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Strain-Gradient Microplasticity and Ductile Fracture of Metals

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Material Strength & Durability Symposium
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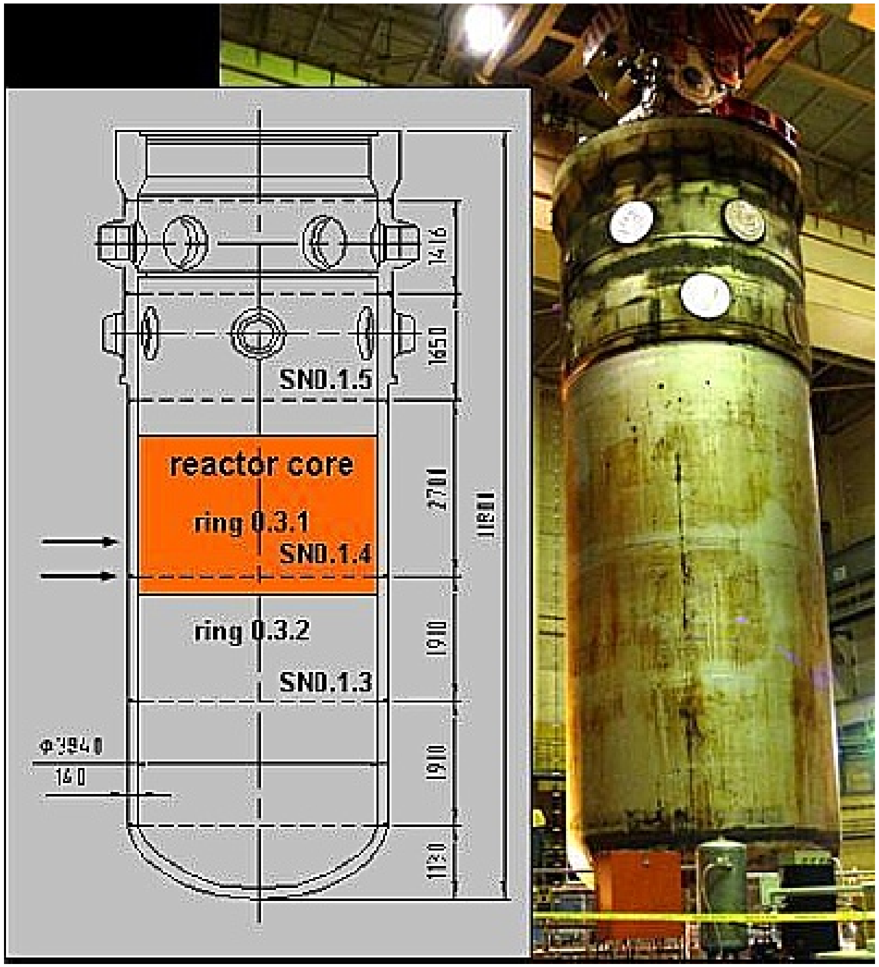
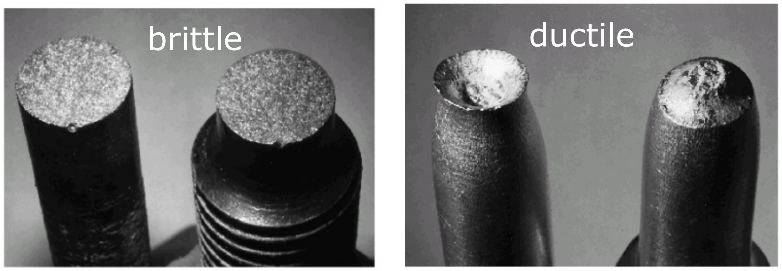
Ductile fracture of metals



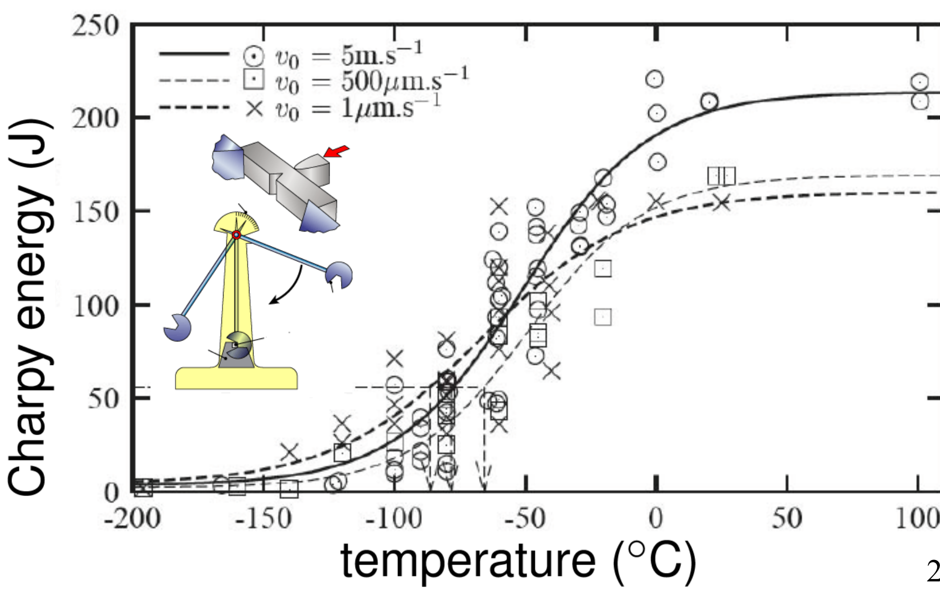
- *Linear-elastic fracture mechanics* proved inadequate for assessing, e.g., safety of mild-steel pressure vessels in nuclear power plants, which spurred the development of *elastic-plastic fracture mechanics* (with focus on Rice's J-integral formalism)

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)

Ductile fracture of metals



(Courtesy NSW HSC online)

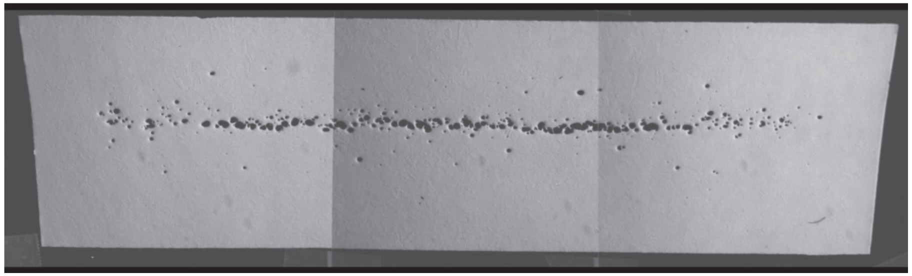


Charpy energy of A508 steel[2]

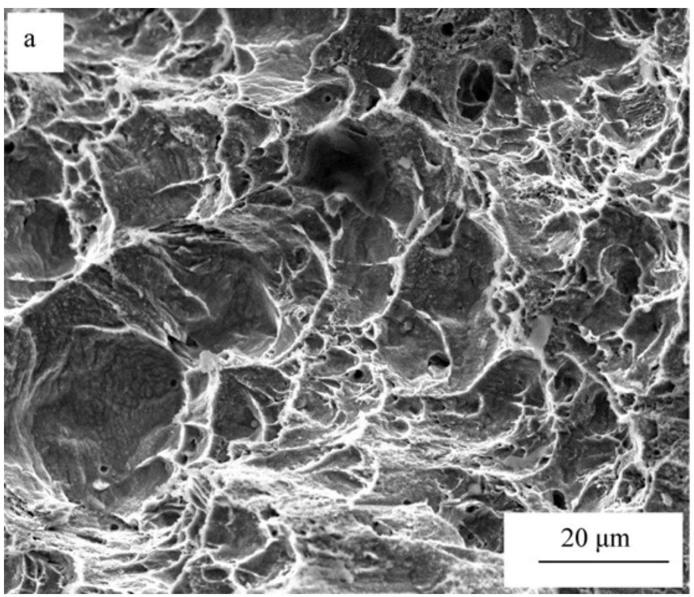
- In general, the *specific fracture energy* for ductile fracture is greatly in excess of that required for brittle fracture…
- A number of *ASTM engineering standards* are in place to characterize ductile fracture properties (J-testing, Charpy test)
- *Can we understand fracture energy, scaling, from micromechanics?*

[2]Tanguy, B., Besson, J., Piques, R. & Pineau, A., *Eng. Frac. Mechanics*, **72** (2005) 49.

Ductile fracture of metals



Spall test in copper disk[1]



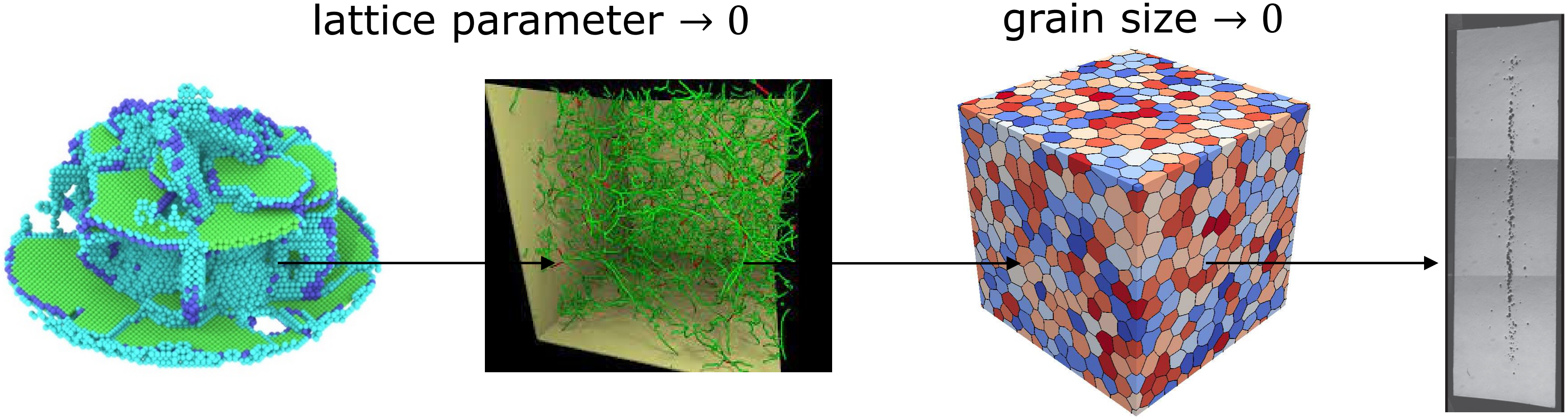
Fracture surface in SA333 steel[2], room temp., $d\varepsilon/dt=3\times10^{-3}s^{-1}$

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

[1]Heller, A., Science & Technology, LLNL, pp. 13-20, July/August, 2002.
[2]S.V. Kamata, M. Srinivasa and P.R. Rao, Mater. Sci. Engr. A, **528** (2011) 4141.

Micro-to-macro: Effective problem

lattice parameter $\rightarrow 0$ grain size $\rightarrow 0$



- Naïve assumptions:
  - Deformation theory of plasticity.
  - *Local* pseudo-energy density $W(F)$.
  - Volume-preserving plasticity.
  - Rigid-plastic behavior.
- Effective macroscopic problem:

unknown!

