Optimal scaling laws in ductile fracture

M. Ortiz

California Institute of Technology

Joint work with: S. Conti, L. Fokoua, S. Heyden, B. Li, K. Weinberg

Workshop on Materials Theories

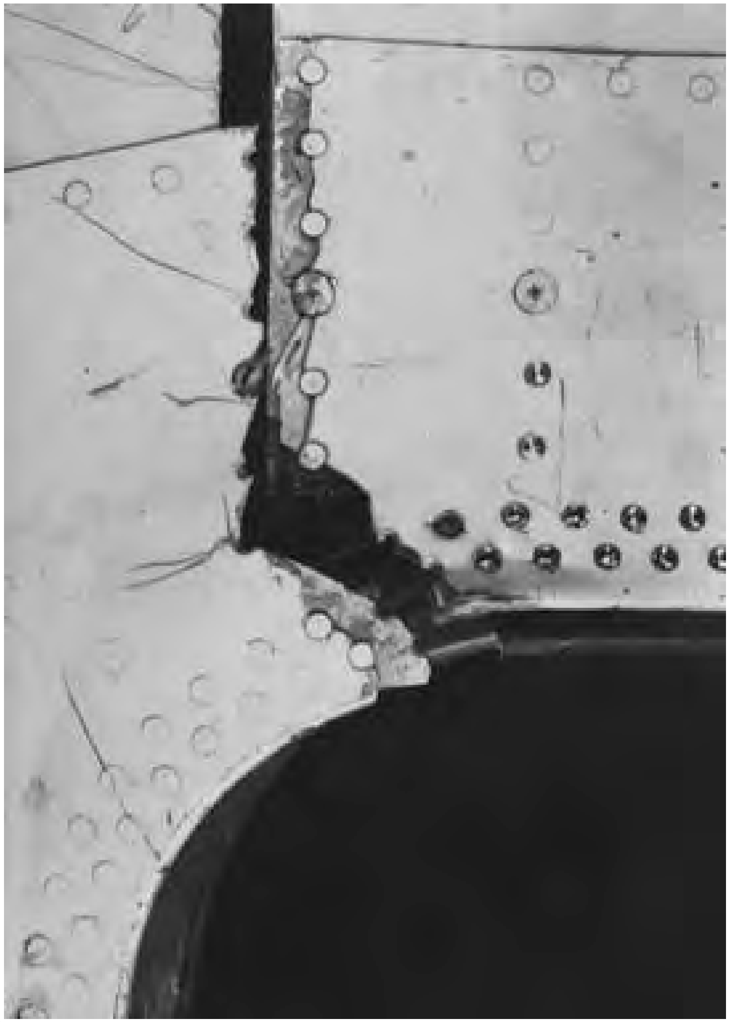
Mathematisches Forschungsinstitut Oberwolfach

December 15-21, 2013

Outline

- Background/phenomenology of ductile fracture
- Metals: mathematical formulation
- Optimal scaling laws
- Numerical approximation
- Applications: Hypervelocity impact and explosively-driven caps
- Extension to polymers
- Application: Taylor anvil tests on polyurea

Background on ductile fracture

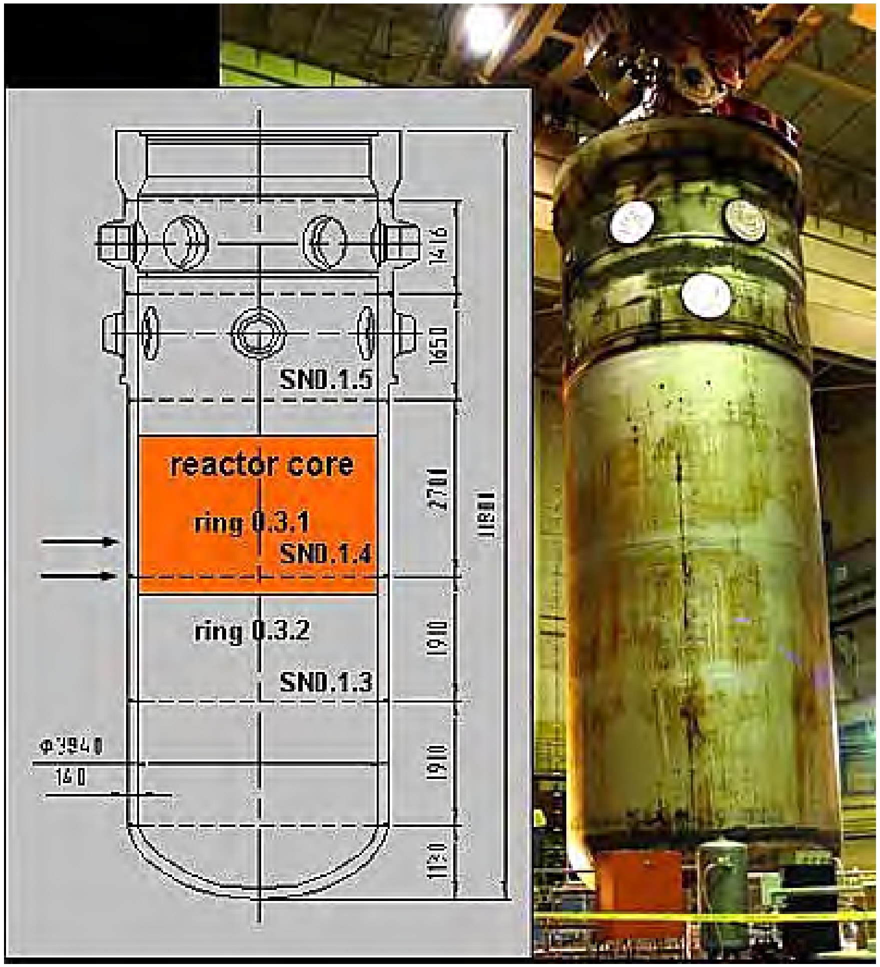


- ***Linear-elastic fracture mechanics*** attained engineering importance as a means of predicting fatigue-crack growth in aircraft structures (focus on Irwin's stress-intensity factor, Paris' fatigue law)

Detail of cabin window crack of a de Havilland Comet G-ALYP recovered from the Mediterranean after its crash in January 1954.

(http://www.ssplprints.com/image.php?imgref=10447442)

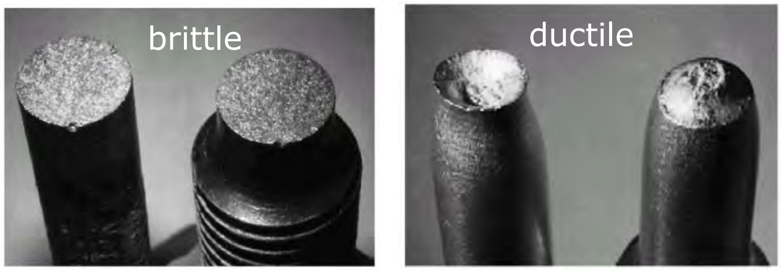
Background on ductile fracture



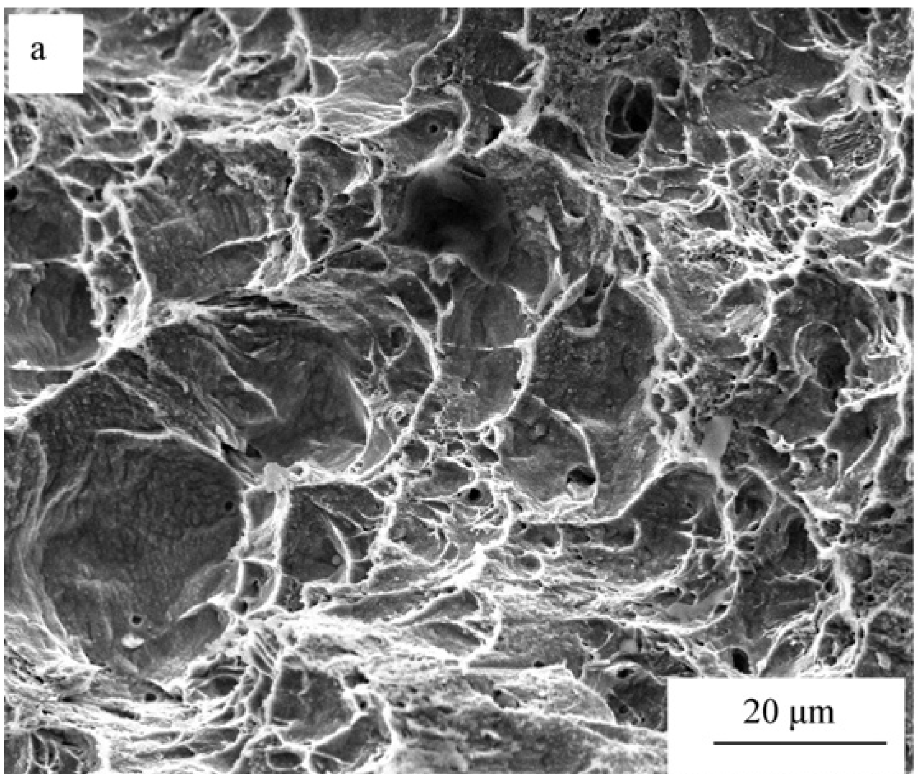
- Linear-elastic fracture mechanics proved inadequate for assessing safety of mild-steel pressure vessels in nuclear power plants, which spurred the development of ***elastic-plastic fracture mechanics*** (with focus on Rice's J-integral formalism)

Reactor Pressure Vessel (RPV) from Greifswald Nuclear Power Plant (courtesy Viehrig, H.W. and Houska, M., Helmholtz Zentrum, Dresden-Rossendorf, https://www.hzdr.de/db/Cms?pNid=2698)

Background on ductile fracture



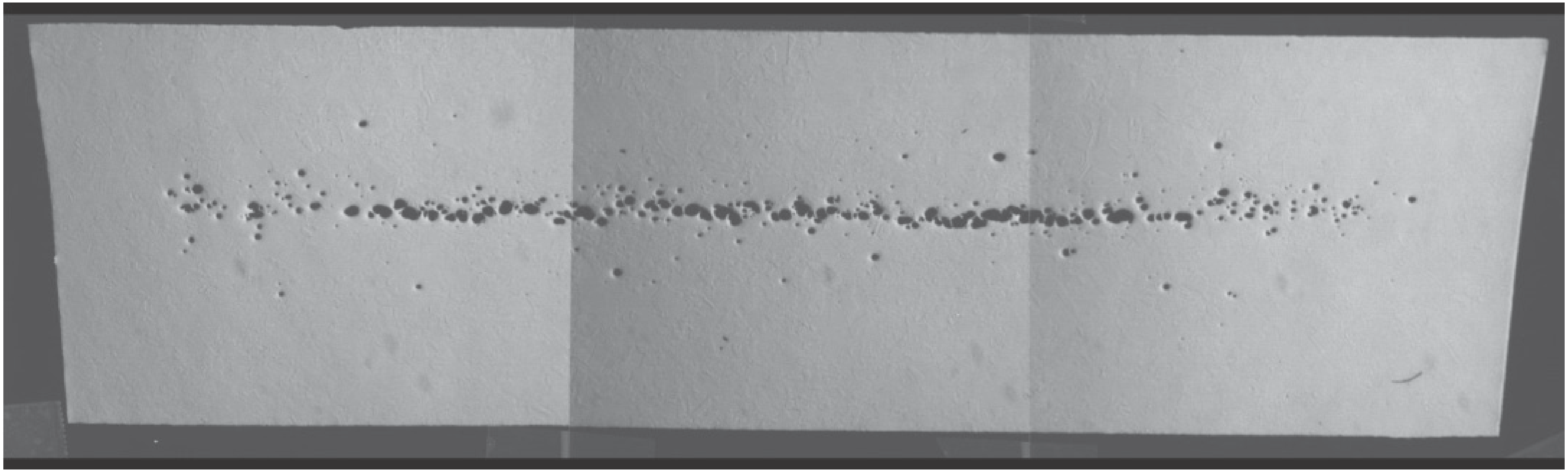
(Courtesy NSW HSC online)



- Ductile fracture in metals occurs by *void nucleation*, *growth and coalescence*
- Fractography of ductile-fracture surfaces exhibits profuse *dimpling*, vestige of microvoids
- Ductile fracture entails large amounts of *plastic deformation* (*vs*. surface energy) and dissipation.

