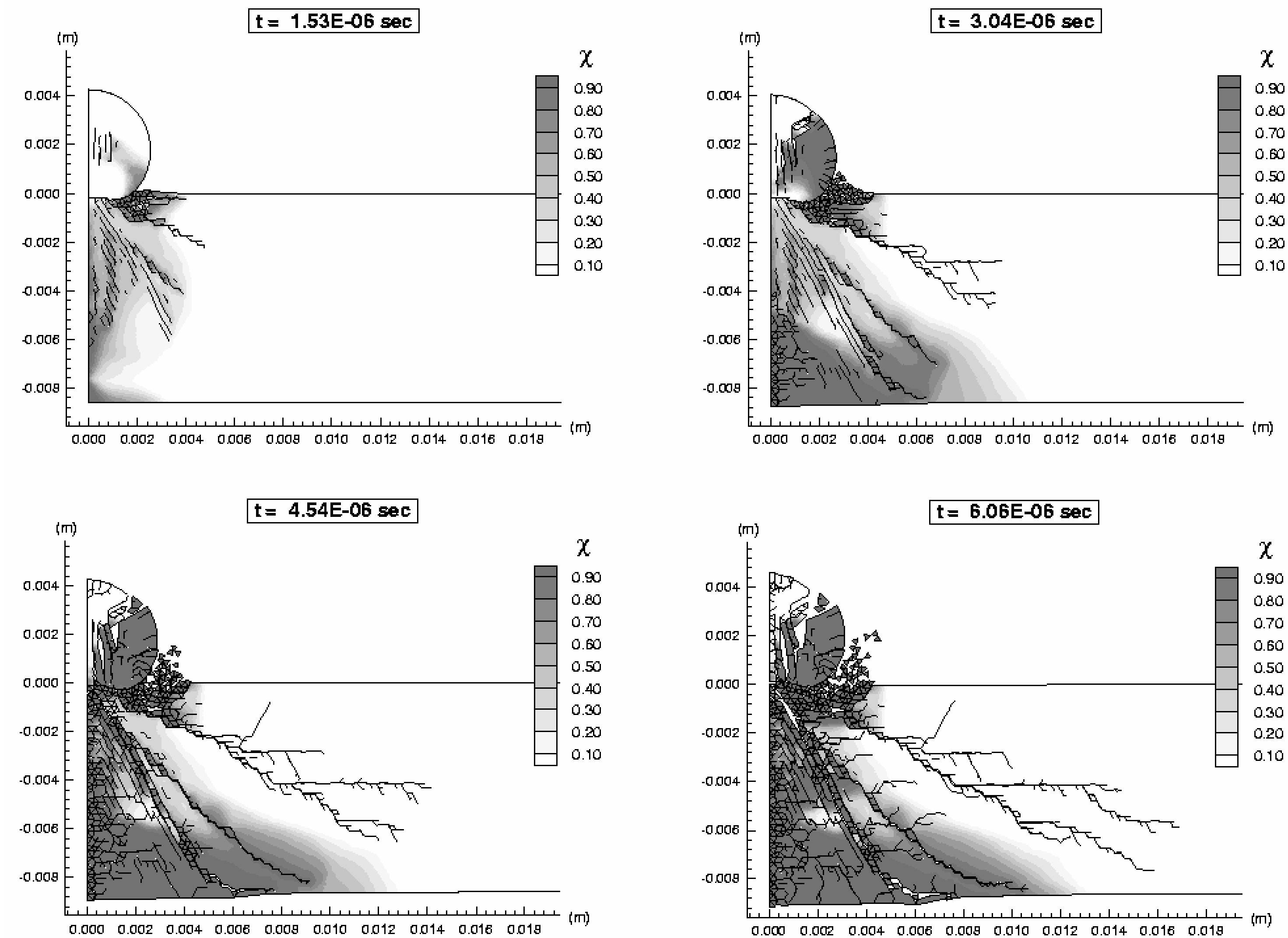
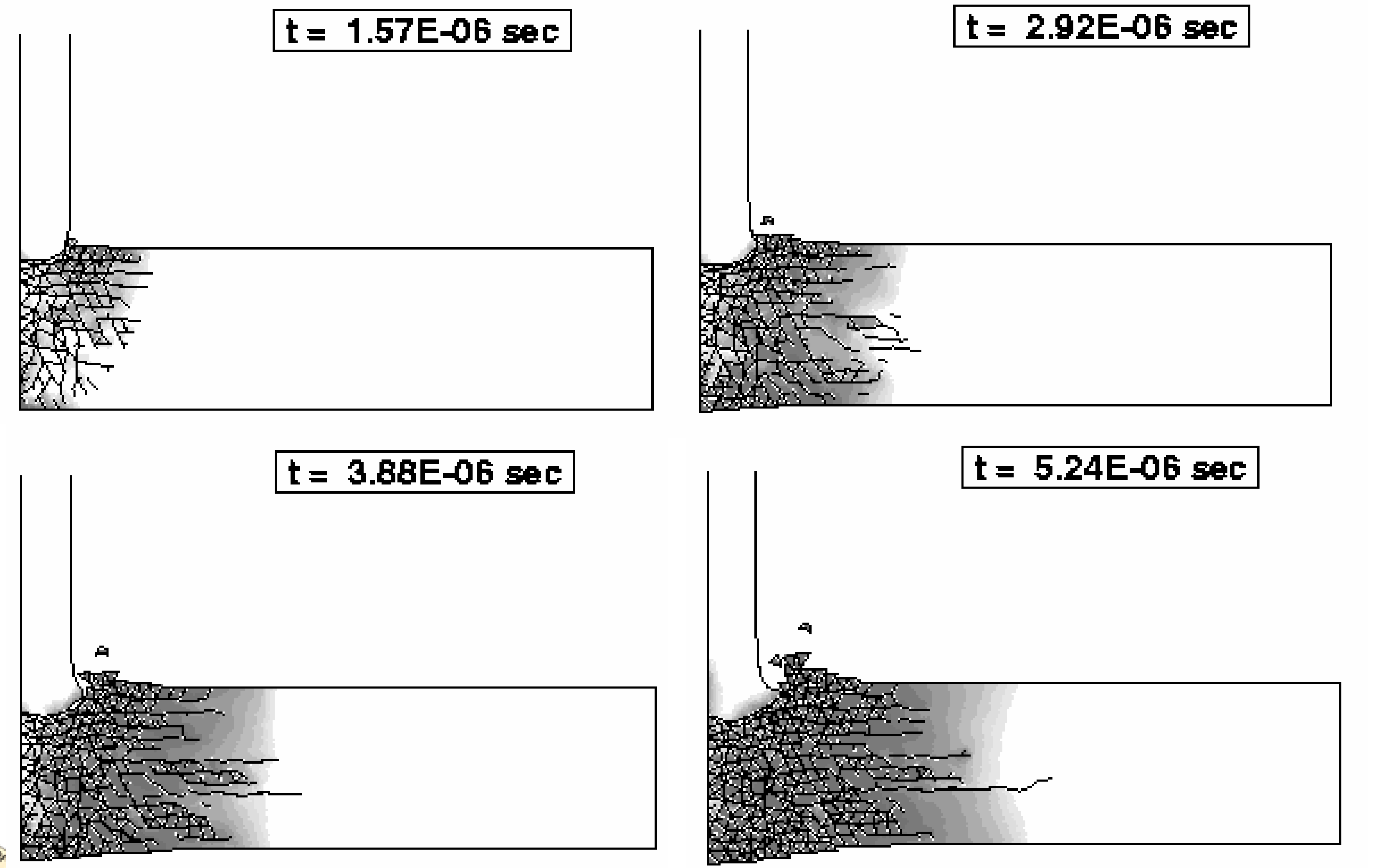
Steel pellet vs. alumina plate