Minimize: $E(y) = \int_\Omega W(Dy(x))\,dx + \text{forcing terms},$

subject to: $\det(Dy(x)) = 1, \quad \text{a. e. in } \Omega.$

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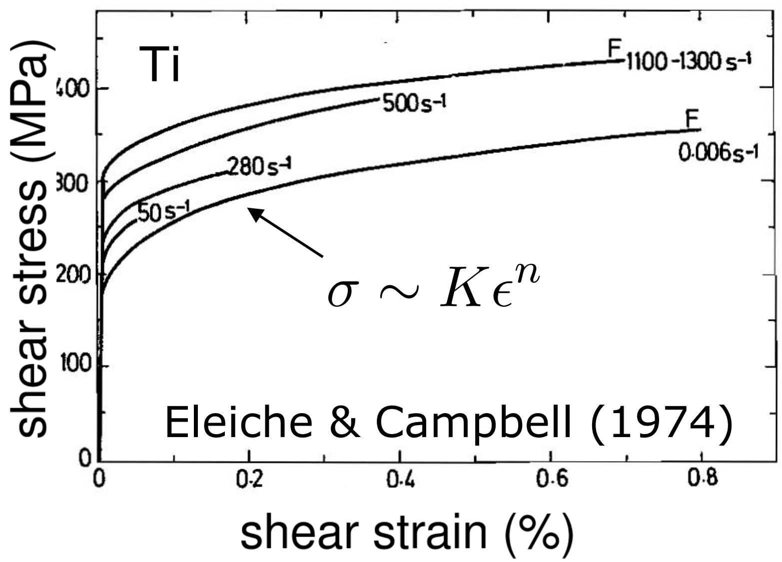
Local deformation theory: Growth

- Deformation theory: Minimize
$$E(y) = \int_\Omega W(Dy(x))\,dx,$$
$y : \Omega \to \mathbb{R}^d$, volume preserving.
- (Observed) growth of $W(F)$?
- Assume 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: $\partial_\lambda W \sim K\lambda^{n-1} \Rightarrow W \sim K\lambda^n$.
- Compare with $W(F) \sim |F|^p$, $p = n \in (0,1)$.
- Considère analysis $\Rightarrow$ *Sublinear growth!* $(p < 1)$.



Necking of bars
Rittel et al. (2014)

Armand Considère, *Annales des Ponts et Chaussées,* **9** (1885) 574-775.

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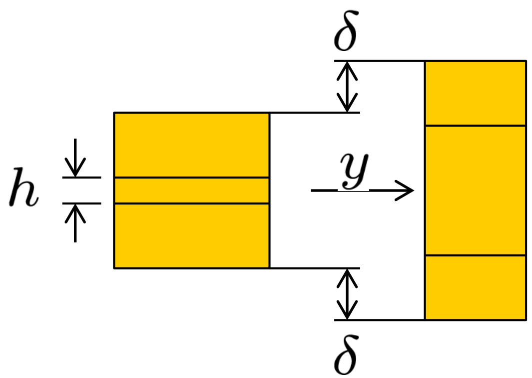
Local deformation theory: Stability



localization of deformations

- 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...

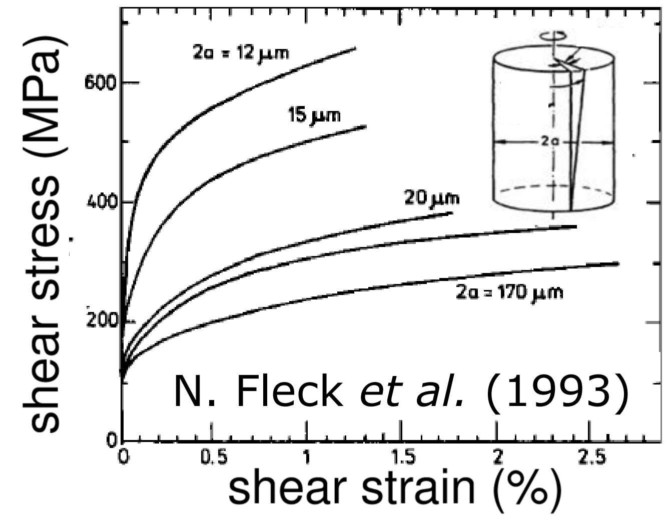
Strain-gradient plasticity

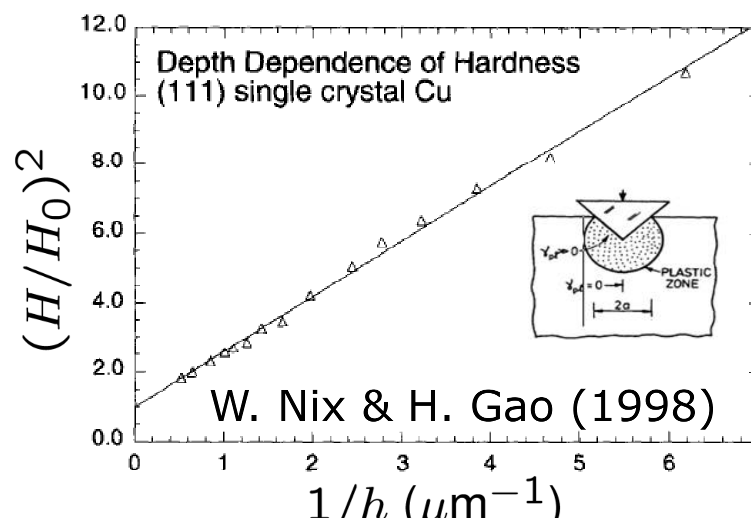
- Local energy relaxes to 0.
- Need additional physics!
- The yield stress of metals is observed to increase in the presence of *strain gradients*.
- *Ansatz*: Minimize

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

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

- Strain-gradient effects may be expected to oppose localization, regularize problem. How?
- NB: Growth of $W(F, \cdot)$?





N.A. Fleck and J.W. Hutchinson, *JMPS*, **41** (1993) 1825.

Strain-gradient plasticity: Growth

- Example: Fence structure,

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

- Across jump set Σ:

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

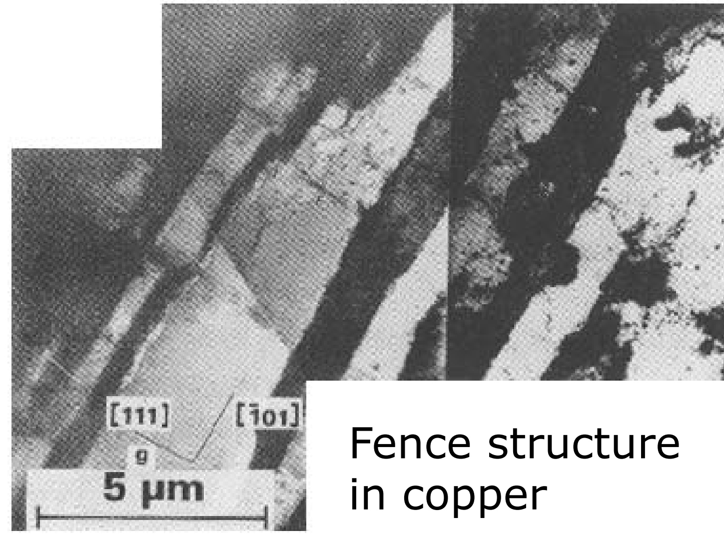
- From line-tension approximation,

$$W = \frac{T}{bL} 2\sin\theta = \frac{T}{bL}|[\![F]\!]|.$$

- Strain-gradient:

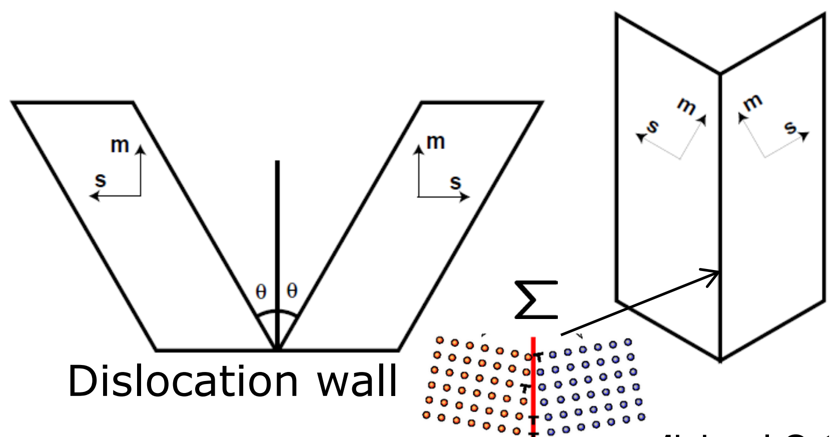
$$|DF| = |[\![F]\!]| \, \mathcal{H}^2 \llcorner \Sigma.$$

