



# Plasticity and fracture of polycrystalline metals

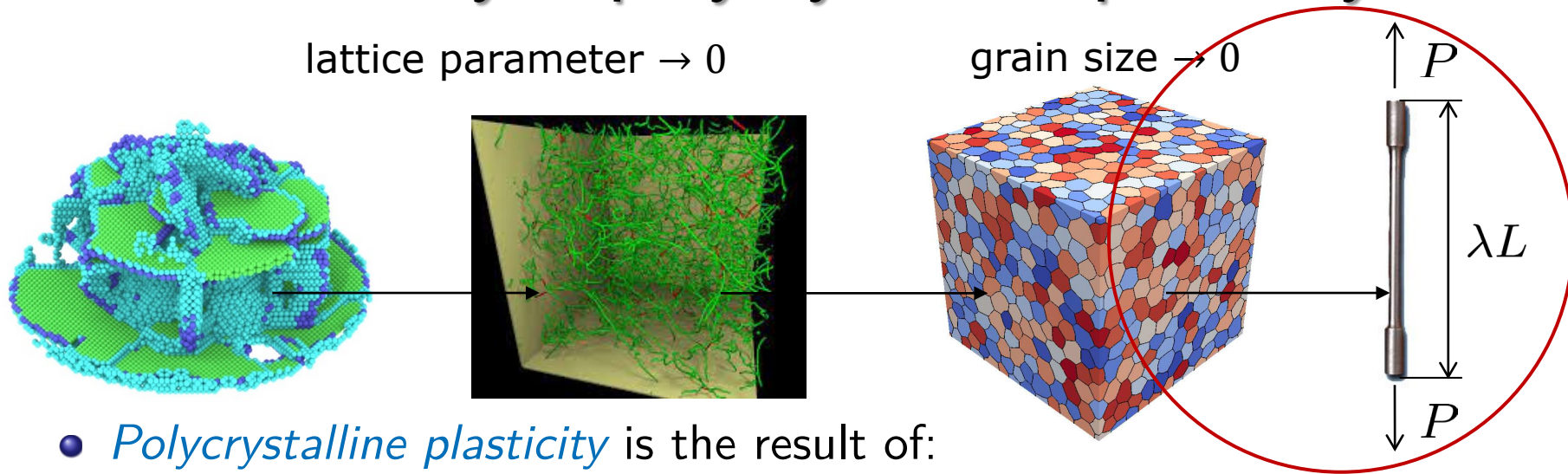
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In collaboration with S. Conti (Universität Bonn)

Workshop on  
Polycrystals: Microstructure and Plasticity  
ICMS, The Bayes Centre, Edinburgh (UK)  
19-22 April 2022

# Taxonomy of polycrystalline plasticity



- *Polycrystalline plasticity* is the result of:
  - Subgrain single-crystal plasticity:
    - Energy: Elasticity, dislocation core (logarithmic divergence).
    - Dissipation: Dislocation motion (Peach-Köhler, crystallography).
    - Confinement: Subgrain dislocation structures (Hall-Petch effect)
  - Texture evolution and polycrystalline averaging.
  - Finite kinematics: *Geometrical softening*, necking, cavitation.
- General *aims and means*:
  - Build *effective theories* of polycrystalline plasticity and fracture.
  - Identify unit mechanisms, multiscale hierarchies (space and time).
  - Apply tools of the *modern Calculus of Variations*

# General problems of evolution

- System with states  $u$  in  $X$ , rates  $v$  in  $Y$ , linear spaces.
- Trajectories  $u : [0, T] \rightarrow X$  in  $X$ ,  $v : [0, T] \rightarrow Y$  in  $Y$ , linear spaces.
- Rate functional:  $G : [0, T] \times X \times Y \rightarrow \overline{\mathbb{R}}$  (energy + dissipation).
- Special case:  $G(t, u, v) = \Psi(v) + \langle DE(t, u), v \rangle$ , with
  - Energy functional:  $E : [0, T] \times X \rightarrow \overline{\mathbb{R}}$ .
  - Dissipation potential:  $\Psi : Y \rightarrow \overline{\mathbb{R}}$ .
- Rate problem: Find  $u \in X$ ,  $v \in Y$ , s. t., for a. e.  $t \in [0, T]$ ,
$$v(t) \in \operatorname{argmin} G(t, u(t), \cdot),$$
$$u(t) = u_0 + \int_0^t v(t') dt'.$$
- Aim: Reformulate (time-dependent) evolutionary problems in a weak form enabling consideration of *evolving microstructures*.

# Weighted Energy-Dissipation functionals

- Aim: Reformulate (time-dependent) evolutionary problems in a weak form enabling consideration of *evolving microstructures*.
- Express the evolutionary problem in variational form: Identify a functional whose minimizers are *entire trajectories* of the system.
- *Weighted energy-dissipation* (WED) functional,

$$F_{\epsilon}(u) = \int_0^T e^{-t/\epsilon} G(t, u(t), \dot{u}(t)) dt$$

- WED functional:
  - 'Strings' all rate problems together into a single functional.
  - Weighs past overwhelmingly more than future (*arrow of time*).
- Causal trajectories:  $u = \lim_{\epsilon \downarrow 0} u_{\epsilon}$ , with  $u_{\epsilon} \in \operatorname{argmin} F_{\epsilon}$ .

# Causal trajectories are energetic solutions

## Theorem (A. Mielke & MO'2008)

Let  $X$  Banach, reflexive, separable,  $X \subset\subset Y$ . Suppose that:

- i)  $\Psi$  convex, 1-homogeneous, coercive in  $Y$ .
- ii)  $E$  weakly lower-semicontinuous and coercive in  $X$ .
- iii) Control of power:  $|\partial_t E(t, u)| \leq cE(t, u) + b$ .

Then:

- iv) Sequences  $(u_\varepsilon)$  of minimizers are weakly precompact in  $X$ .
- v) Limit points  $u \in X$  are solutions of the *energetic formulation*:

$$(S) \quad \forall y \in X: E(t, u(t)) \leq E(t, y) + \Psi(y - u(t)),$$

$$(E) \quad E(t, u(t)) + \int_{[0,t]} \Psi(du) = E(0, u(0)) + \int_0^t \partial_s E(s, u(s)) ds.$$

# Deformation theory of plasticity

- The problem of microstructure evolution for arbitrary loading histories, including changes in loading direction, is largely open.
- Suppose that there is  $M \subset X$  and a function  $E : [0, T] \times X \rightarrow \overline{\mathbb{R}}$  such that

$$u \in M \Rightarrow G\left(t, u(t), \dot{u}(t)\right) = \frac{d}{dt} E\left(t, u(t)\right).$$