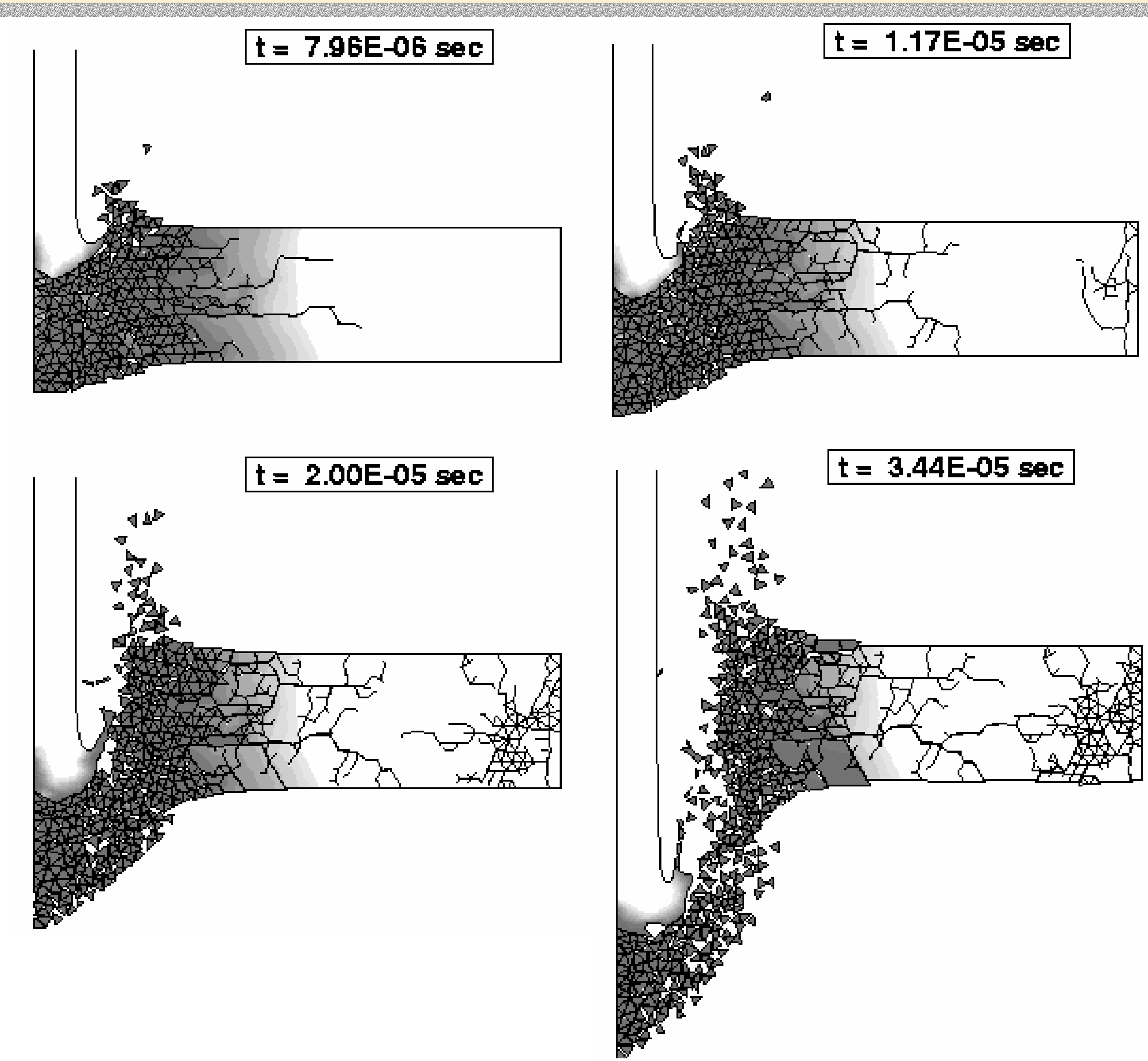
(Camacho and Ortiz, 1996; Field, 1988)

WHA long rod vs. alumina plate



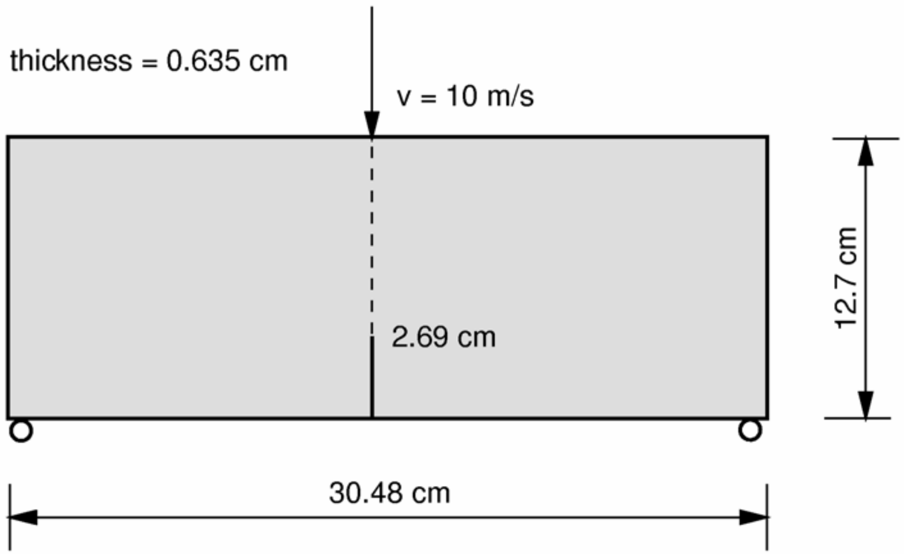
(Camacho and Ortiz, 1996; Woodward et al., 1994)

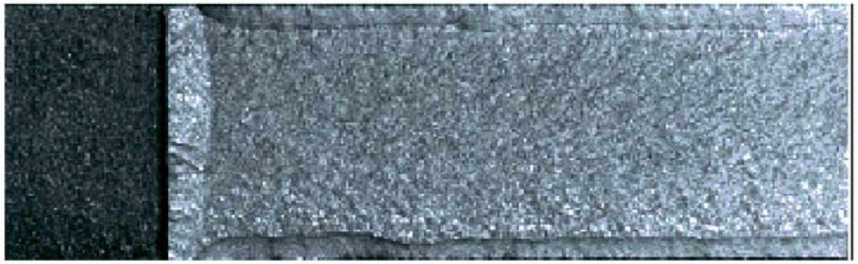
WHA long rod vs. alumina plate

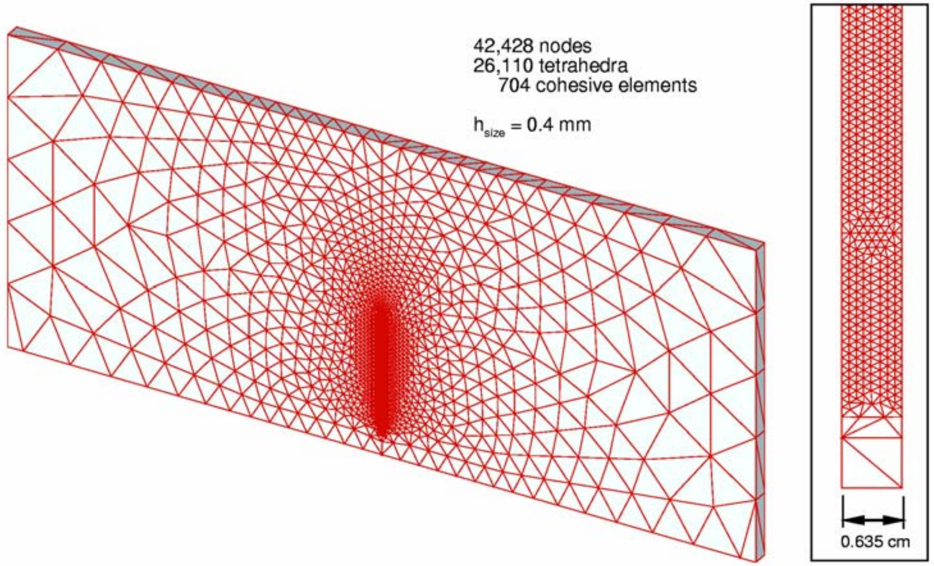


Michael Ortiz
Stanford 04/04

Drop-weight test - C300 steel

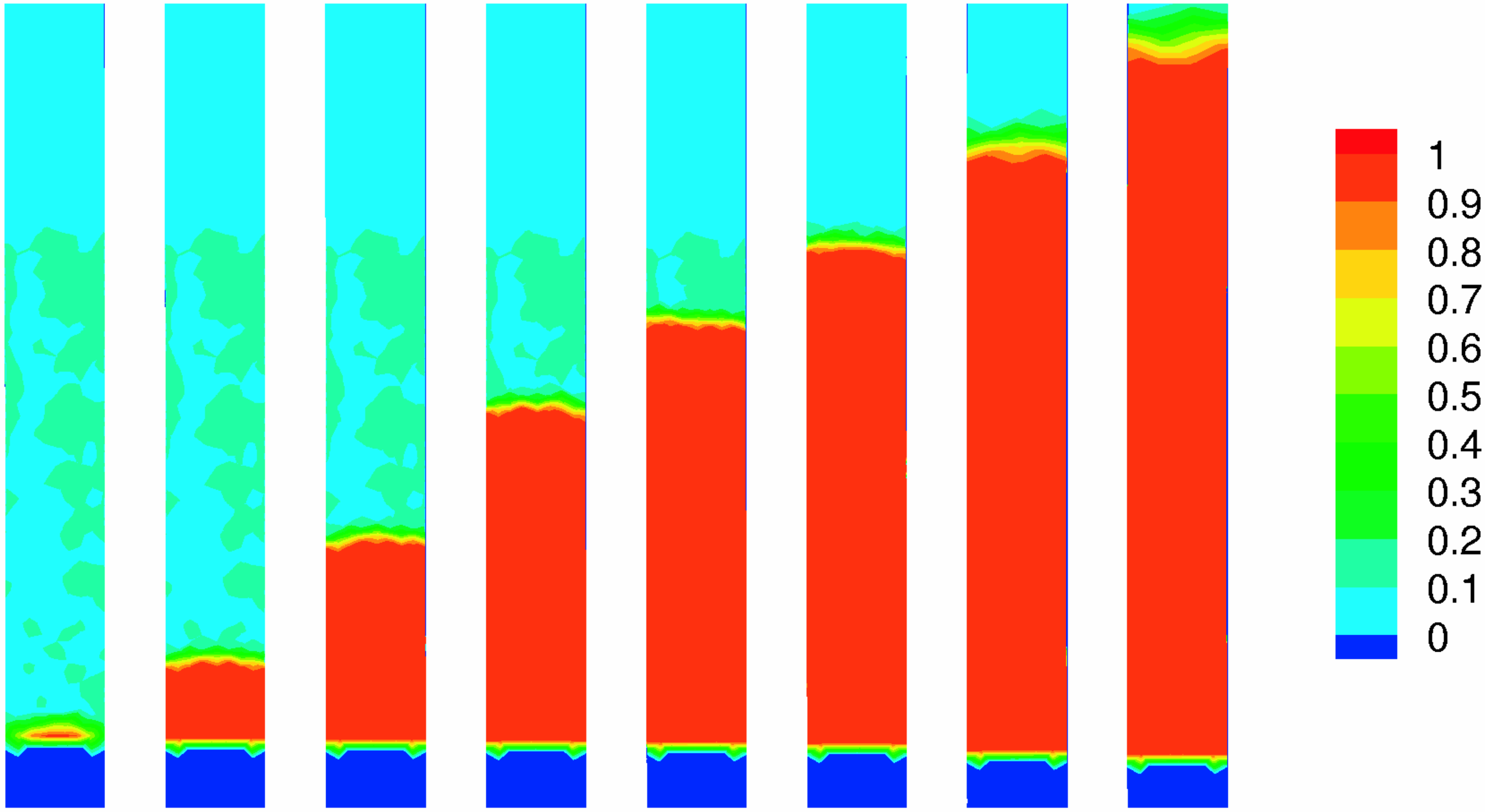






(Pandolfi, Guduru, Ortiz and Rosakis, 2000)