Fracture surface in SA333 steel, room temp., $d\varepsilon/dt=3\times10^{-3}s^{-1}$ (S.V. Kamata, M. Srinivasa and P.R. Rao, Mater. Sci. Engr. A, ***528*** *(2011) 4141–4146)*

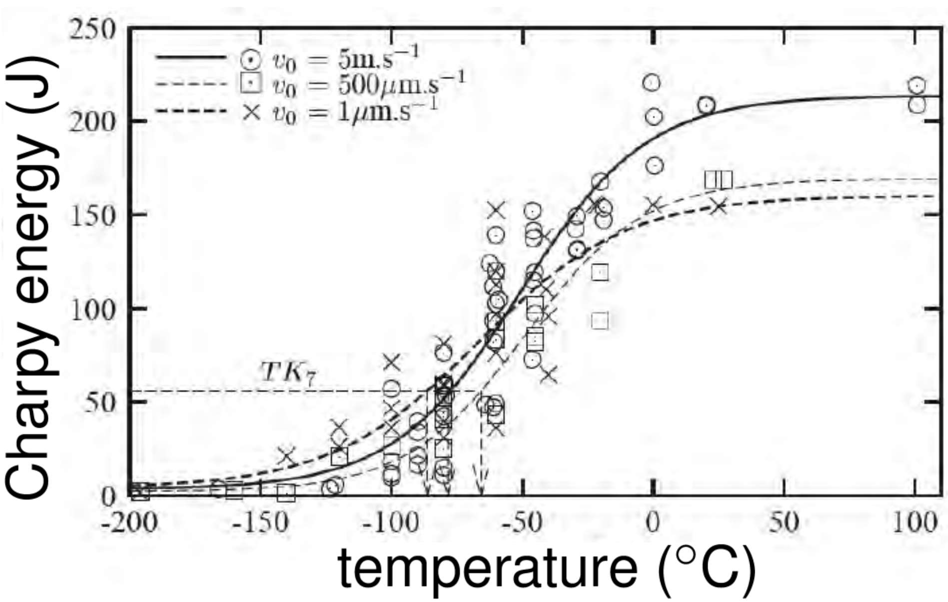
Background on ductile fracture



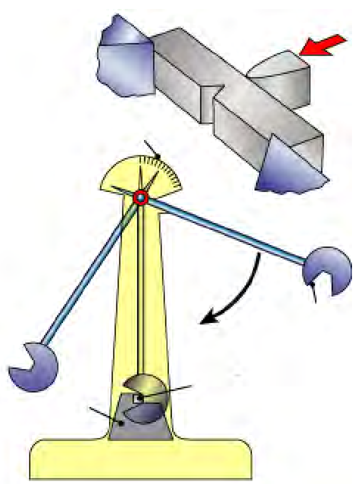
Photomicrograph of a copper disk tested in a gas-gun experiment showing the formation of voids and their coalescence into a fracture plane

Heller, A., How Metals Fail,
Science & Technology Review Magazine,
Lawrence Livermore National Laboratory,
pp. 13-20, July/August, 2002

Background on ductile fracture



Charpy energy of A508 steel (Tanguy *et al.*, *Eng. Frac. Mechanics*, 2005)



- A number of ASTM engineering standards are in place to characterize ductile fracture properties (J-testing, Charpy test)
- The Charpy test data reveals a brittle-to-ductile transition temperature
- In general, the specific fracture energy for ductile fracture is greatly in excess of that required for brittle fracture…

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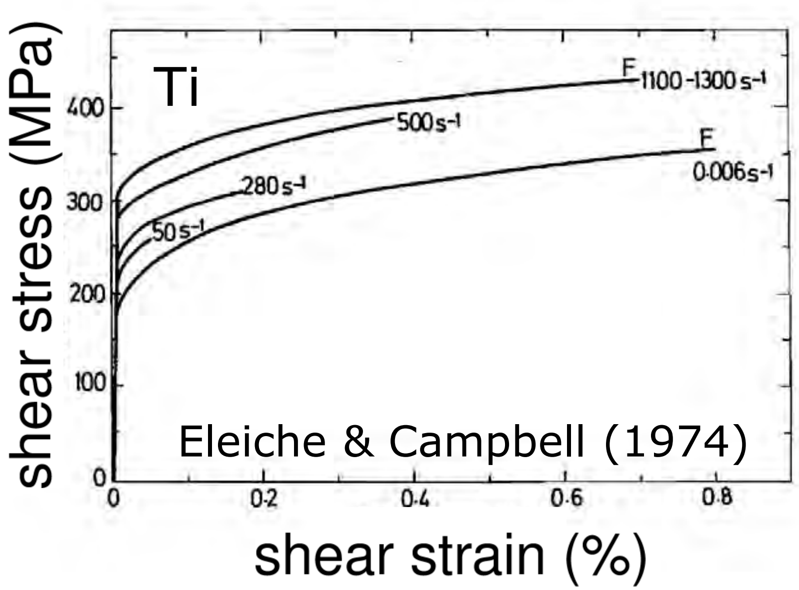
Naïve model: Local plasticity

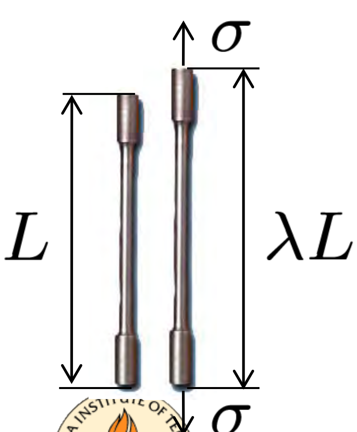


- Deformation theory: Minimize

$$E(y) = \int_\Omega W\Big(Dy(x)\Big)\,dx$$

- Growth of $W(F)$?
- Asume power-law hardening:

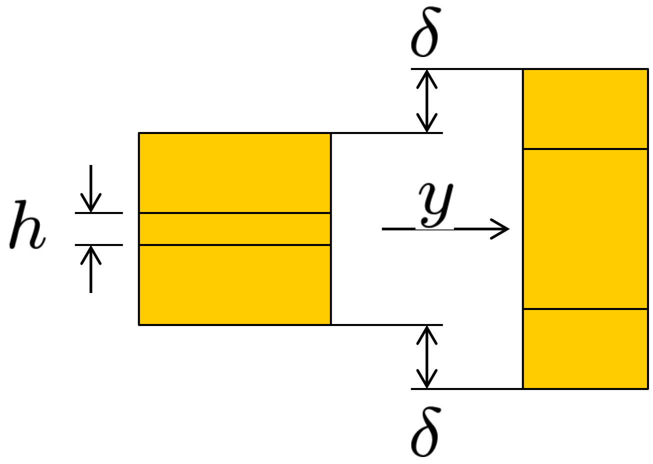
$$\sigma \sim K\epsilon^n = K(\lambda - 1)^n$$



- Nominal stress: $\partial_\lambda W = \sigma/\lambda = K(\lambda-1)^n/\lambda$
- For large λ: $\partial_\lambda W \sim K\lambda^{n-1} \Rightarrow W \sim K\lambda^n$
- In general: $W(F) \sim |F|^p,\ p = n \in (0,1)$

$\Rightarrow$ Sublinear growth!

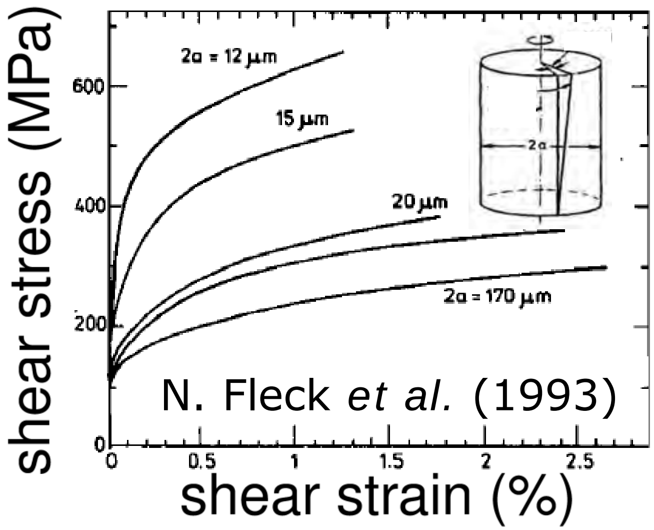
Naïve model: Local plasticity

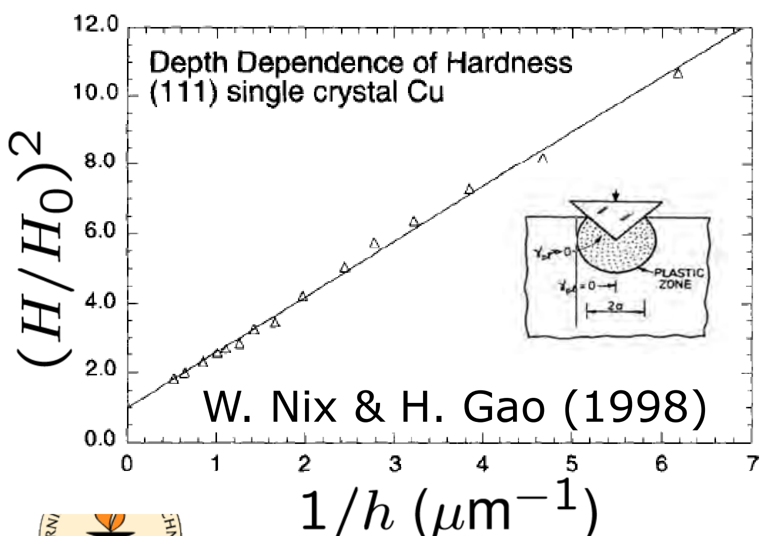


- Example: Uniaxial extension
- Energy: $E_h \sim h \left(\frac{2\delta}{h} \right)^p$
- For $p < 1$: $\lim_{h \to 0} E_h = 0$

- Energies with sublinear growth relax to 0.
- For hardening exponents in the range of experimental observation, local plasticity yields no useful information regarding ductile fracture properties of materials
- Need additional physics, structure…

Strain-gradient plasticity





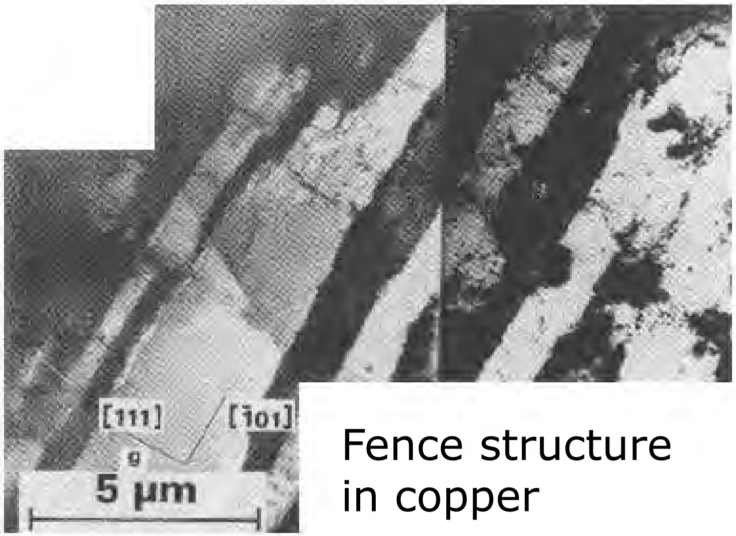
- The yield stress of metals is observed to increase in the presence of strain gradients
- Deformation theory of strain-gradient plasticity:

$$E(y) = \int_\Omega W\Big(Dy(x), D^2y(x)\Big)\, dx$$

$y : \Omega \to \mathbb{R}^n$, volume preserving

- Strain-gradient effects may be expected to oppose localization
- Growth of *W* with respect to the second deformation gradient?