- $W(F,\cdot)$: *Linear growth!*



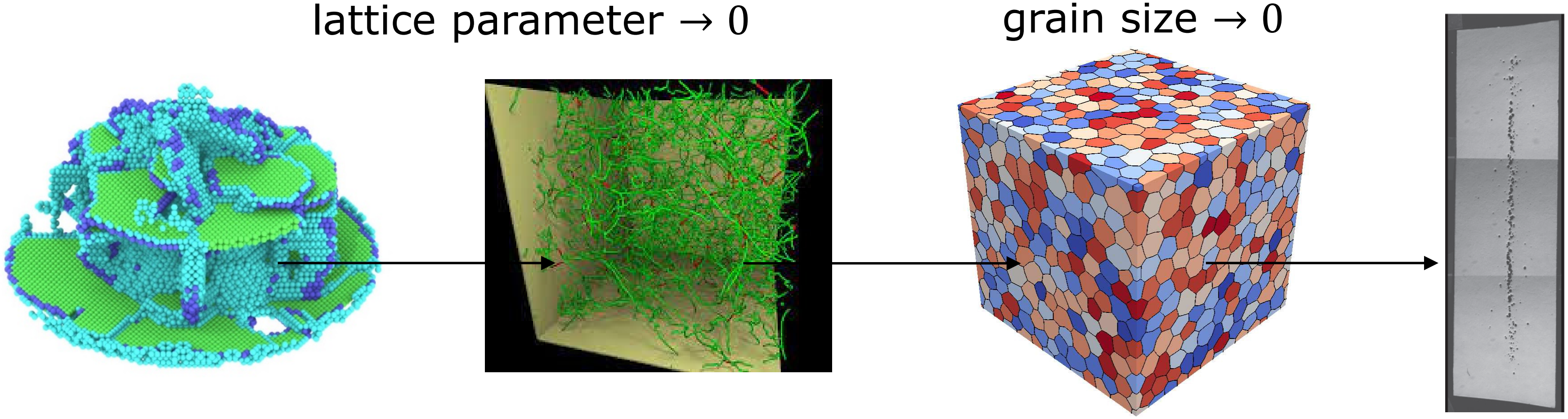
Fence structure in copper

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



Micro-to-macro: Effective problem

lattice parameter → 0 grain size → 0



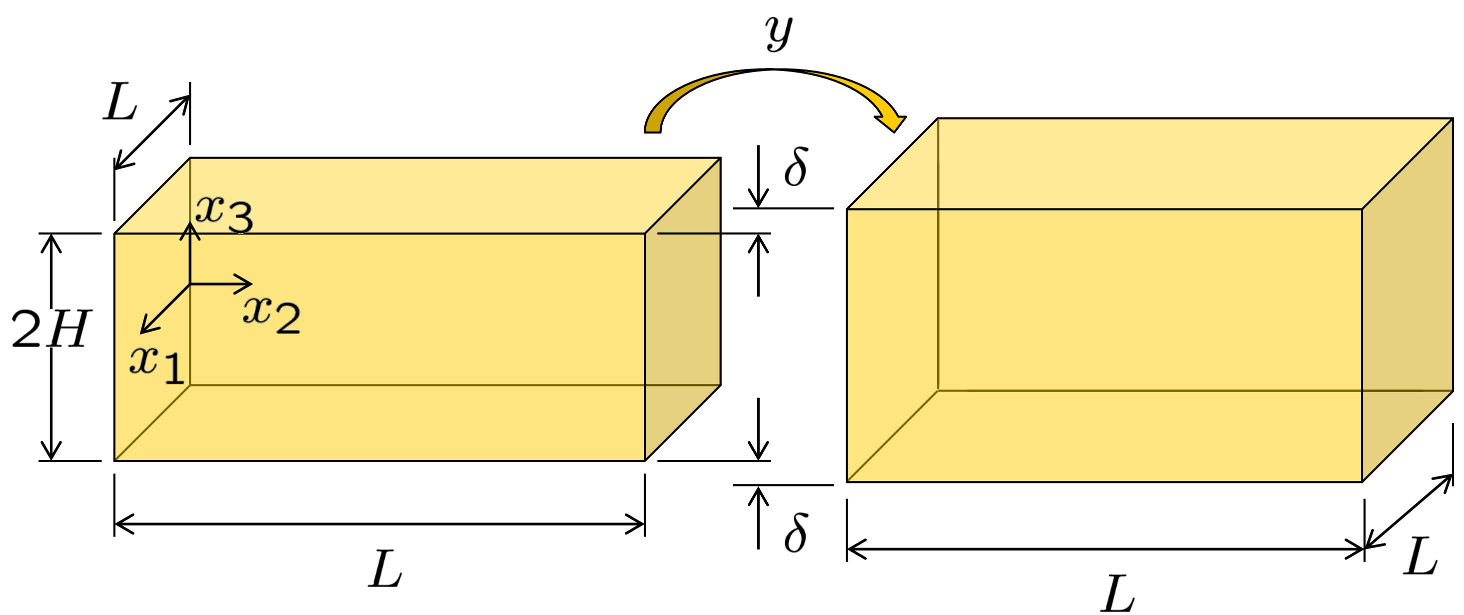
- *Ansatz*: Macroscopic deformation-theoretical problem of the form

  Minimize: $E(y) = \int_\Omega W\Big(Dy(x), D^2y(x)\Big)\, dx +$ forcing terms,

  subject to: $\det(Dy(x)) = 1$, a. e. in Ω.

- Expected growth properties (experimental, heuristics):
  - $W(\cdot, DF)$ sublinear: Promotes localization.
  - $W(F, \cdot)$ linear: Opposes localization.
- What is the net macroscopic result of the competition between local and non-local energies?

Model problem: Uniaxial extension of slab



- Slab: $\Omega = [0, L]^2 \times [-H, H]$, in-plane periodic.
- Deformation $y : \Omega \to \mathbb{R}^3$, $\det Dy(x) = 1$.
- Uniaxial extension: $y_3(x_1, x_2, \pm H) = \pm(H + \delta)$.
- Growth: $E(y) \sim \int_\Omega \Big(|Dy(x)|^p + \ell|D^2 y(x)|\Big)\, dx$, $0 < p < 1$.

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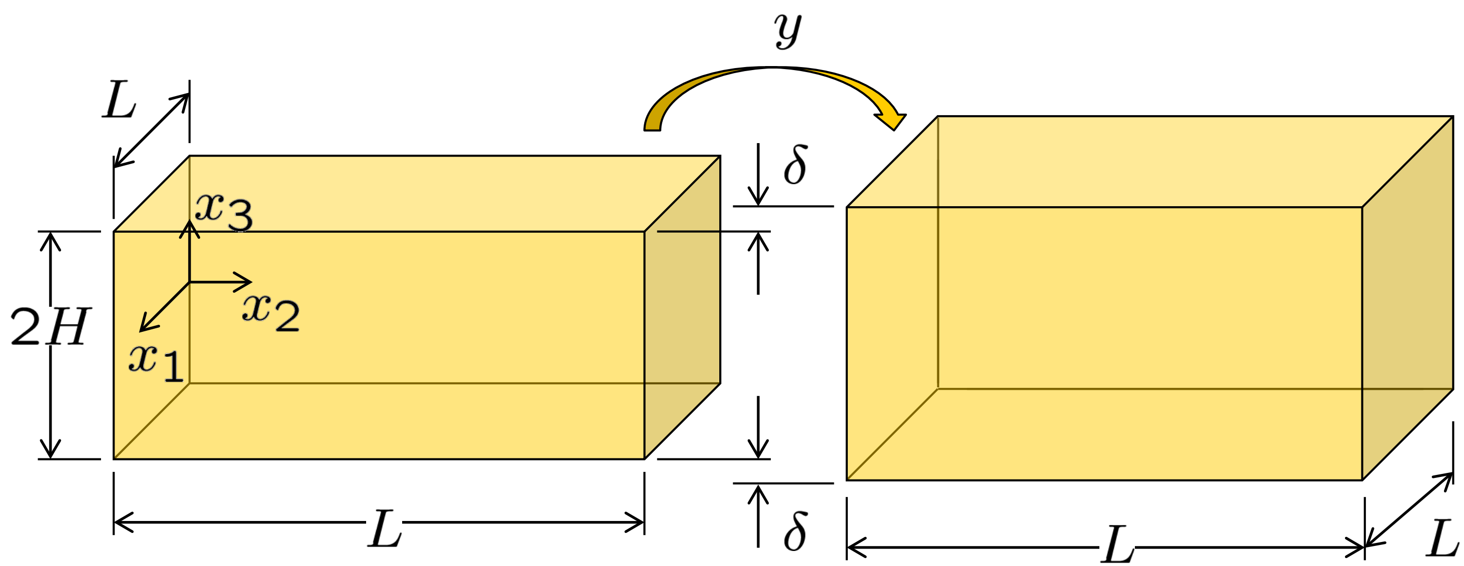
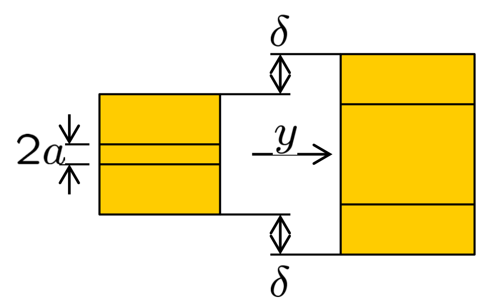
Optimal scaling: Heuristics



- Ignore volume constraint, localize def to band of thickness $2a$.
- Trial energy: $E \sim \delta^p a^{1-p} + \ell(\delta/a)$.
- Optimize thickness: $a \sim \ell^{\frac{1}{2-p}} \delta^{\frac{1-p}{2-p}}$.
- Optimal energy: $E \sim \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$.



- To show: i) Same scaling can also be achieved by means of volume-preserving map; ii) scaling is optimal.

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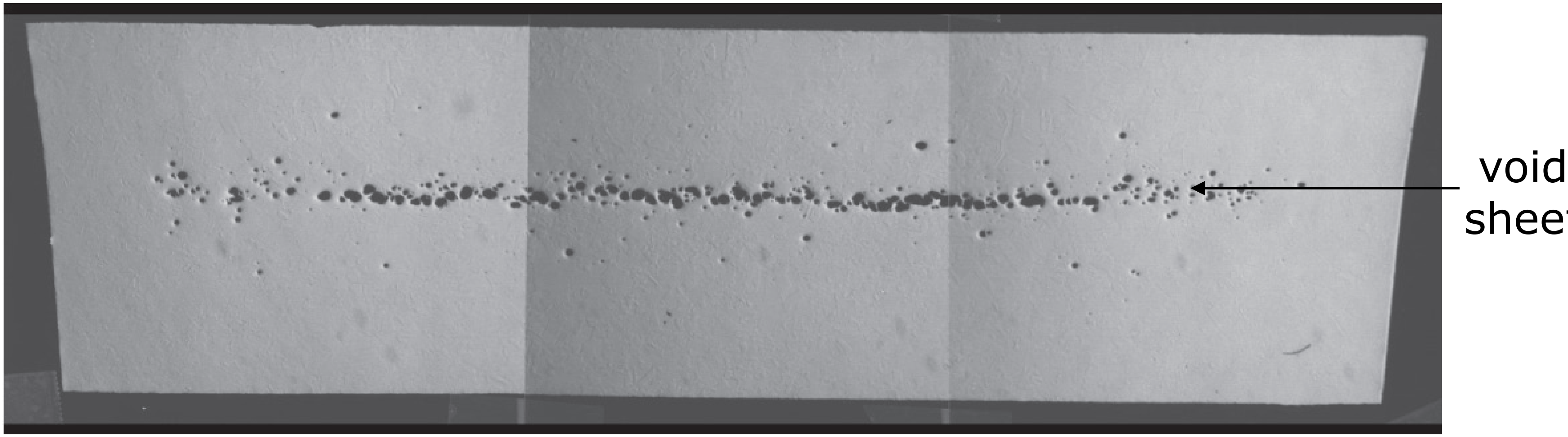
Ductile fracture: Void sheets



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

- Volume conservation is restored by opening *voids* in the band, i. e., by means of a void-sheet construction.
- The void-sheet construction is related to constructions used in the mathematical literature of *cavitation* (Sverak'88; Ball'92; Müller & Spector'95; Conti & de Lellis'03; Henau & Mora-Corral'10).

Ductile fracture: Upper bound

Theorem (L. Fokoua, S. Conti & MO'2014)

Let $\Omega = L\,\mathbb{T}^2 \times (-H, H)$, $H > 1$, $\ell \in (0, 1)$, $p \in (0, 1)$, *and*

$$E(y) \sim \int_\Omega \Big(|Dy(x)|^p + \ell |D^2 y(x)| \Big)\, dx.$$

Fix $\delta > 0$. *For every* ℓ *sufficiently small, there is a map* $y : \Omega \to \mathbb{R}^3$ *such that* $y_3(x_1, x_2, \pm H) = \pm(H + \delta)$ *for all* $(x_1, x_2) \in L\,\mathbb{T}^2$ *and such that*

$$E(y) \leq C(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}},$$

independently of H, *where, explicitly,*

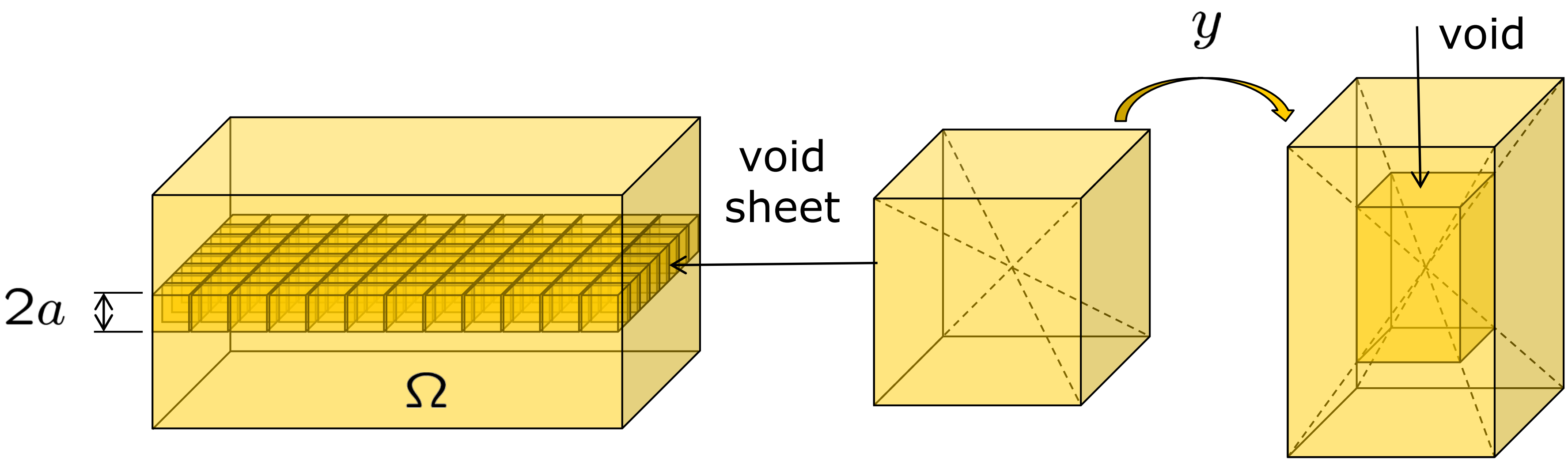
$$C(p) = C \left((1-p)^{\frac{1}{2-p}} + (1-p)^{\frac{p-1}{2-p}} \right),$$

and $C > 0$ *is a universal constant.*

L. Fokoua, S. Conti & MO, *ARMA*, **212** (2014) 331–357.

Upper bound: Sketch of proof

- Void-sheet construction:



- Calculate, estimate: $E \leq CL^2 \left(a^{1-p}\delta^p + \ell\delta/a\right)$.
- Optimize thickness: $a_{\rm opt} \sim \ell^{\frac{1}{2-p}} \delta^{\frac{1-p}{2-p}}$ (coarsening).
- Optimal bound: $E \leq CL^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$. QED

Ductile fracture: Lower bound

Theorem (L. Fokoua, S. Conti & MO'2014)

Let $\Omega = L\,\mathbb{T}^2 \times (-H, H)$, $H > 1$, $\ell \in (0,1)$, $p \in (0,1)$, *and*

$$E(y) \sim \int_\Omega \Big(|Dy(x)|^p + \ell |D^2 y(x)| \Big)\, dx.$$

Fix $\delta > 0$. *For every* ℓ *sufficiently small, there is a map* $y : \Omega \to \mathbb{R}^3$ *such that* $y_3(x_1, x_2, \pm H) = \pm(H + \delta)$ *for all* $(x_1, x_2) \in L\,\mathbb{T}^2$ *and such that*

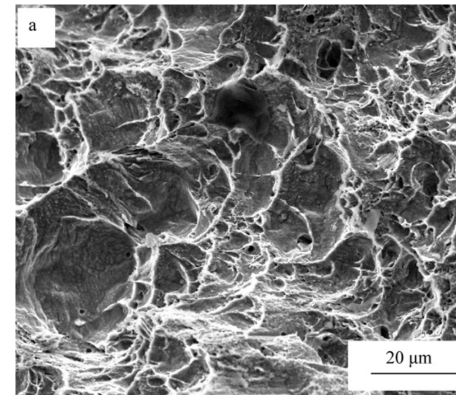
$$E(y) \geq C(p) L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}},$$

independently of H, *where, explicitly,*

$$C(p) = 2 \left(1 - \left(\frac{\sqrt{3}}{2} \right)^p \right) \left((1-p)^{\frac{1}{2-p}} + (1-p)^{\frac{p-1}{2-p}} \right).$$

L. Fokoua, S. Conti & MO, *ARMA*, **212** (2014) 331–357.

Micro-plasticity to ductile fracture: Discussion



- Optimal (matching) upper and lower bounds:

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

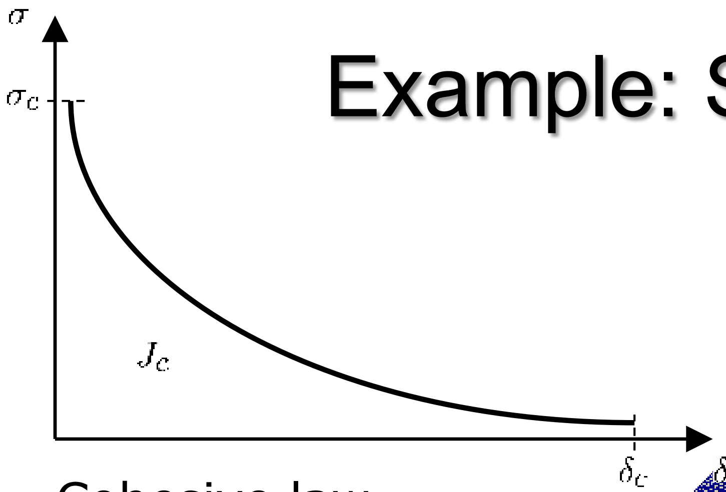
- Bounds apply to classes of materials having the same growth, specific model details immaterial!
- Energy scales with area (L^2): Fracture scaling!
- Energy scales with power of opening displ (δ): Cohesive behavior!
- Bounds degenerate when the intrinsic length ℓ decreases to zero...
- Bounds on specific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

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

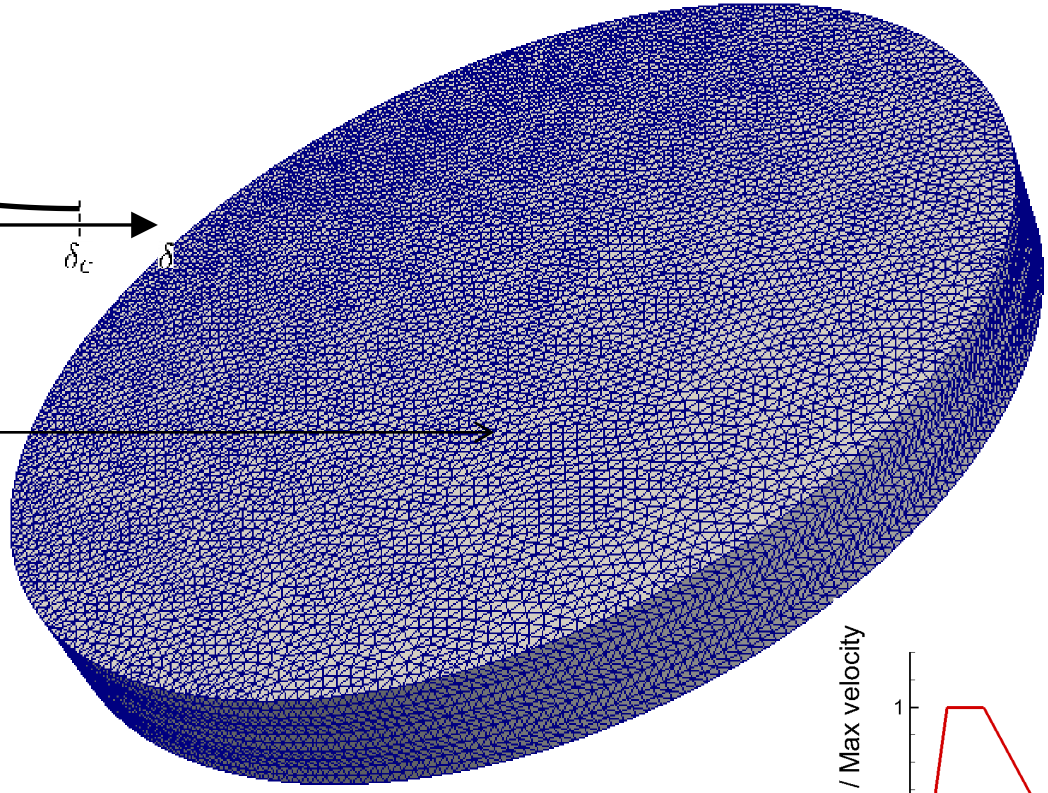
- Theory provides a link between micro-plasticity (ℓ, constants) and macroscopic fracture (J_c).

L. Fokoua, S. Conti & M. Ortiz, *JMPS*, **62** (2014) 295.

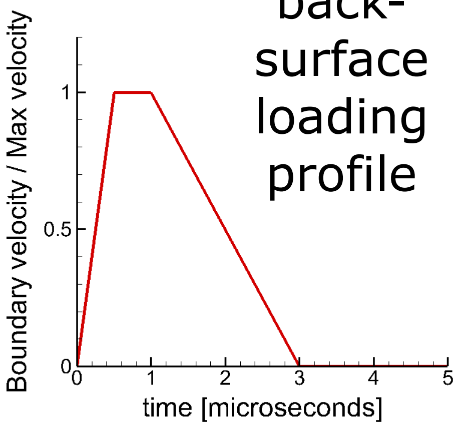
Example: Spall fracture simulations



Cohesive law determined from optimal scaling inserted using cohesive elements



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



back-surface loading profile

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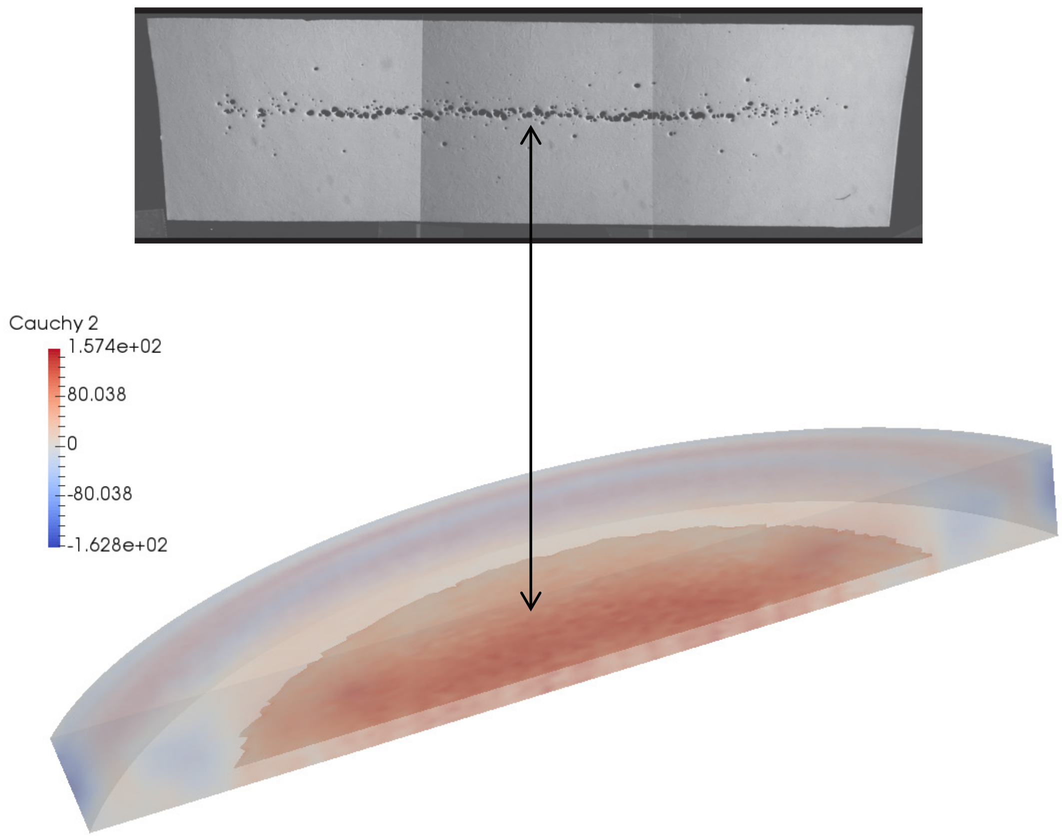
Example: Spall fracture simulations



- Visualization of cohesive element set at the end of the calculations
- Upscaled cohesive law accounts for void sheet in an effective sense