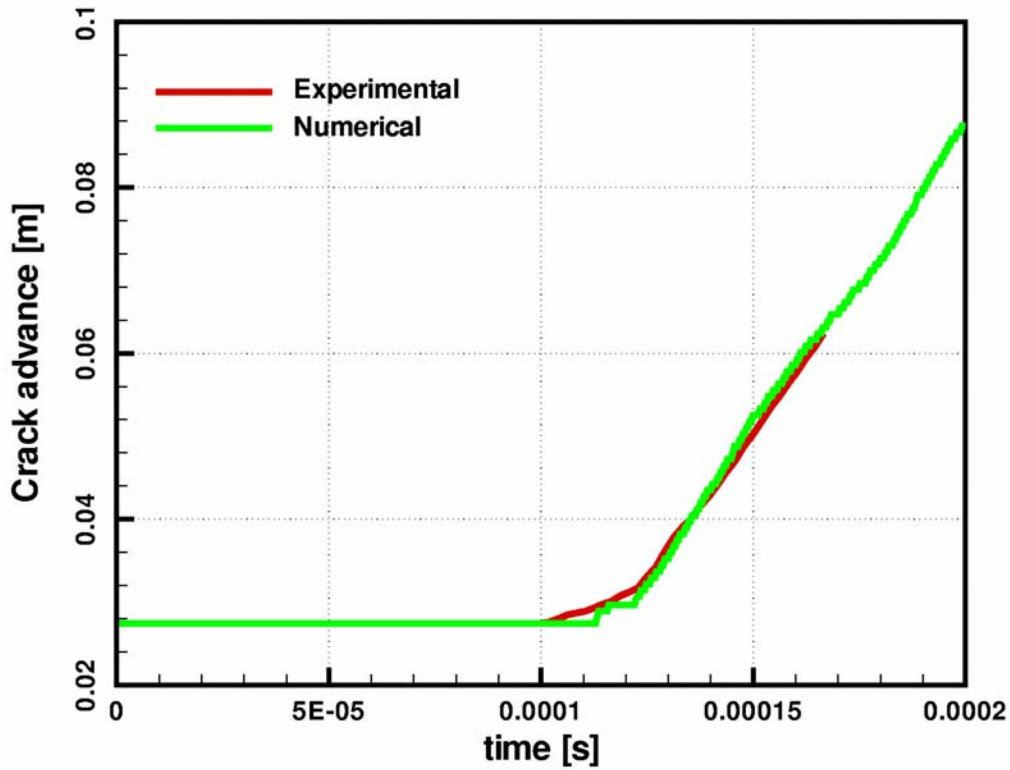
Drop-weight test - C300 steel



Crack geometry as a function of time

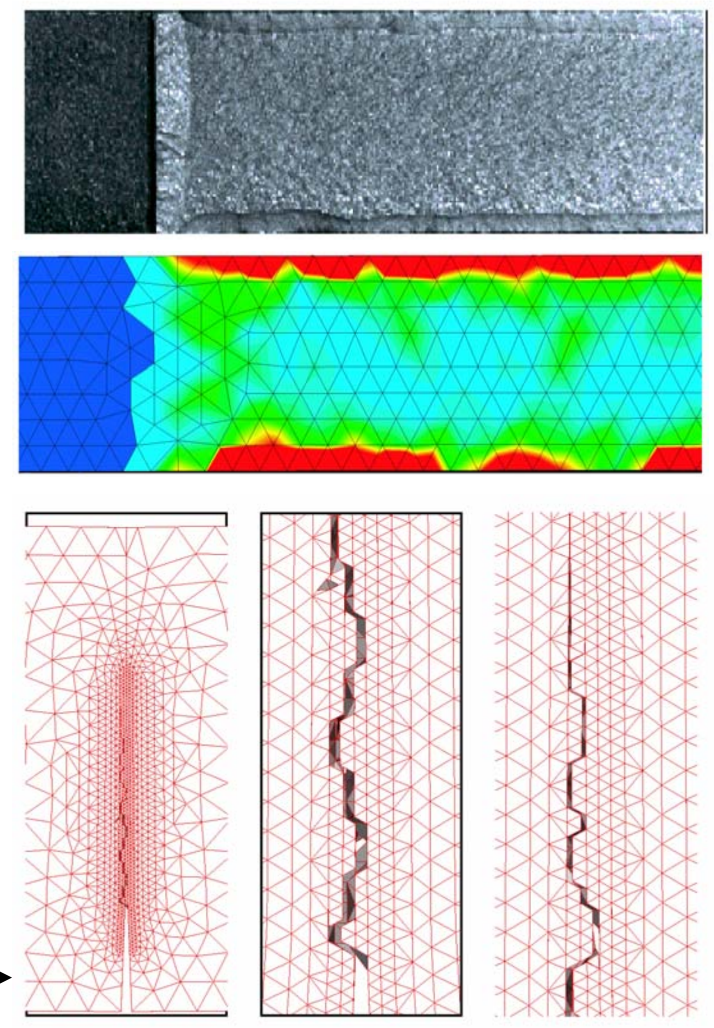
(Pandolfi, Guduru, Ortiz and Rosakis, 2000)

Drop-weight test - C300 steel



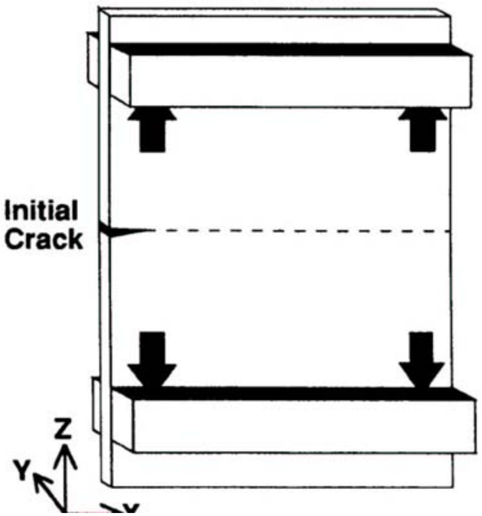
Computed vs. experimential
crack-tip trajectory.

Plastic zone and shear-lip formation
(Impact velocity = 10 m/s) →



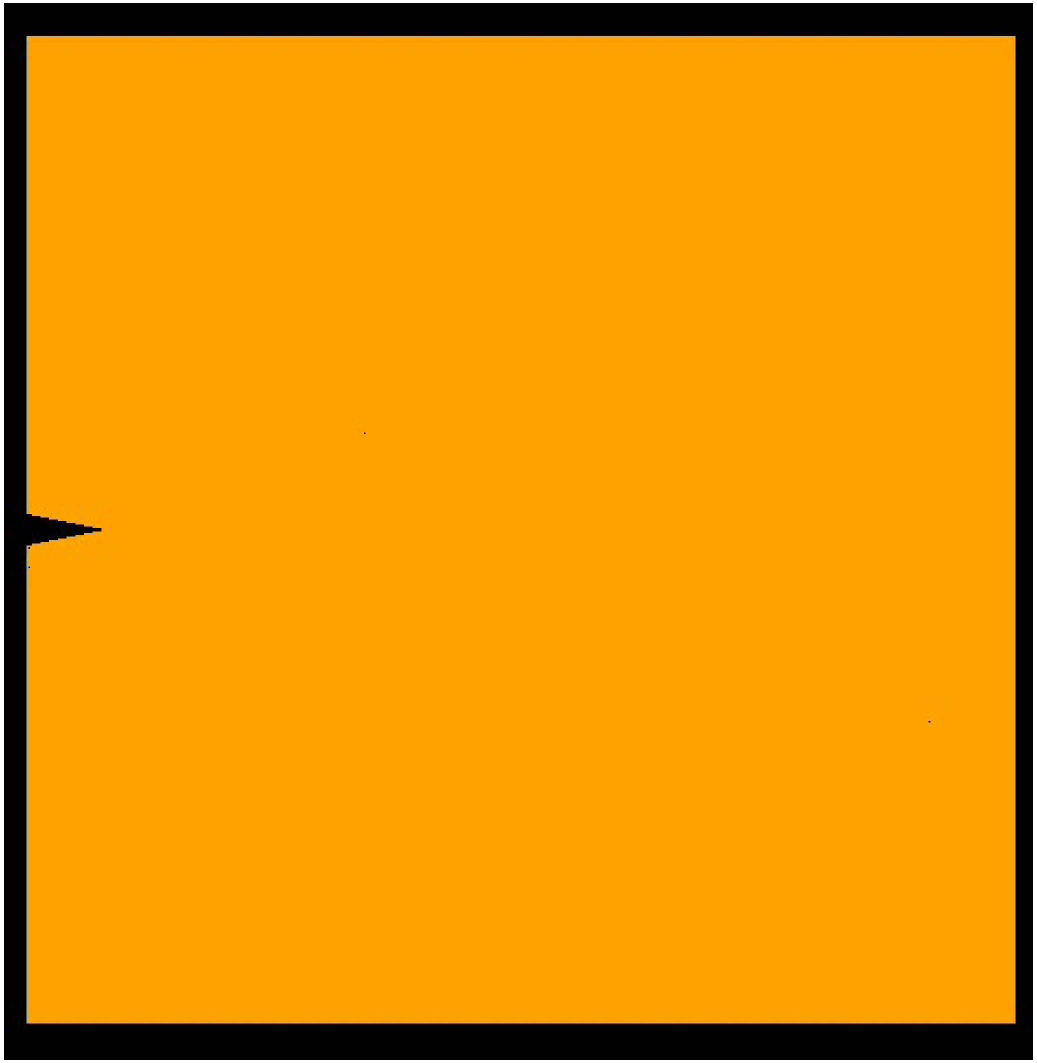
(Pandolfi, Guduru, Ortiz and Rosakis, 2000)

