Optimal scaling laws in ductile fracture

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Joint work with: S. Conti, S. Heyden and A. Pandolfi

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Variational Models of Fracture
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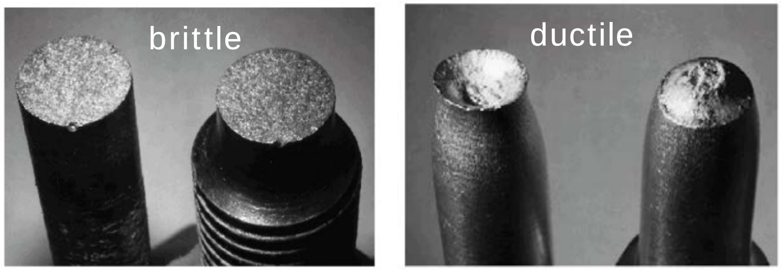
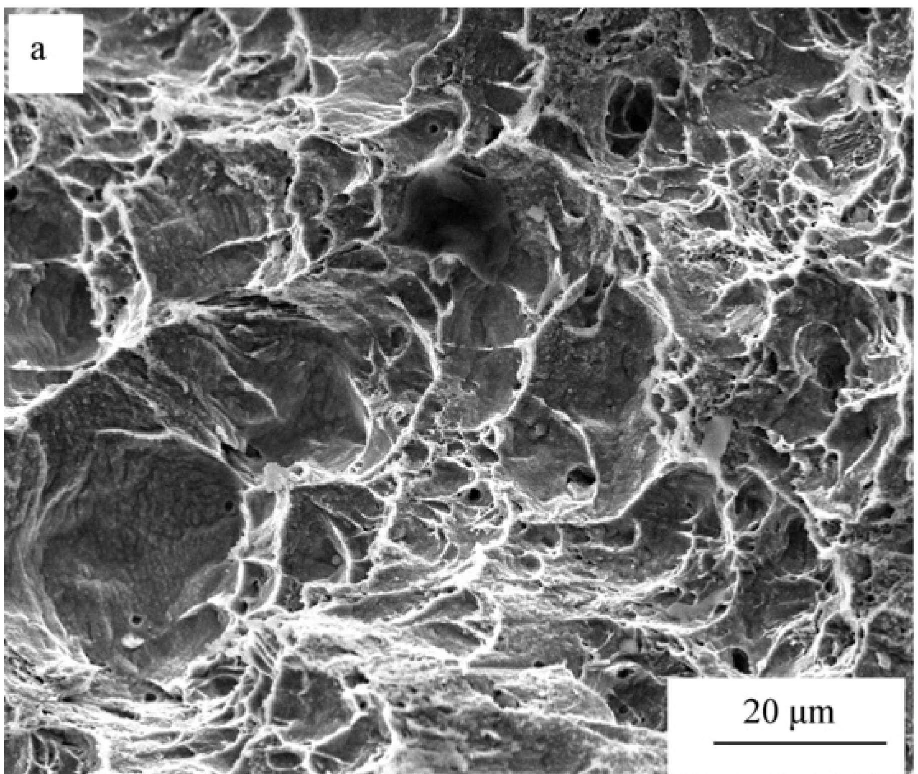
Contents

- Two mathematical results:
  - *Optimal scaling for ductile fracture of metals*
  - *Optimal scaling for ductile fracture of polymers*
- Attempts at connections with microscale:
  - *Verification of optimal scaling in atomic Ni*
  - *Nanovoid plastic cavitation*
- Attempts at connections with macroscale:
  - *Spall tests in metals*
  - *Taylor anvil impact tests for polyurea*

Background on ductile fracture



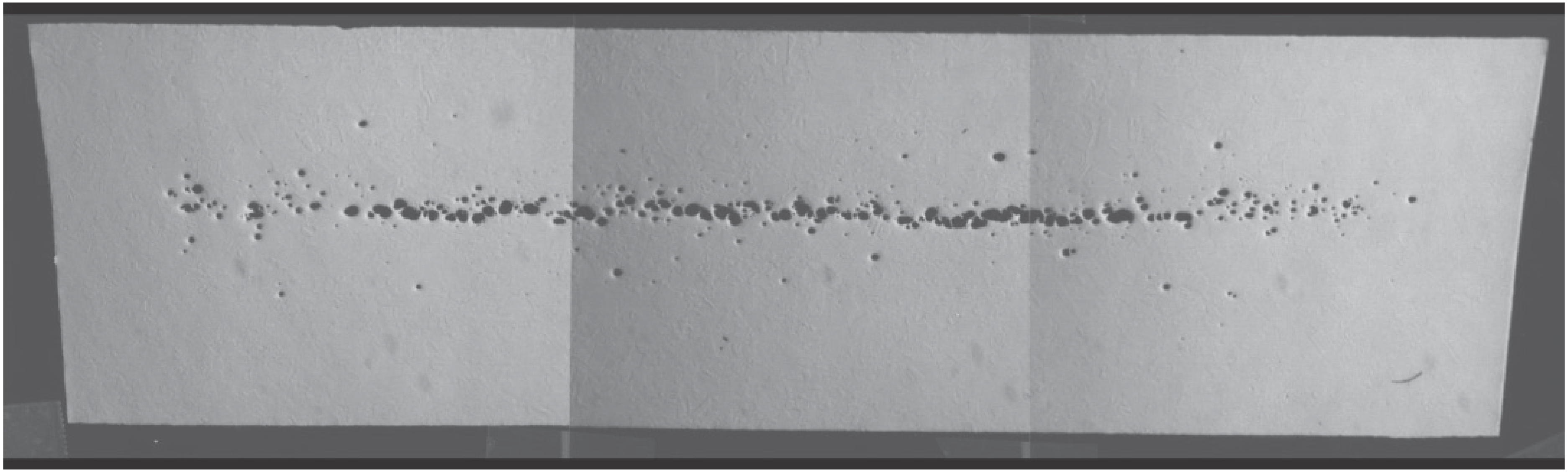
(Courtesy NSW HSC online)



- 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



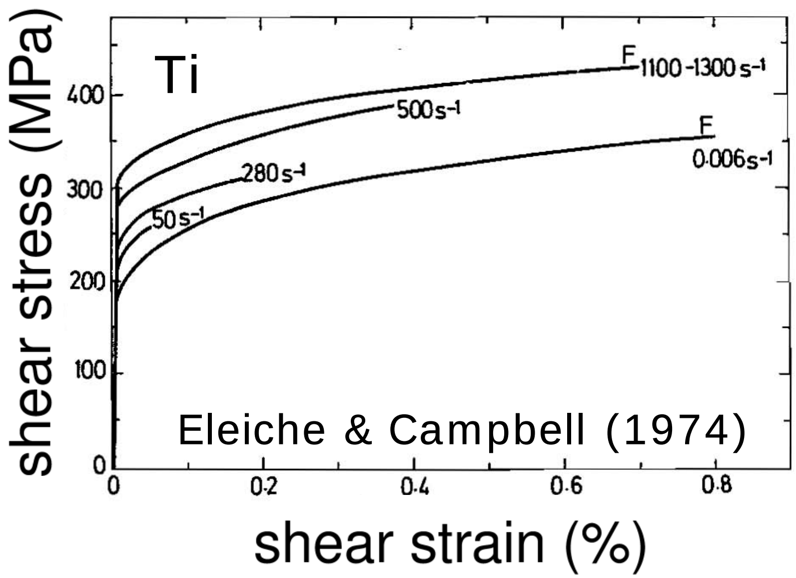
Photomicrograph of a copper disk tested in a gas-gun experiment showing the formation of voids and their coalescence into a fracture plane

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

Background on ductile fracture

- Ductile fracture is a multiscale phenomenon:
  - *Void nucleation occurs at the microscale*
  - *Void growth and coalescence occurs at the mesoscale*
  - *Fracture occurs at the macroscale*
- Challenges:
  - *Bridging of scales (micro-to-macro)*
  - *Upscaling of material properties from lower scales*
  - *Determination of macroscopic effective behavior*
- Approach:
  - *Mathematize the problem! (entry level requirement)*
  - *Micro-to-macro optimal scaling relations*
  - *Calibration of relevant properties from microscale*
  - *Application of effective laws at macroscale*

Naïve model: Local plasticity

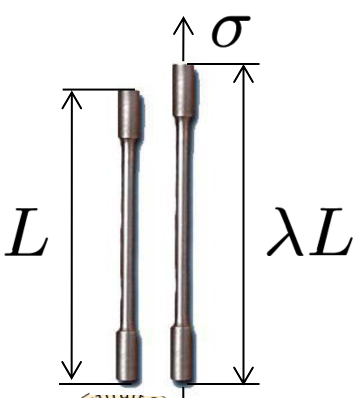


- Deformation theory: Minimize

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

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

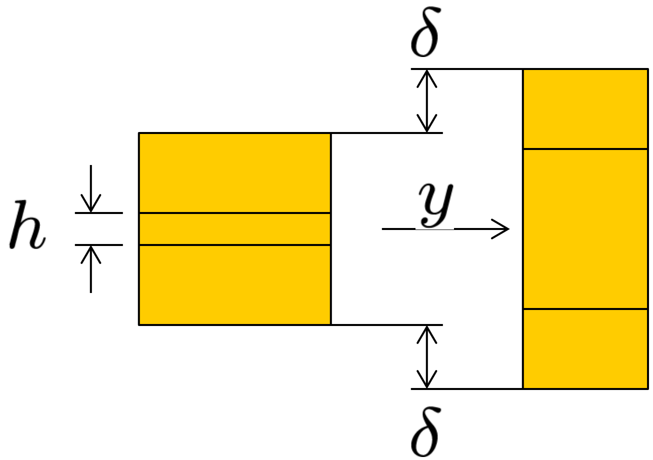
$$\sigma \sim K\epsilon^n = K(\lambda - 1)^n$$



- 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!

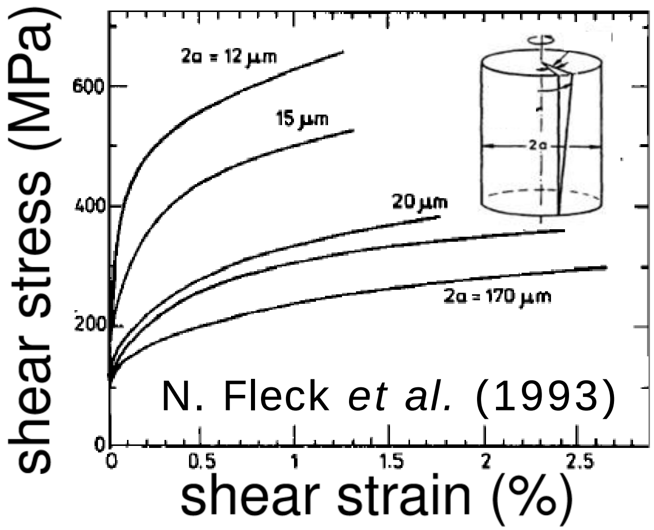
Naïve model: Local plasticity

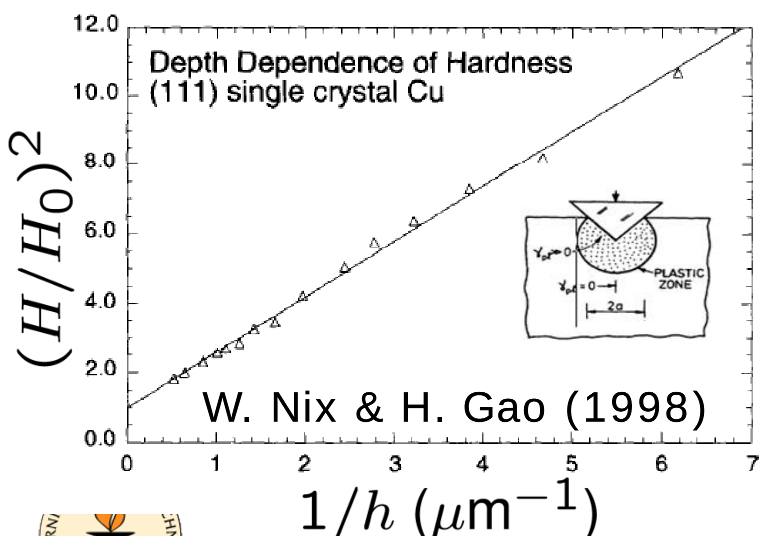


- Example: Uniaxial extension
- Energy: $E_h \sim h \left(\frac{2\delta}{h} \right)^p$
- For $p < 1$: $\lim_{h \to 0} E_h = 0$

- 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





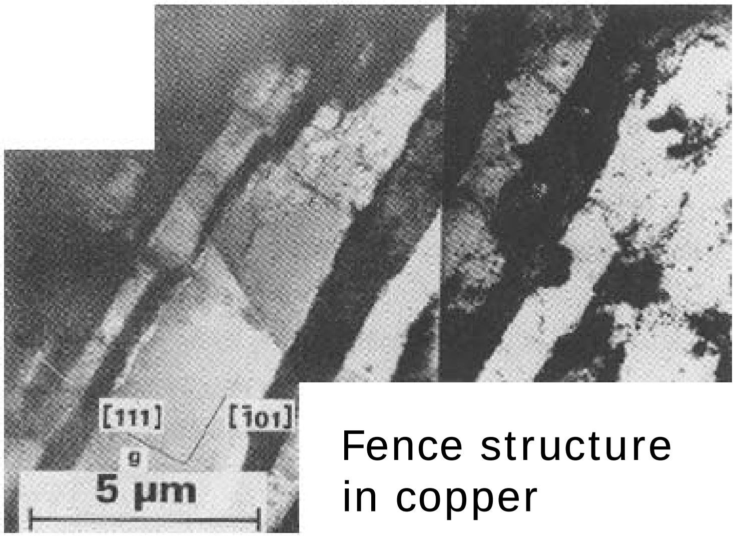
- The yield stress of metals is observed to increase in the presence of strain gradients
- Deformation theory of strain-gradient plasticity:

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

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

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

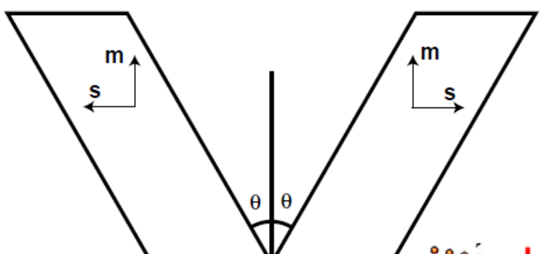
- Across jump planes:

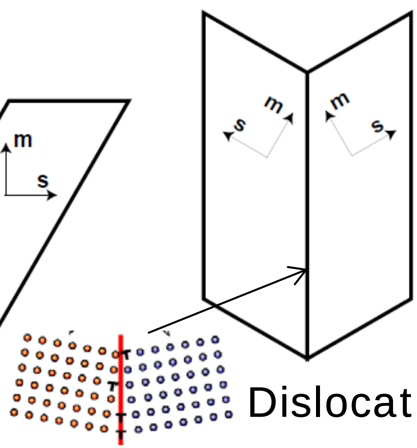
$$|[\![F]\!]| = 2\sin\theta$$

- 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

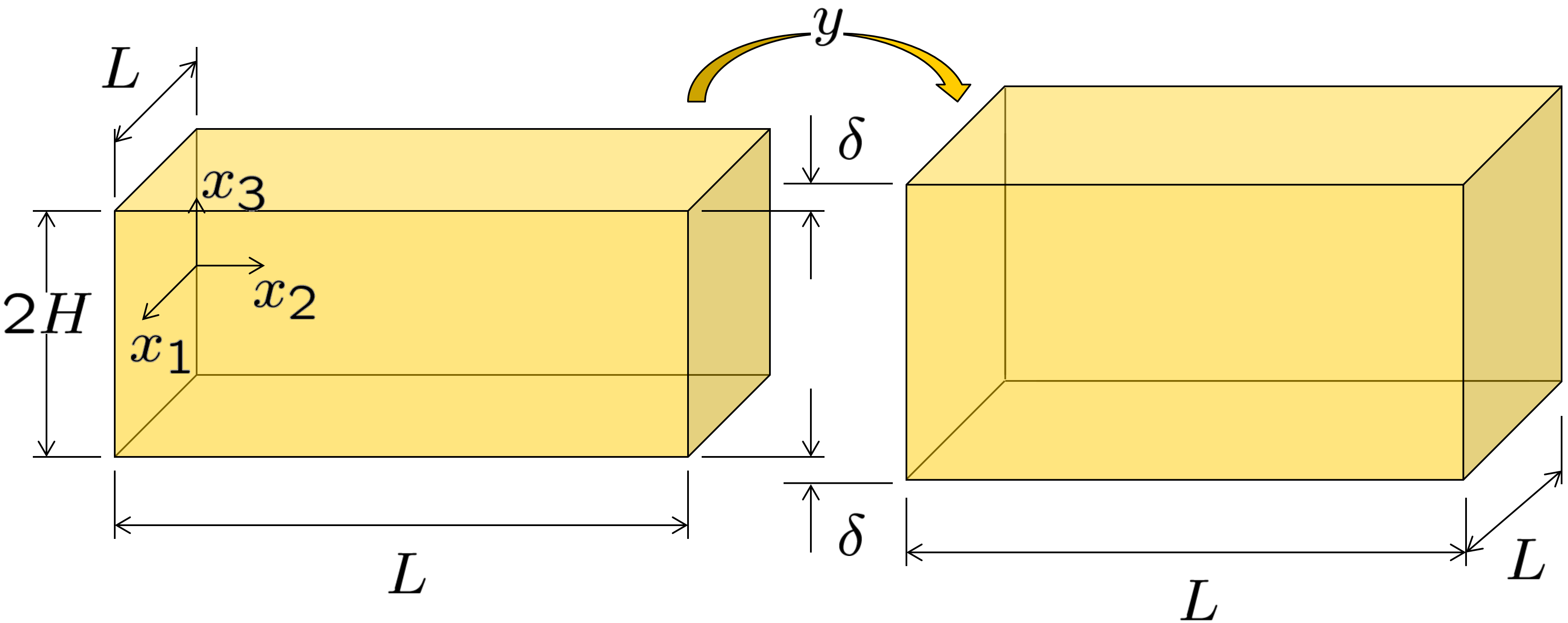
- Mathematical model: Minimize

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

$y : \Omega \to \mathbb{R}^n$, 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?*

Optimal scaling – Uniaxial extension



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

L. Fokoua, S. Conti & M. Ortiz, *ARMA*, **212**: 331-357, 2014.

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* $\ell > 0$,

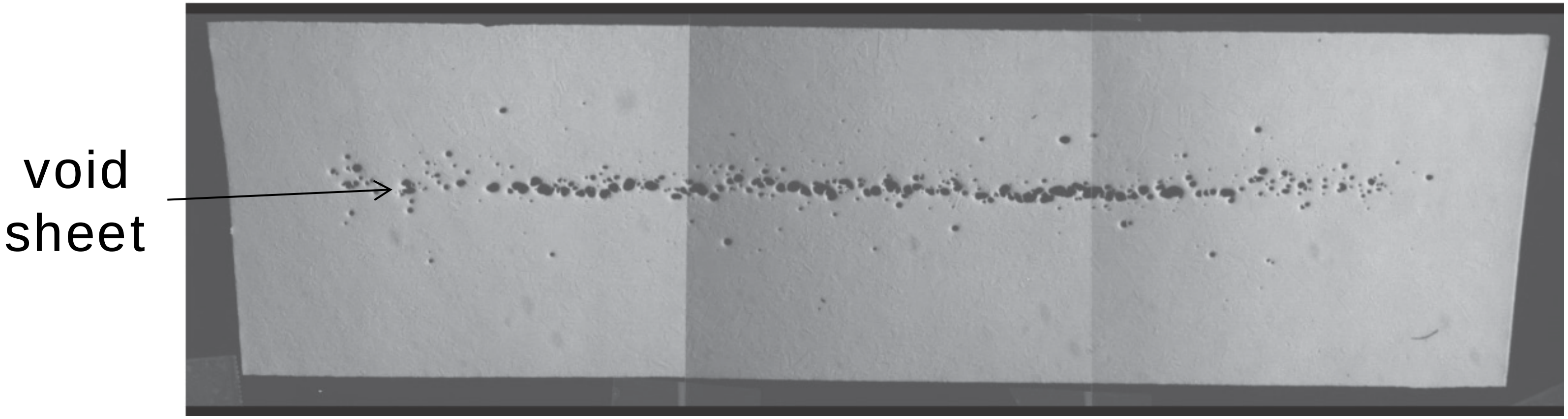
$$E(y) \geq K_L \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell \int_\Omega |D^2 y|\, dx \right)$$
$$E(y) \leq K_U \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell \int_\Omega |D^2 y|\, dx \right)$$

Theorem [Fokoua, Conti & MO, ARMA, 2014]. For ℓ sufficiently small, $p \in (0, 1)$, $0 < C_L(p) < C_U(p)$,

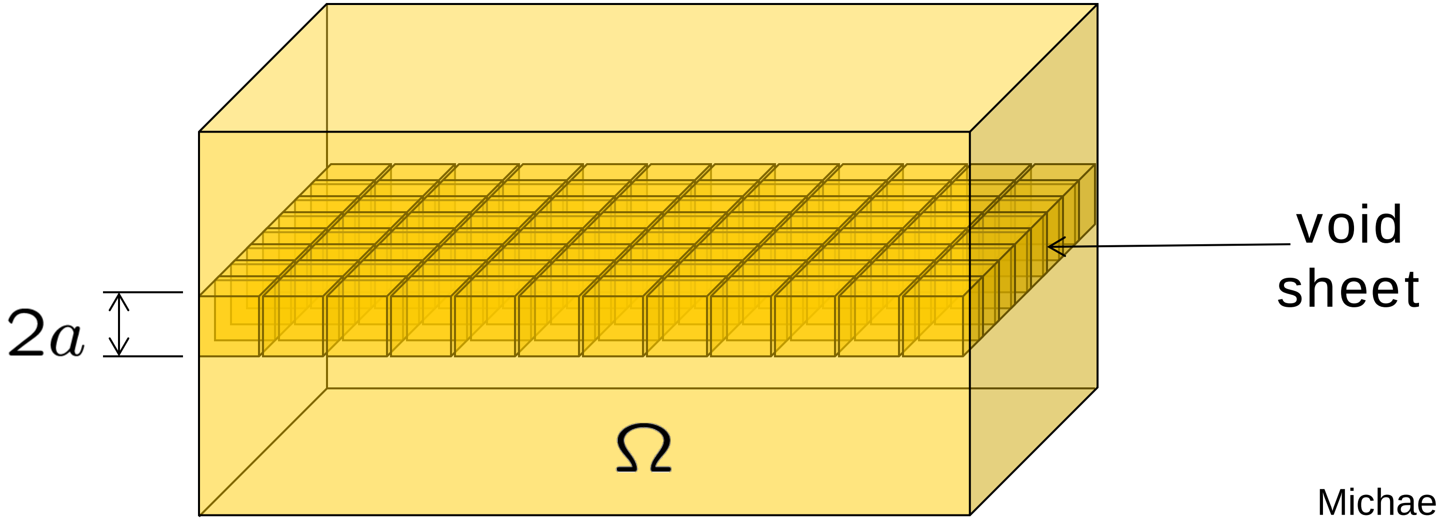
$$C_L(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}} \leq \inf E \leq C_U(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$$

L. Fokoua, S. Conti & M. Ortiz, *ARMA*, **212**: 331-357, 2014.

Sketch of proof – Upper bound

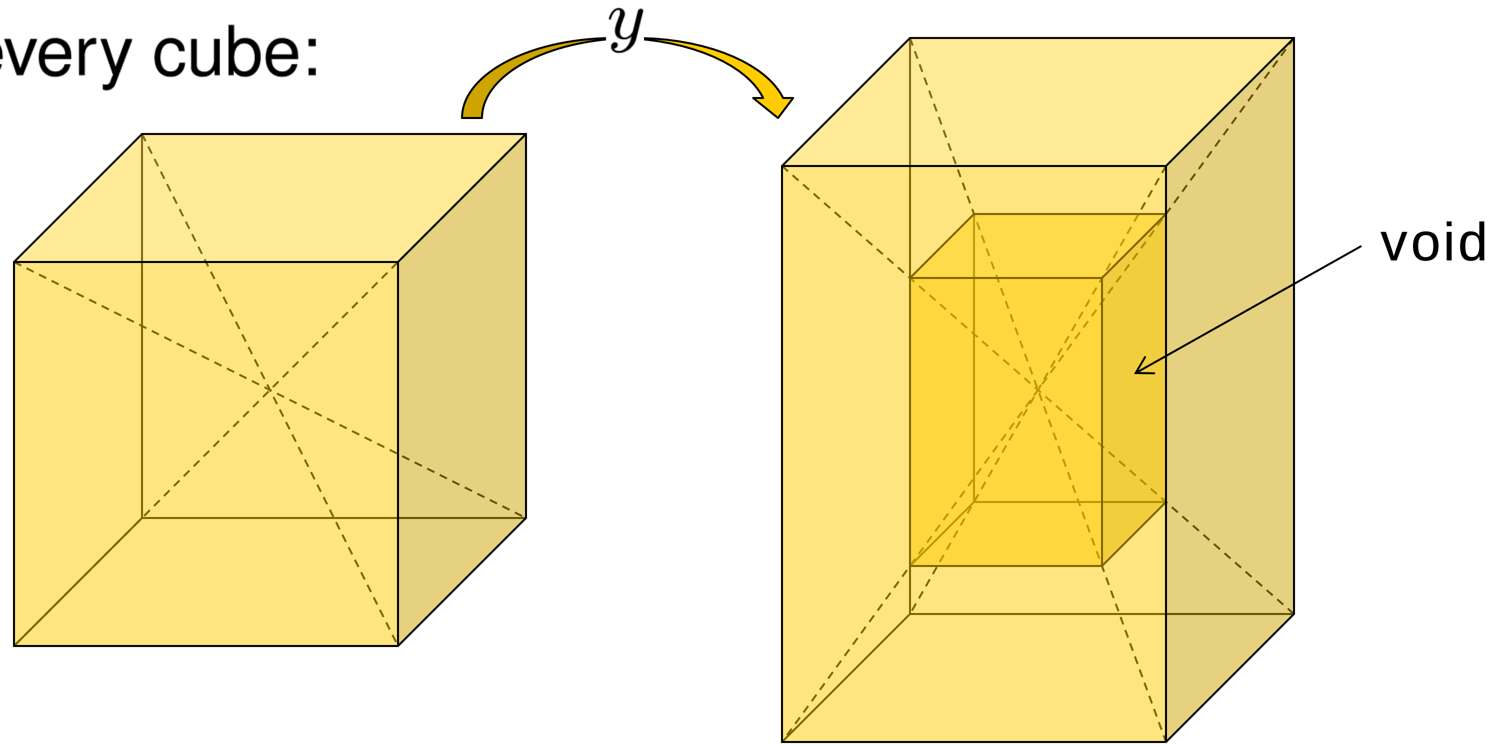


Heller, A., Science & Technology Review Magazine, LLNL, pp. 13-20, July/August, 2002