- For  $u \in M$ , an integration by parts gives

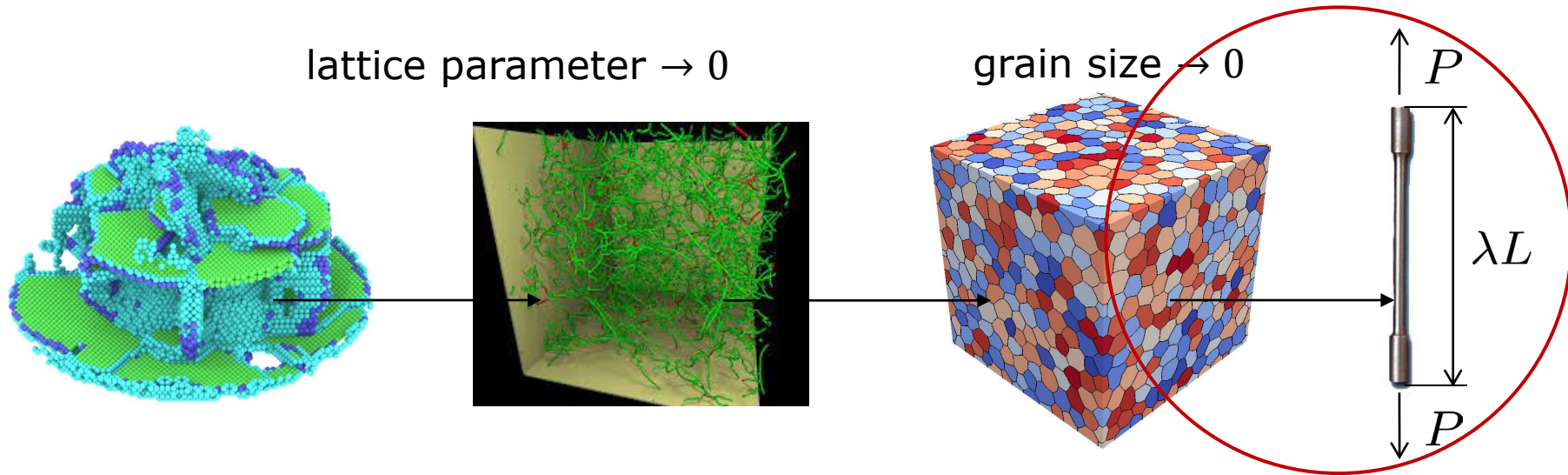
$$F_\epsilon(u) = \int_0^T \frac{1}{\epsilon} e^{-t/\epsilon} E(u(t), t) dt + \left[ e^{-t/\epsilon} E(u(t), t) \right]_0^T.$$

- *Deformation-theory problem:*

- Time-wise minimization:  $u(t) \in \operatorname{argmin}\{E(t, \cdot)\}$ ,  $t \in [0, T]$ .
- Verify monotonicity condition  $u \in M$  *a posteriori*.

Then,  $u$  causal trajectory and solution of the evolutionary problem.

# Micro-to-macro: Effective problem



- Multiscale hierarchy: Complete  $\Gamma$ -limit  $E(y)$  not known.
- *Ansatz* for effective macroscopic problem (deformation theory):

Minimize:  $E(y) = \int_{\Omega} W(Dy(x)) dx + \text{forcing terms},$   
 subject to:  $\det(Dy(x)) = 1, \quad \text{a. e. in } \Omega.$

- NB: For *optimal scaling*, need only know growth  $W(F) \sim |F|^p$ .
- NB: Existence of solutions for  $p > d$  (Mielke & Müller'2006).



# Local deformation theory: Growth

- Deformation theory: Minimize

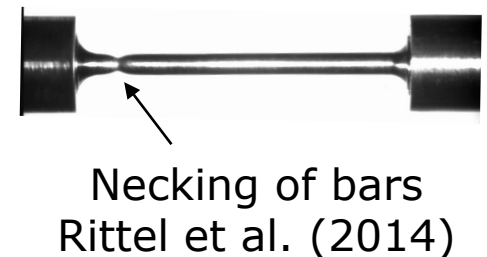
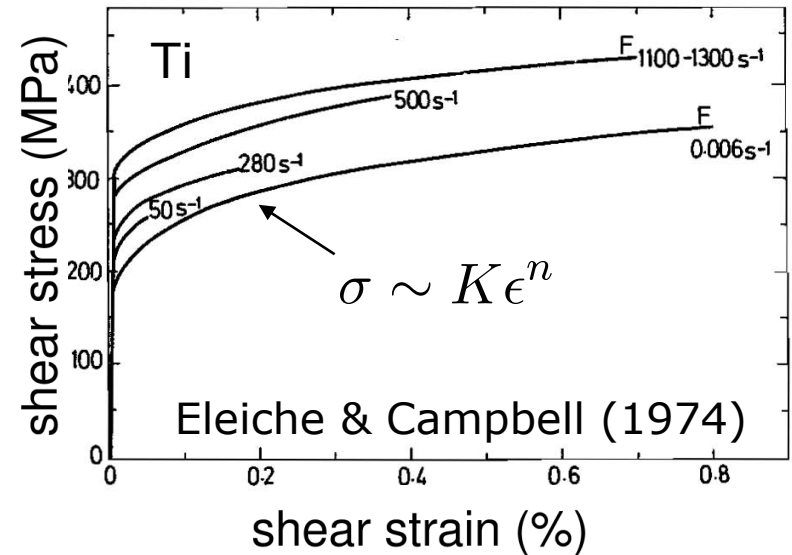
$$E(y) = \int_{\Omega} W(Dy(x)) \, dx,$$

$y : \Omega \rightarrow \mathbb{R}^d$ , 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  $\lambda$ :  $\partial_{\lambda} W \sim K \lambda^{n-1} \Rightarrow W \sim K \lambda^n$ .
- Compare with  $W(F) \sim |F|^p$ ,  $p = n \in (0, 1)$ .
- Considère analysis  $\Rightarrow$  **Sublinear growth!** ( $p < 1$ ).





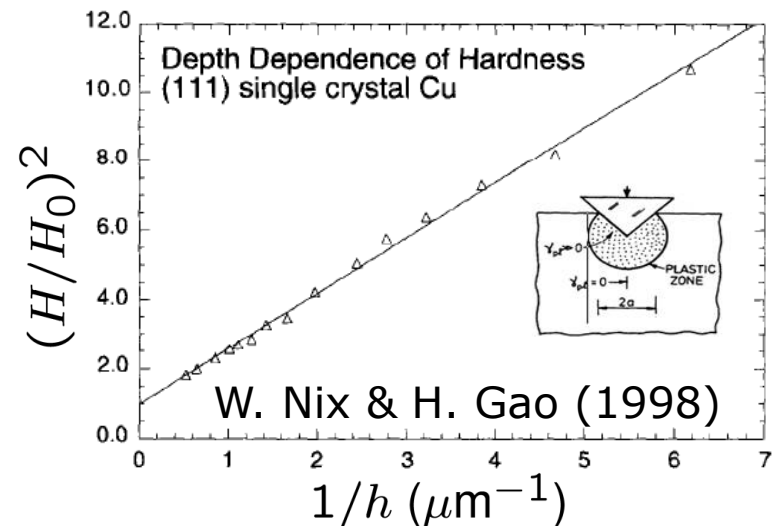
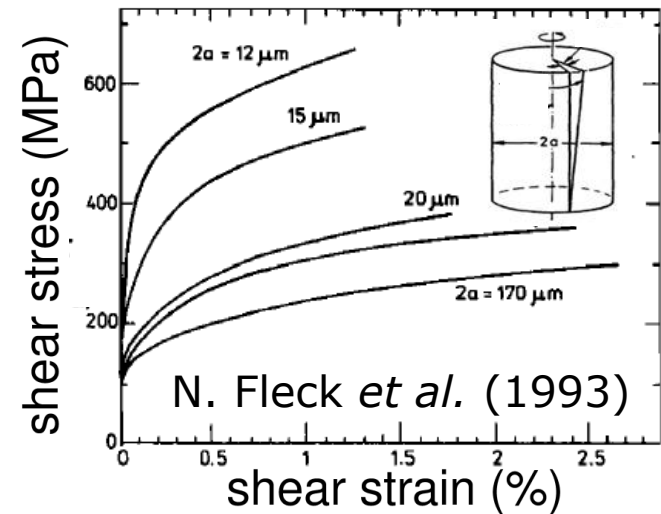
# Strain-gradient plasticity