Fracture – Dynamic branching



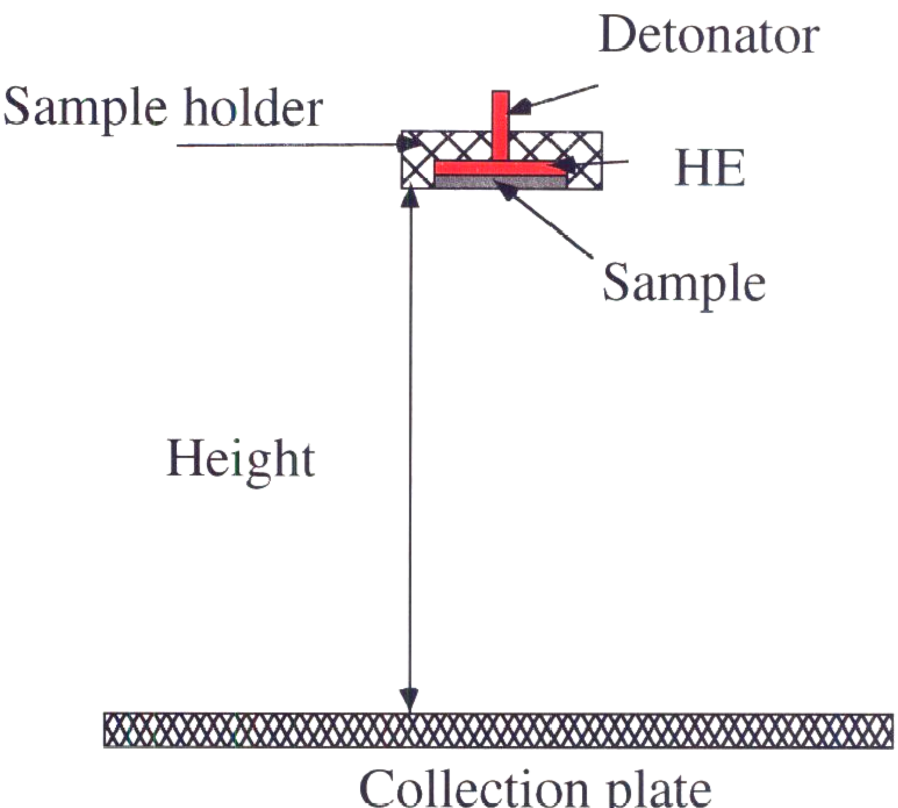
$\dot{\varepsilon} = 4000 \text{ s}^{-1}$

(Fineberg and Sharon, 1992)



(Arias, Knap and Ortiz '04)

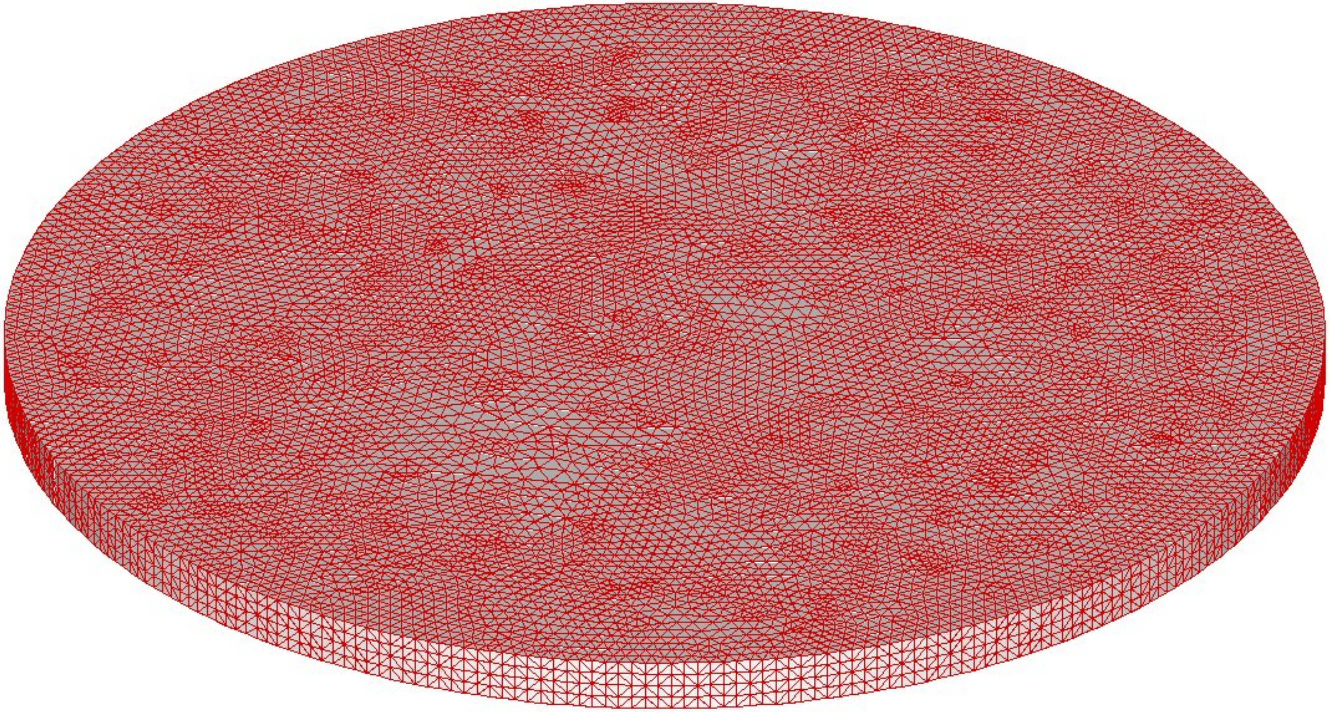
Fracture – Dynamic fragmentation



Collection plate with fragments

(Courtesy Griswold, LLNL, '04)

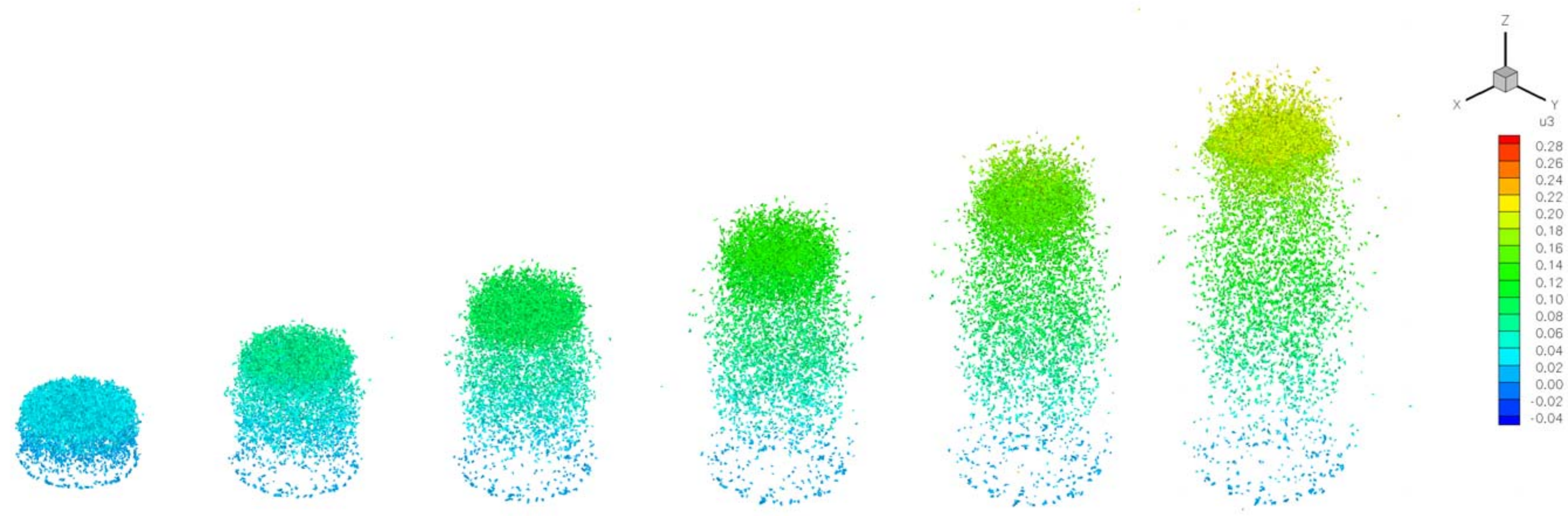
Fracture – Dynamic fragmentation



26574 nodes; 13107 elements; 32 processors

(Mota, Knap and Ortiz '04)