Sketch of proof – Upper bound

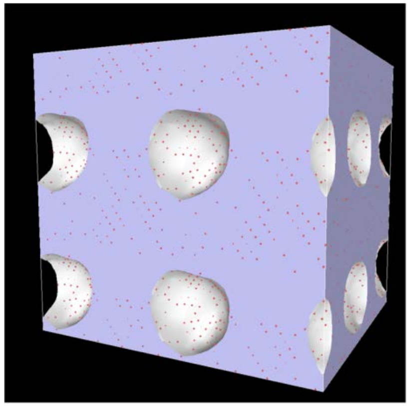
- In every cube:



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

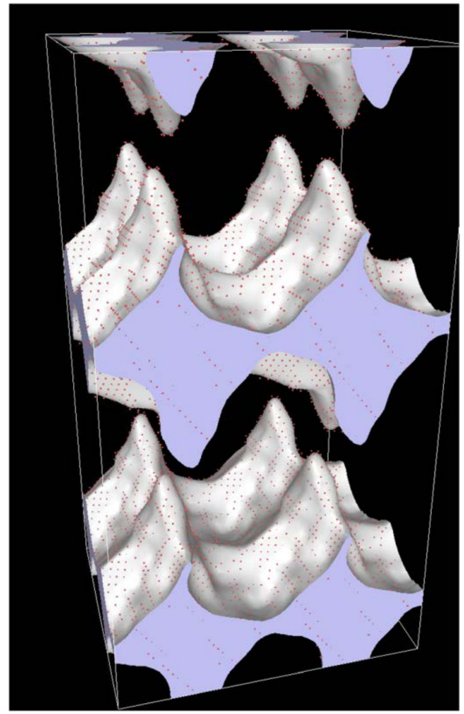
- Optimize: $a = \left(\frac{\ell\delta^{1-p}}{1-p} \right)^{1/(2-p)} \Rightarrow E \leq C_U L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$

Optimal scaling – Atomic Ni

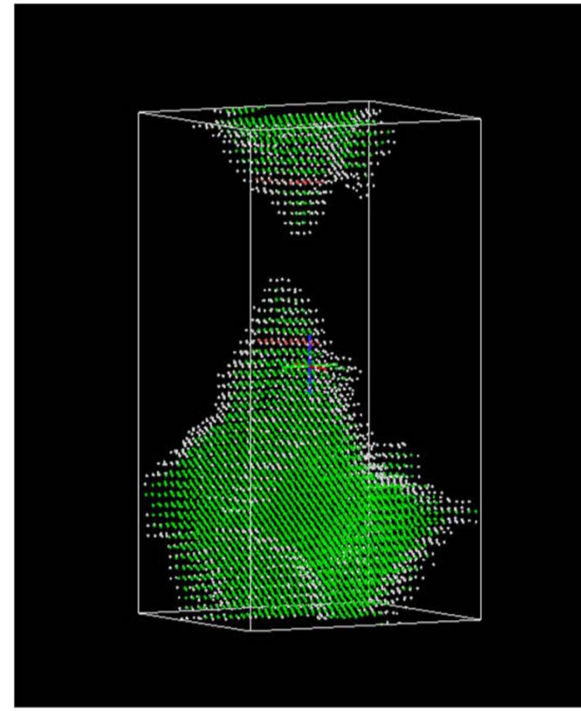


(a)

EAM Nickel,
[111] loading,
NPT 300K[1]



(b)

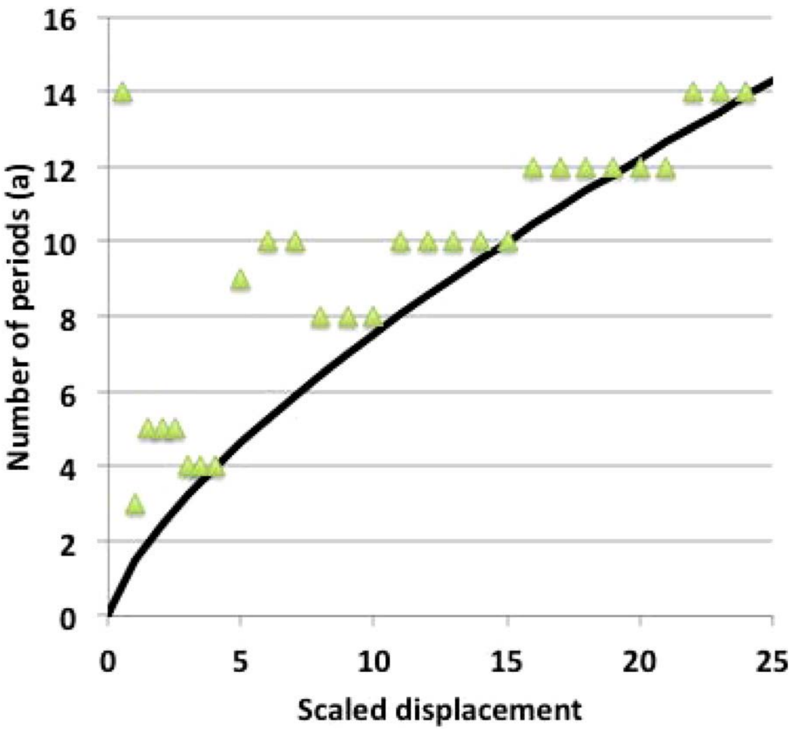


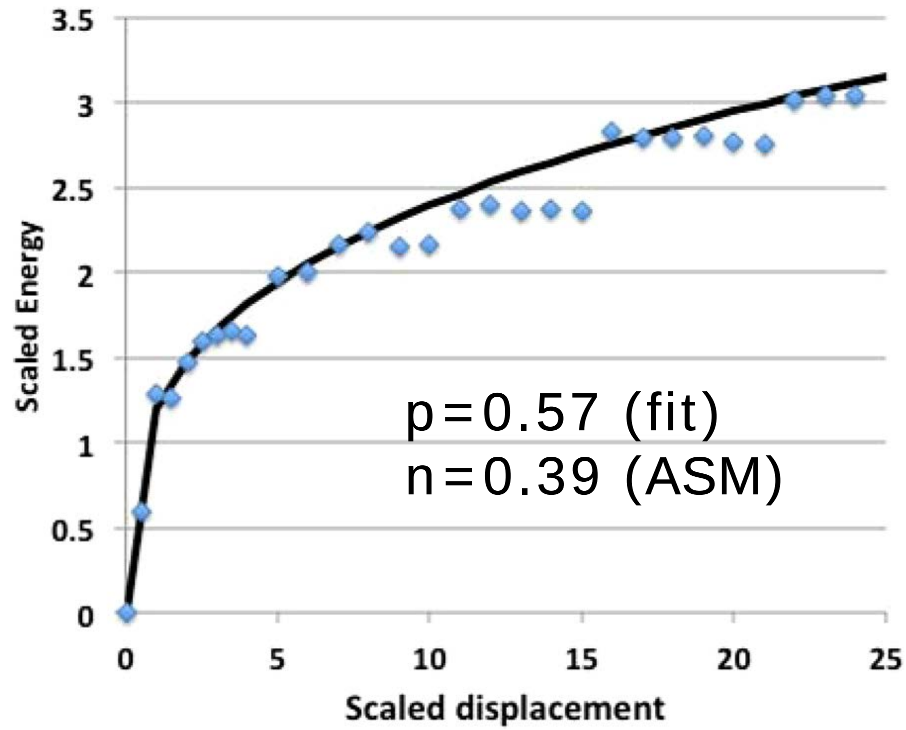
(c)

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

[1]M.I. Baskes and M. Ortiz, *JAM*, **82**: 071003-1-071003-5, 2015

Optimal scaling – Atomic Ni





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Optimal scaling – Uniaxial extension

- Optimal (matching) upper and lower bounds:

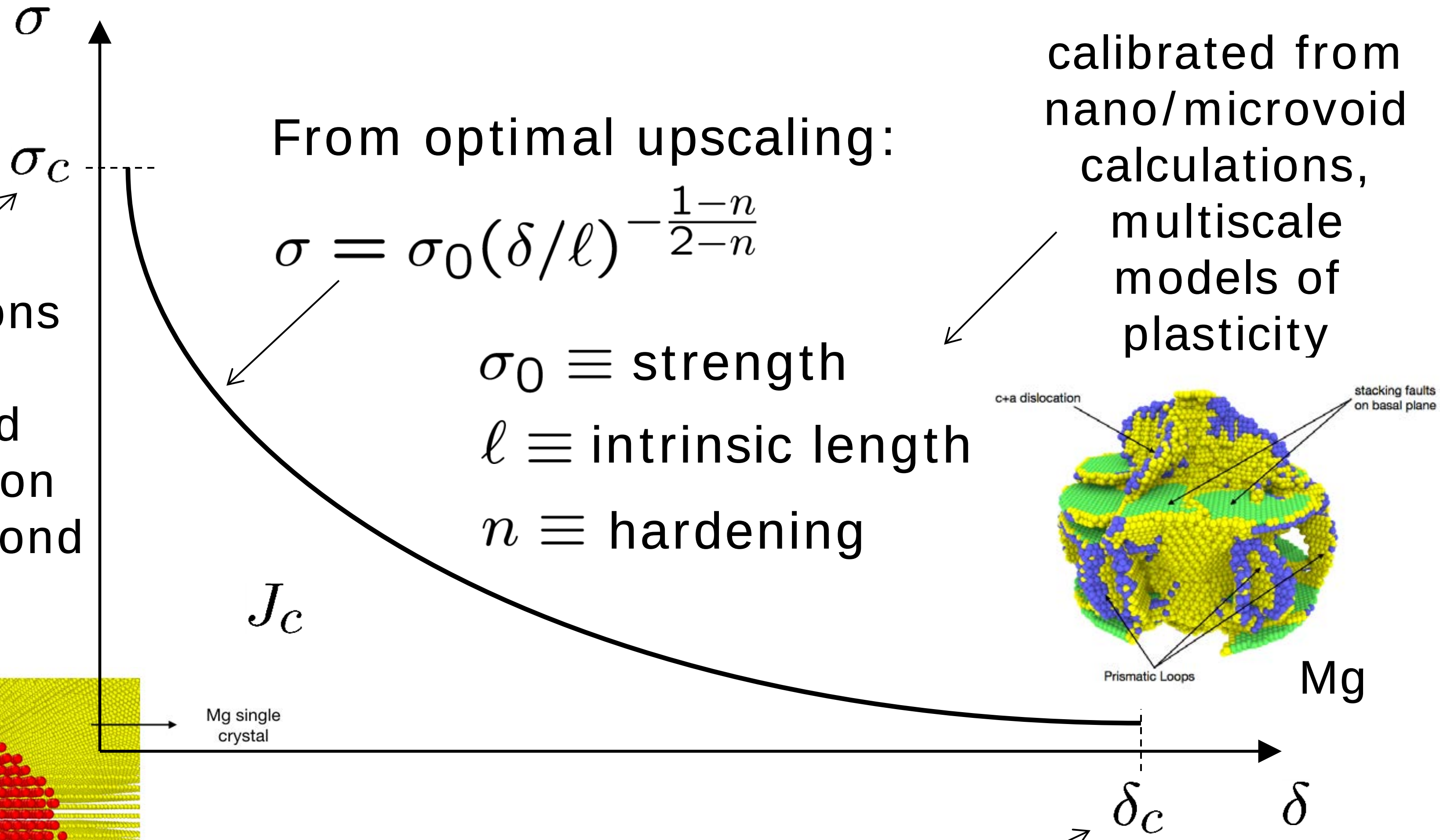
$$C_L(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}} \leq \inf E \leq C_U(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$$

- 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 cohesive energy:

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

Upscaling: Effective cohesive law

from simulations of nano/ microvoid decohesion from second phase particles



From optimal upscaling:

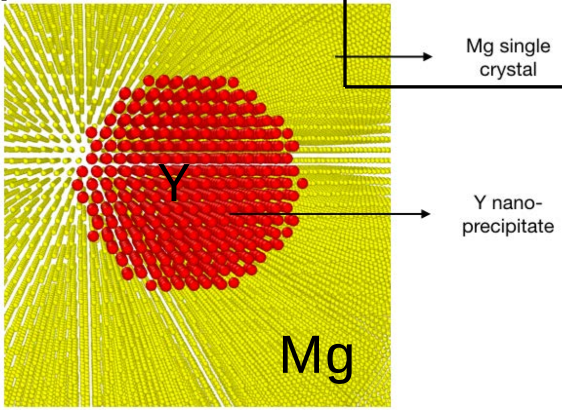
$$\sigma = \sigma_0(\delta/\ell)^{-\frac{1-n}{2-n}}$$