- 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

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

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

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



# Growth w.r.t. strain gradient: Heuristics

- Example: Fence structure,

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

- Across jump set  $\Sigma$ :

$$||F|| = 2 \sin \theta.$$

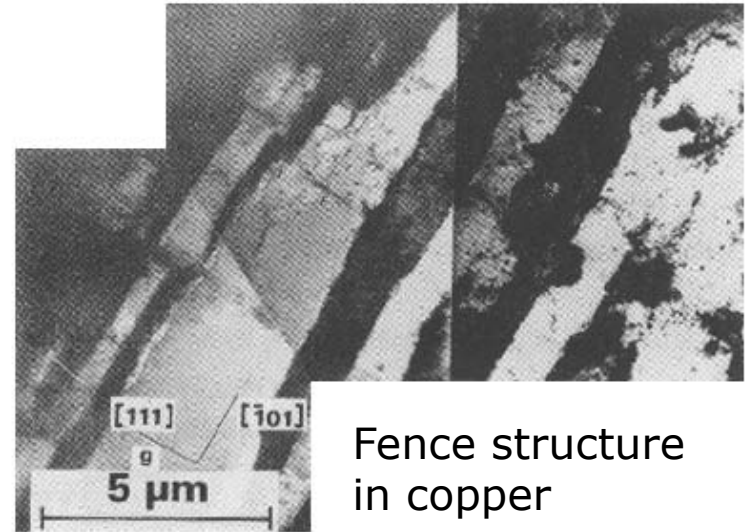
- From line-tension approximation,

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

- Strain-gradient:

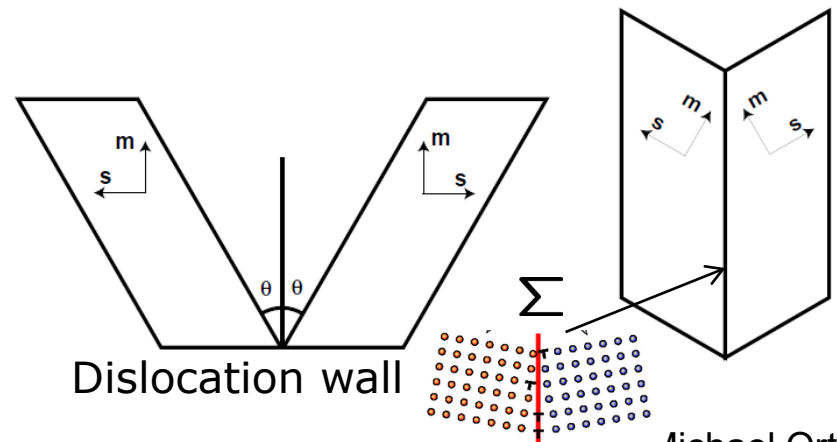
$$|DF| = ||F|| \mathcal{H}^2 \llcorner \Sigma.$$