Fracture – Dynamic fragmentation



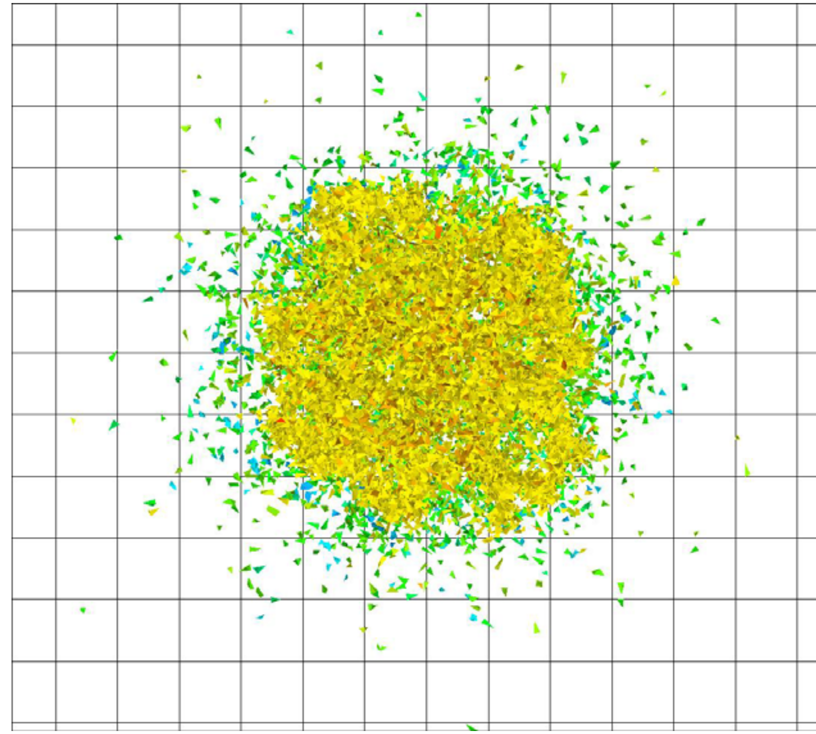
100 μs 200 μs 300 μs 400 μs 500 μs 600 μs

Contours of vertical displacement (m) (animation)

(Mota, Knap and Ortiz '04)

Fracture – Dynamic fragmentation

Experiment



Simulation

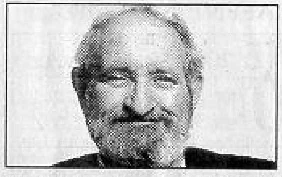
Vertical view of final configuration (680 ms)

Approximate same size (0.30m x 0.30m)

(Mota, Knap and Ortiz '04)

Firearm trauma to the human skull

Friday, September 27, 2002 | LOCAL / REGION | Pasadena Star-News A3



CHARLES CHERNISS

Smoke, ashes, weeping

FIRE and flood have been among the greatest boons and greatest fears of mankind since the cave days.

We have little to fear from flood in Our Valley — though I can recall incidents from my childhood when the San Gabriel River and/or the L.A. River overflowed their banks.

That, of course, was before the Corps of Engineers covered their beds with concrete.

Pasadenans in such areas as Kinneloa have wrestled with

When the bullet hits the bone

Program created to study gunshots to head

By Becky Oskin
Staff Writer

PASADENA — As a bullet pierces the skull, fragments of bone fly into the air and into the brain. What's left behind is a small, neat hole.

This scenario, shown in a computer simulation, matches forensic data taken from thousands of soldiers killed during 20th-century wars.

Caltech postdoctoral scholar Alejandro Mota, 35, created the computer model for two reasons: to help forensic scientists piece together where a killer bullet came from when all that's left is a skull with a gunshot wound; and to prevent bullets ever reaching the brain, including using the model to design better helmets for police and soldiers.

An engineer by training, Mota started the project by boning up on gunshot wounds.

"It's very, very morbid stuff because the statistics mean people are dying and getting shot," Mota said. "But in some way it's good for me, because the aim of the project is to actually help people."

Gunshot wounds to the head have become the leading or second-leading cause of head injury in most U.S. cities, Mota said. They also have a more than 90-percent fatality rate.

The simulation focuses on a pistol shot to the skull's parietal bone, on the side of the head.

Information about the properties of bone came from a Japanese group trying to create synthetic bone and input on the curve of the parietal bone was bought from a company that does laser scanning of objects.

It took about a year to combine all the information and write software to run the simulation. Mota relied on complicated physics to account for the bullet's impact.

"In the end, bone is a solid material, so you can model it with more or less the same equations you use for modeling a piece of steel or rock," Mota said.

The model itself took two months to run on a desktop computer.

The results show a bullet from a 9 mm pistol produces a hole 18 millimeters in diameter — less than three-quarters of an inch.

Forensic data is similar — the average diameter wound for a 9 mm pistol is 12 millimeters, but the holes can range from 8 millimeters to 18 millimeters.

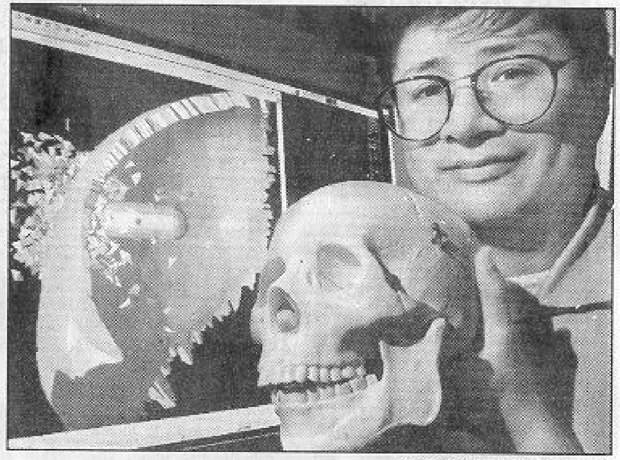
"Our result is a little bit bigger than average but we know, more or less, why that happens. We need more computational power," Mota said.

Mota and his colleagues have submitted their results to the Journal of Biomechanics.

Mota works with Michael Ortiz, a Caltech professor of aeronautics and mechanical engineering. Ortiz has similar projects in the works, including developing software for the Department of Defense that simulates the ballistic penetration of hard targets, to be used in designing structures to withstand direct attacks.

Mota's other collaborators include Caltech graduate student William Klug and Anna Pandolfi, a professor of structural engineering at the Politecnico di Milano in Italy.

Becky Oskin can be reached at (626) 578-6300, Ext. 4451, or by e-mail at becky.oskin@sgvn.com.

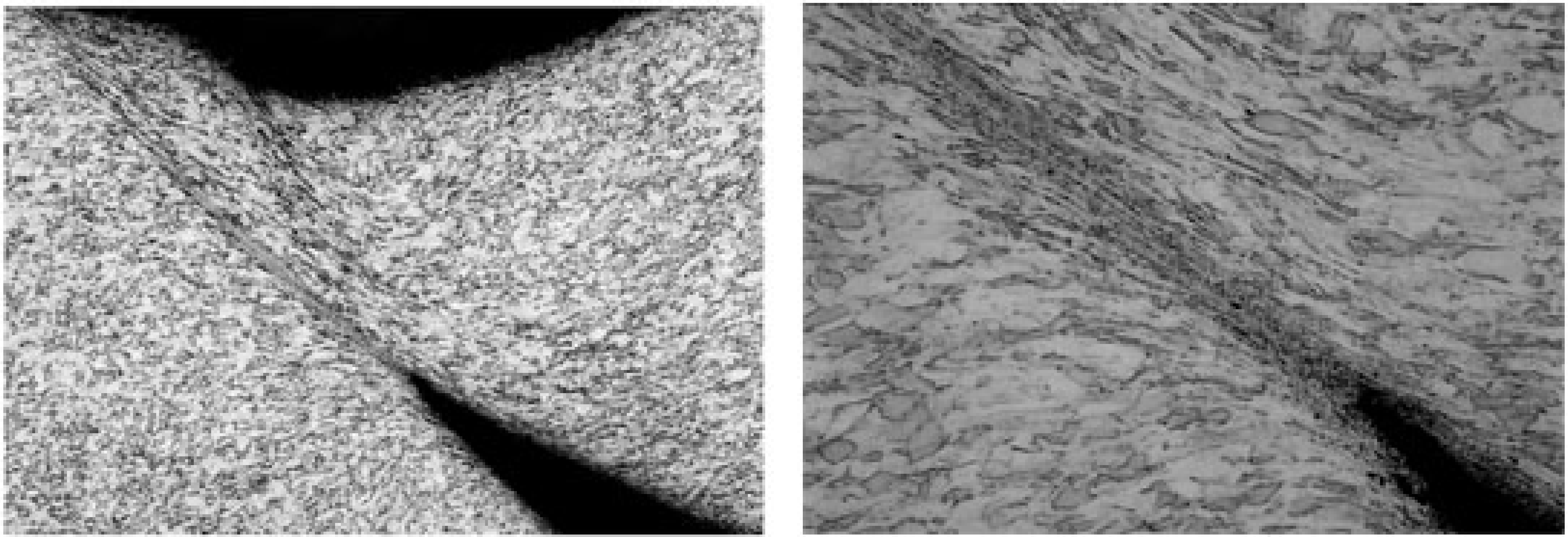


Staff photo by WALT MANCINI

ALEJANDRO MOTA, 35, has created a computer simulation of how the skull fractures when hit by a bullet.