Strain-gradient plasticity



Fence structure in copper

(J.W. Steeds, *Proc. Roy. Soc. London*, **A292**, 1966, p. 343)

- Growth of $W(F, \cdot)$?
- For fence structure:

$$F^{\pm} = R^{\pm}(I \pm \tan\theta \, s \otimes m)$$

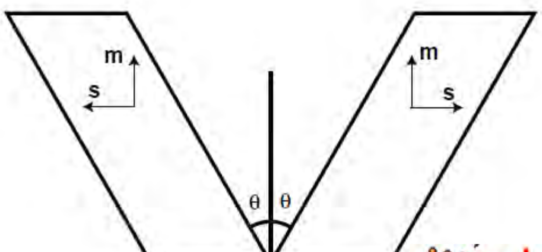
- Across jump planes:

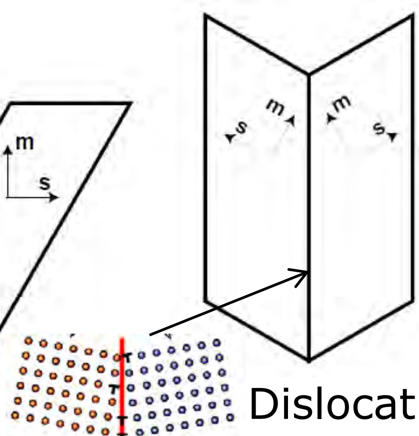
$$|[\![F]\!]| = 2\sin\theta$$

- Dislocation-wall energy:

$$E = \frac{T}{b} 2\sin\theta = \frac{T}{b}|[\![F]\!]|$$

$\Rightarrow W(F, \cdot)$ has linear growth!





Dislocation wall

Strain-gradient plasticity

- Mathematical model: Minimize

$$E(y) = \int_\Omega W\Big(Dy(x), D^2y(x)\Big)\,dx$$

$y : \Omega \to \mathbb{R}^n$, volume preserving

- For metals, local plasticity exhibits sub-linear growth, which favors localization of deformations
- Strain-gradient plasticity may be expected to exhibit linear growth, which opposes localization
- *Question: Can ductile fracture be understood as the result of a competition between sublinear growth and strain-gradient plasticity?*

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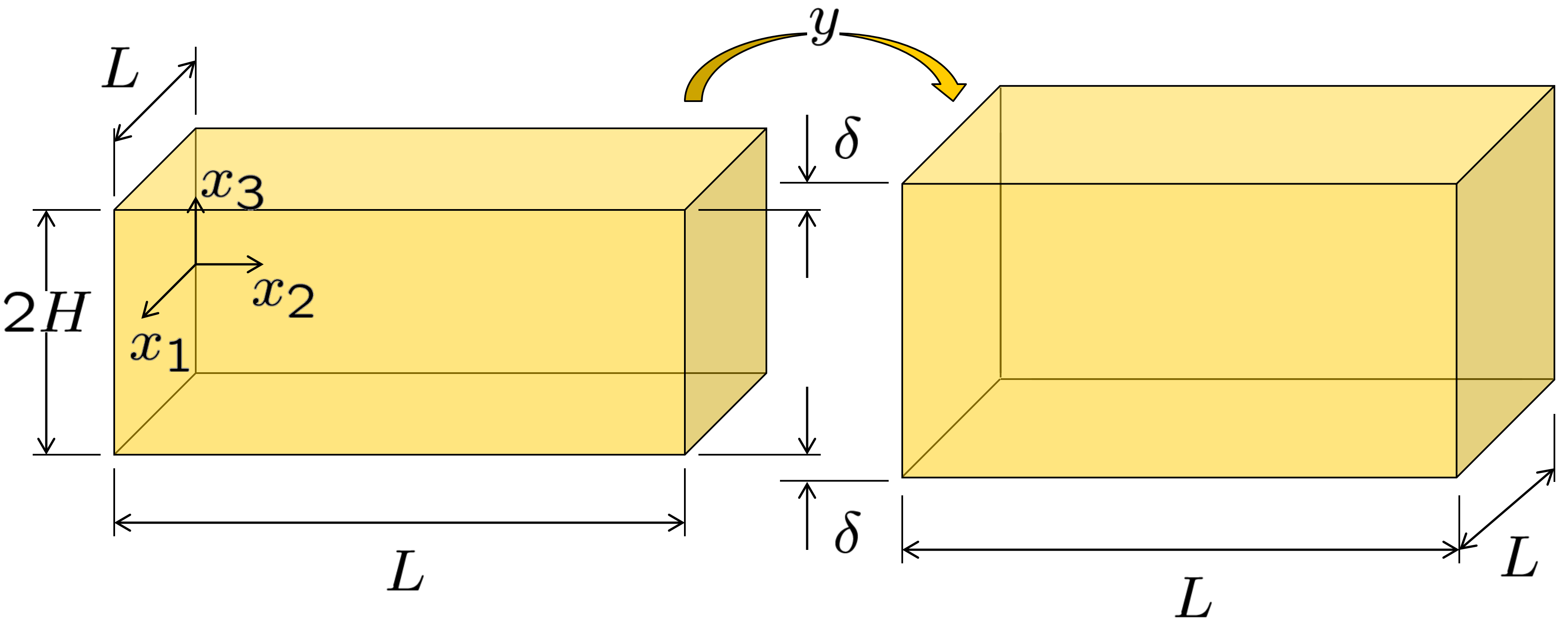
Optimal scaling – Uniaxial extension



- Approach: Optimal scaling
- Slab: $\Omega = [0, L]^2 \times [-H, H]$, periodic
- Uniaxial extension: $y_3(x_1, x_2, \pm H) = x_3 \pm \delta$

Optimal scaling – Uniaxial extension

- $y : \Omega \to \mathbb{R}^3$, $[0, L]^2$-periodic, volume preserving
- $y \in W^{1,1}(\Omega; \mathbb{R}^3)$, $Dy \in BV(\Omega; \mathbb{R}^{3\times 3})$
- Growth: For $0 < K_L < K_U$, *intrinsic length* $\ell > 0$,

$$E(y) \geq K_L \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell \int_\Omega |D^2 y|\, dx \right)$$
$$E(y) \leq K_U \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell \int_\Omega |D^2 y|\, dx \right)$$

Theorem [Fokoua, Conti & MO, ARMA, 2013]. For ℓ sufficiently small, $p \in (0,1)$, $0 < C_L(p) < C_U(p)$,

$$C_L(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}} \leq \inf E \leq C_U(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$$

Optimal scaling – Uniaxial extension

- Optimal (matching) upper and lower bounds:

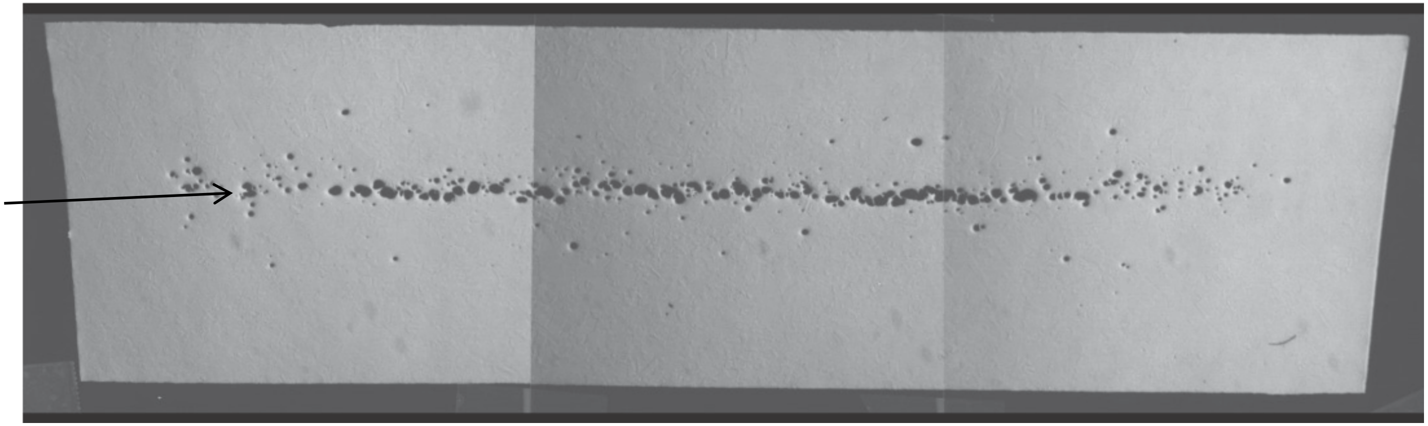
$$C_L(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}} \leq \text{inf}\, E \leq C_U(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$$

- Bounds apply to *classes of materials* having the same growth, specific model details immaterial
- Energy scales with *area* (L^2): Fracture scaling!
- Energy scales with power of *opening displacement* (δ): Cohesive behavior!
- Lower bound degenerates to 0 when the intrinsic length (ℓ) decreases to zero…
- Bounds on specific fracture energy:

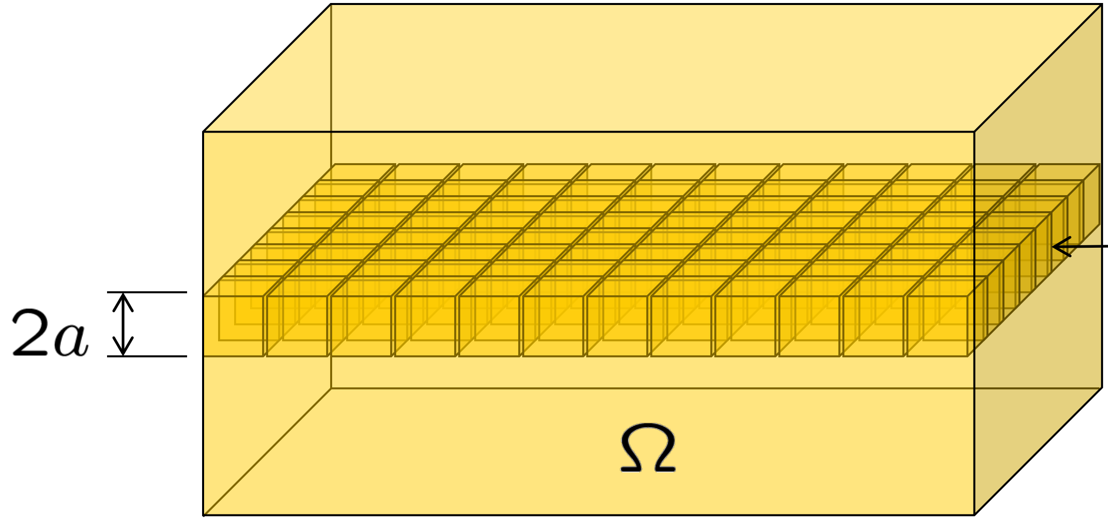
$$C_L(p) \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}} \leq J_c \leq C_U(p) \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$$