$\sigma_0 \equiv$ strength

$\ell \equiv$ intrinsic length

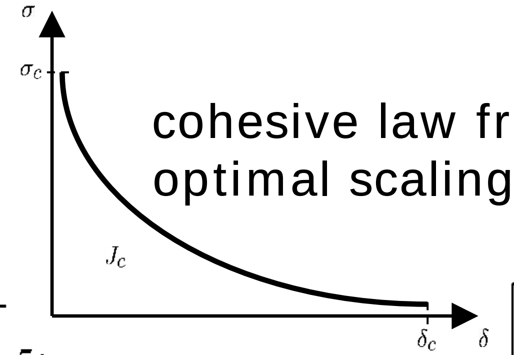
$n \equiv$ hardening

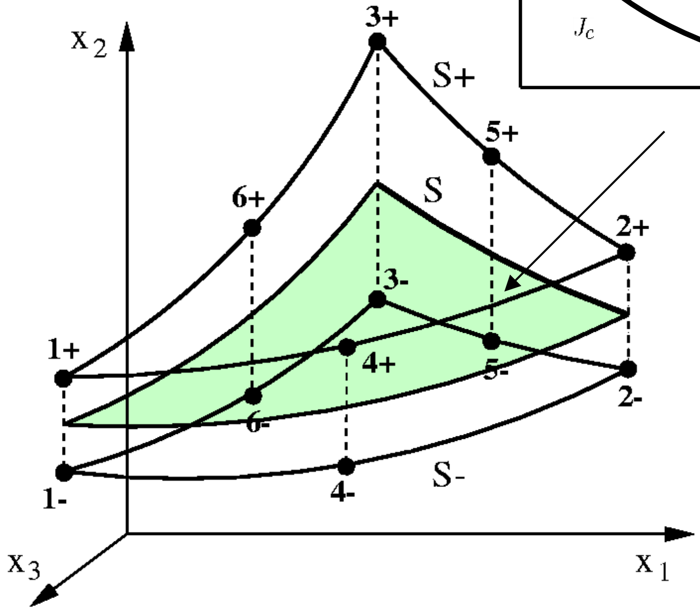
calibrated from nano/microvoid calculations, multiscale models of plasticity

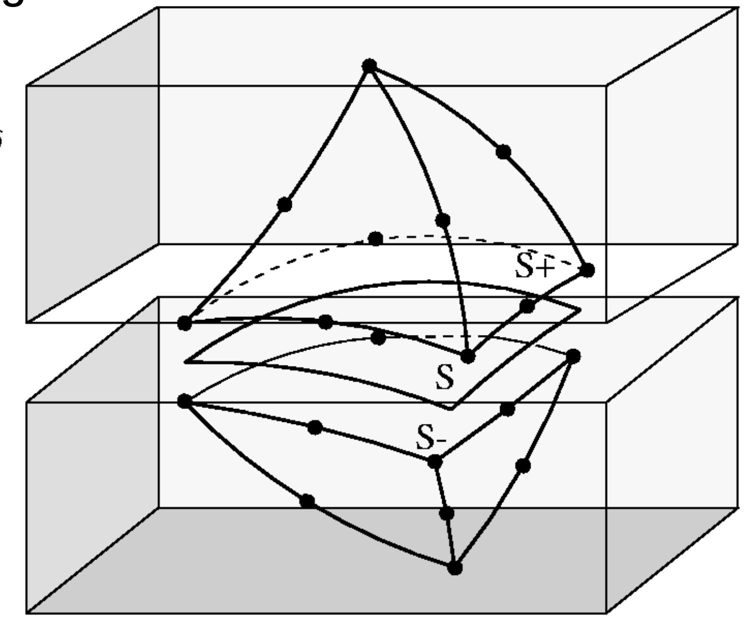


Failure of ligaments?

Implementation: Cohesive elements





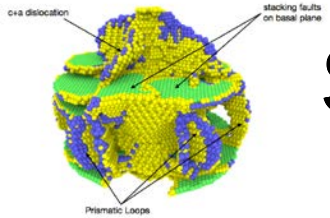


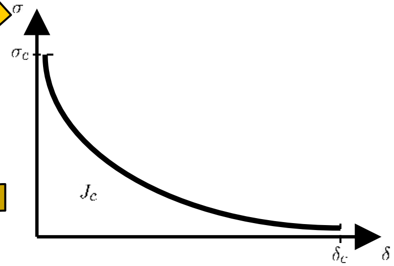
12-node quadratic cohesive elements

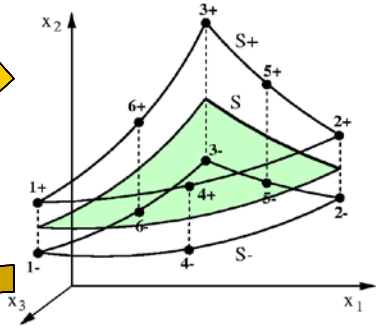
Insertion of cohesive element between two volume elements

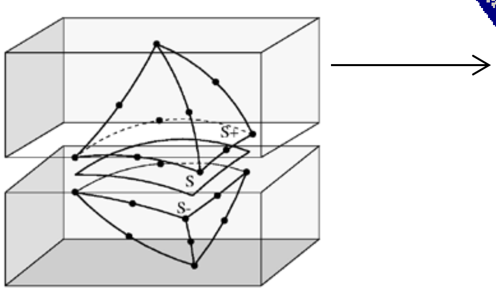
Ortiz, M. and Pandolfi, A., I*JNME*, **44** (9): 1267-1282, 1999.

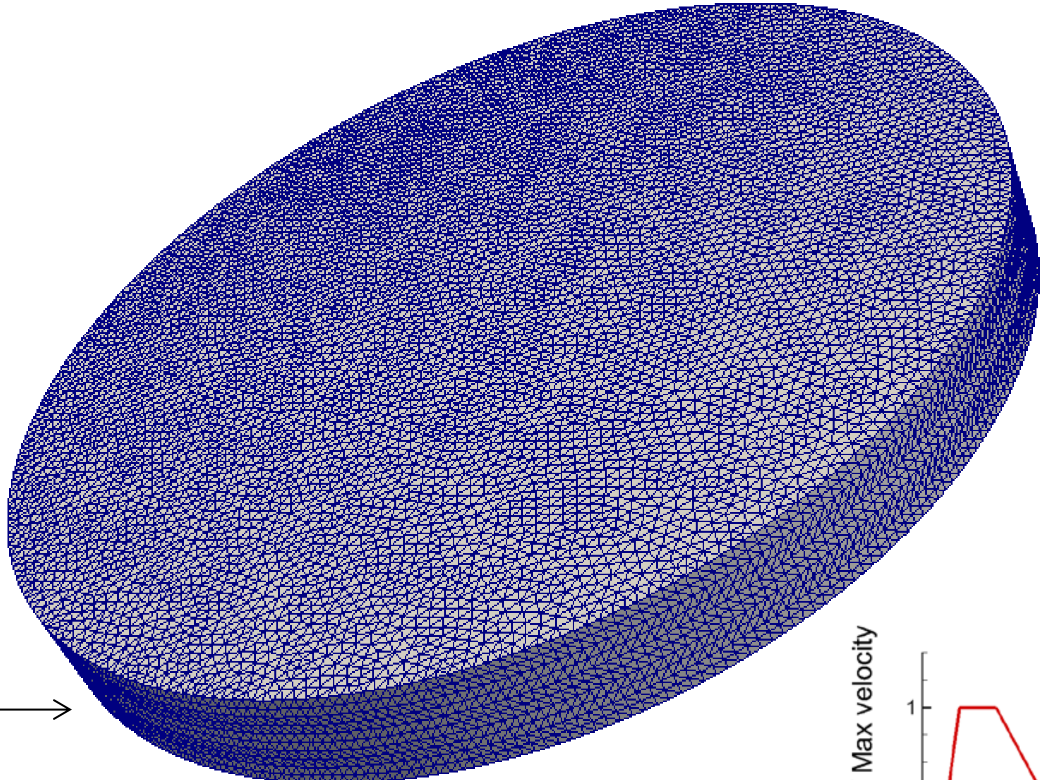
Spall fracture simulations

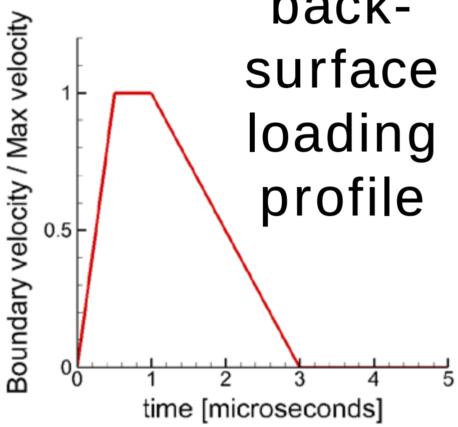












back-surface loading profile

- Ni specimen, D = 50 mm, t = 4.95 mm
- J2 plasticity, power-law hardening
- h= 0.49 mm, 191,960 tets, 456,262 nodes

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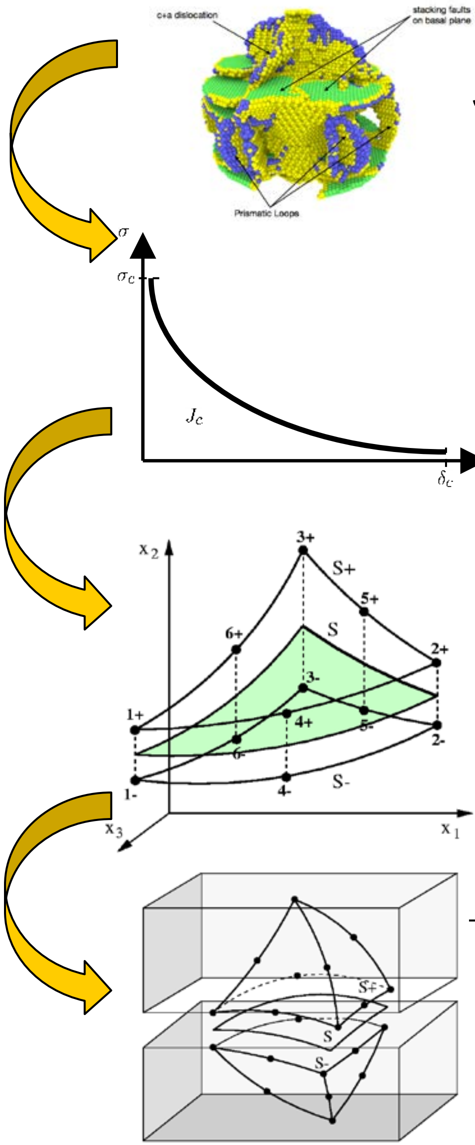
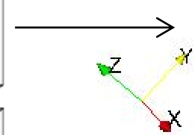
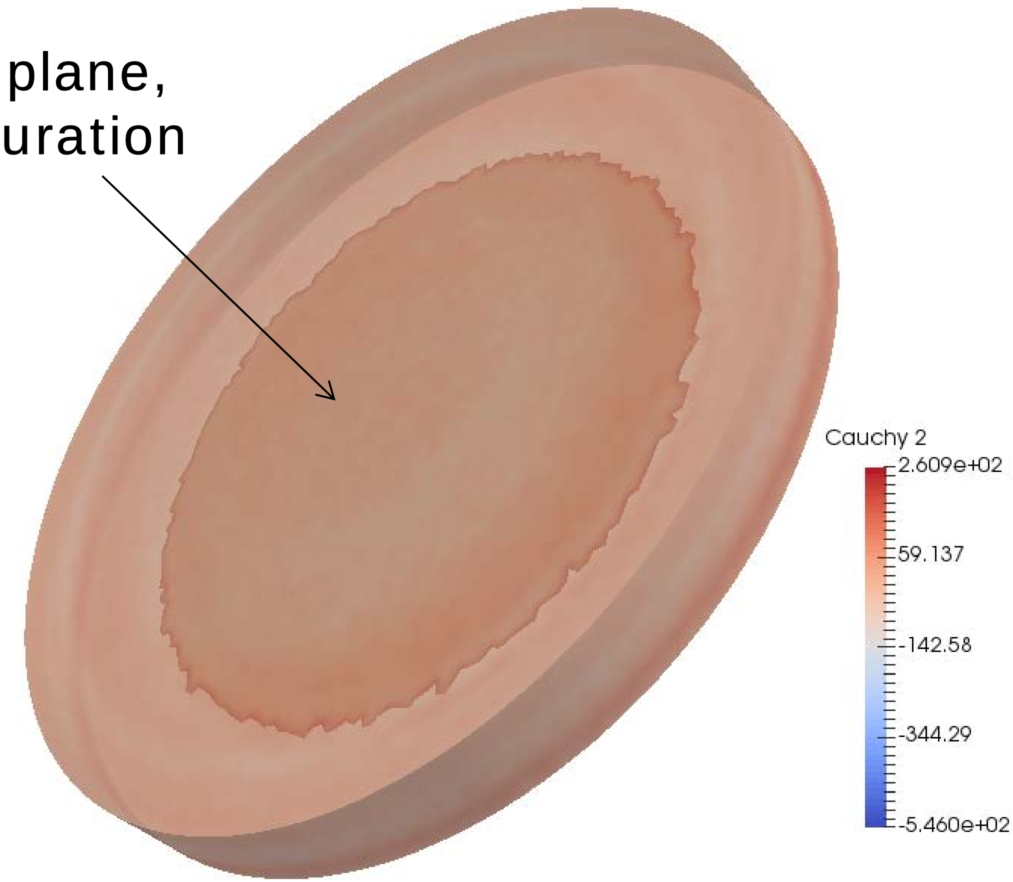
BANFF0516