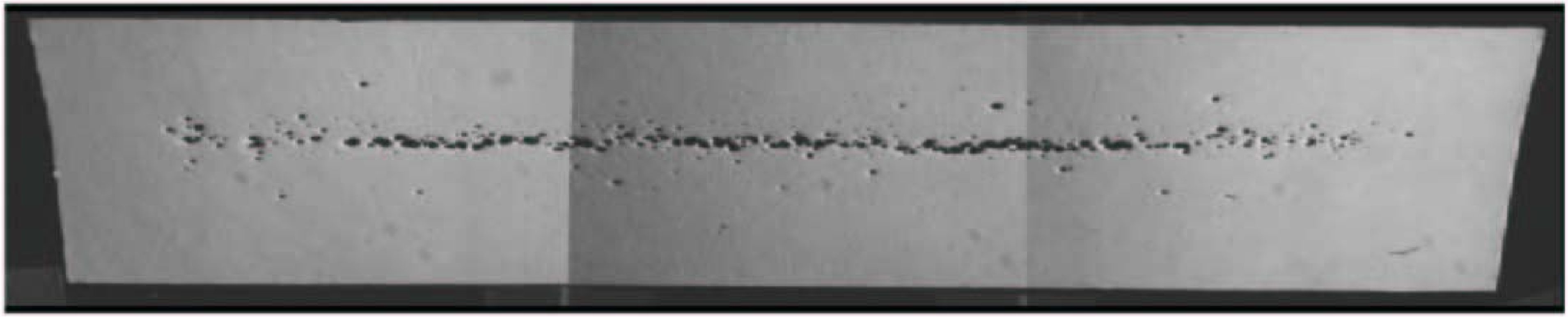
Localization as free-discontinuity problem

(a) (b)



(a) Micrograph of a tantalum–tungsten alloy cylinder driven by a gas gun showing that the material breaks along shear bands (darker diagonal line). (b) The crack tip at a higher magnification. (R. Becker, “How Metals Fail”, UCRL-52000-02-7/8 | July 12, 2002; Micrograph produced by Anne Sunwoo) .

Localization as free-discontinuity problem



Shock-driven spall fracture
(R. Becker, “How Metals Fail”, UCRL-52000-02-7/8 | July 12, 2002

Detonation-driven Al-tube fracture
(Shepherd et al., 2003)

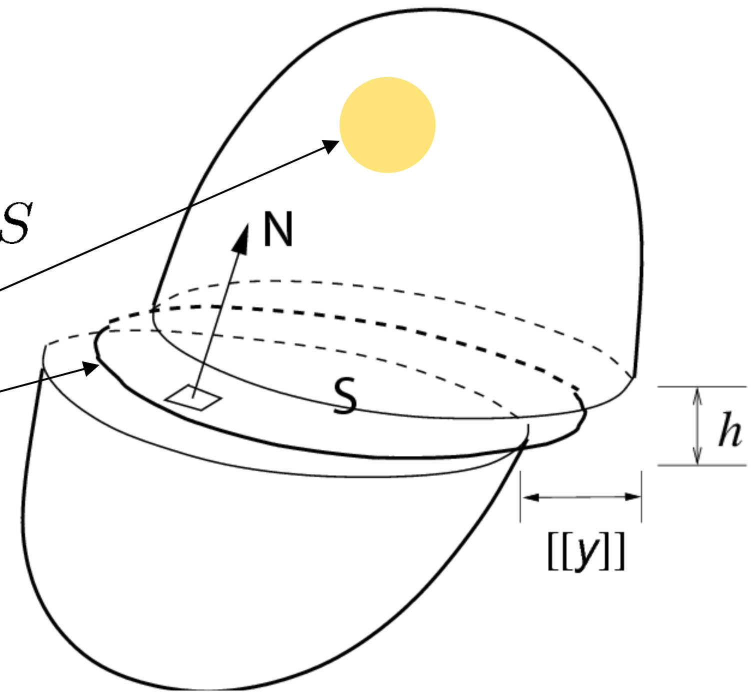
Michael Ortiz
Stanford 04/04

Localization as free-discontinuity problem

- Deformation gradient:

$$Dy = \nabla y + h^{-1}[\![y]\!] \otimes N\delta_S$$

$$\begin{cases} \nabla y \text{ absolutely continuous} \\ \text{Singular set } S \equiv \text{ band} \end{cases}$$



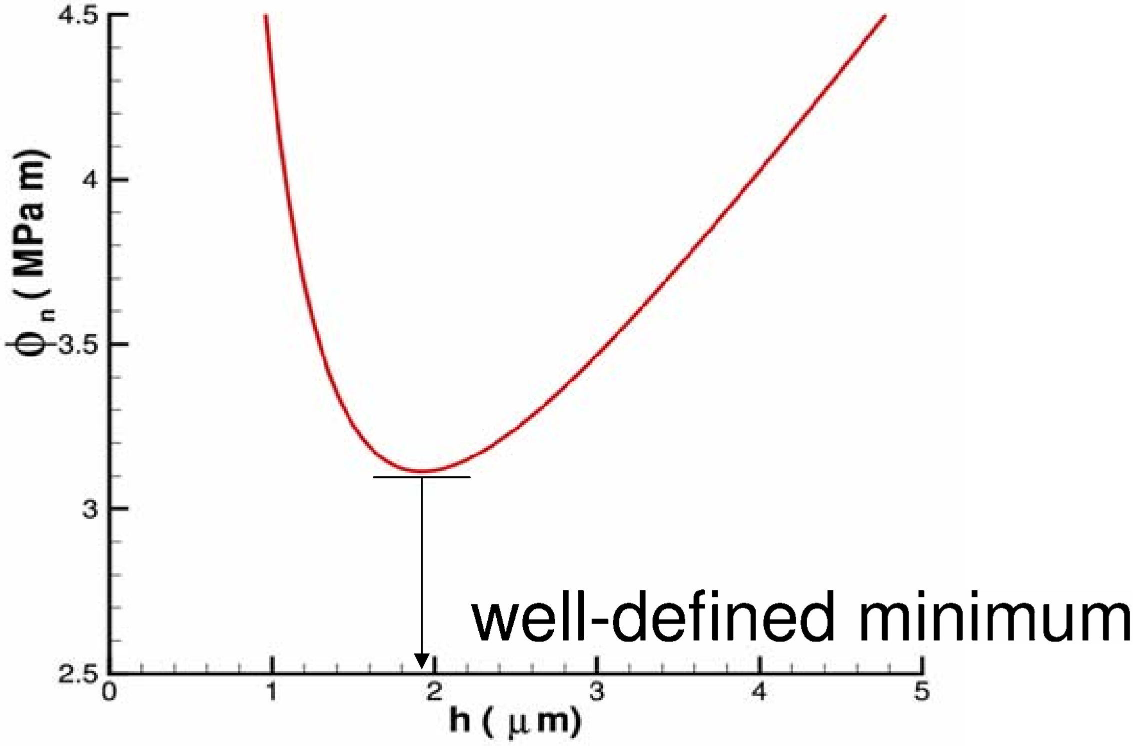
- Energy (incremental):

$$E(y) = \underbrace{\int W(\nabla y)dx}_{\text{Bulk energy}} + \underbrace{\int_S \phi([\![y]\!], N, h)dS}_{\text{Localized energy}}$$

$\phi \equiv$ Localized energy density.