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



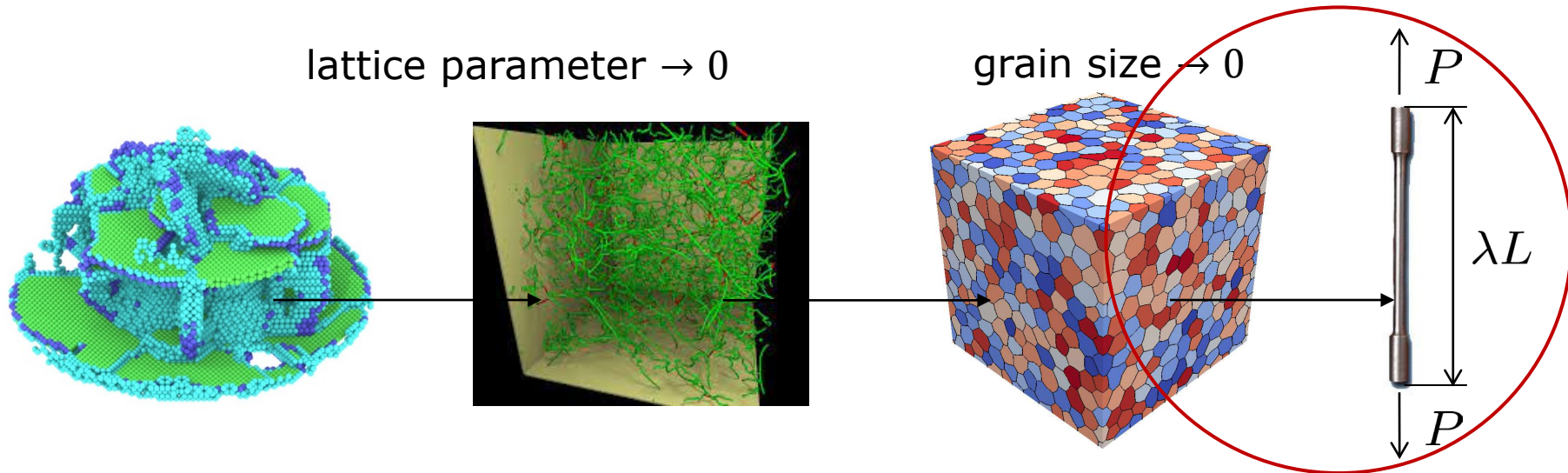
Fence structure  
in copper

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



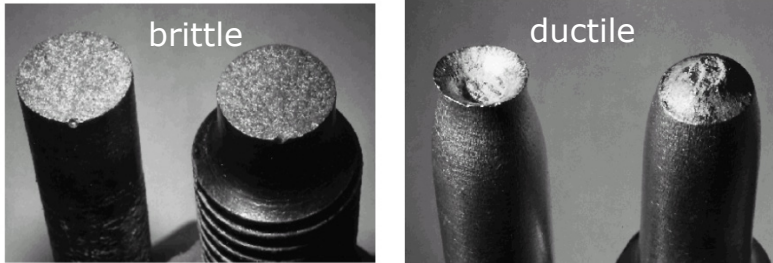
Dislocation wall

# Micro-to-macro: Effective problem

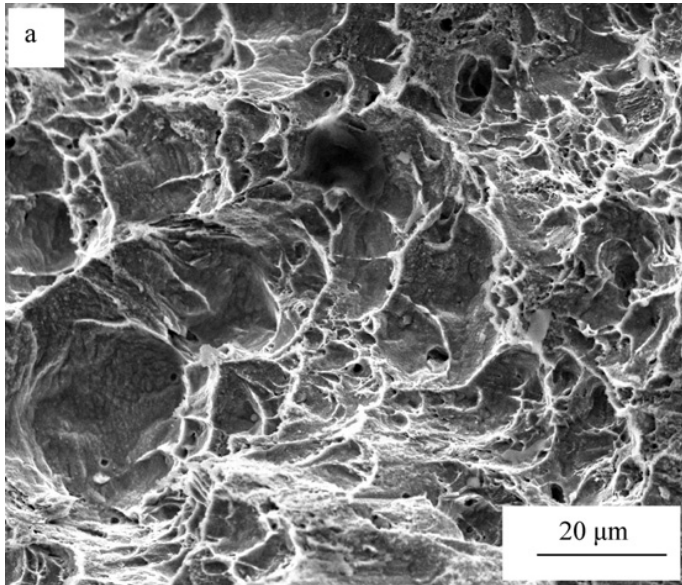


- *Ansatz*: Macroscopic deformation-theoretical problem of the form  
 Minimize:  $E(y) = \int_{\Omega} W(Dy(x), D^2y(x)) dx + \text{forcing terms},$   
 subject to:  $\det(Dy(x)) = 1, \quad \text{a. e. in } \Omega.$
- Expected growth properties (experimental, heuristics):
  - $W(\cdot, DF)$  sublinear: Promotes localization.
  - $W(F, \cdot)$  linear: Opposes localization.
- What is the net macroscopic result of the competition between local and non-local energies?

# Strain-gradient plasticity and fracture



(Courtesy NSW HSC online)



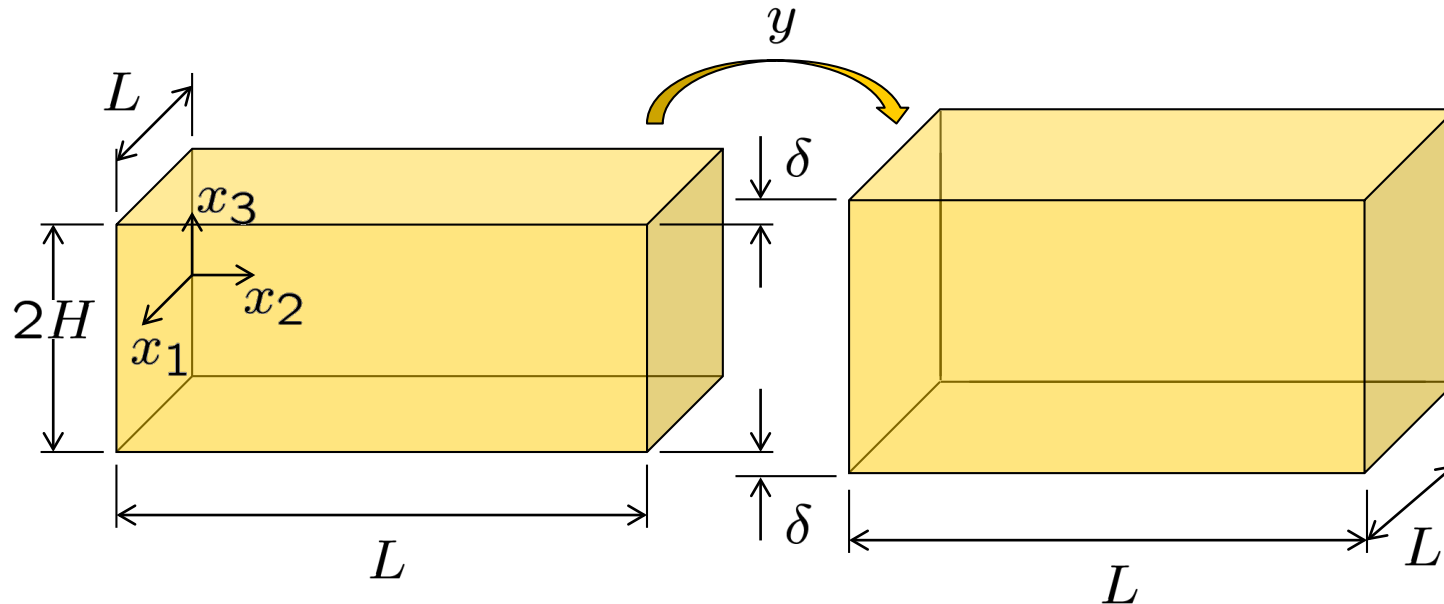
Fracture surface in SA333 steel,  
room temp.,  $d\epsilon/dt = 3 \times 10^{-3} s^{-1}$

(S.V. Kamata, M. Srinivasa and P.R. Rao,  
*Mater. Sci. Engr. A*, **528** (2011) 4141–4146)

- 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 and dissipation.
- Can ductile fracture be understood as the result of a competition between sublinear growth and strain-gradient plasticity?