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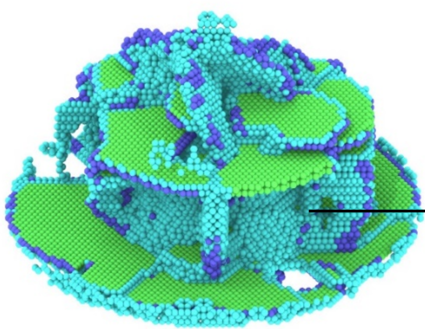
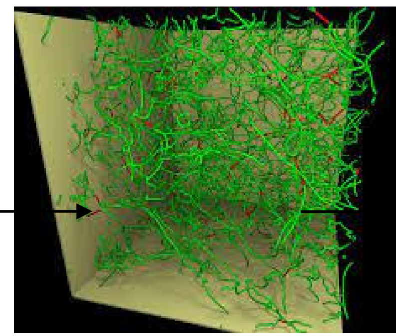
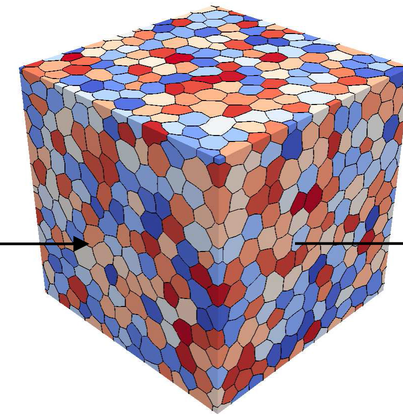
Micro-plasticity to ductile fracture: Discussion

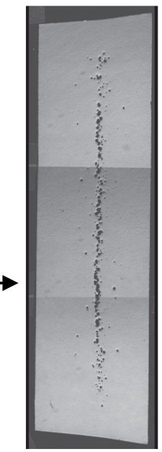
lattice parameter → 0

grain size → 0









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Critique of SGP (I): Size effect

Extreme Mechanics Letters 1 (2014) 62–69

Contents lists available at ScienceDirect

Extreme Mechanics Letters

journal homepage: www.elsevier.com/locate/eml

Micro-pillar measurements of plasticity in confined Cu thin films

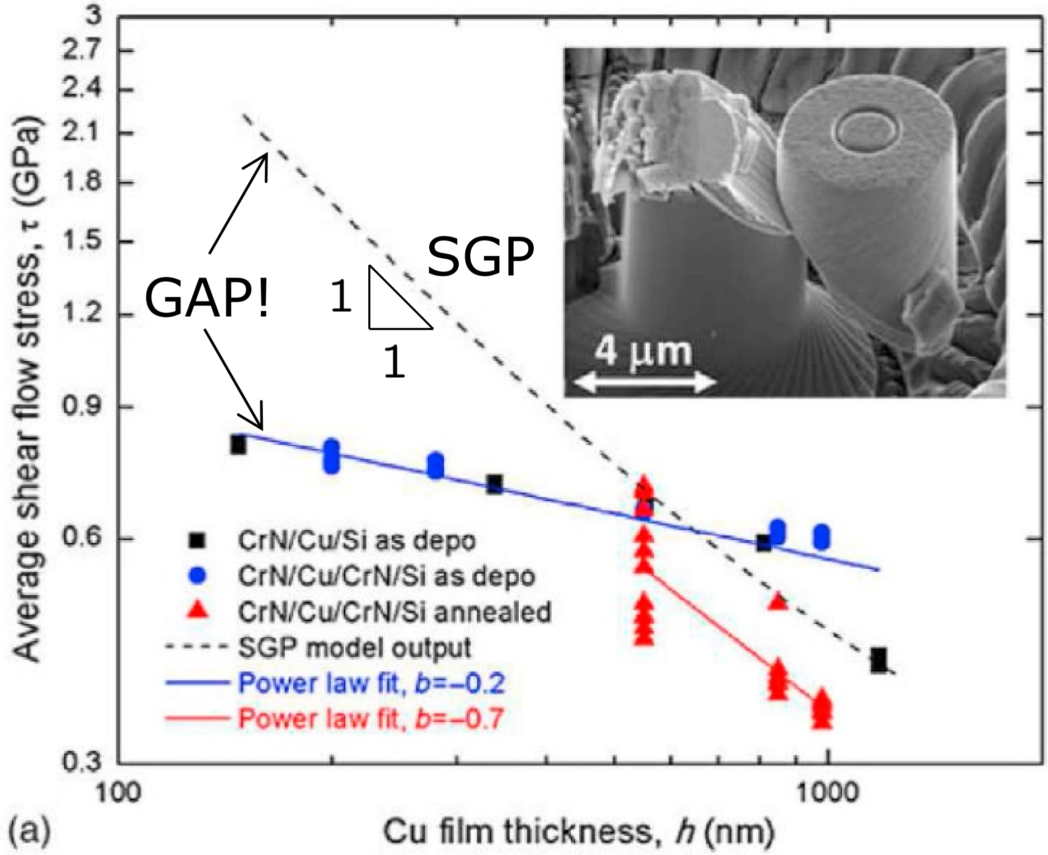
Yang Mu [a], J.W. Hutchinson [b], W.J. Meng [a,*]

[a] Department of Mechanical and Industrial Engineering, Louisiana State University, Baton Rouge, LA 70803, United States

[b] School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, United States

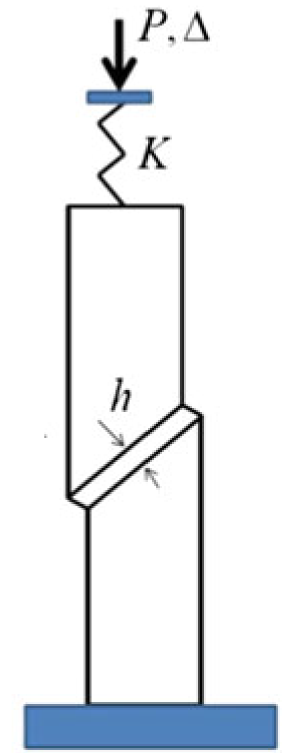
Mu, Y., Chen, K., Meng, W.J., 2014. MRS Commun. Res. Lett. 4, 126–133.
Mu, Y., Zhang, X., Hutchinson, J.W., Meng, W.J., 2016. MRS Commun. Res. Lett.20, 1–6.
Mu, Y., Zhang, X., Hutchinson, J.W., Meng, W.J., 2017. J. Mater. Res. 32 (8), 1421–1431.

Strain-gradient plasticity misses size effect!



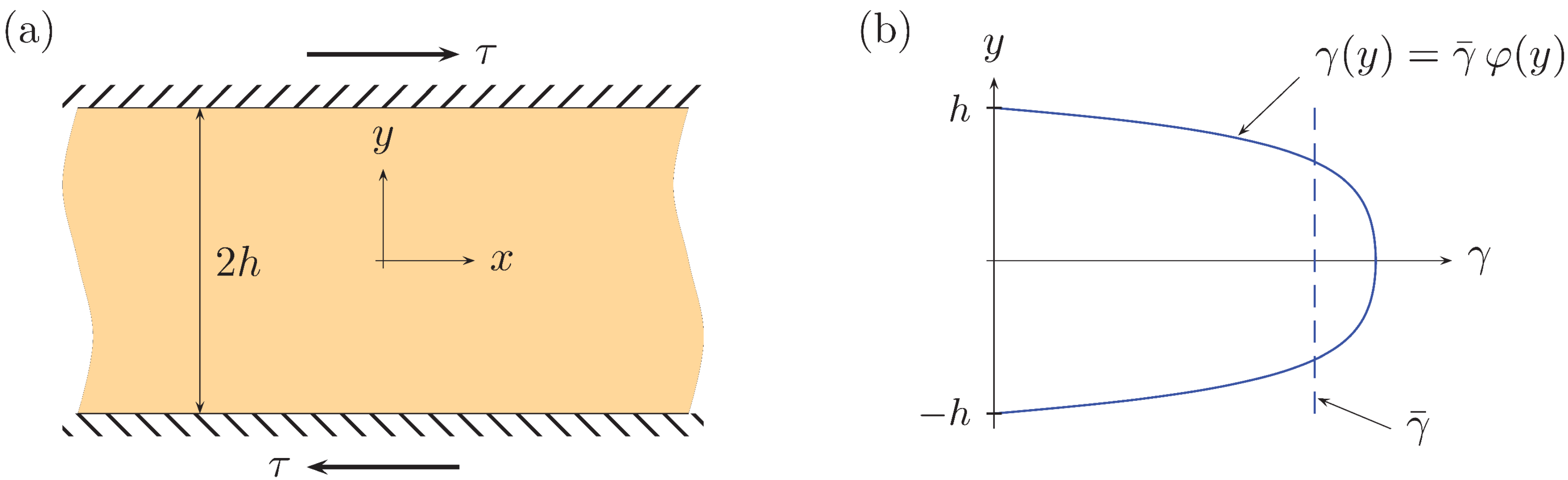
Shear flow stress as a function of thickness for Cu layers[1].
SGP model prediction shown as dashed line.
Insert shows SEM image of experimental setup.

[1]Mu, Y., Zhang, X., Hutchinson, J.W., Meng, W.J., 2016. MRS Commun. Res. Lett. 20, 1–6.



Mu, Y., Zhang, X., Hutchinson, J.W., Meng, W.J., 2017. J. Mater. Res. 32 (8), 1421–1431.

Confined layer under prescribed simple shear



- Confined layer of thickness $2h$ under prescribed simple shear:

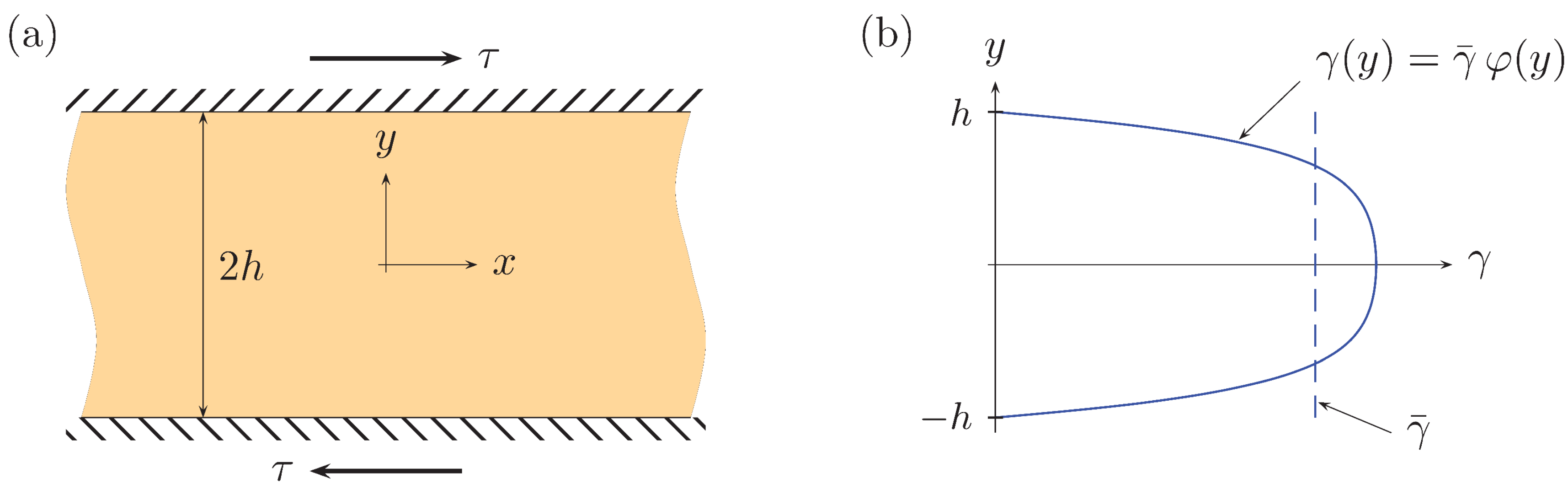
$$\text{minimize:} \quad E(\gamma) = \int_{-h}^{+h} \Big(\psi_p(\gamma(y)) + \psi_g(\gamma_{,y}(y)) \Big)\, dy,$$

$$\text{subject to:} \quad \frac{1}{2h} \int_{-h}^{+h} \gamma(y)\, dy = \bar{\gamma}, \quad \gamma(-h) = \gamma(h) = 0.$$