Spall fracture simulations





spall plane,
final configuration



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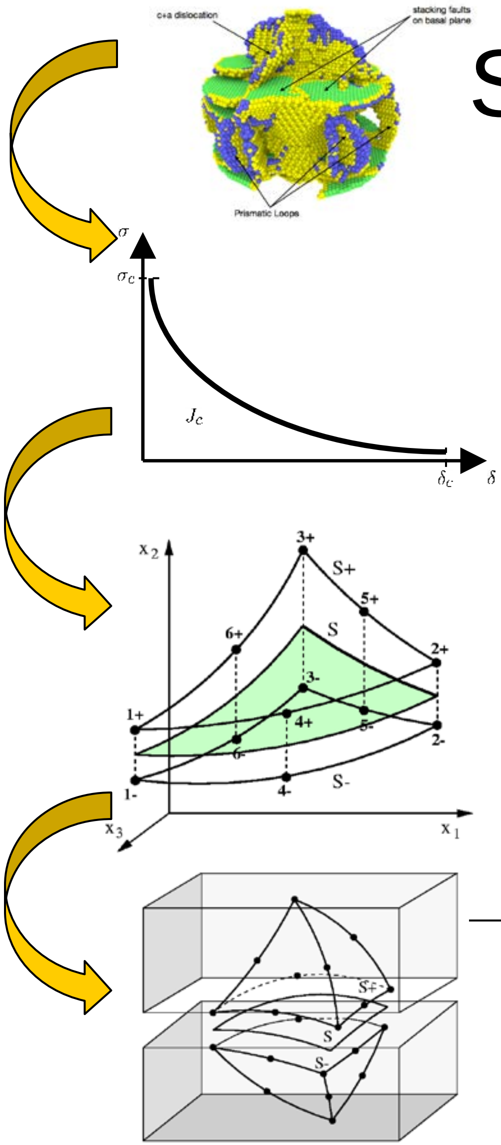

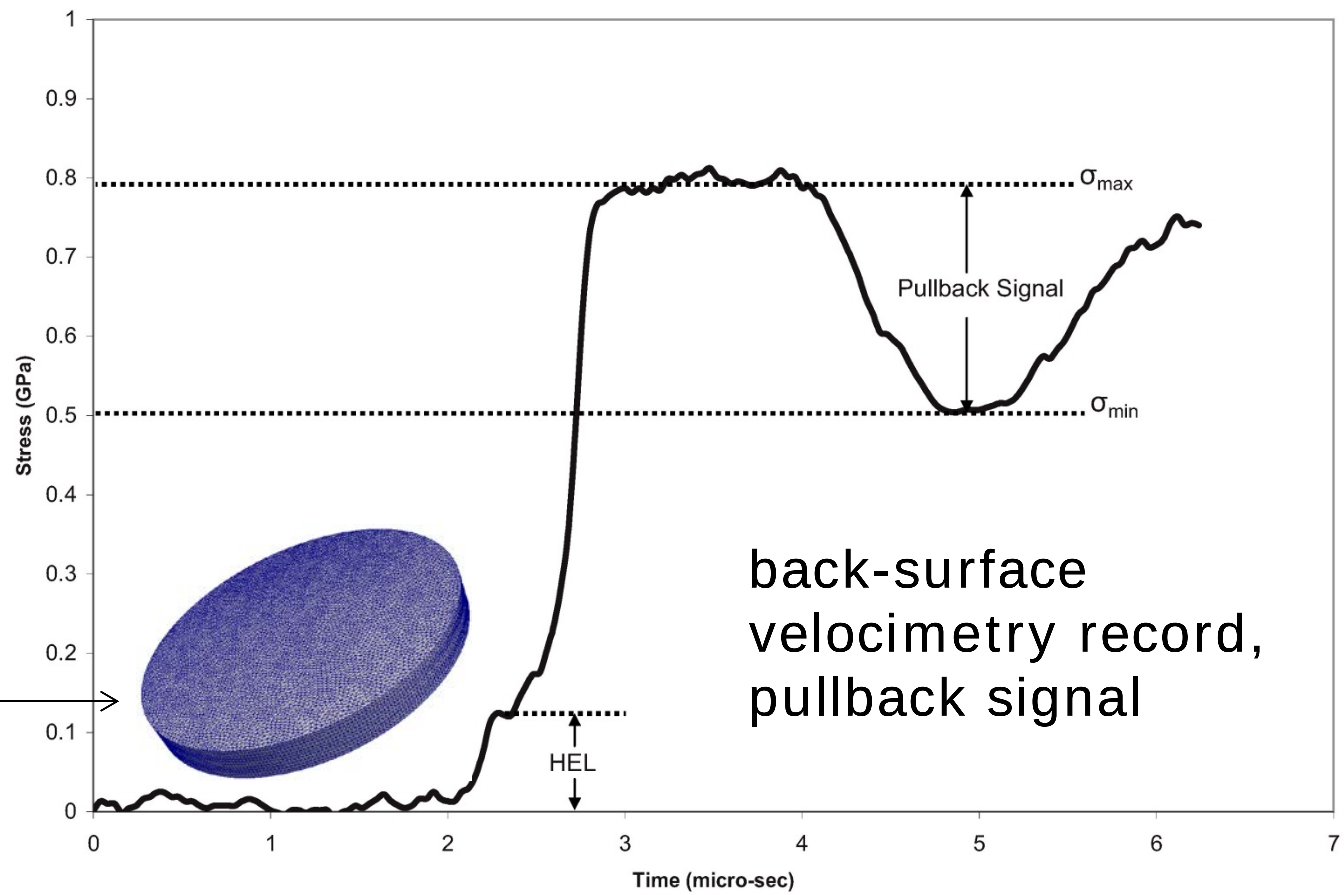

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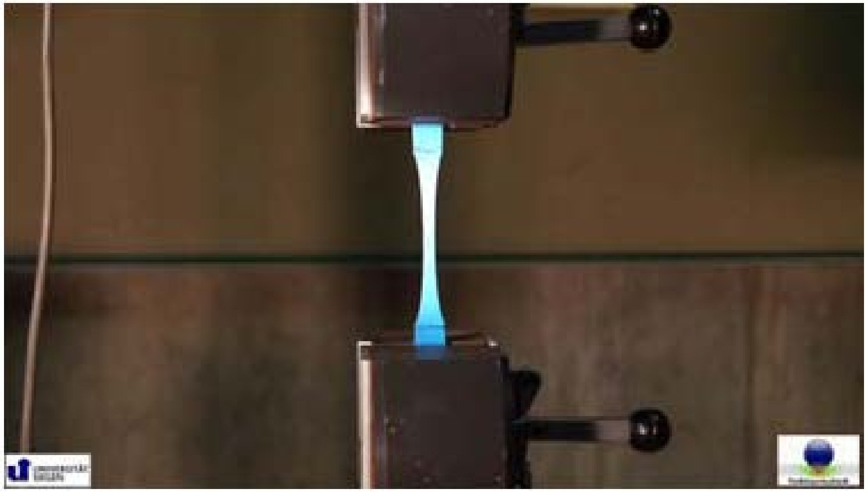
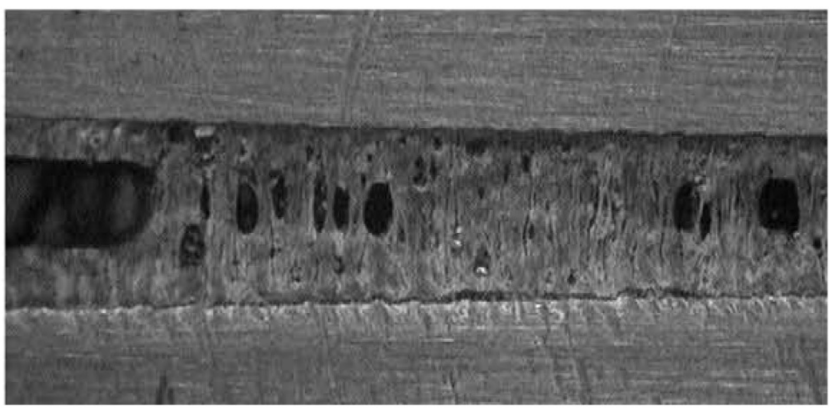
INTERMISSION

Fracture of polymers



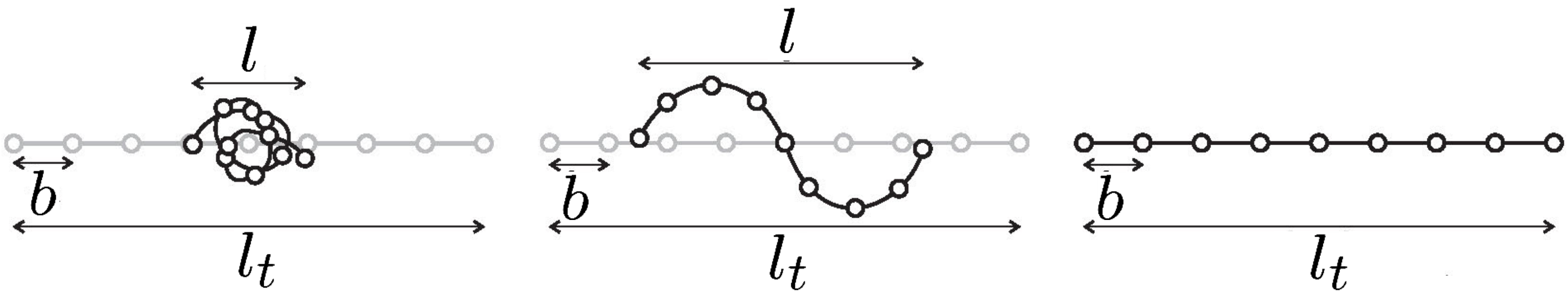
T. Reppel, T. Dally, T. and K. Weinberg, Technische Mechanik, 33 (2012) 19-33.



Crazing in steel/polyurea/steel sandwich specimen (Zhu *et al*., 2008).

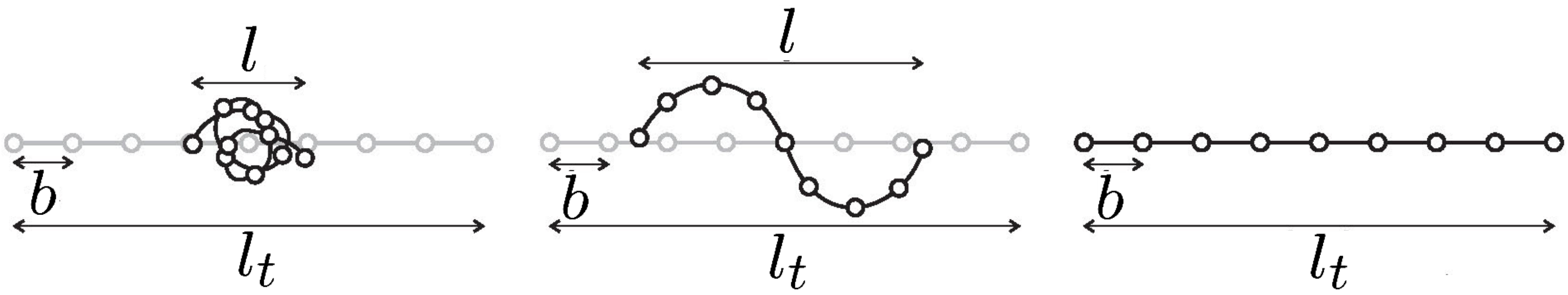
- Polymers undergo entropic elasticity and damage due to chain stretching and failure
- Polymers fracture by means of the crazing mechanism consisting of fibril nucleation, stretching and failure
- The free energy density of polymers saturates in tension once the majority of chains are failed: p=0!
-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