Sketch of proof – Upper bound

void
sheet



Heller, A., Science & Technology Review Magazine, LLNL, pp. 13-20, July/August, 2002



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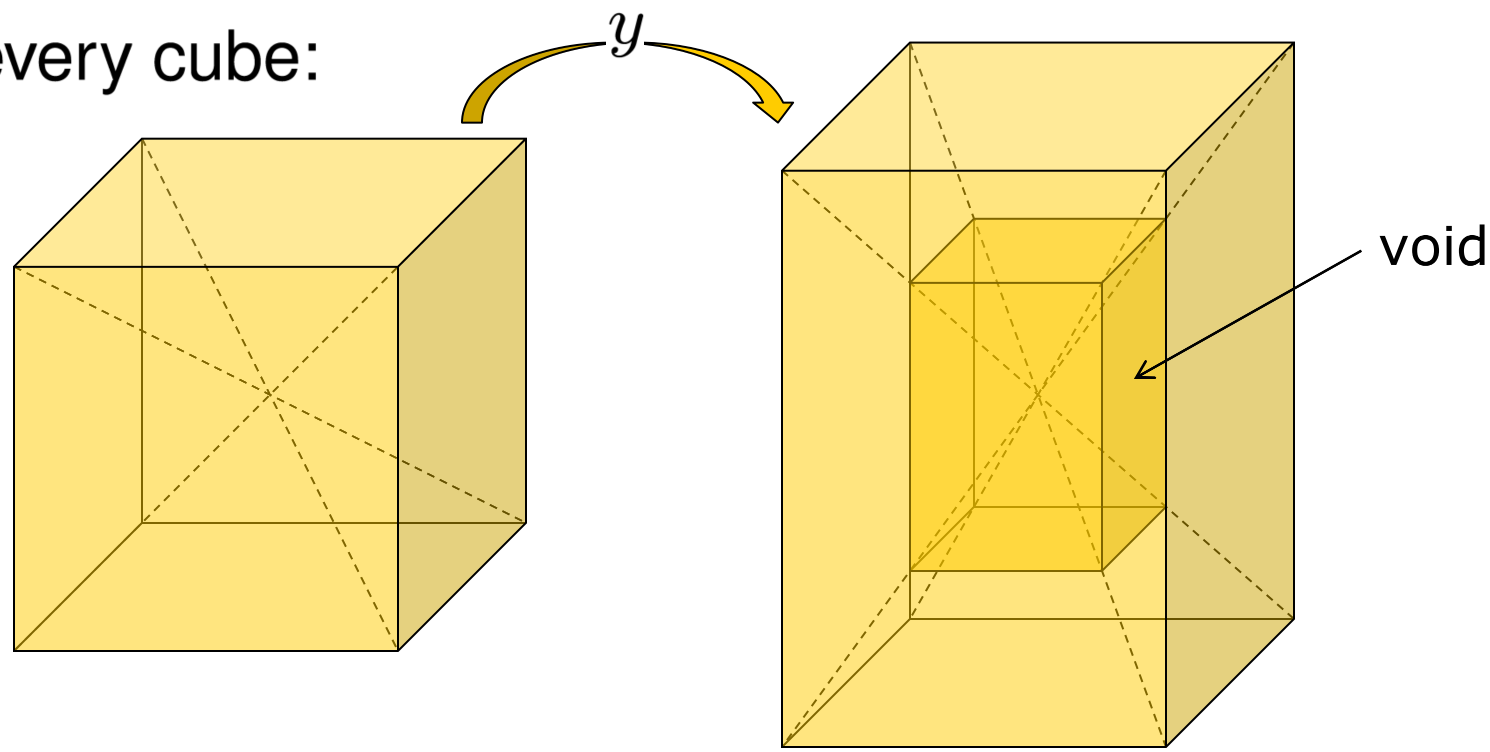
Sketch of proof – Upper bound

- In every cube:



- Calculate, estimate: $E \leq CL^2 \left(a^{1-p} \delta^p + \ell \delta / a \right)$
- Optimize a: $E \leq C_U L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$

Sketch of proof – Lower bound

- Lower bound: 1D arguments in x_3-direction
- For fixed (x_1, x_2): $f(x_3) \equiv |D_3 y(x_1, x_2, x_3)|$
- Then: $|D^2 y| \geq |D_3^2 y| \geq |D_3 |D_3 y|| = |Df|$

$$\bar{f} \equiv \frac{1}{2H} \int_{-H}^{H} f(x_3) dx_3 \geq \frac{1}{2H} \int_{-H}^{H} \frac{\partial u_3}{\partial x_3} dx_3 = 1 + \frac{\delta}{H}$$

- Define reduced energy density:

$$W(\lambda) = \min\{|F|^p - 3^{p/2},\ \det F = 1,\ |Fe_3| = \lambda\}$$

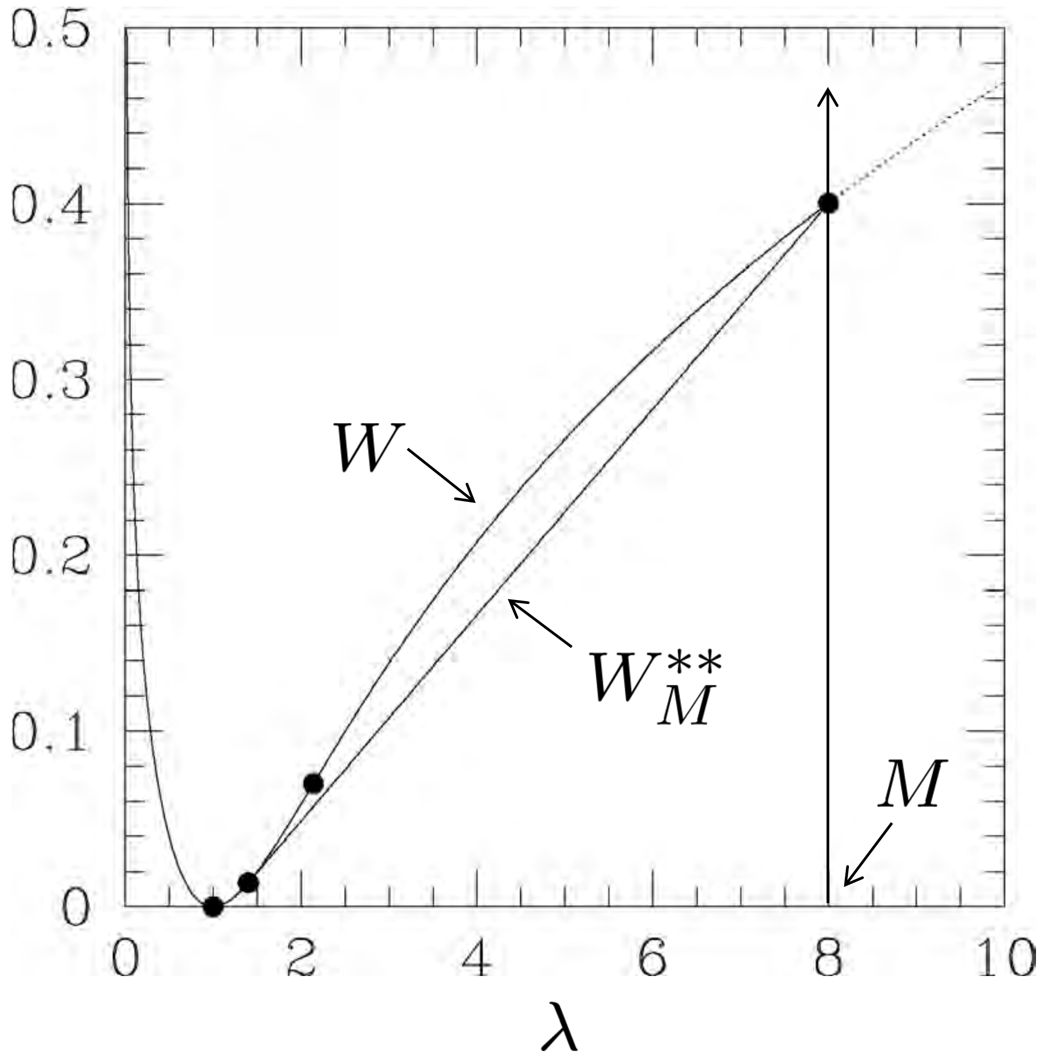
- Then: $\int_{-H}^{H} (|Dy|^p - 3^{p/2} + \ell |D^2 y|)\, dx_3 \geq$

$$\int_{-H}^{H} (W(f(x_3)) + \ell |Df(x_3)|)\, dx_3$$

Sketch of proof – Lower bound

- $W(\lambda)$: Minimized at $\lambda = 1$, p-growth
- Let: $M = \max f$, $N = \min f$
- Then: $\int_{-H}^{H} |Df| \, dx_3 \geq M - N$