- Power-law hardening (growth):

$$\psi_p(\gamma) = \frac{A}{m+1} \Big|\frac{\gamma}{\gamma_0}\Big|^{m+1} + \tau_0 \gamma, \quad \psi_g(\gamma_{,y}) = \frac{B}{n+1} \Big|\frac{\ell \gamma_{,y}}{\gamma_0}\Big|^{n+1}$$

Confined layer under prescribed simple shear



- Assume $n = 0$ (nonlocal energy with linear growth):

$$E(\bar{\gamma}, \varphi) = 2h(\tau_0|\bar{\gamma}| - \tau\bar{\gamma}) + 2h\frac{AC(\varphi)}{m+1}\left|\frac{\bar{\gamma}}{\gamma_0}\right|^{m+1} + 2hB\left|\frac{\ell\bar{\gamma}}{h\gamma_0}\right|$$

- Yield condition: $\bar{\gamma} \neq 0 \Rightarrow |\tau| \geq \tau_0 + \frac{B\ell}{\gamma_0 h} \Rightarrow$ wrong size effect!
- Conventional strain-gradient plasticity over-predicts size effect!

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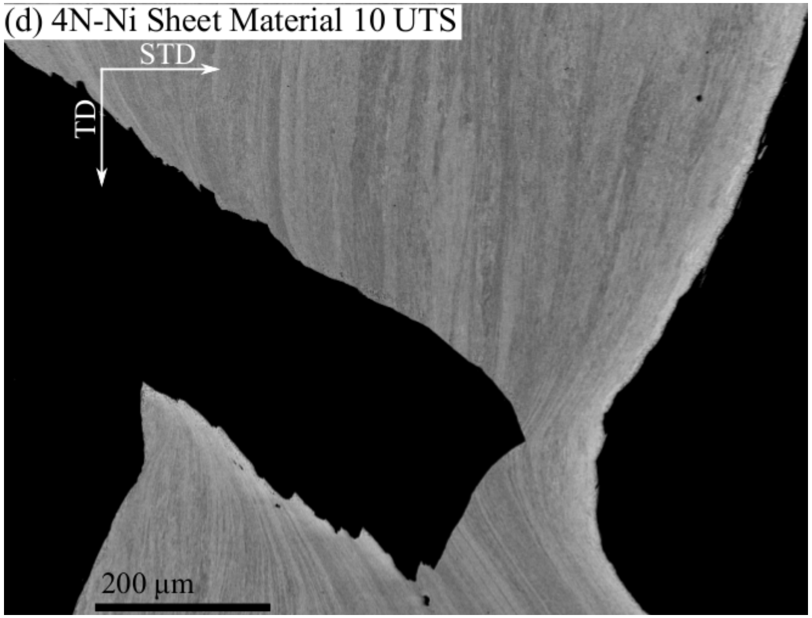
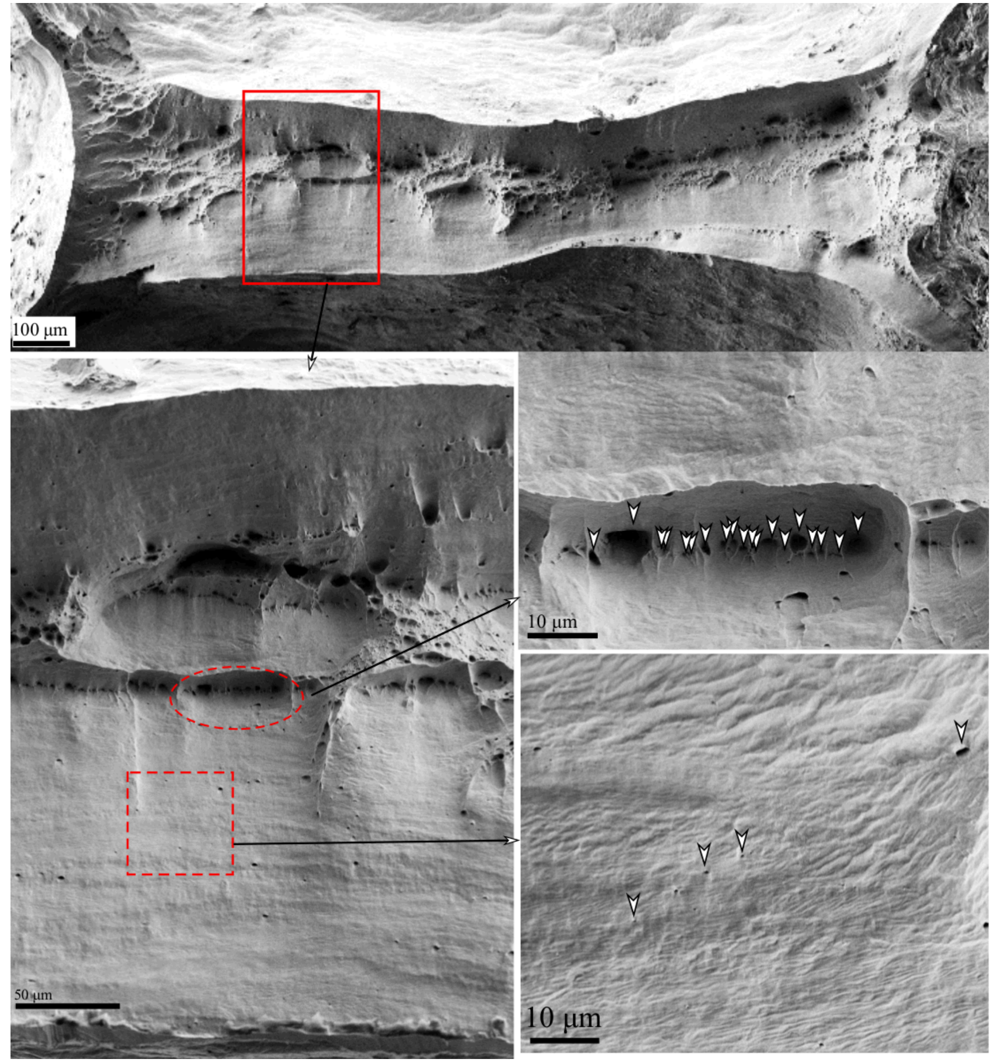
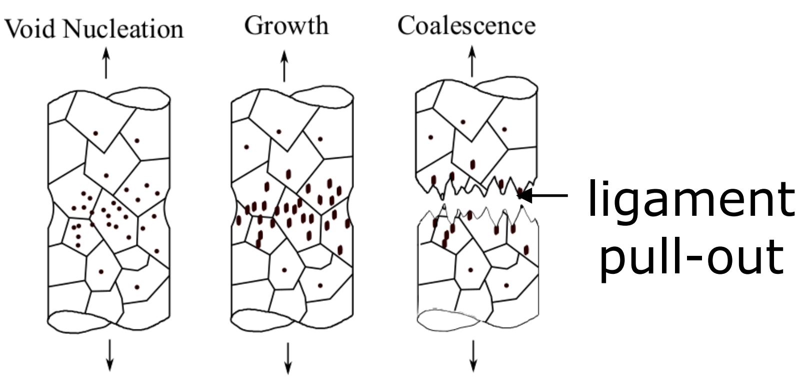
Critique of SBP (II): Final stages of fracture



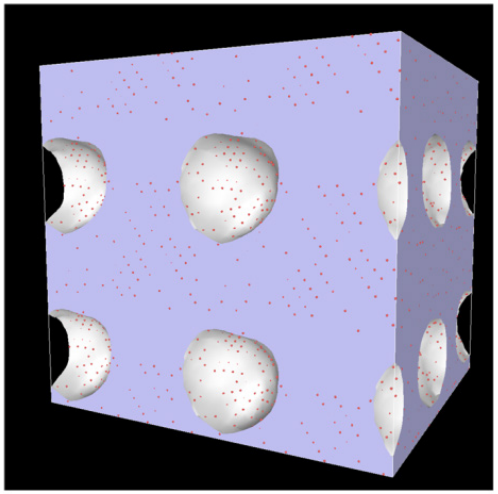


Final fracture of high-purity Ni



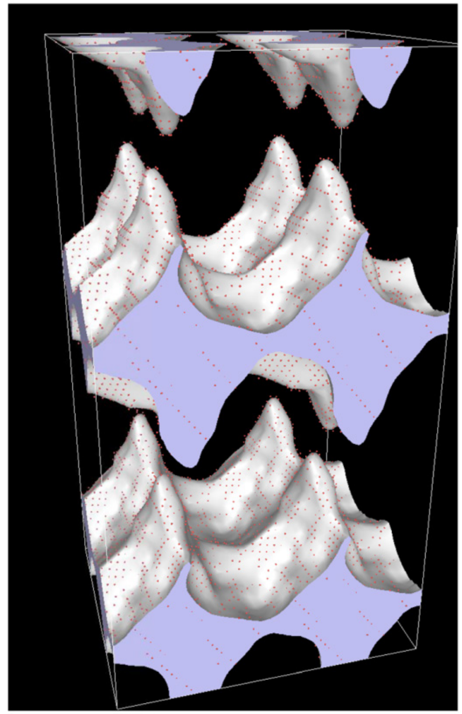
P. Noell, J. Carroll, B. Boyce, K. Hattar & B. Clark, SAND2018-2431C

Final stages of fracture in metals

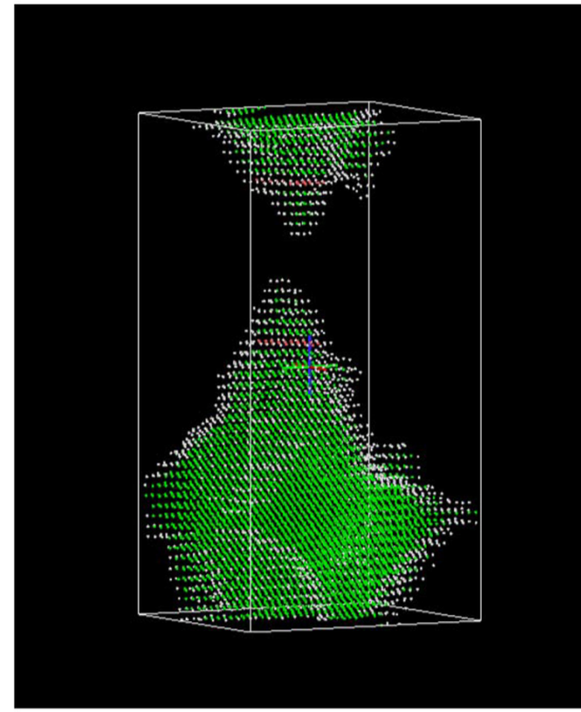


(a)

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



(b)