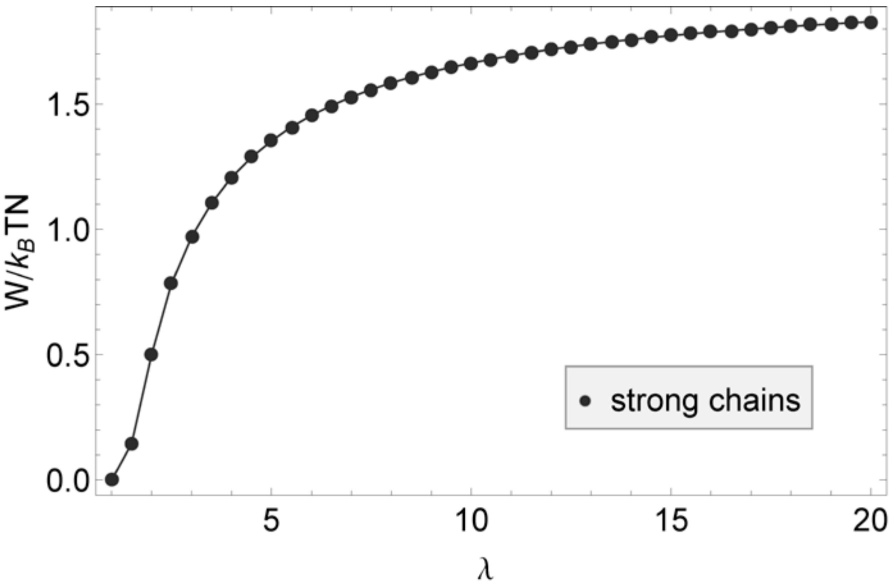
Network theory of polymer elasticity

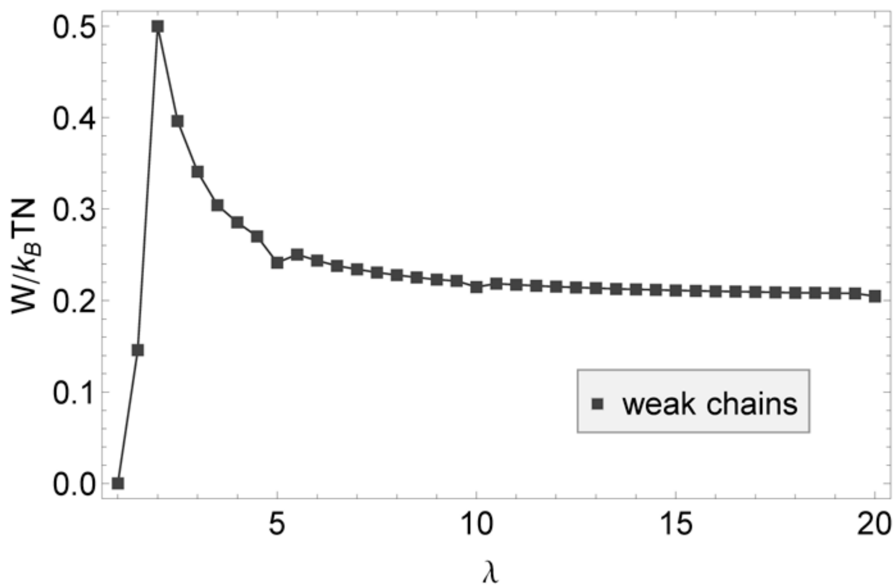


- Polymer: Cross-linked long-chain molecules
- Chains: Freely jointed, far from full extension
- Cross-linking points follow macroscopic def.
- Polymer nearly incompressible
- *Chain links break at critical elongation*

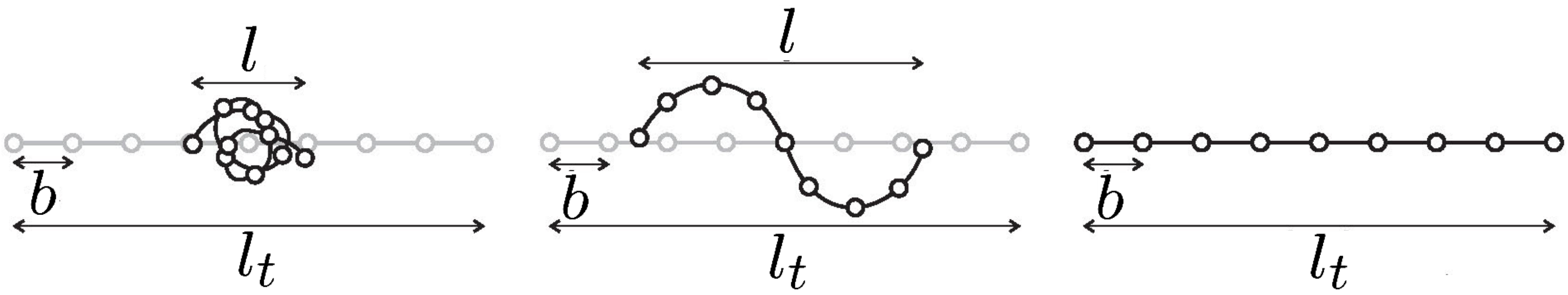
Network theory of polymers

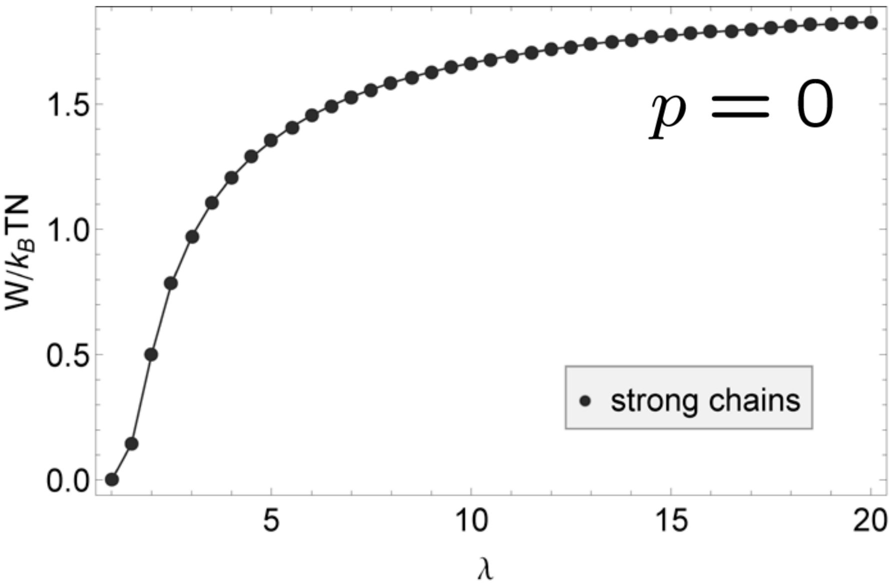


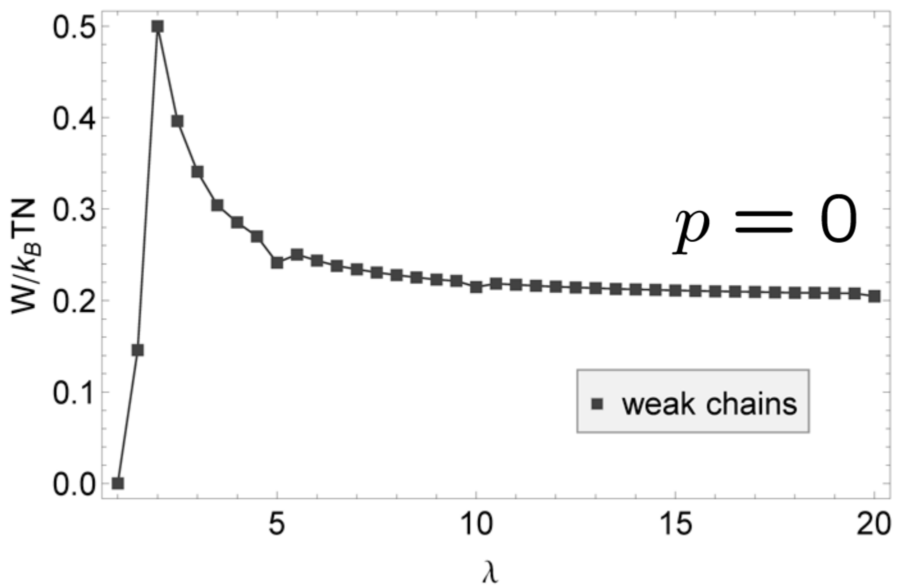




Network theory of polymers







Energy has zero growth!

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Fracture of polymers

- Suppose: For $K_L > 0$, *intrinsic length* $\ell > 0$, $p \approx 0$,

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

- If $E(y) < +\infty$: $y \in W^{1,1}(\Omega) \Rightarrow$ No crazing!

Strain-gradient elasticity precludes crazing!

Michael Ortiz
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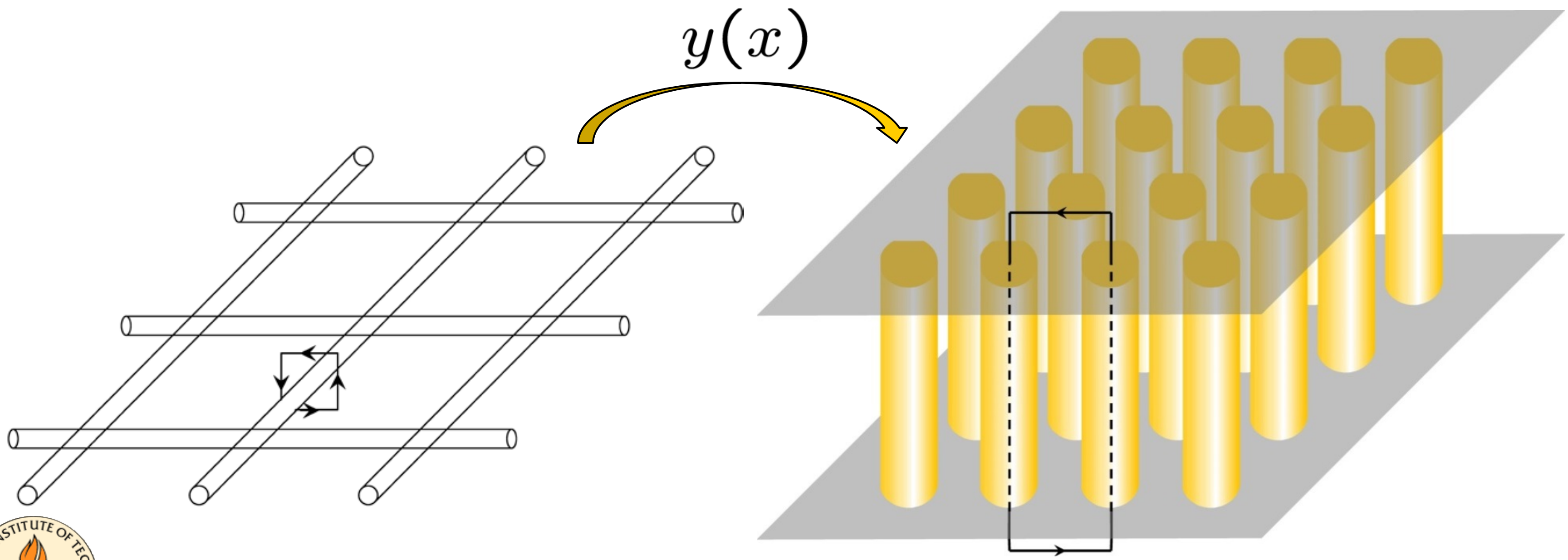
Fracture of polymers

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

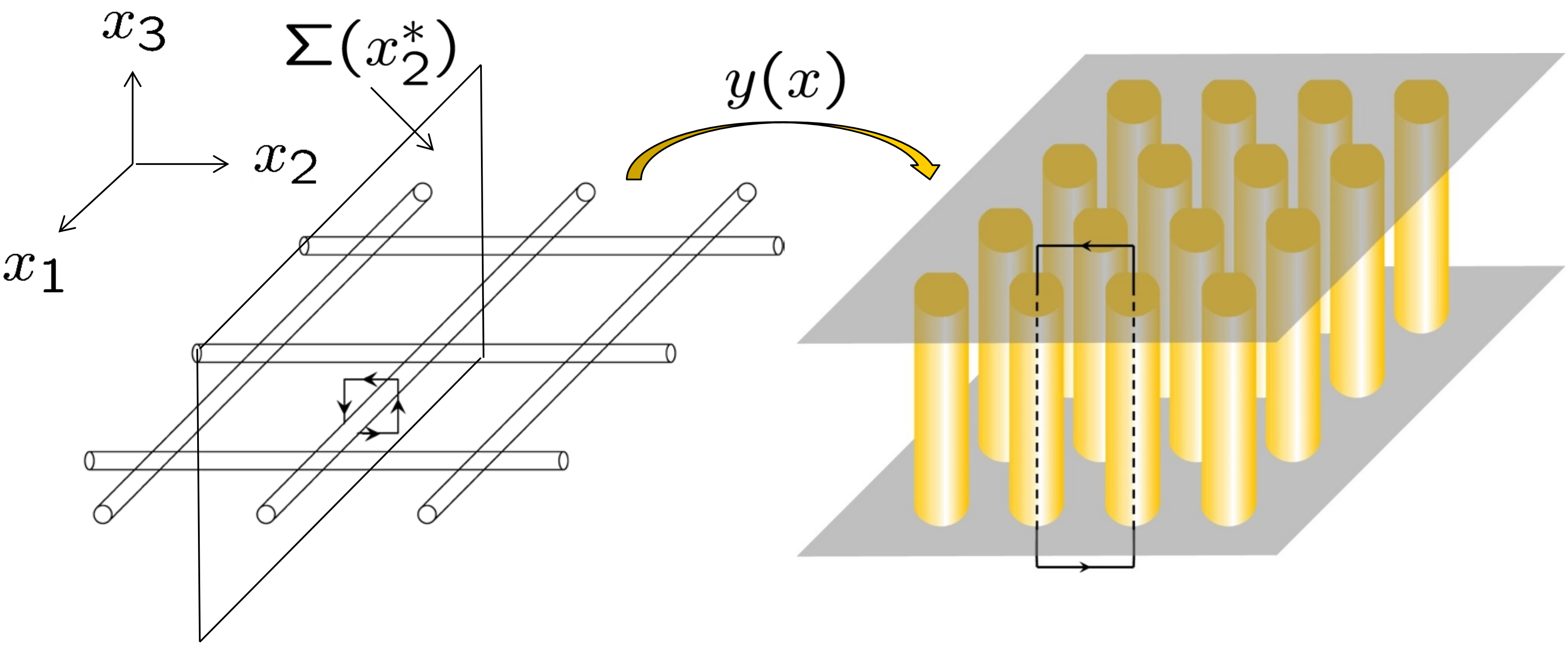
$$E(y) \geq K_L \left(\int_\Omega (|Dy|^p - 3^{p/2})\, dx + \ell \int_\Omega |D^2 y|\, dx \right)$$

- If $E(y) < +\infty$: $y \in W^{1,1}(\Omega) \Rightarrow$ No crazing!