Sketch of proof – Lower bound

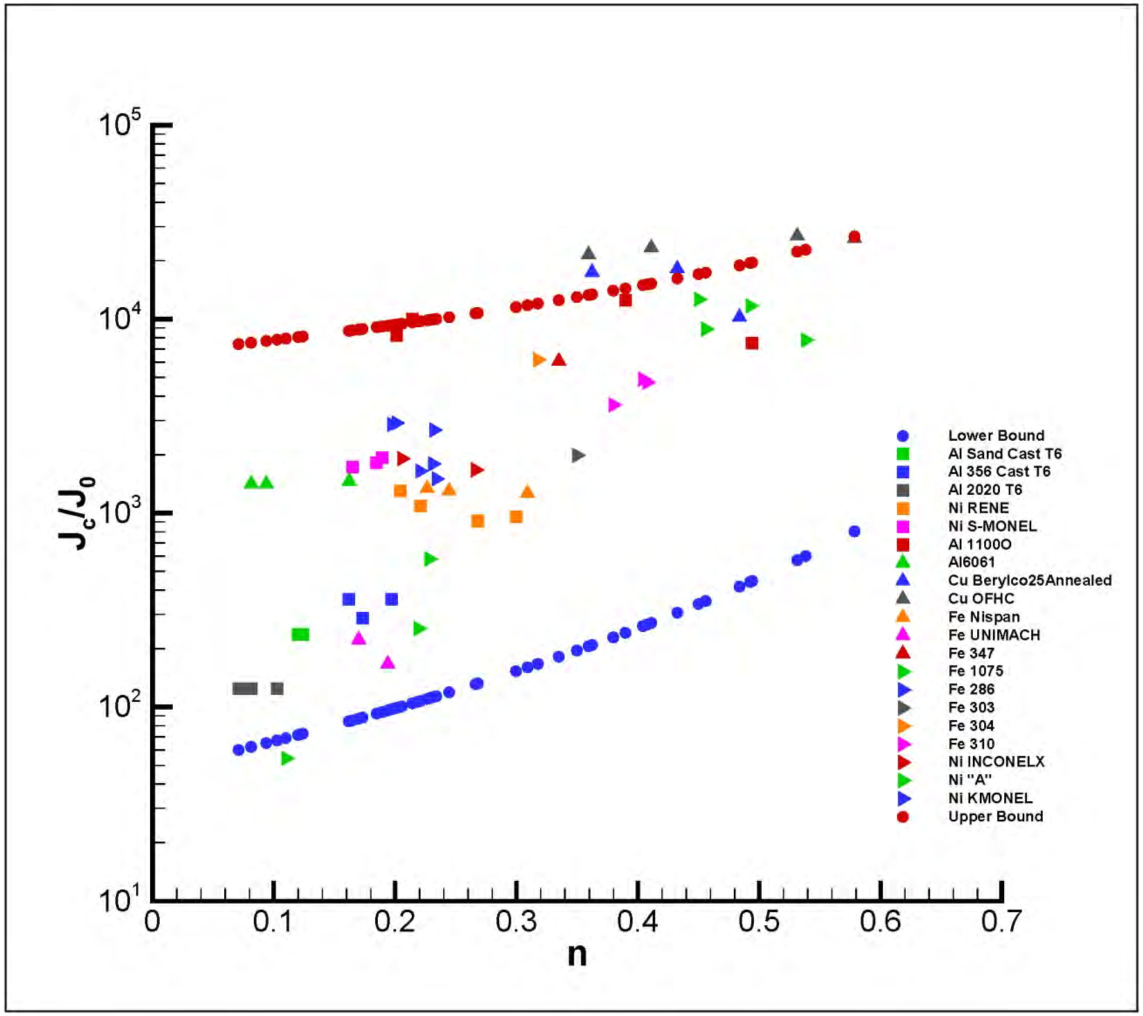


Sketch of proof – Lower bound

- $W(\lambda)$: Minimized at $\lambda = 1$, p-growth
- Let: $M = \max f$, $N = \min f$
- Then: $\int_{-H}^{H} |Df| \, dx_3 \geq M - N$
- By Jensen: $\frac{1}{2H} \int_{-H}^{H} W(f(x_3)) \, dx_3 \geq W_M^{**}(\bar{f})$
- Suffices to bound: $G(\bar{f}) = H W_M^{**}(\bar{f}) + \ell(M - N)$

  subject to: $N \leq \bar{f} \leq M$, $\bar{f} \geq 1 + \frac{\delta}{H} > 1$
- From estimates for W_M^{**}: $G(\bar{f}) \geq C_L \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$
- Integrating: $E \geq C_L L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$ q. e. d.

Comparison with experiment



L. Fokoua, S. Conti & MO,
J. Mech. Phys. Solids, **62** (2014) 295–311

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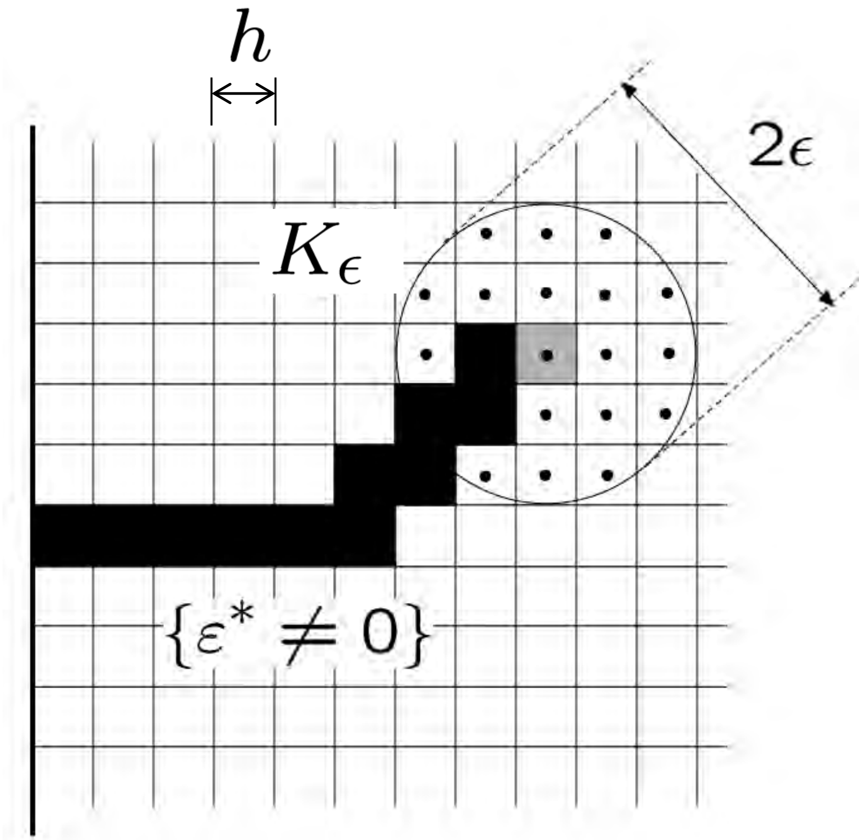
Numerical implementation

- Optimal scaling laws hint at the existence of a well-defined specific fracture energy J_c (in uniaxial tension)
- Ideally, we would like to have (but we don't) a full Γ-limit of the sequence of scaled functionals

$$F_\ell(y) = \ell^{-\frac{1-p}{2-p}} \int_\Omega W\Big(Dy(x), \ell D^2 y(x)\Big)\, dx$$

- Conjecture: The Γ-limit is Griffith-like with specific fracture J_c
- In numerical calculations: *Material-point erosion algorithm*

Material-point erosion



schematic of
ε-neighborhood
construction

- ε-neighborhood construction: Choose h << ε << L
- Erode material point if

$$\frac{h^2}{|K_\epsilon|}\int_{K_\epsilon} W(\nabla u)\,dx \geq J_c$$

- Proof of Γ-convergence to Griffith fracture:
  - *Schmidt, B., Fraternali, F. & MO, SIAM J. Multiscale Model. Simul.*, **7**(3):1237-1366, 2009.

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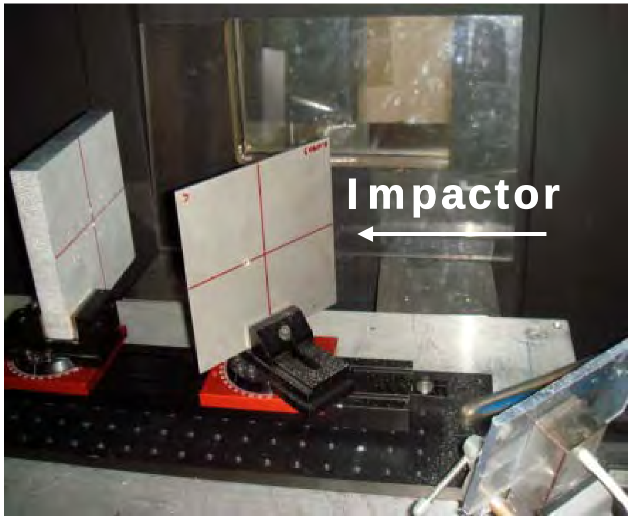
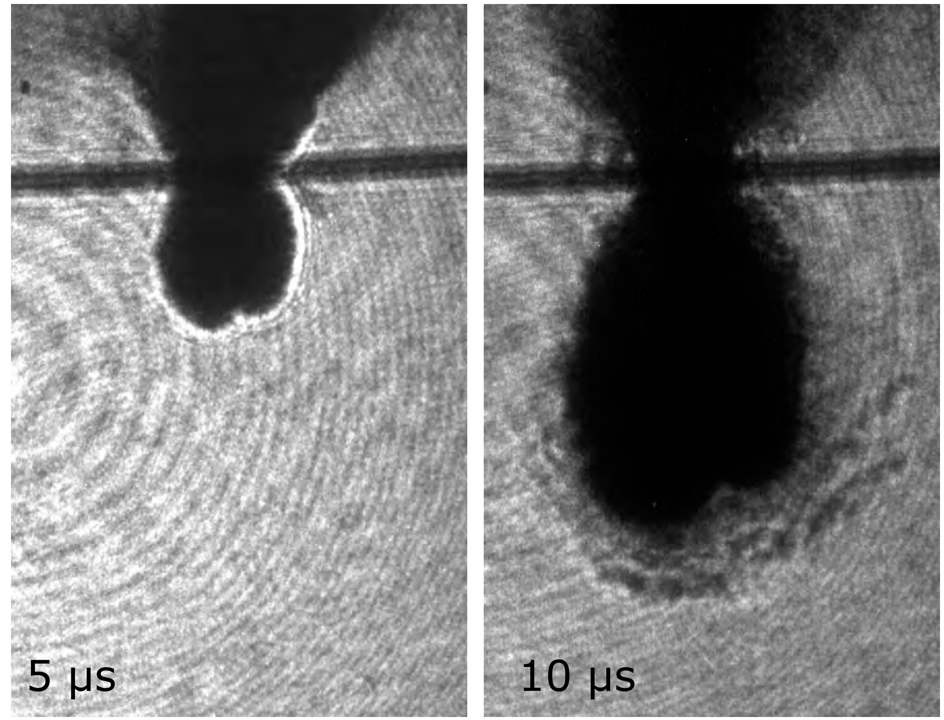
Application to hypervelocity impact