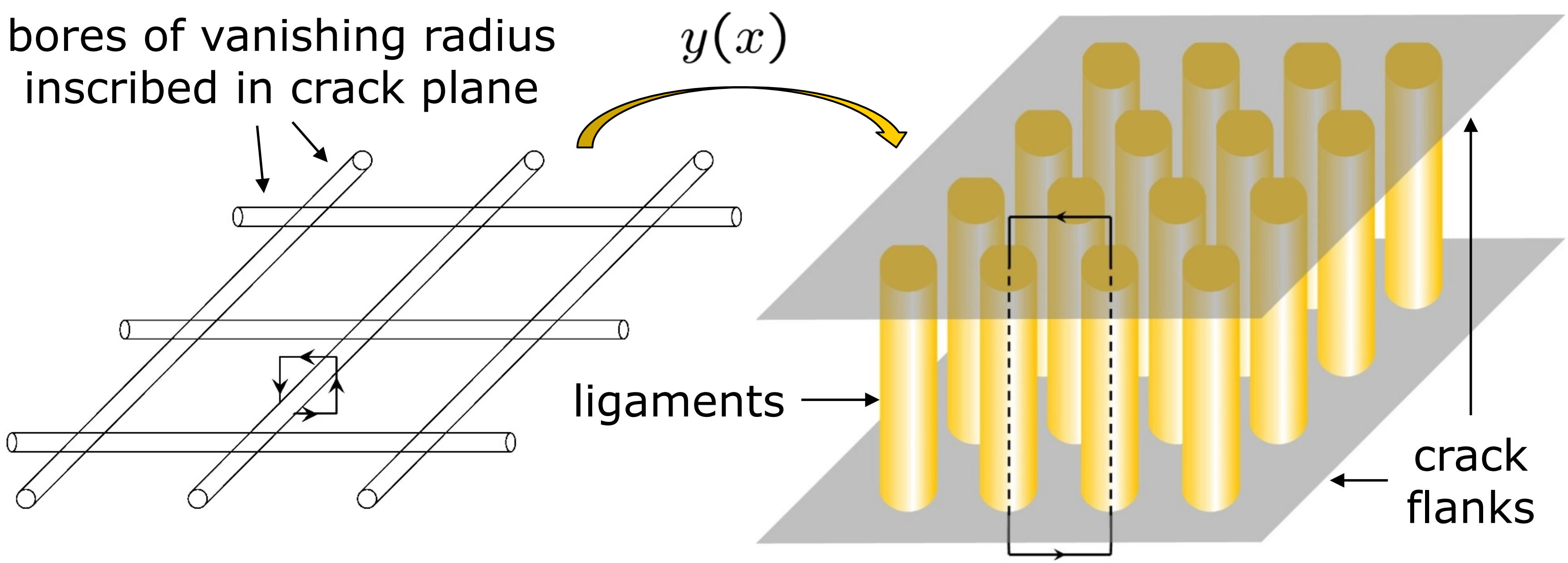


(c)

- Molecular Dynamics calculations of nano-void growth and coalescence in EAM-Ni single crystals.
- Voids coalesce to form ligaments. Final failure occurs by ligament stretching and necking to a point.

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

Ligament formation as topological transition



Lemma (S. Conti & MO'2016)

Assume Strain-gradient plasticity (SGP). Suppose bounded energy $E(y) < +\infty$. Then, the deformation mapping y is continuous.

- No topological transitions, in particular, no ligament formation.

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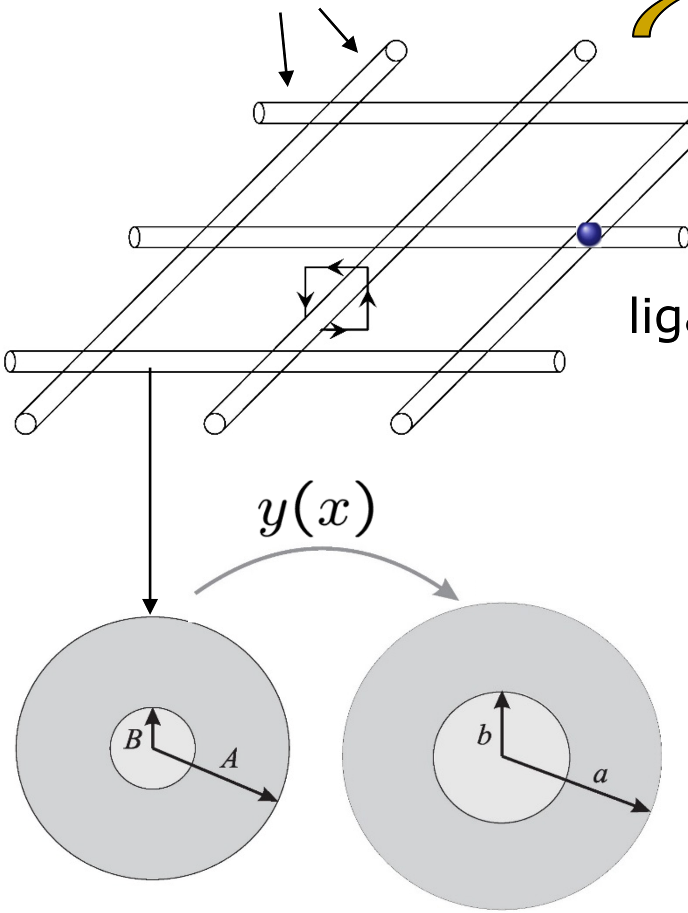
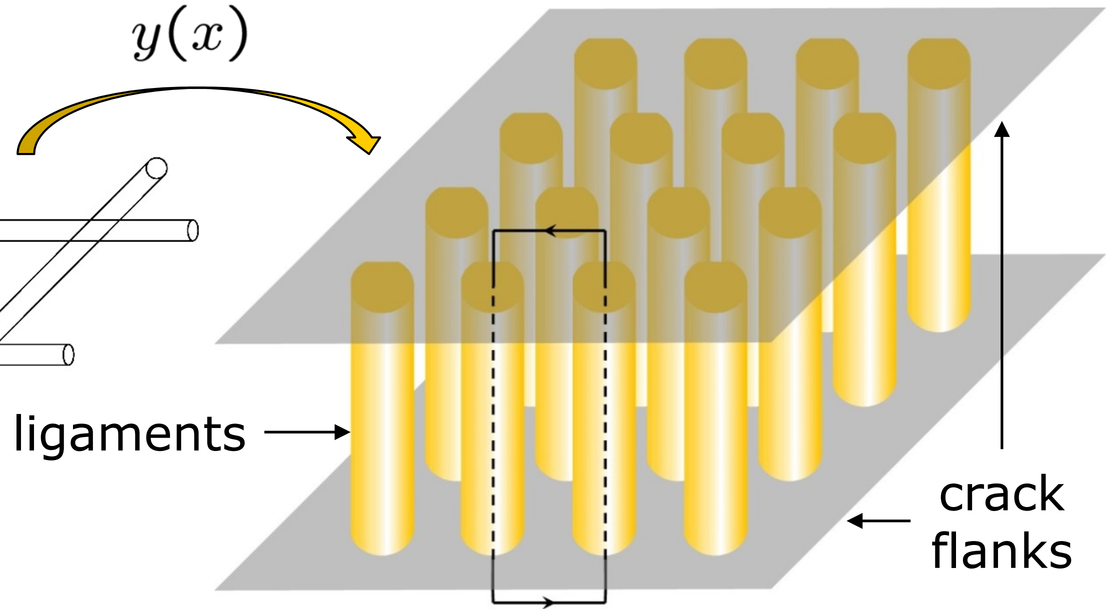
S. Conti & MO, *ARMA*, **219**(2) (2016) 607-636.

Ligament formation as topological transition

bores of vanishing radius
inscribed in crack plane





- Introduce core cutoff, radius B.
- By incompressibility, non-local energy

$$E_{\text{non}} \sim \log \frac{A}{B}$$

- Logarithmic divergence as $B \to 0$!

S. Heyden, S. Conti & MO, *Mechanics of Materials*, **90** (2015) 131.

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Fractional strain-gradient plasticity

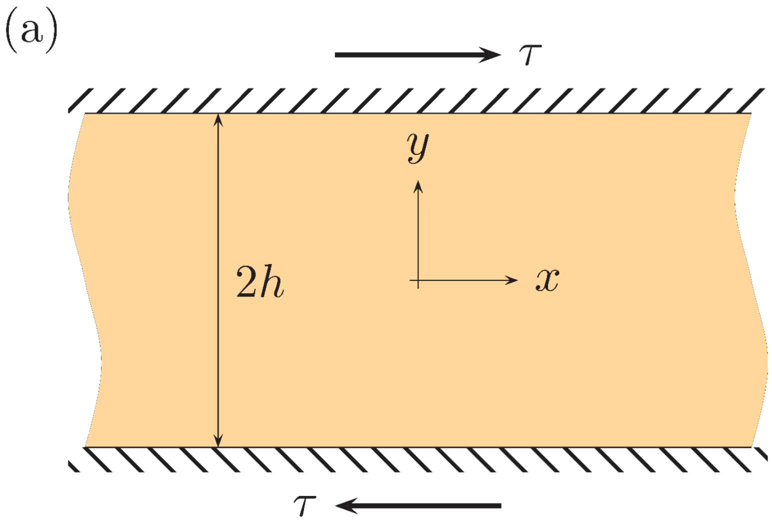
- Conventional strain-gradient plasticity (SGP) is *too stiff*:
  - Overestimates size effect relative to experiments.
  - Introduces topological obstruction that prevents ligament formation.
- Tip: Size scaling, continuous embedding, directly related to order of derivatives assumed in nonlocal energy.
- Ergo: Can eliminate the stiffness of conventional SGP by allowing for *fractional derivatives*.
- *Fractional strain-gradient plasticity* (FSGP): Assume energy growth

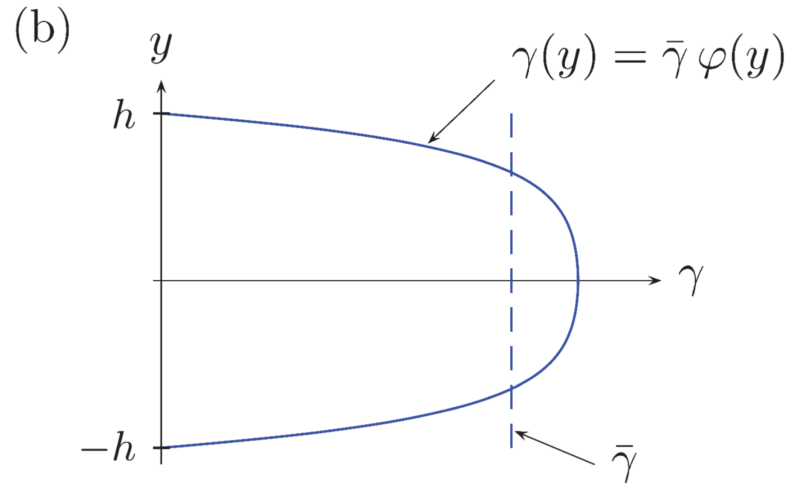
$$E(y) \sim \int_\Omega |Dy(x)|^p \, dx + \ell \, \|y\|_{1+\sigma,1}, \quad 0 \leq p < 1, \quad 0 < \sigma < 1.$$

- Recall: Gagliardo's formula,

$$\|y\|_{1+\sigma,1} \sim \int_\Omega \int_\Omega \frac{|Dy(x') - Dy(x'')|}{|x' - x''|^{d+\sigma}} \, dx' \, dx''.$$

Confined layer under prescribed simple shear





- Fractional nonlocal energy from Gagliardo's formula ($n = 0$):

$$\Psi_{\mathrm{g}}(\varepsilon) = \int_\Omega \int_\Omega B \frac{\ell^\sigma}{\varepsilon_0} \frac{|\varepsilon(x') - \varepsilon(x'')|}{|x' - x''|^{d+\sigma}}\, dx'\, dx''.$$

- Assume $n = 0$ (nonlocal energy with linear growth):

$$E(\bar{\gamma}, \varphi) = 2h(\tau_0|\bar{\gamma}| - \tau\bar{\gamma}) + 2h\frac{AC(\varphi)}{m+1}\left|\frac{\bar{\gamma}}{\gamma_0}\right|^{m+1} + 2hB\left|\frac{\ell^\sigma \bar{\gamma}}{h^\sigma \gamma_0}\right|$$

- Yield condition: $\bar{\gamma} \neq 0 \Rightarrow |\tau| \geq \tau_0 + \dfrac{B\ell^\sigma}{\gamma_0 h^\sigma}$

can match size scaling exactly!