Topology of crazing

The topology of crazing



- Suppose $y \in W^{1,1}(\Omega)$, $|D^2 y|(\Omega) < +\infty$.

$\Rightarrow$ For every $x_2^* \in (0, L)$: $v(x_1, x_3) = y(x_1, x_2^*, x_3)$,

$$v \in W^{1,1} \text{ and } |D^2 v|\Big(\Sigma(x_2^*)\Big) < +\infty,$$

$\Rightarrow$ v continuous and $v\Big(\Sigma(x_2^*)\Big)$ simply connected!

Fracture of polymers

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

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

- If $E(y) < +\infty$: $y \in W^{1,1}(\Omega) \Rightarrow$ No crazing!

- Instead suppose: For $\sigma \in (0,1)$,

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

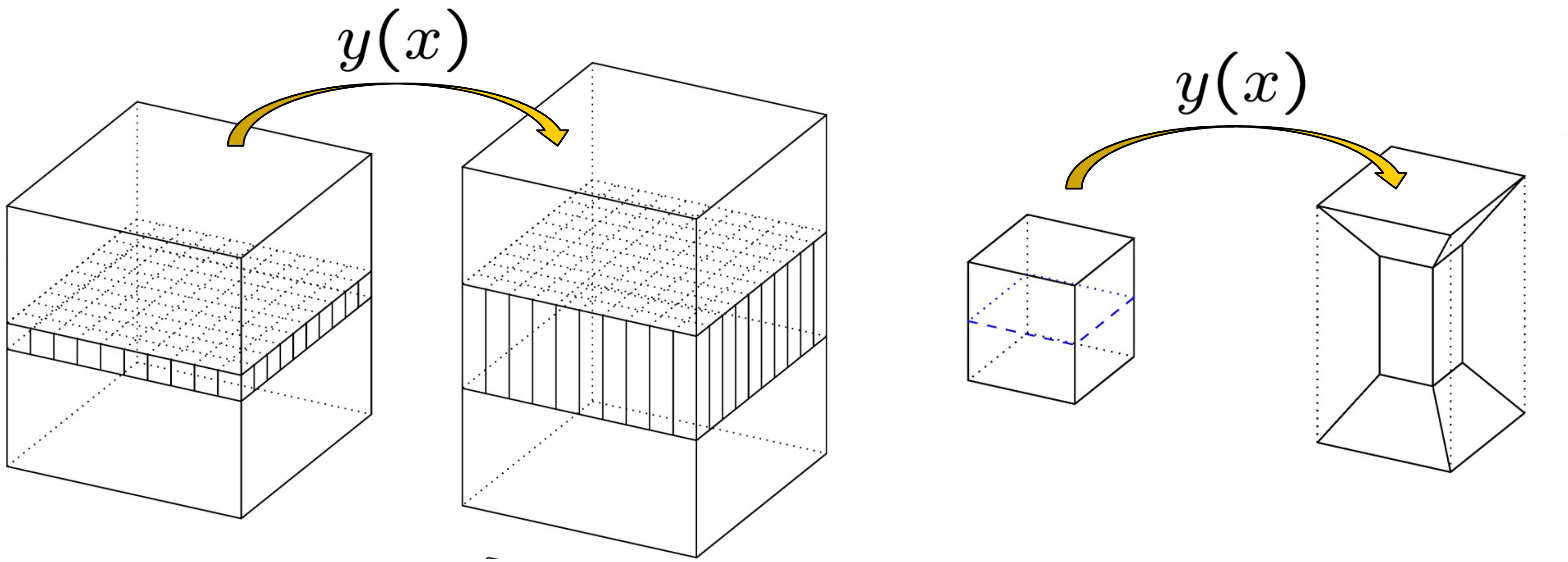
$\Rightarrow$ *Fractional strain-gradient elasticity!*

Theorem [Conti & MO, 2016]. For ℓ sufficiently small,

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

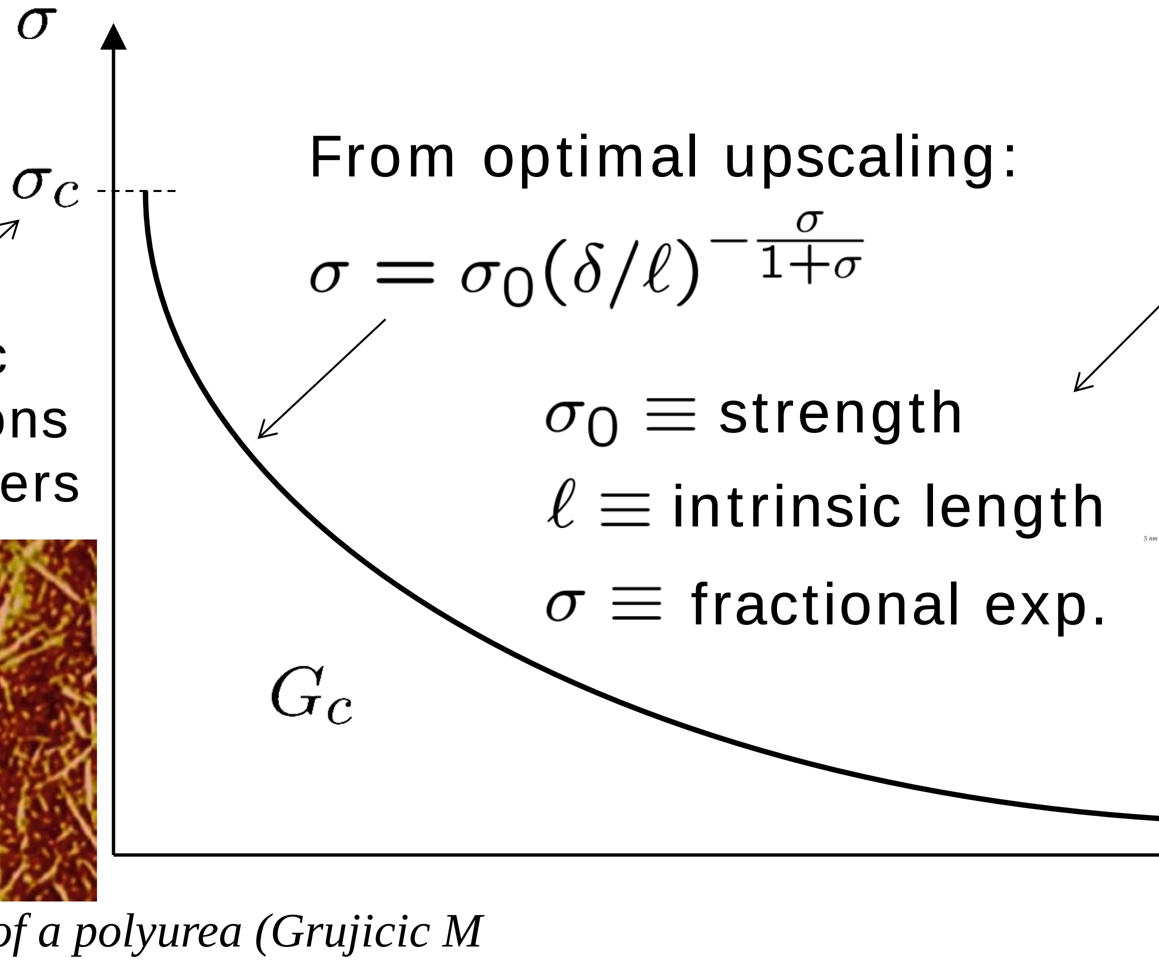
$$C_L L^2 \ell^{\frac{\sigma}{1+\sigma}} \delta^{\frac{1}{1+\sigma}} \leq \inf E \leq C_U L^2 \ell^{\frac{\sigma}{1+\sigma}} \delta^{\frac{1}{1+\sigma}}$$

Sketch of proof: Upper bound



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

Upscaling: Effective cohesive law



From optimal upscaling:

$$\sigma = \sigma_0(\delta/\ell)^{-\frac{\sigma}{1+\sigma}}$$

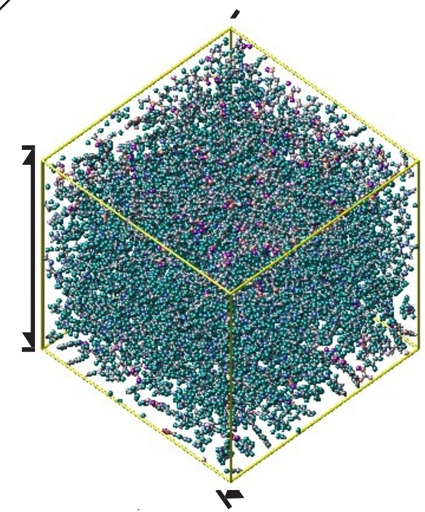
$\sigma_0 \equiv$ strength

$\ell \equiv$ intrinsic length

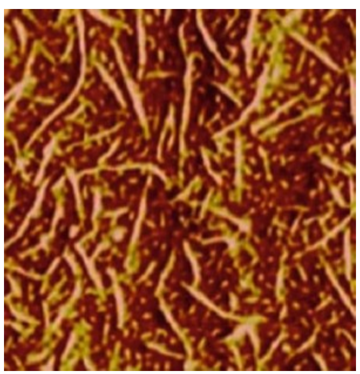
$\sigma \equiv$ fractional exp.

from atomistic simulations of polymers

calibrated from atomistic calculations of polymers



Failure of ligaments?

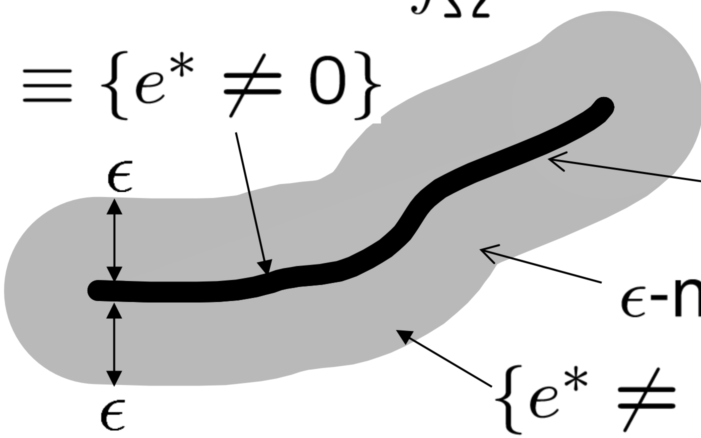


AFM image of a polyurea (Grujicic M et al, MMMS, 9(2013):548-578).

Implementation: Eigenfracture

- Regard fracture as an energy-relaxation process!
- Total incremental energy[1]: Elastic + fracture,

$$E_\epsilon(u, e^*) = \int_\Omega W(e(u) - e^*)\, dx + \frac{G_c}{2\epsilon}|\{e^* \neq 0\}_\epsilon|$$

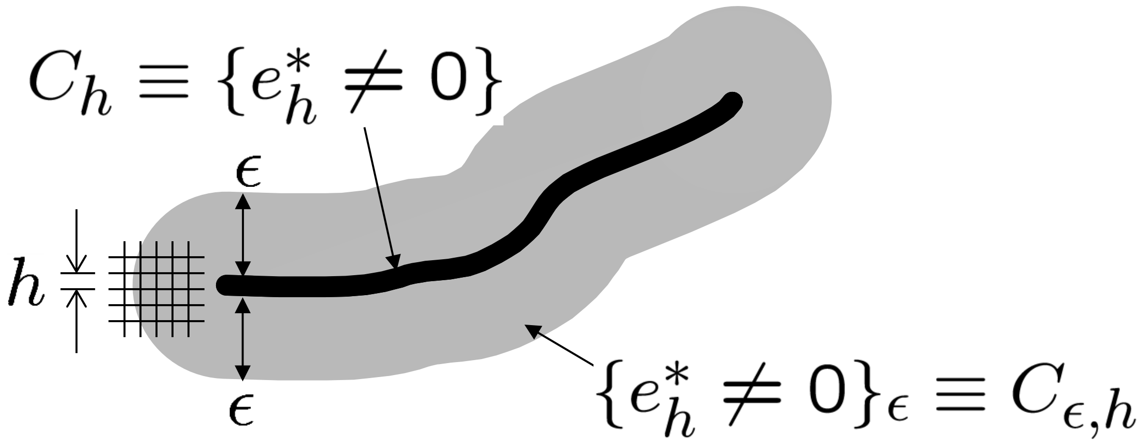


- Energy-minimizing cracks: $E_\epsilon(u, e^*) \to \inf$!
- **<u>Theorem</u>**[1]: $\Gamma - \lim_{\epsilon \to 0} E_\epsilon =$ Griffith energy

[1]Schmidt, B., *et al.*, *SIAM Multi. Model.*, **7** (2009) 1237.