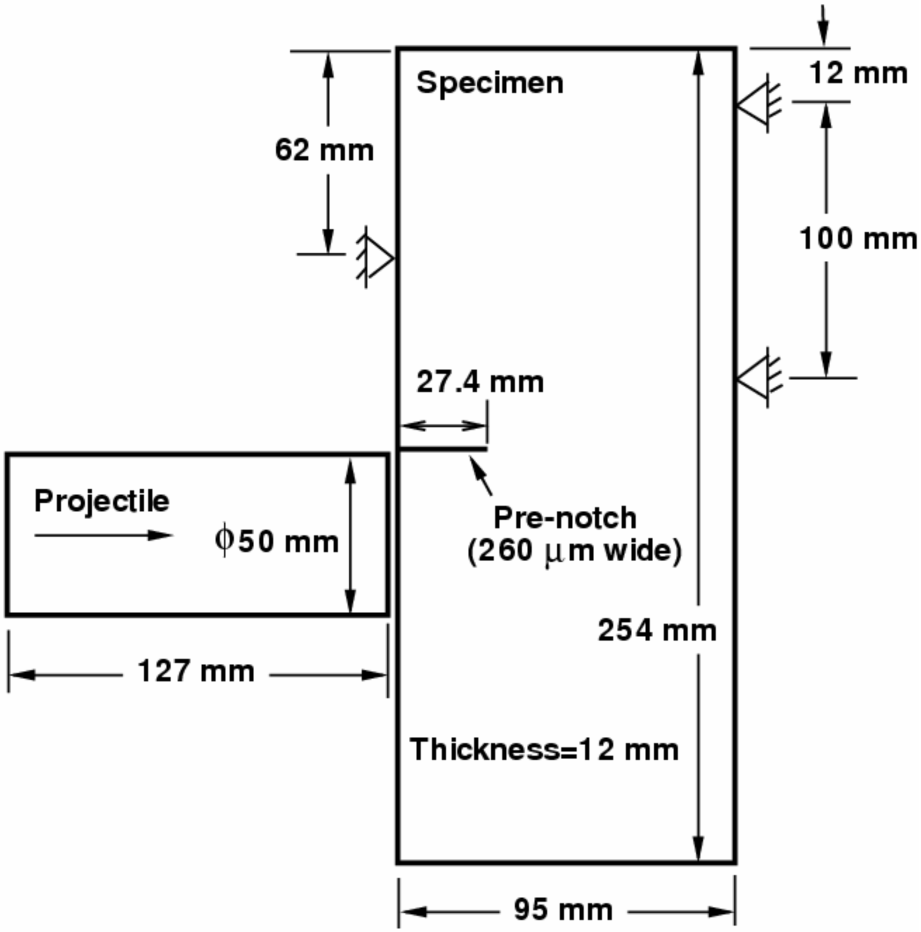
Michael Ortiz
Stanford 04/04

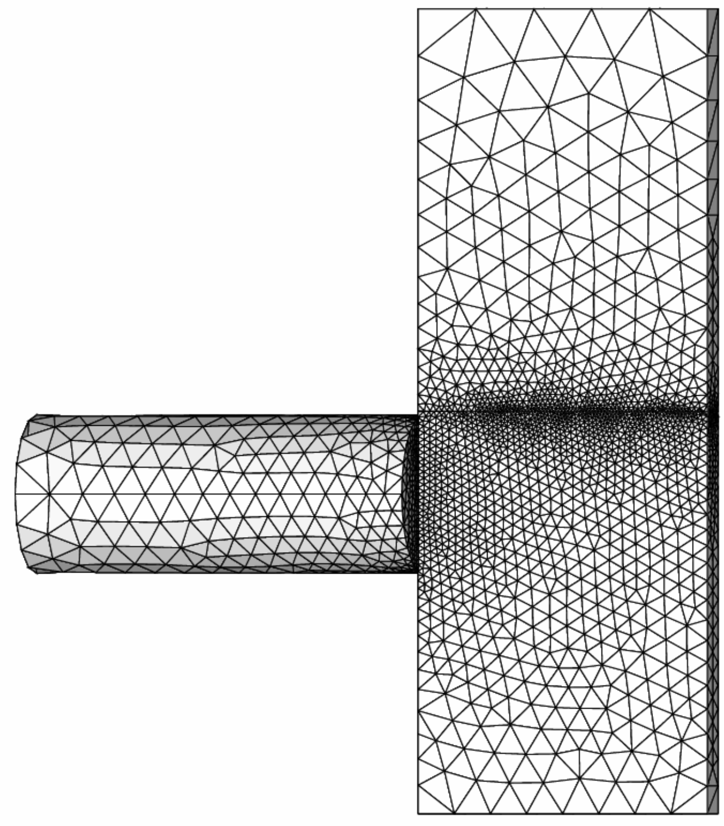
Localization – Band thickness



$$\int_S \phi([\![y]\!], N, h)\, dS \sim \underbrace{Ah}_{\text{(local)}} + \underbrace{\frac{B}{h}}_{\text{(nonlocal)}}$$

Localization – Plate impact

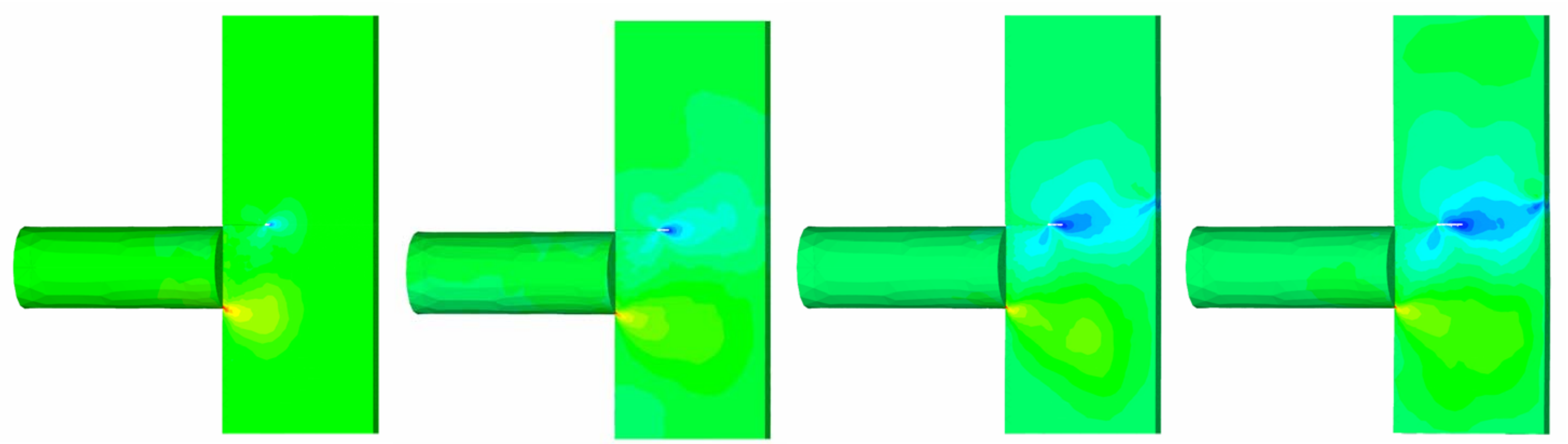




Pre-notched C300 steel plates

(Guduru it et al. ’01)

Localization – Plate impact

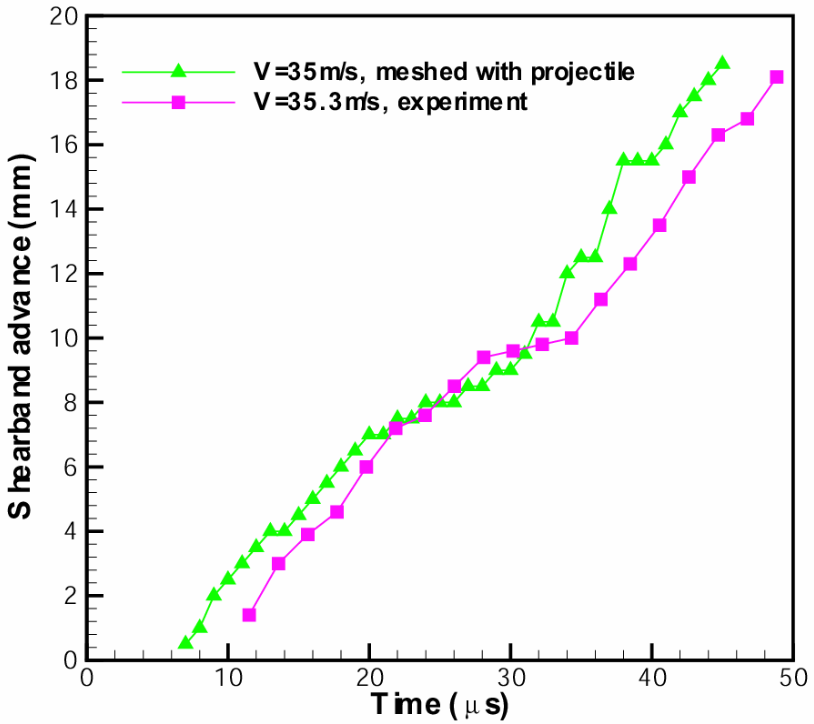


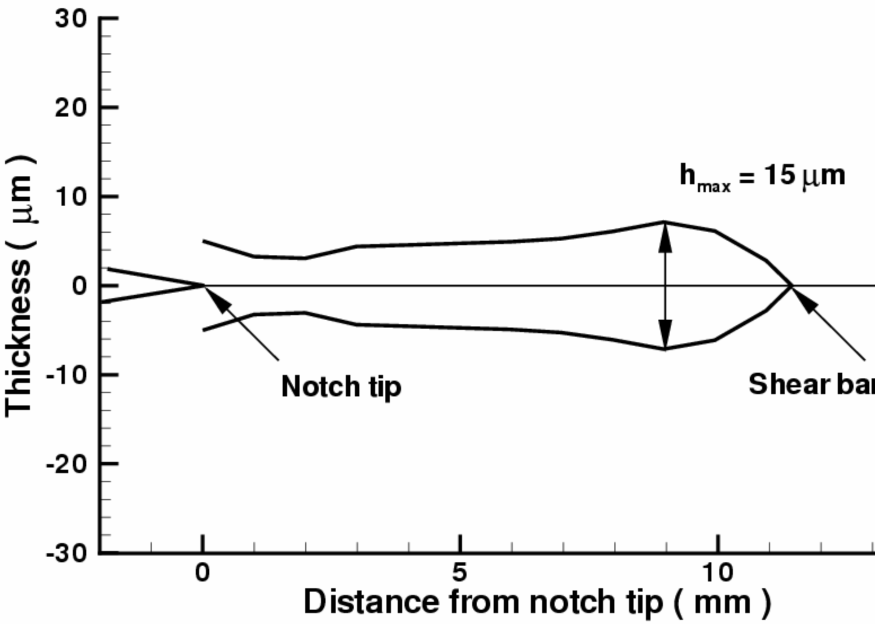
10 μs 20 μs 30 μs 40 μs

Dynamic shear band propagation

(Yang, Mota and Ortiz '04)