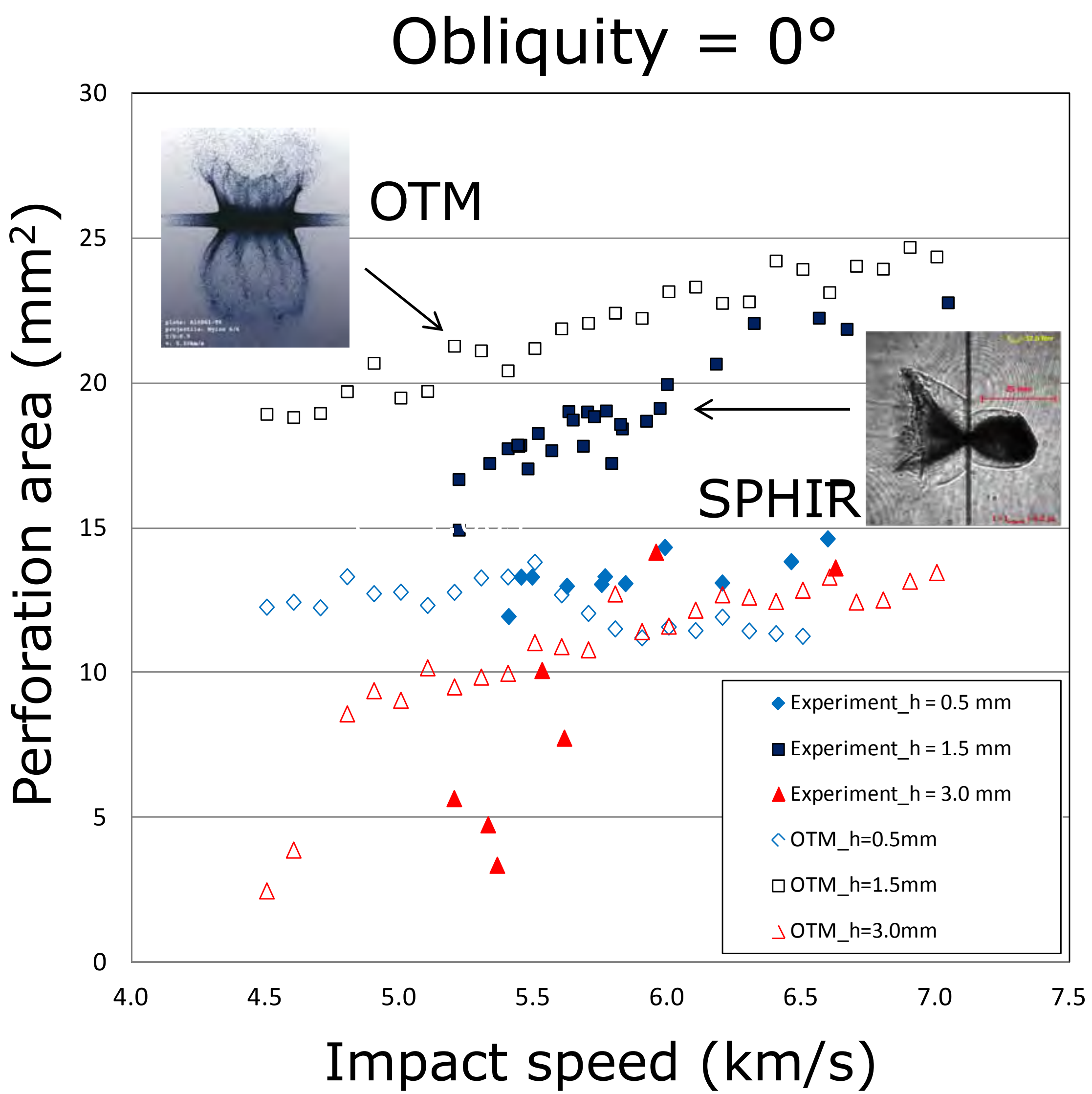


Caltech's hypervelocity
Impact facility



Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

Application to hypervelocity impact



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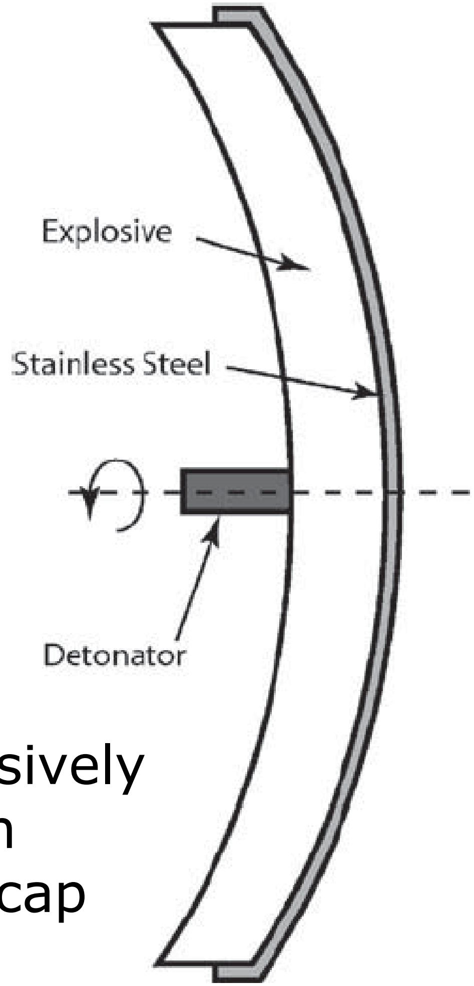
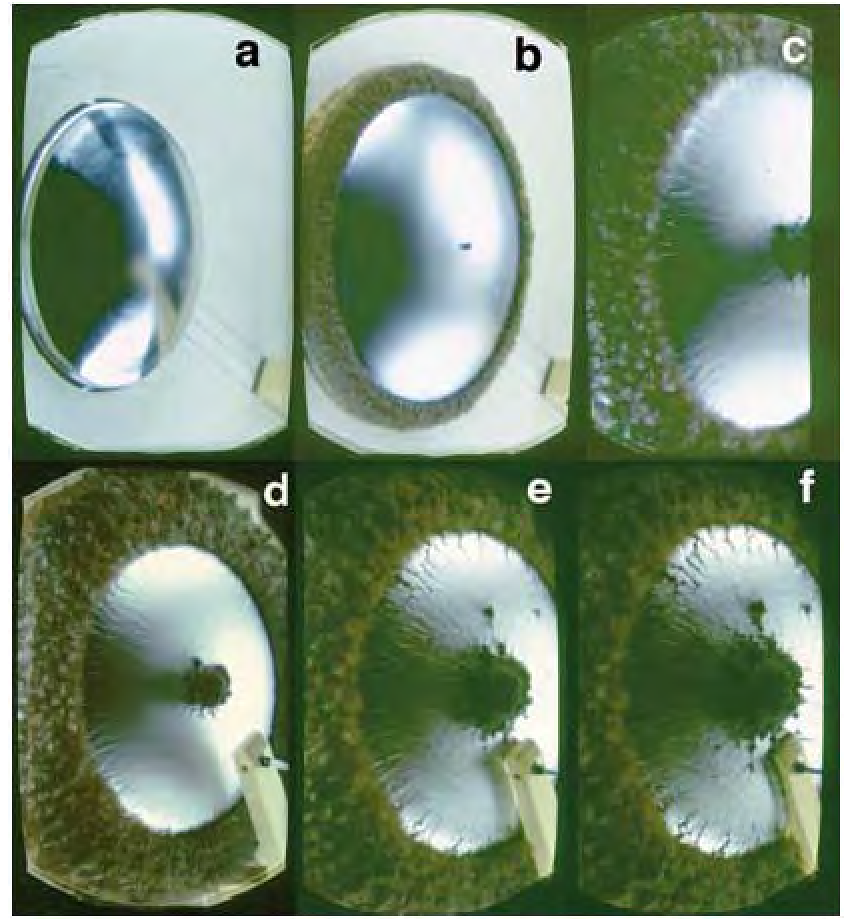
Application to explosively driven cap



Explosively driven steel cap

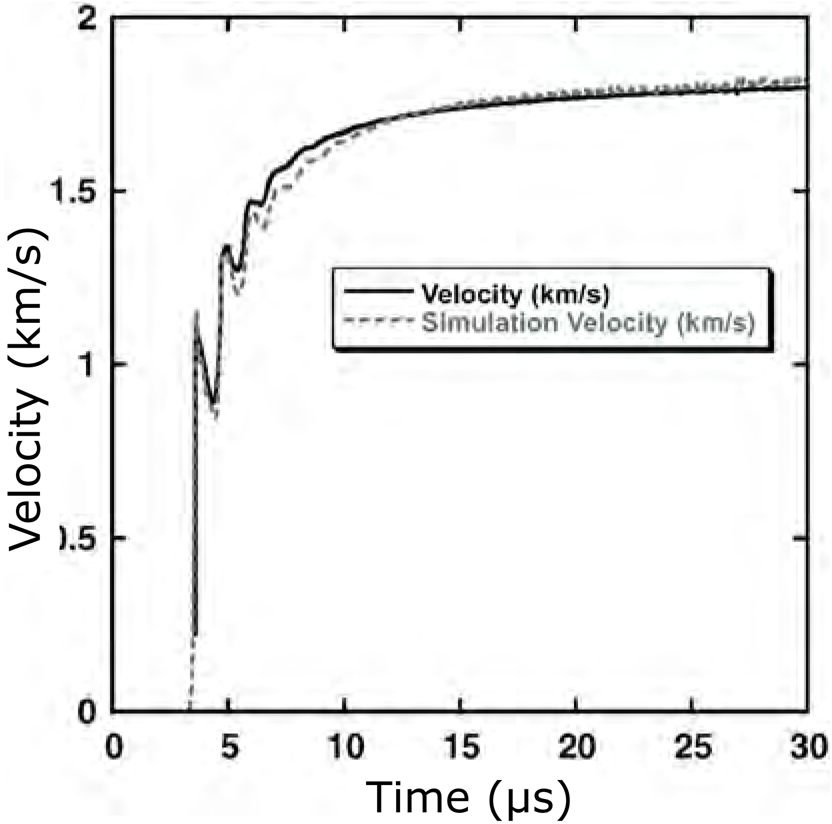


Optical framing camera records

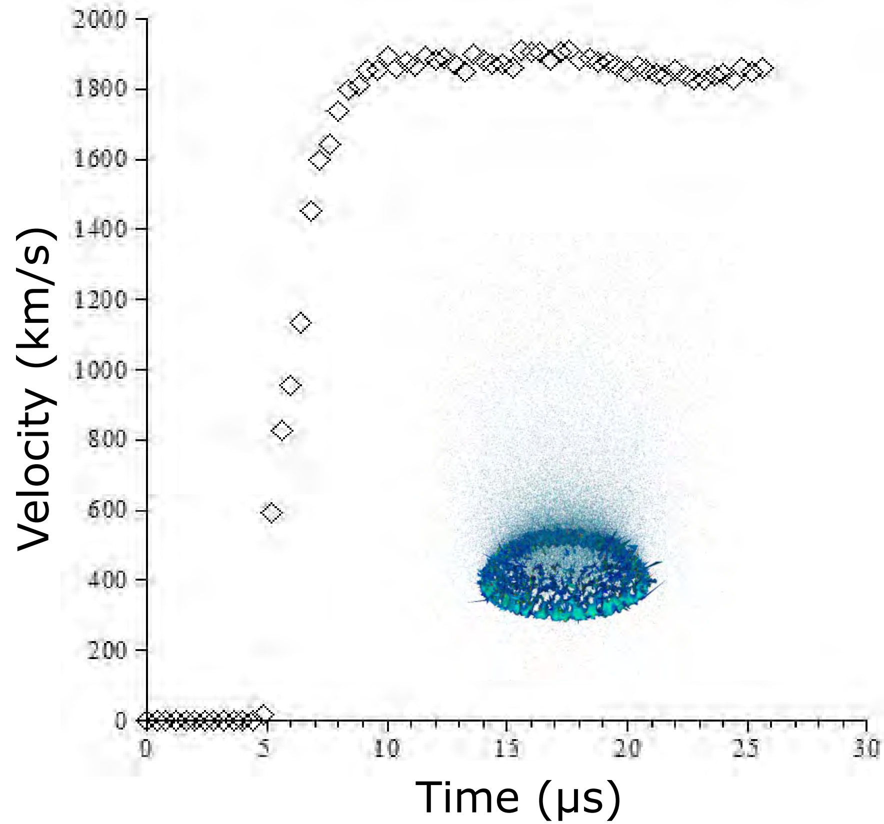
G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