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ICMS 2022

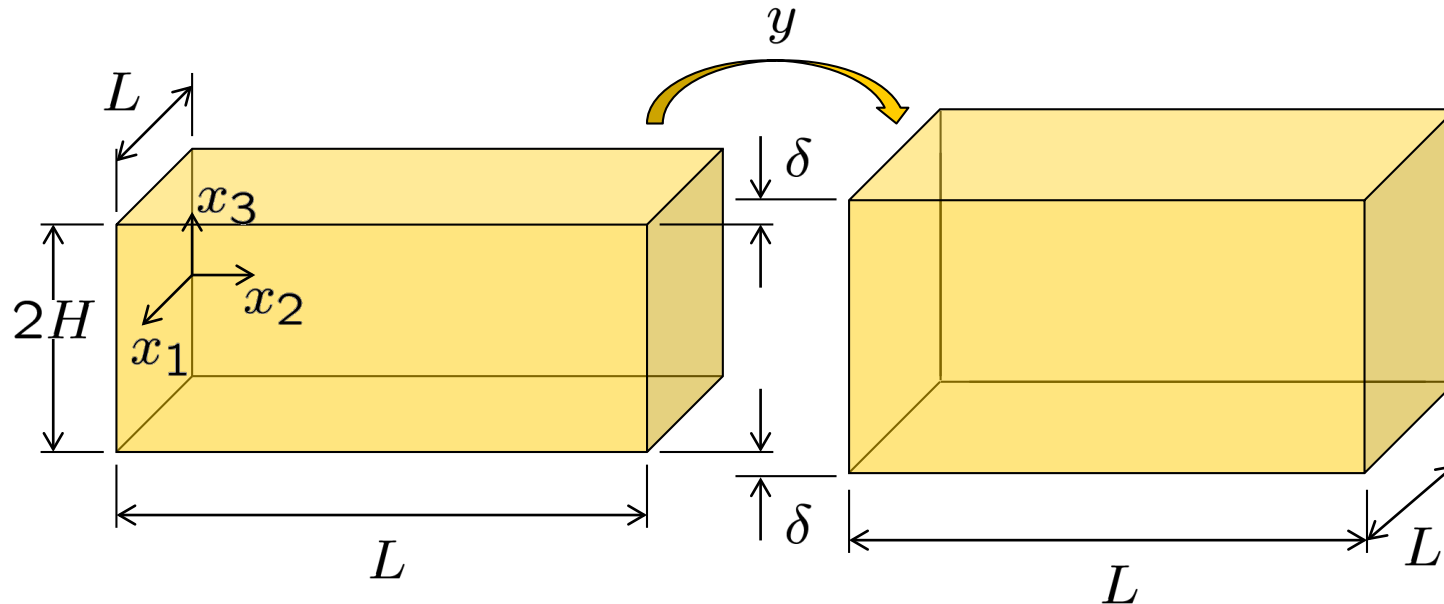
# Ductile fracture: Optimal scaling



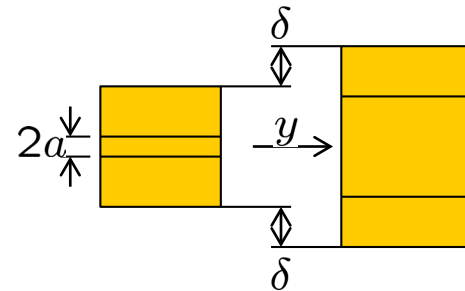
- Slab:  $\Omega = [0, L]^2 \times [-H, H]$ , in-plane periodic.
- Deformation  $y \in W^{1,1}(\Omega; \mathbb{R}^3)$  and  $Dy \in BV(\Omega; \mathbb{R}^{3 \times 3})$ ,  

$$\det Dy(x) = 1, \quad \text{a. e. in } \Omega.$$
- Uniaxial extension:  $y_3(x_1, x_2, \pm H) = \pm(H + \delta)$ .
- Growth:  $E(y) \sim \int_{\Omega} (|Dy(x)|^p + \ell |D^2 y(x)|) dx, \quad 0 < p < 1.$

# Optimal scaling: Heuristics

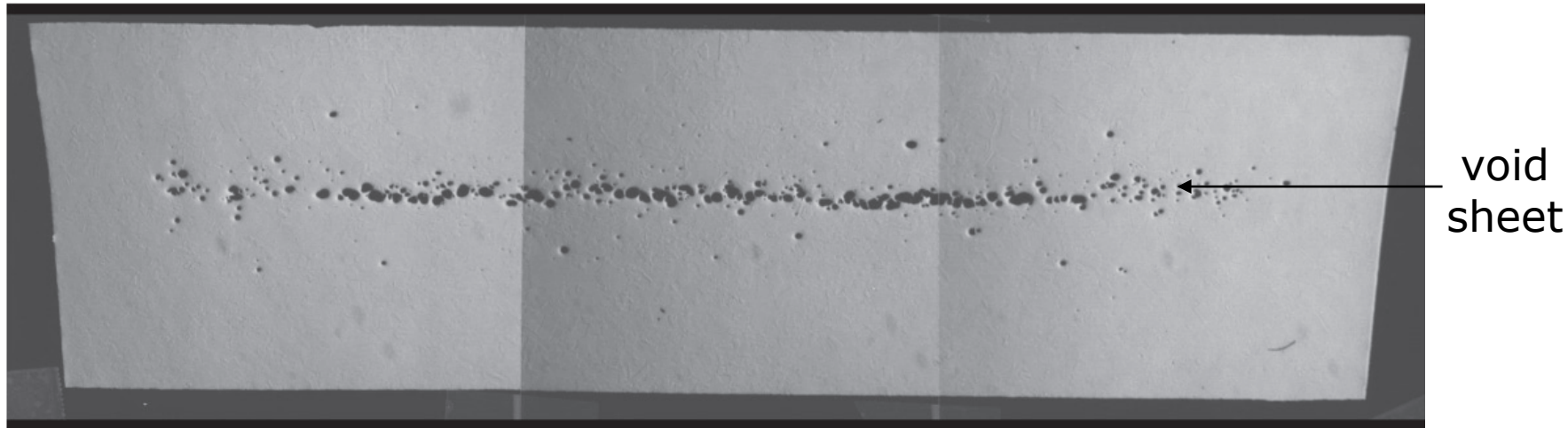


- Ignore volume constraint, localize def to band of thickness  $2a$ .
- Trial energy:  $E \sim \delta^p a^{1-p} + \ell(\delta/a)$ .
- Optimize thickness:  $a \sim \ell^{\frac{1}{2-p}} \delta^{\frac{1-p}{2-p}}$ .
- Optimal energy:  $E \sim \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$ .
- To show: i) Same scaling can also be achieved by means of volume-preserving map; ii) scaling is optimal.





# 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

$$E(y) \sim \int_{\Omega} \left( |Dy(x)|^p + \ell |D^2y(x)| \right) dx.$$

Fix  $\delta > 0$ . For every  $\ell$  sufficiently small, there is a map  $y : \Omega \rightarrow \mathbb{R}^3$  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

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

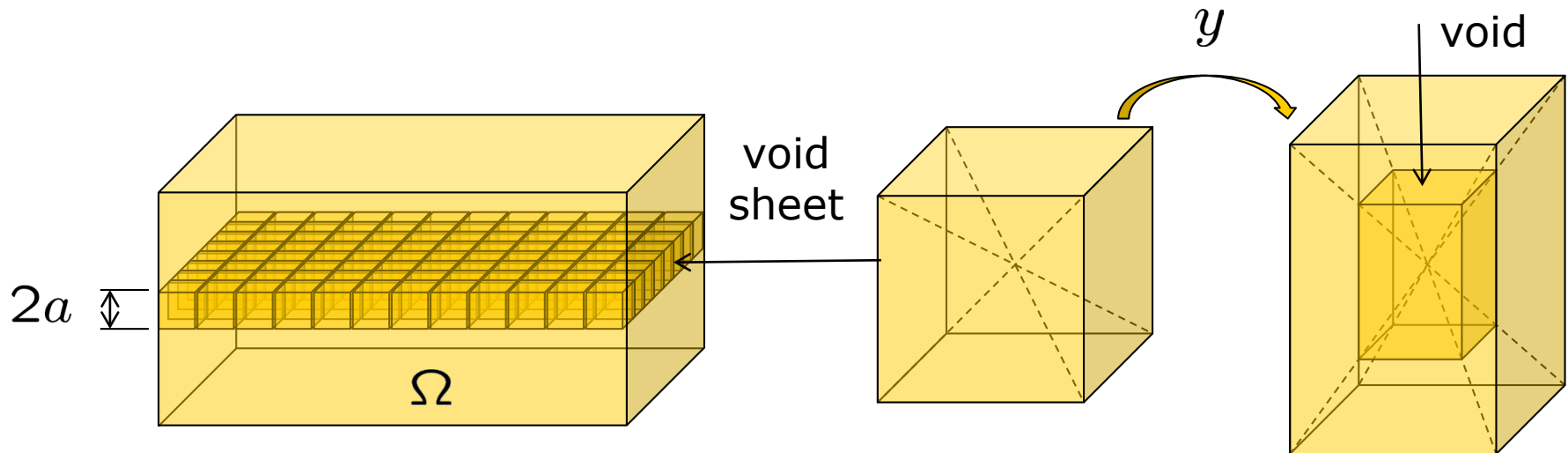
independently of  $H$ , where, explicitly,

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

and  $C > 0$  is a universal constant.