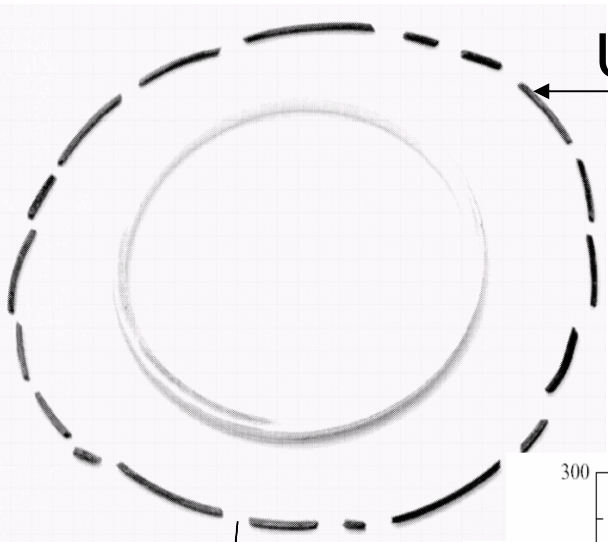
Localization – Plate impact





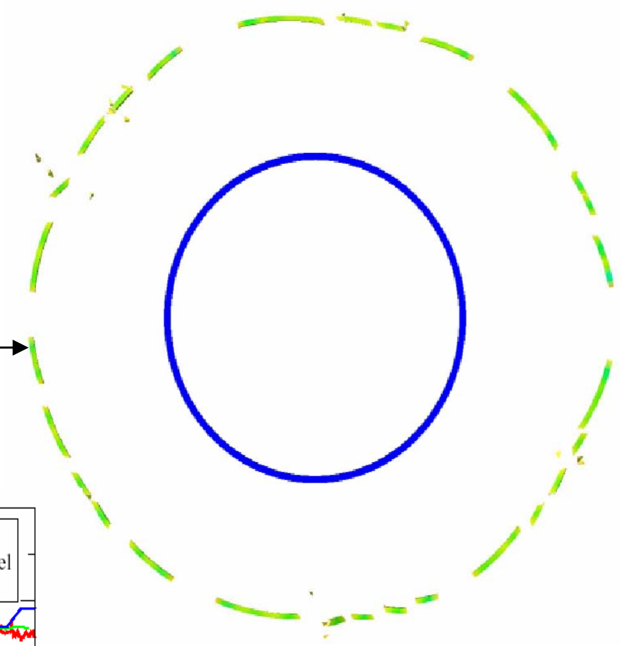
(Yang, Mota and Ortiz '04)

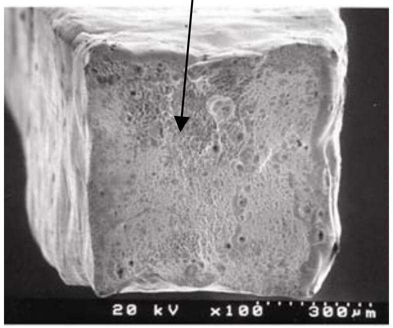
Localization – Ring expansion tests



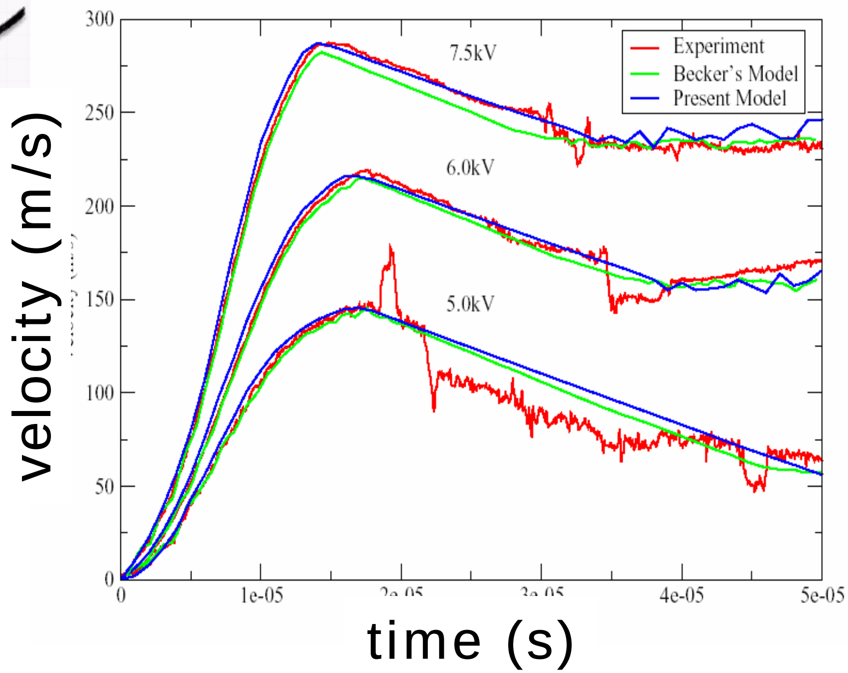
U6Nb ring expansion
(Becker LLNL '02)

FE simulation
(Mota *et al* '03)





Rich Becker, LLNL)



(animation)

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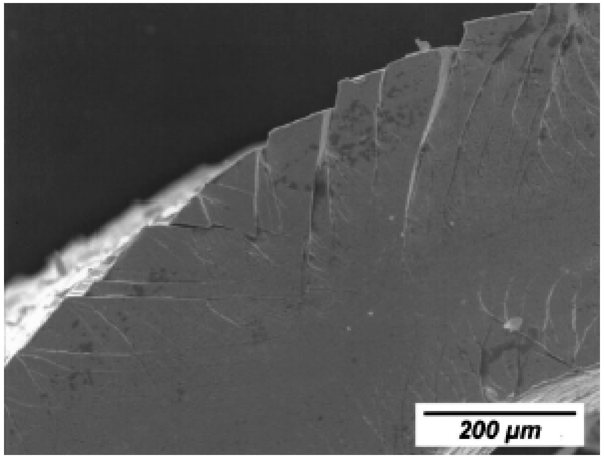
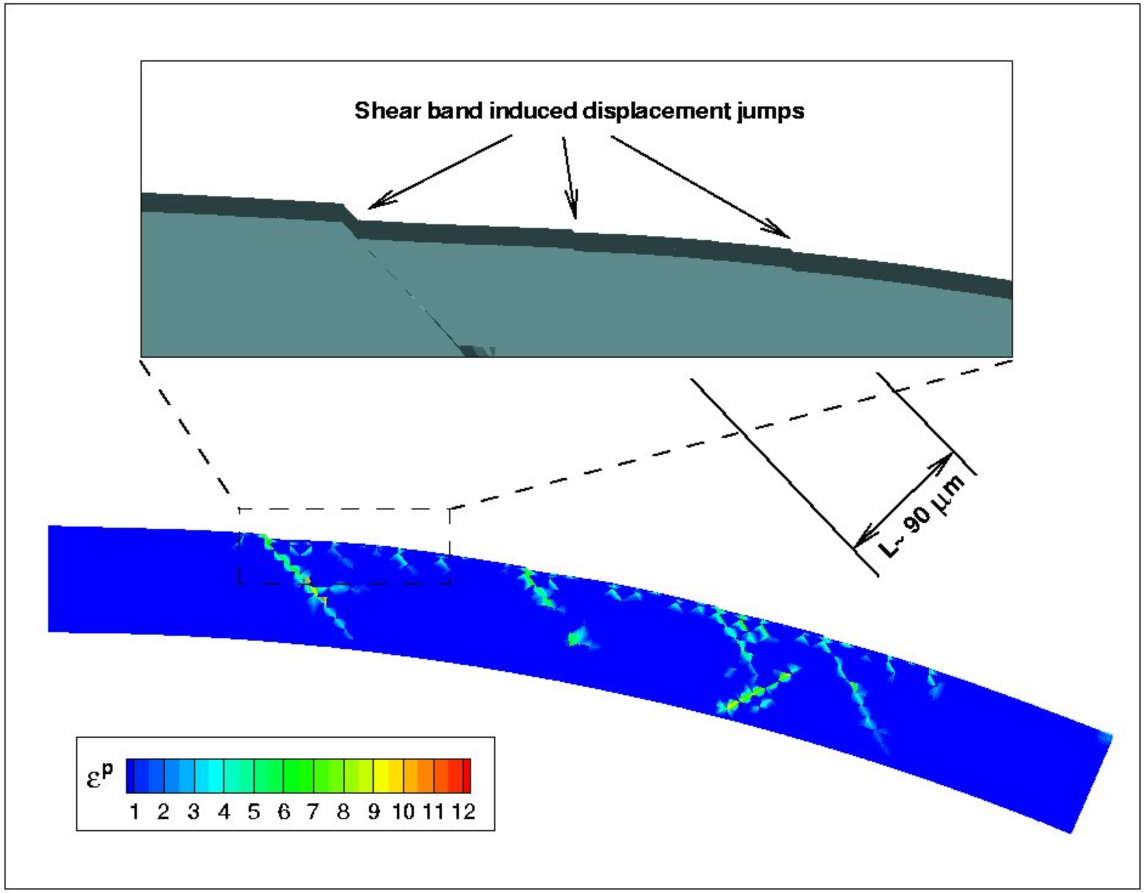
Localization – BMG bending tests



Bending experiments
(Conner et al. ‘03)

(Yang, Mota & Ortiz ‘04)



Finite element simulation of bulk metallic glass in bending. The computed shear band spacing is about 15% of the specimen’s thickness. Experimental observations report a spacing about 10% of the thickness.

Concluding remarks

- Many problems in solid mechanics can be formulated as ‘free-discontinuity’ problems.
- The free-discontinuity concept provides a `recipe’ for formulating problems involving localization
- Modeling focuses on physics of the ‘singular set’ (slip, cohesive fracture, adiabatic heating, void sheets…).
- There are powerful mathematical tools (e.g., relaxation, Gamma-convergence, in SBV) for analyzing problems.
- Cohesive/localization elements provide a simple and effective means of approximating free-discontinuity solutions.