Application to explosively driven cap

Experiment



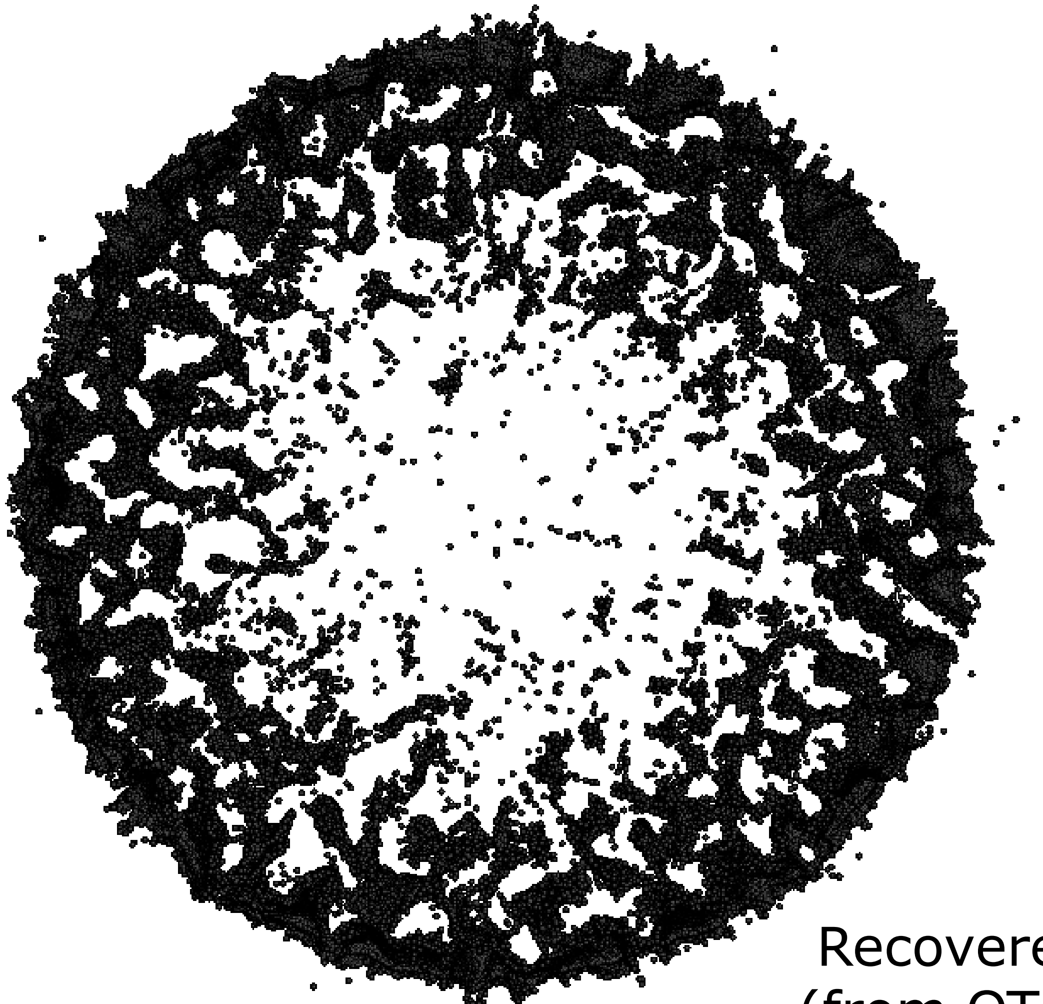
OTM simulation



Surface velocity for spot midway between pole and edge

G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

Application to explosively driven cap



Recovered fragments
(from OTM simulation)

G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

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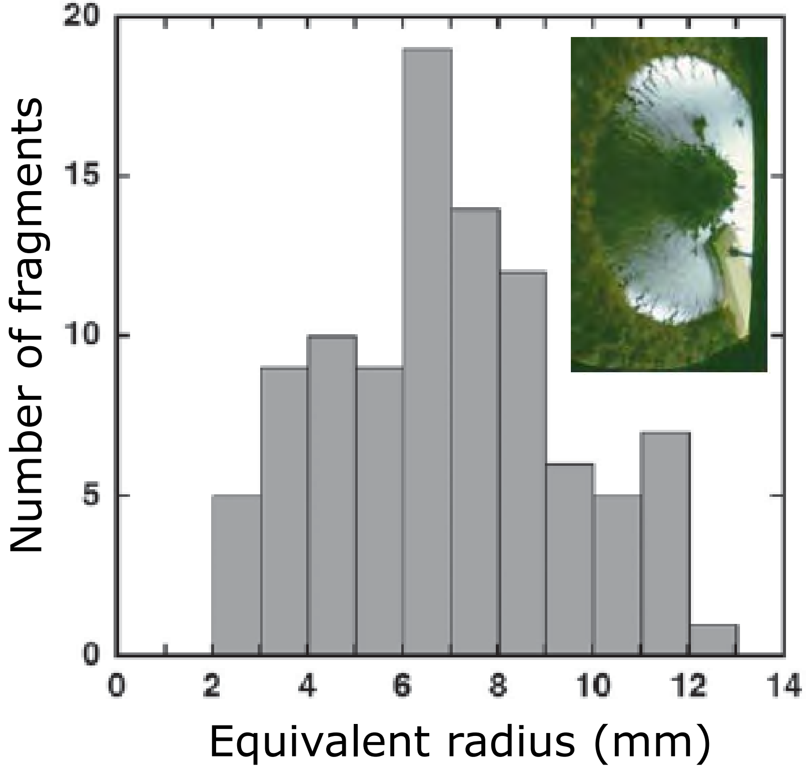
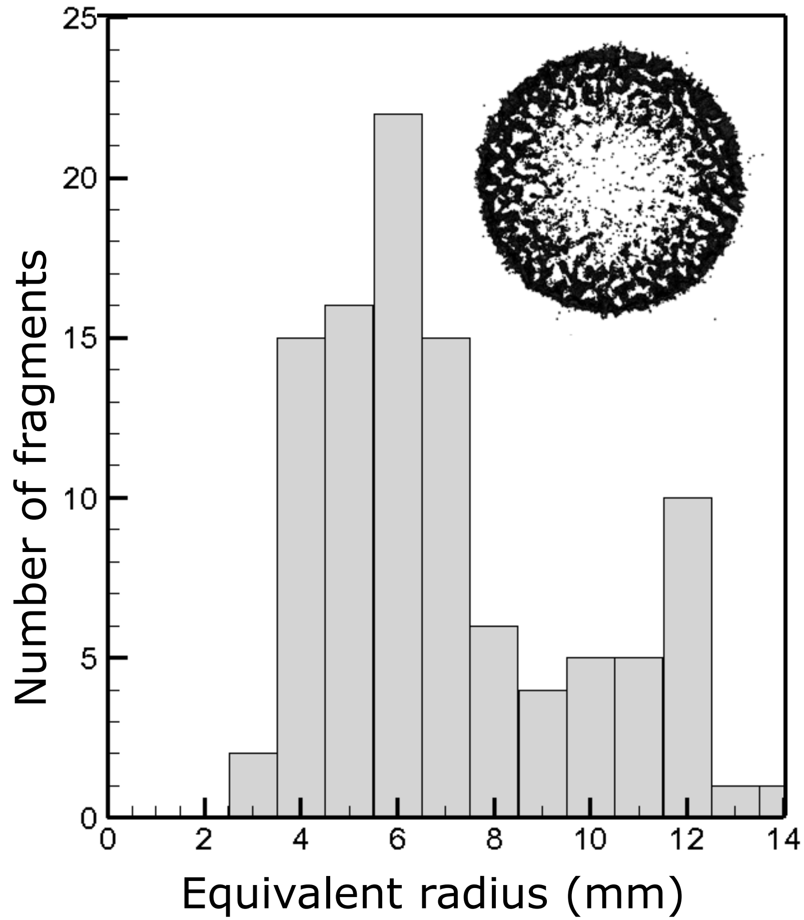
Application to explosively driven cap

Experiment



OTM simulation



Histograms of equivalent fragment radii

G.H. Campbell, G. C. Archbold, O. A. Hurricane and P. L. Miller, *JAP*, **101**:033540, 2007

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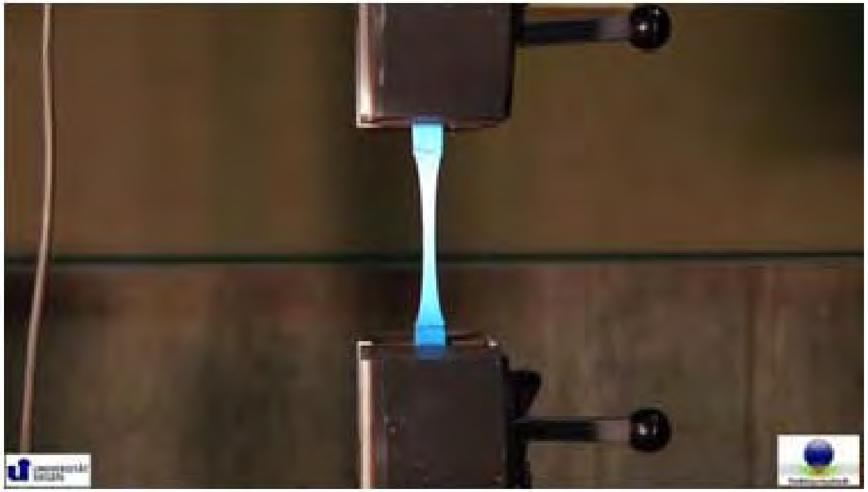
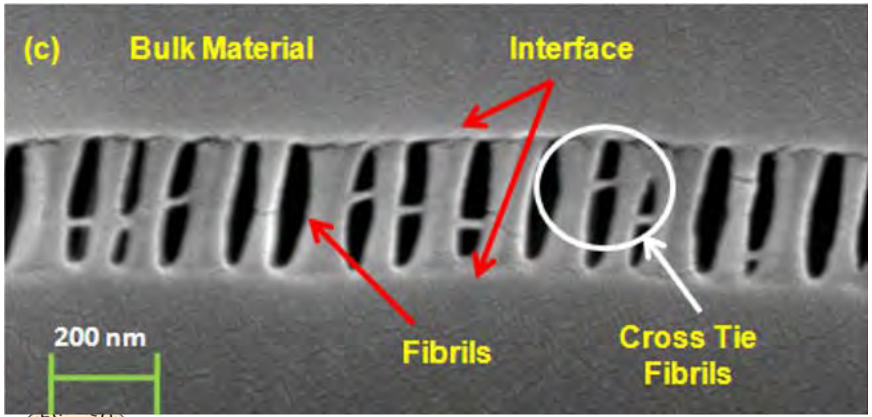
Fracture of polymers



T. Reppel, T. Dally, T. and K. Weinberg, Technische Mechanik, 33 (2012) 19-33.



Crazing in 800 nm polystyrene thin film (C. K. Desai *et al.*, 2011)

- Polymers undergo entropic elasticity and damage due to chain stretching and failure
- Polymers fracture by means of the crazing mechanism consisting of fibril nucleation, stretching and failure
- The free energy density of polymers saturates in tension once the majority of chains are failed: p=0!
- Crazing mechanism is incompatible with strain-gradient elasticity…

Fracture of polymers

- Suppose: For $K_U > 0$, *intrinsic length* $\ell > 0$,

$$E(y) \leq K_U \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell \int_\Omega |D^2 y|\, dx \right)$$

- If $E(y) < +\infty$: $y \in W^{2,1}(\Omega) \Rightarrow y$ continuous
- Crazing is precluded by the continuity of y!
- Instead suppose: For $\sigma \in (0,1)$,

$$E(y) \leq K_U \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell^\sigma |y|_{W^{1+\sigma,1}(\Omega)} \right)$$

Theorem [Conti, Heyden & MO]. For ℓ sufficiently small,

$$p = 0,\ \ \sigma \in (0,1),\ \ 0 < C_L < C_U,$$

$$C_L L^2 \ell^{\frac{\sigma}{1+\sigma}} \delta^{\frac{1}{1+\sigma}} \leq \inf E \leq C_U L^2 \ell^{\frac{\sigma}{1+\sigma}} \delta^{\frac{1}{1+\sigma}}$$