# Upper bound: Sketch of proof

- Void-sheet construction:



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

$$E(y) \sim \int_{\Omega} \left( |Dy(x)|^p + \ell |D^2y(x)| \right) dx.$$

Fix  $\delta > 0$ . For every  $\ell$  sufficiently small, there is a map  $y : \Omega \rightarrow \mathbb{R}^3$  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,

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

# Lower bound: Sketch of proof

General strategy: 1D arguments in  $x_3$ -direction (normal).

(i) Fix  $(x_1, x_2)$ , let  $f(x_3) \equiv |D_3 y(x_1, x_2, x_3)|$ .

Then:  $|D^2 y| \geq |D_3^2 y| \geq |D_3 |D_3 y|| = |Df|$ .

(ii) Define the reduced energy density:

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

(iii) From (i) and (ii),

$$\int_{-H}^H W(Dy, D^2 y) dx_3 \geq \int_{-H}^H (W_{1D}(f(x_3)) + \ell |Df(x_3)|) dx_3.$$

(iv) From Jensen and duality estimates,

$$\int_{-H}^H (W_{1D}(f(x_3)) + \ell |Df(x_3)|) dx_3 \geq CL^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}.$$

Integrating over the periodic cell:  $E \geq CL^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}} . \text{QED}$

# From micro-plasticity to ductile fracture

- 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 ( $\delta$ ): Cohesive behavior!
- Bounds degenerate when the intrinsic length  $\ell$  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 ( $\ell$ , constants) and macroscopic fracture ( $J_c$ ).

SUCCESS! ODER?

# 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](http://www.elsevier.com/locate/eml)



## Micro-pillar measurements of plasticity in confined Cu thin films



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<sup>a</sup> Department of Mechanical and Industrial Engineering, Louisiana State University, Baton Rouge, LA 70803, United States

<sup>b</sup> School of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, United States

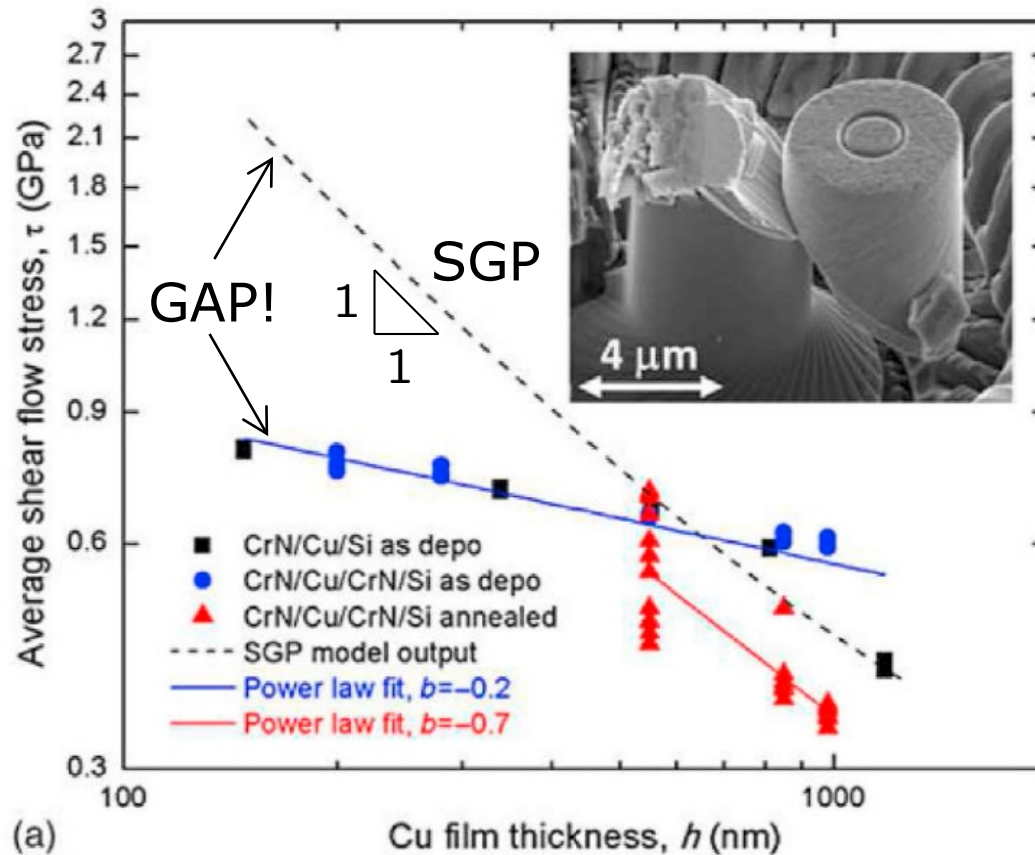
Mu, Y., Chen, K., Meng, W.J., 2014. MRS Commun. Res. Lett. 4, 126–133.

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!

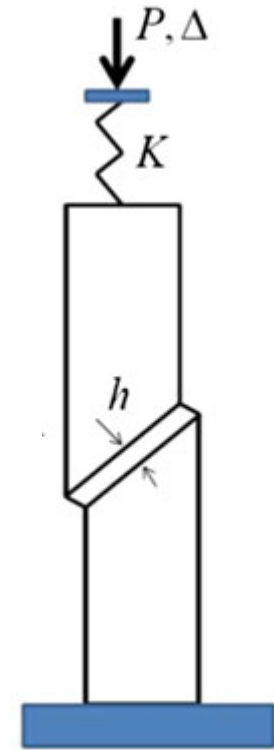


Shear flow stress as a function of thickness for Cu layers<sup>1</sup>.

SGP model prediction shown as dashed line.

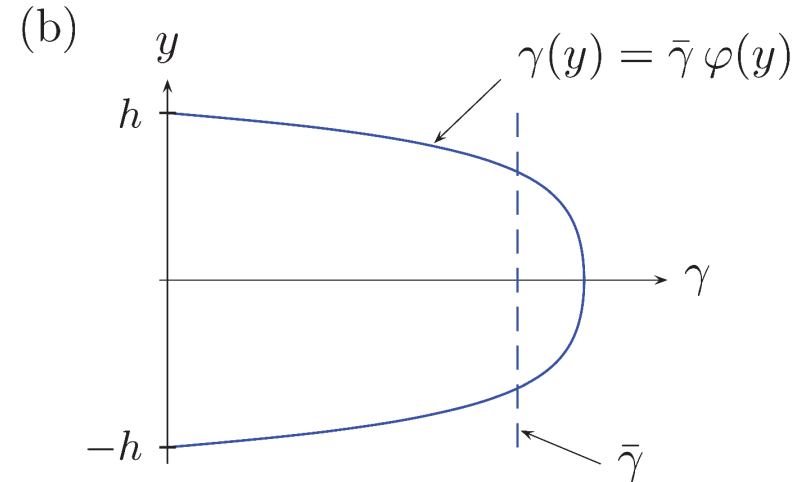
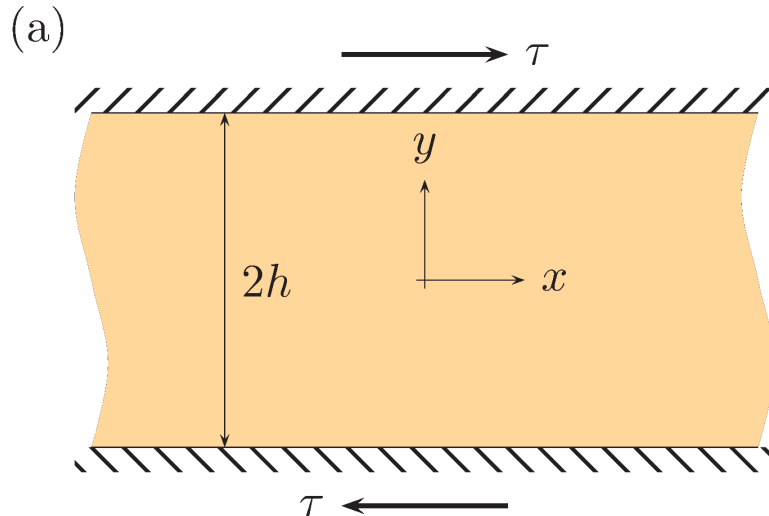
Insert shows SEM image of experimental setup.