Implementation: Eigenfracture

- Spatial discretization:



- Discretized incremental energy:

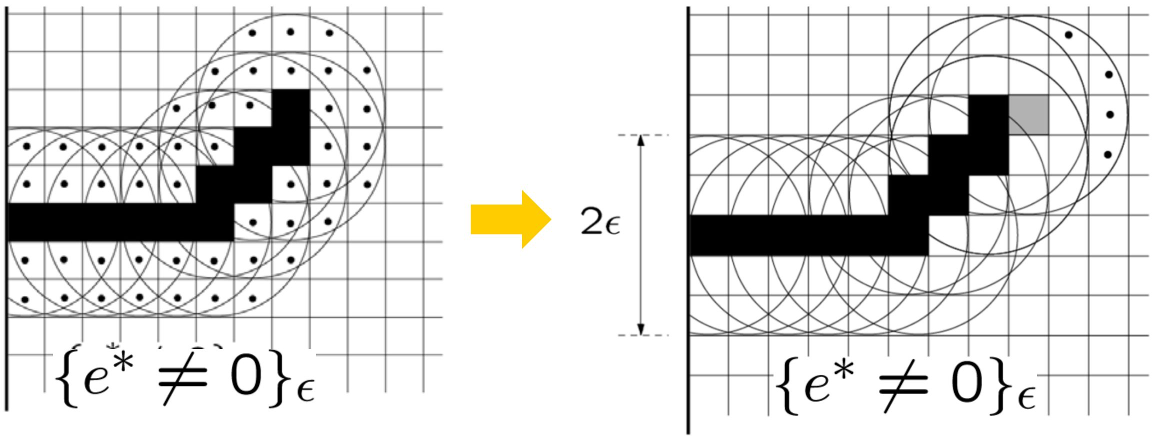
$$E_{\epsilon,h}(u, e^*) = \begin{cases} E_\epsilon(u, e^*), & \text{if } u \in V_h,\ e^* \in W_h, \\ +\infty, & \text{otherwise.} \end{cases}$$

- **<u>Theorem</u>**[1]: Suppose $\epsilon = \epsilon(h)$ and $h/\epsilon(h) \to 0$ as $h \to 0$. Then, $\Gamma-\lim_{h\to 0} E_{h,\epsilon(h)} =$ Griffith energy

[1]Schmidt, B., *et al.*, *SIAM Multi. Model.*, **7** (2009) 1237.

Implementation: Eigenerosion

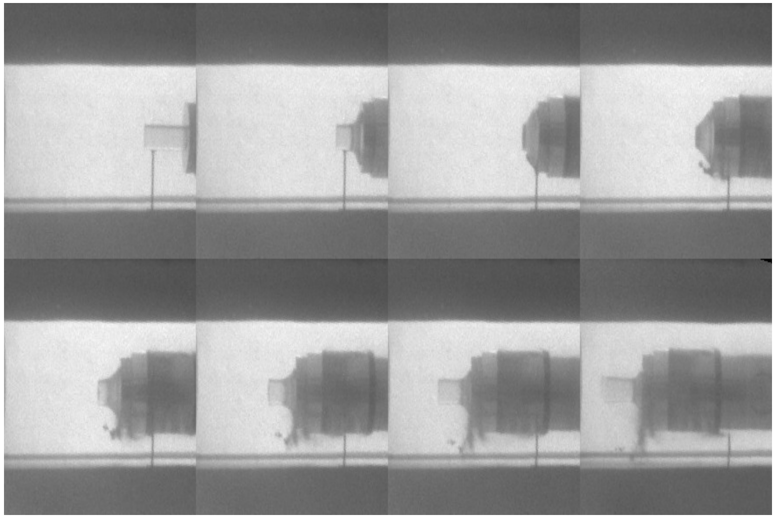
- For every element K, choose[1,2]
  - either: $e_K^* = e(u_K) \Rightarrow$ element erosion,
  - or: $e_K^* = 0 \Rightarrow$ intact element.
- Erosion criterion: $-\Delta E_K \geq \frac{G_c}{2\epsilon}\underbrace{|(C \subset K)_\epsilon \backslash C_\epsilon|}$

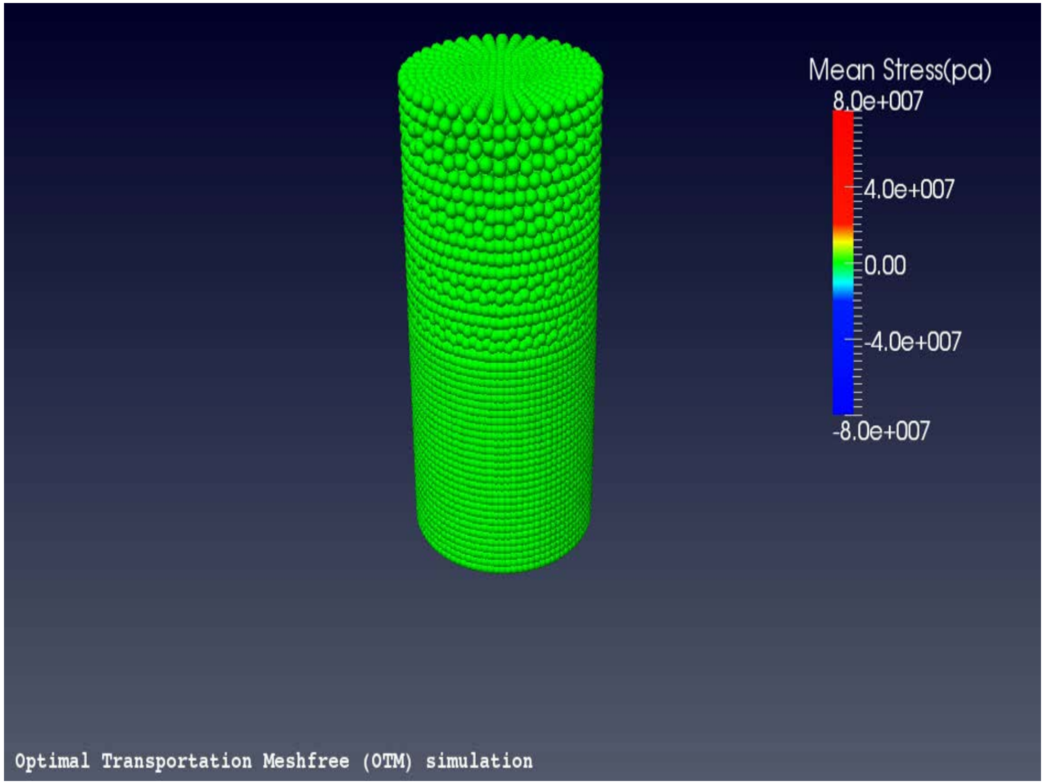


- To first order[1,2]: $-\Delta E_K \sim$ energy in element K

[1]Pandolfi, A. & Ortiz, M. , *IJNME*, **92** *(*2012) 694.
[2]Pandolfi, A., Li, B. & Ortiz, M. , *Int. J. Fract.*, **184** *(*2013) 3.

Taylor-anvil tests on polyurea

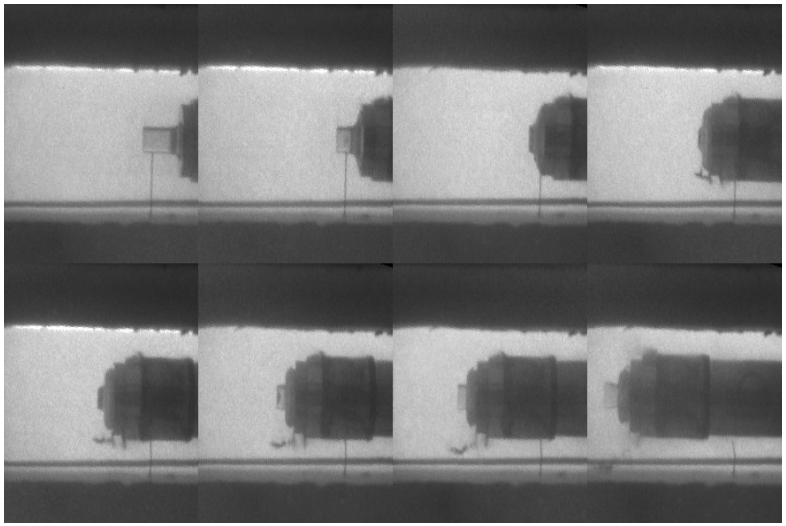




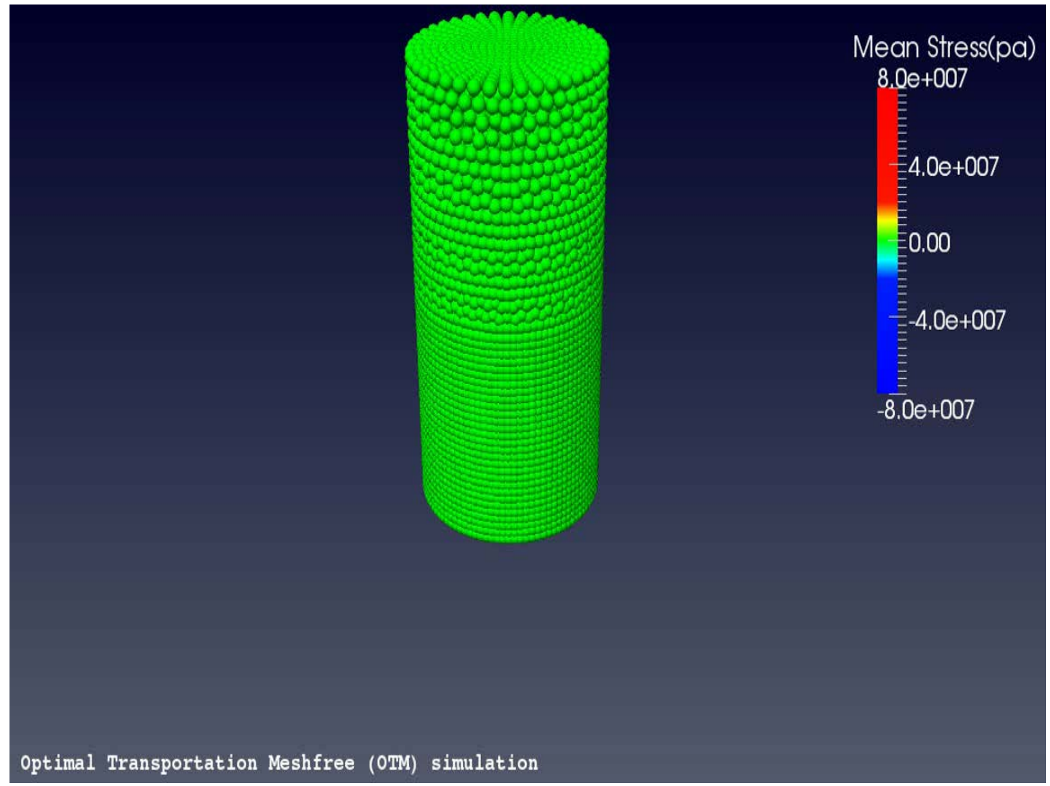
Shot #854:
R0 = 6.3075 mm,
L0 = 27.6897 mm,
v = 332 m/s

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,
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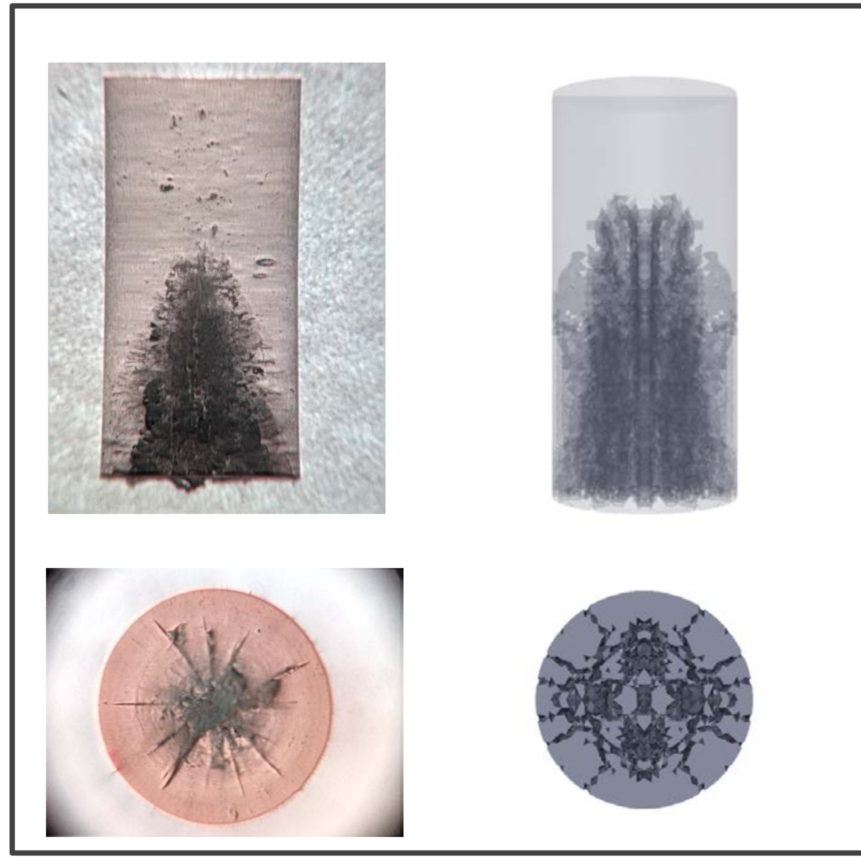
Taylor-anvil tests on polyurea

Shot #854



Shot #861

Comparison of damage and fracture patterns
in recovered specimens and simulations

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...)
- Upscaled properties can be efficiently implemented through cohesive or material-point erosion schemes
- Highly to be desired: Full Γ-limit as $\ell \to 0$, evolution...

Concluding remarks

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