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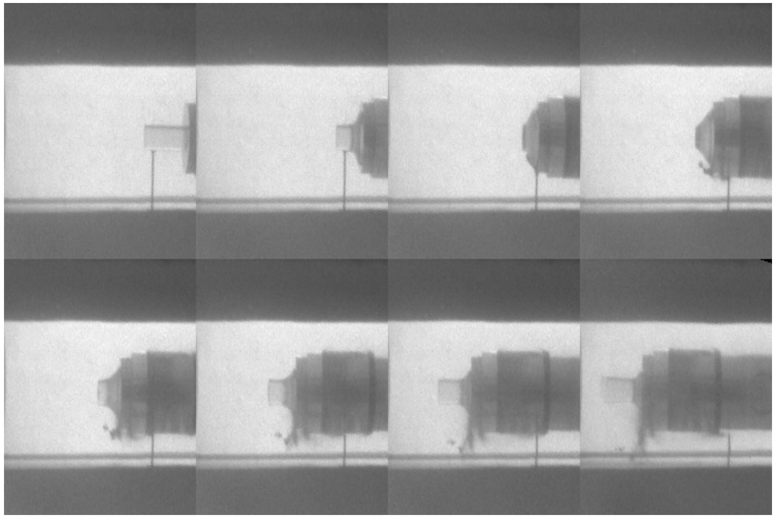
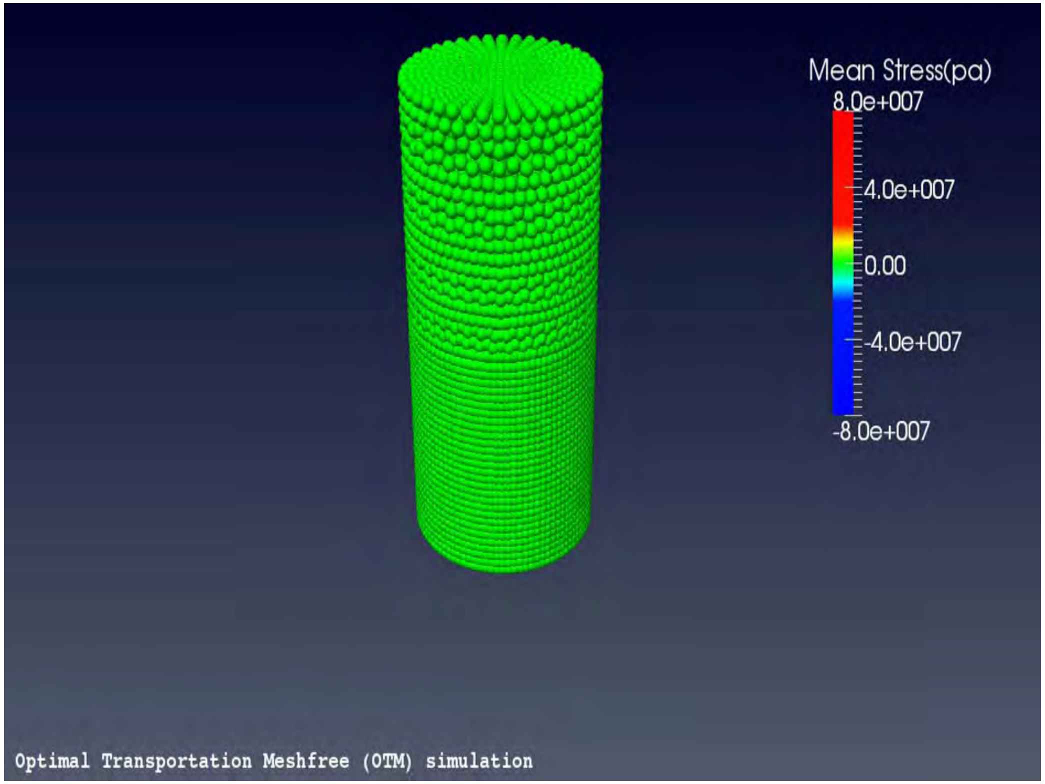
Taylor-anvil tests on polyurea

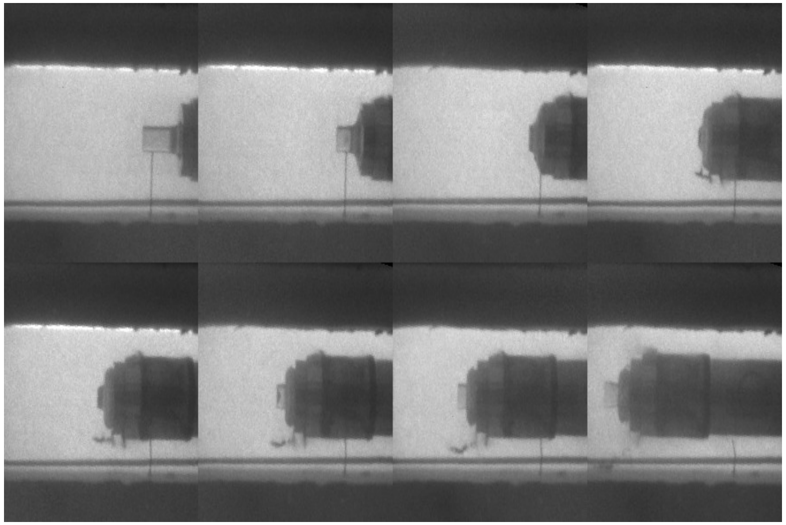


Shot #854:
R0 = 6.3075 mm,
L0 = 27.6897 mm,
v = 332 m/s

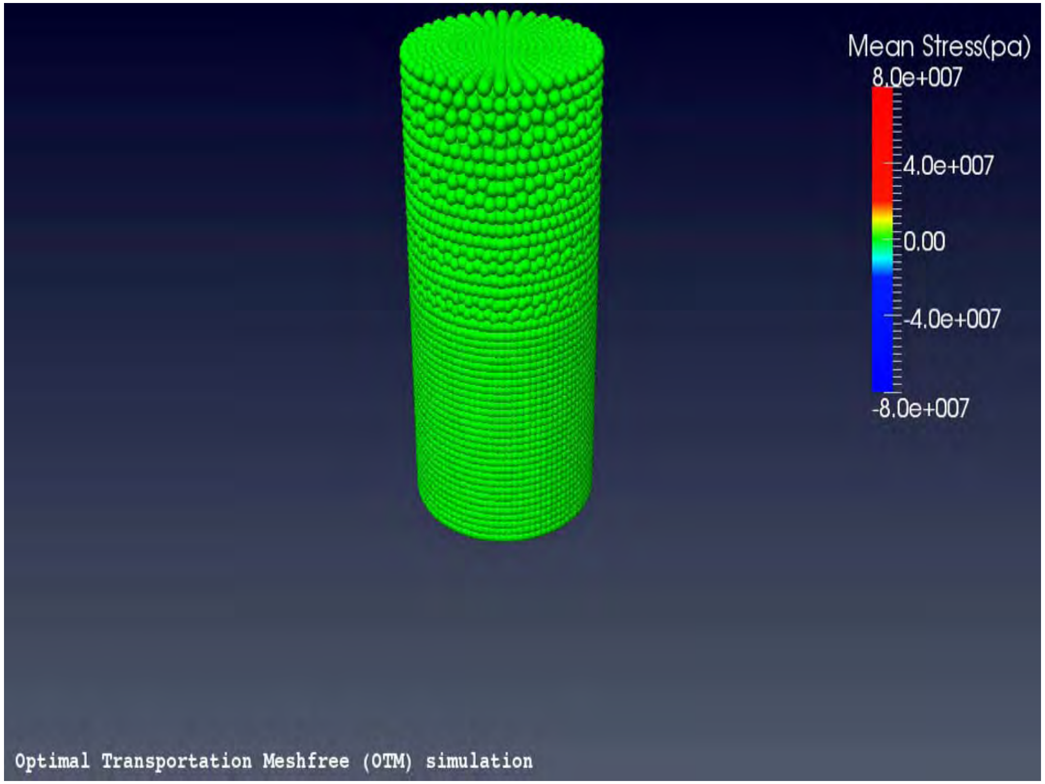


Experiments conducted by W. Mock, Jr. and J. Drotar,
at the Naval Surface Warfare Center (Dahlgren Division)
Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA

Experiments and simulations



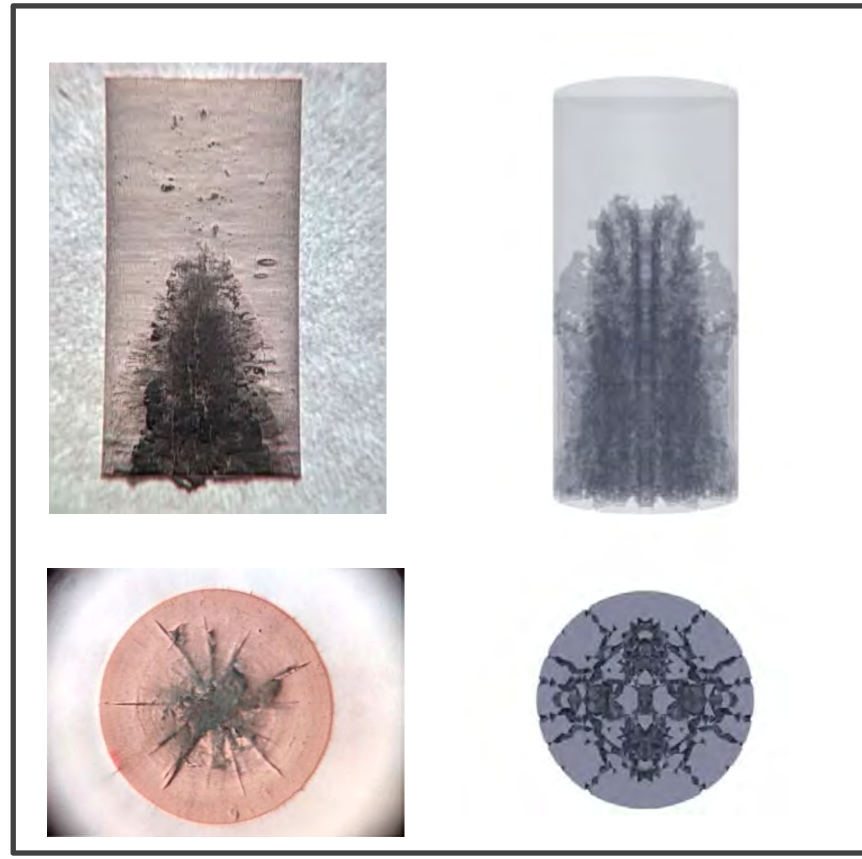
Shot #861:
R0 = 6.3039 mm,
L0 = 27.1698 mm,
v = 424 m/s



Experiments conducted by W. Mock, Jr. and J. Drotar,
at the Naval Surface Warfare Center (Dahlgren Division)
Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA

Taylor-anvil tests on polyurea

Shot #854



Shot #861

Comparison of damage and fracture patterns
in recovered specimens and simulations

Michael Ortiz
OW12/13

Concluding remarks

- Ductile fracture can indeed be understood as the result of the competition between sublinear growth and (possibly fractional) strain-gradient effects
- Optimal scaling laws are indicative of a well-defined specific fracture energy, cohesive behavior, and provide a (multiscale) link between macroscopic fracture properties and micromechanics (intrinsic micromechanical length scale, void-sheet and crazing mechanisms…)
- Ductile fracture can be efficiently implemented through material-point erosion schemes
- Highly to be desired: Full Γ-limit as $\ell \to 0$…