<sup>1</sup>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.,  
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# Confined layer under prescribed simple shear



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

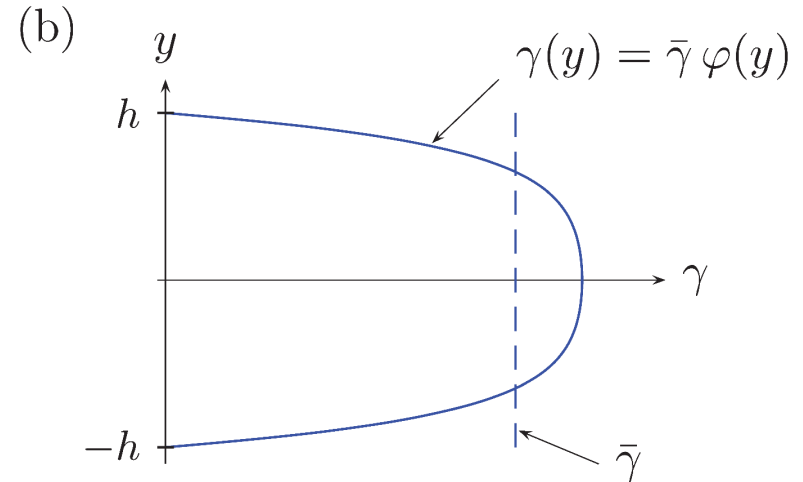
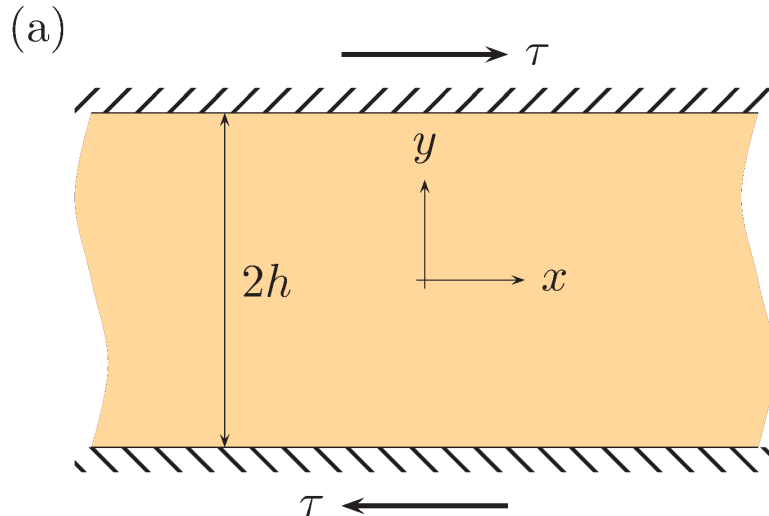
$$\text{minimize: } E(\gamma) = \int_{-h}^{+h} \left( \psi_p(\gamma(y)) + \psi_g(\gamma, y(y)) \right) dy,$$

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

- Power-law hardening (growth):

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

# Confined layer under prescribed simple shear



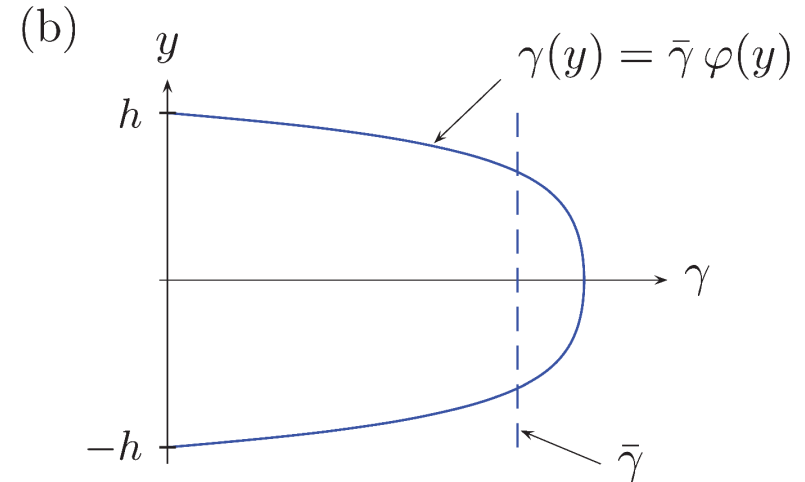
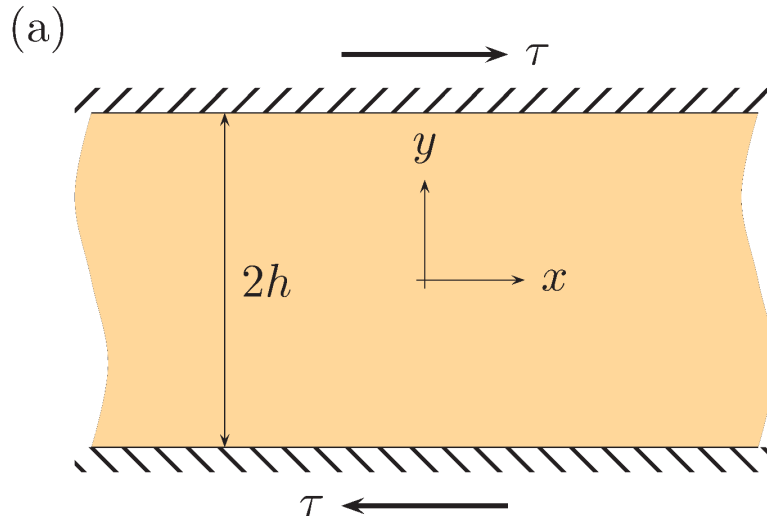
- Separate average strain and profile across thickness:

$$\gamma(y) = \bar{\gamma} \varphi(y), \quad \frac{1}{2h} \int_{-h}^{+h} \varphi(y) dy = 1 \Rightarrow$$

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

- For  $n > 0$ ,  $\bar{\gamma} \neq 0$  requires  $|\tau| \geq \tau_0 \Rightarrow$  no size effect!