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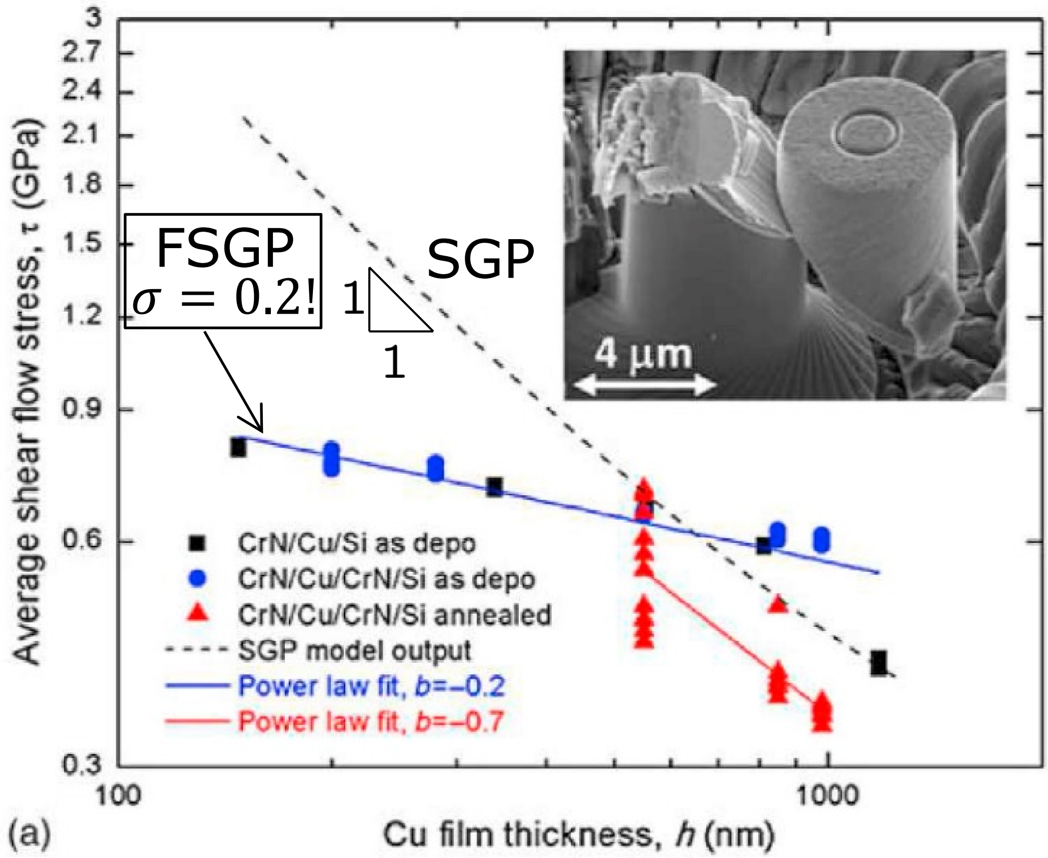
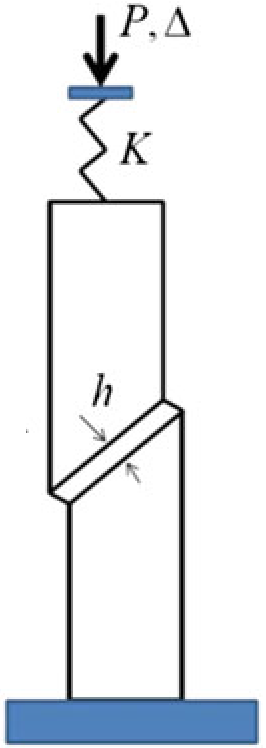
Fractional strain-gradient plasticity can match size scaling



Shear flow stress as a function of thickness for Cu layers[1].
SGP model prediction shown as dashed line.
Insert shows SEM image of experimental setup.



Mu, Y., Zhang, X., Hutchinson, J.W., Meng, W.J., 2017. J. Mater. Res. 32 (8), 1421–1431.

[1]Mu, Y., Zhang, X., Hutchinson, J.W., Meng, W.J., 2016. MRS Commun. Res. Lett. 20, 1–6.

Ductile fracture revisited: FSGP

Theorem (Upper bound, adapted from S. Conti & MO'2016)

Let $p \in [0,1)$, $\sigma \in (0,1)$, $H, L, \delta > 0$, with $0 \leq \ell \leq \delta \leq L$. Then, there is $y \in W^{1,1}_{\text{loc}}(\mathbb{R}^3;\mathbb{R}^3)$ such that $y(x) = x \pm \delta e_3$ for $\pm x_3 \geq H$, y is $(0,L)^2$-periodic in the first two variables and

$$E(y) \leq C L^2 \ell^{\frac{\sigma(1-p)}{1+\sigma-p}} \delta^{\frac{1-(1-\sigma)p}{1+\sigma-p}} .$$

The constant C depends only on p and σ.

Theorem (Lower bound, adapted from S. Conti & MO'2016)

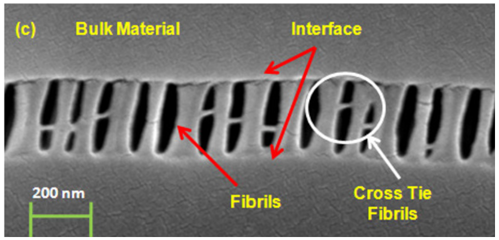
Let $p \in [0,1)$, $\sigma \in (0,1)$, $H, L, \delta > 0$, let $\Omega = (0,L)^2 \times (-H,H)$. Then for sufficiently small ℓ we have

$$C L^2 \ell^{\frac{\sigma(1-p)}{1+\sigma-p}} \delta^{\frac{1-(1-\sigma)p}{1+\sigma-p}} \leq E(y),$$

for any $y : \Omega \to \mathbb{R}^3$ such that $y_3(x) = \pm(H+\delta)$ for $x_3 = \pm H$. The constant $C > 0$ depends only on p.

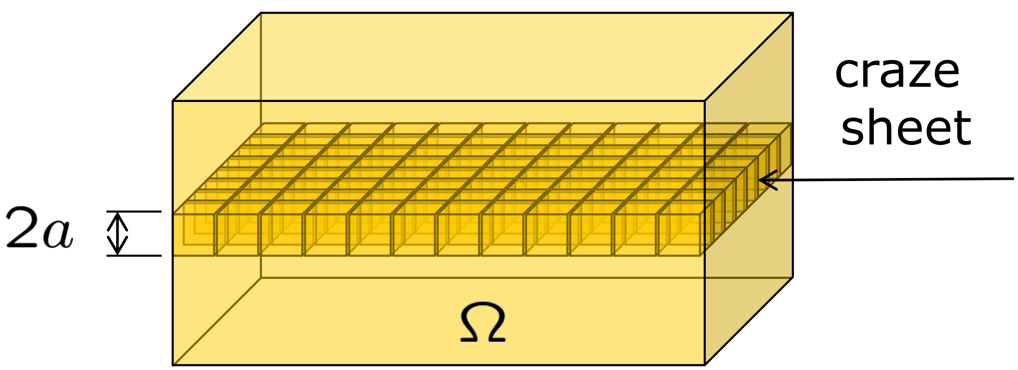
S. Conti & MO, *ARMA*, **219** (2016) 607–636

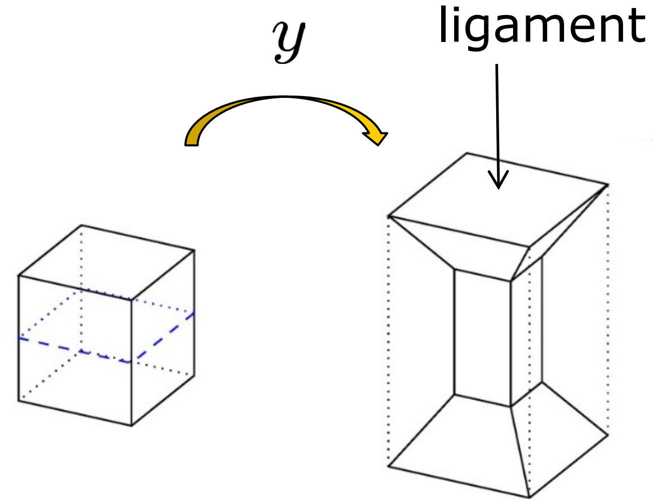
Upper bound: Sketch of proof



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

- Crazing construction:





- Calculate, estimate: $E \leq CL^2\left(a^{1-p}\delta^p + \ell^\sigma \delta / a^\sigma\right).$
- Optimize thickness: $a_{\text{opt}} \sim \ell^{\frac{\sigma}{\sigma+1-p}}\,\delta^{\frac{1-p}{\sigma+1-p}}$ (coarsening).
- Optimal bound: $E \leq CL^2 \ell^{\frac{\sigma(1-p)}{1+\sigma-p}}\,\delta^{\frac{1-(1-\sigma)p}{1+\sigma-p}}.$ QED

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Fractional micro-plasticity to ductile fracture

- Optimal (matching) upper and lower bounds:

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

- Bounds apply to classes of materials having the same growth, fractional differentiation order.
- Energy scales with area (L^2): Fracture scaling!
- Energy scales with power of opening displ (δ): Cohesive behavior!
- Bounds degenerate when the intrinsic length ℓ decreases to zero.
- Bounds degenerate when $\sigma \to 0$ and $\sigma \to 1$.
- Bounds on specific fracture energy:

$$C_L(p,\sigma)\ell^{\frac{\sigma(1-p)}{1+\sigma-p}}\delta^{\frac{1-(1-\sigma)p}{1+\sigma-p}} \leq J_c \leq C_U(p,\sigma)\ell^{\frac{\sigma(1-p)}{1+\sigma-p}}\delta^{\frac{1-(1-\sigma)p}{1+\sigma-p}}.$$

- Theory provides a link between micro-plasticity (ℓ, σ, constants) and macroscopic fracture (J_c).

Concluding remarks

- *Optimal scaling provides a practical avenue for traversing length scales, from micro-plasticity to ductile fracture.*
- Optimal scaling exponents depend only on the *growth properties* of the constitutive equations, other details get 'buried' in the upper and lower-bound constants
- *Fractional strain-gradient plasticity* (FSGP) provides a way of removing the excessive rigidity of conventional strain-gradient plasticity (SGP) and match observed *size scaling*
- *Physical origin of fractional derivatives? Connections to dislocation mechanics?*
- *Numerical implementation of FSGP?*

Thank you!

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