# Confined layer under prescribed simple shear

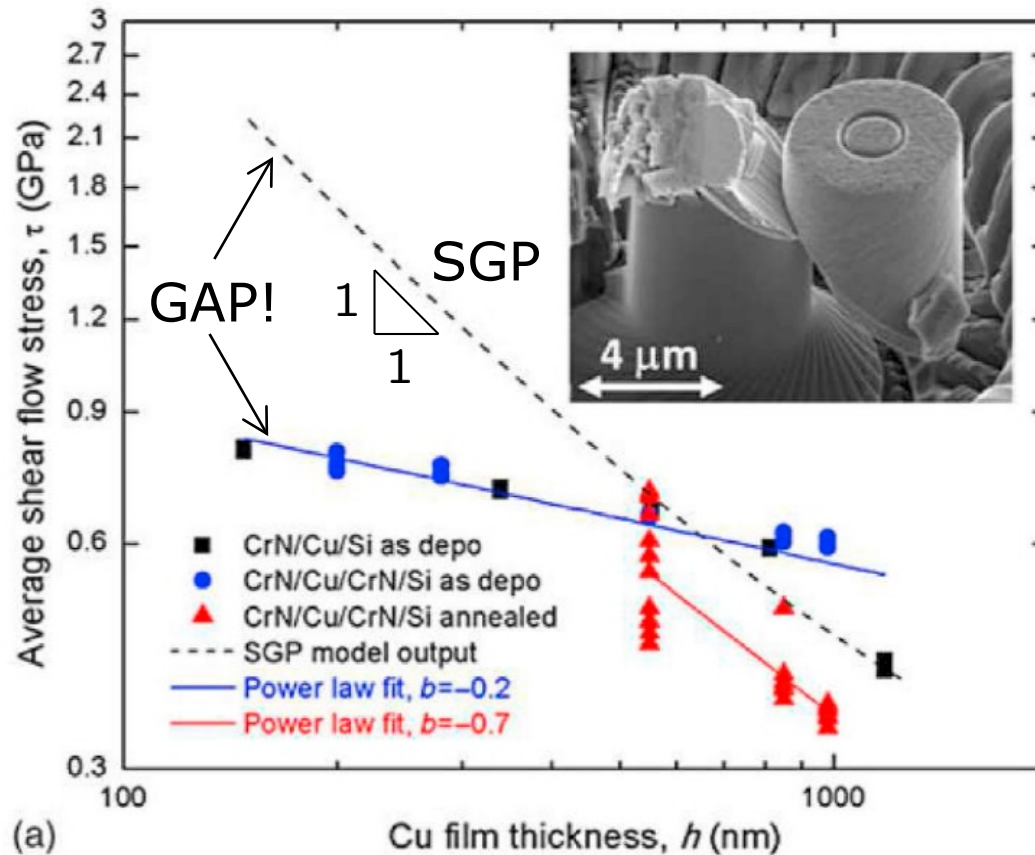


- Assume  $n = 0$  (nonlocal energy with linear growth):

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

- 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!

# Strain-gradient plasticity misses size effect!

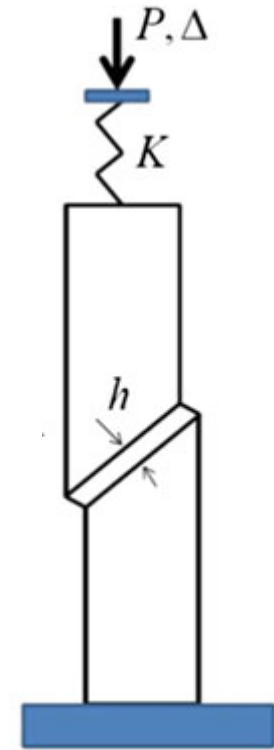


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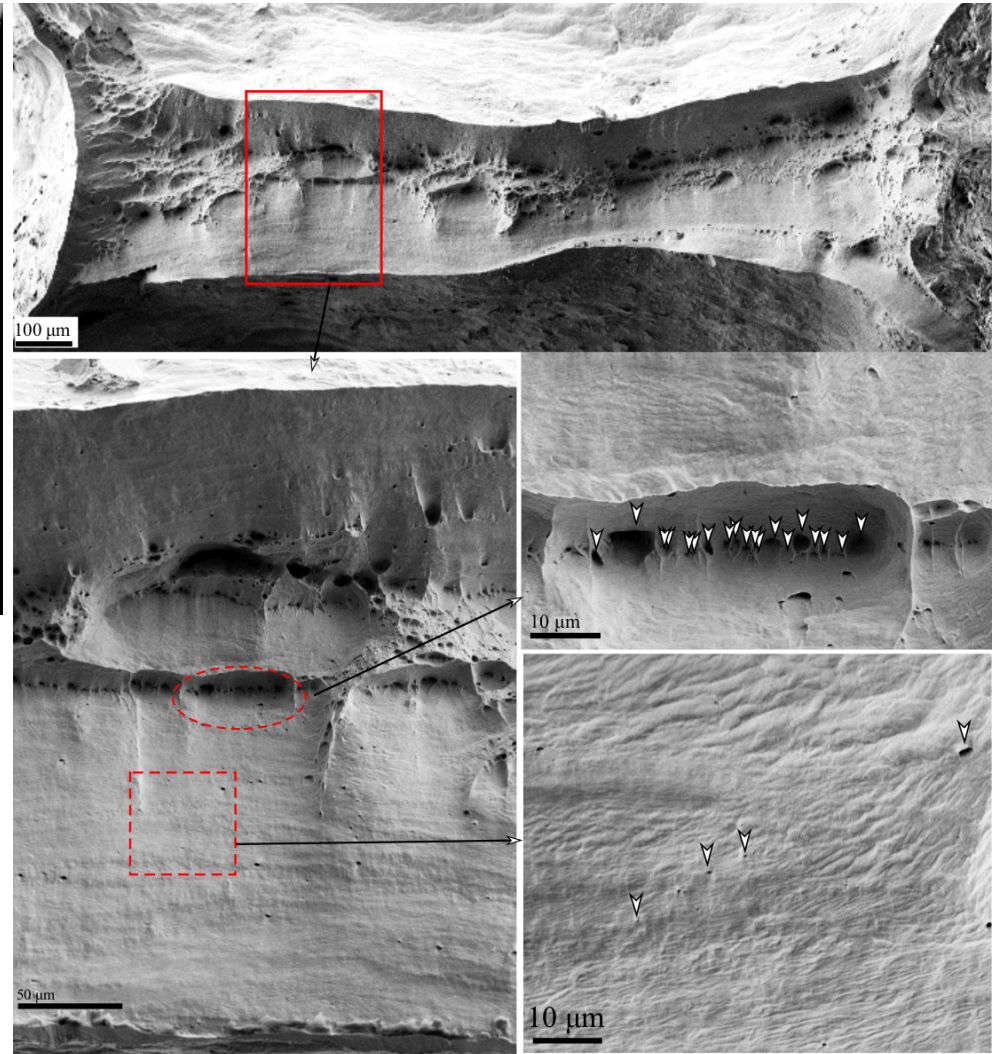
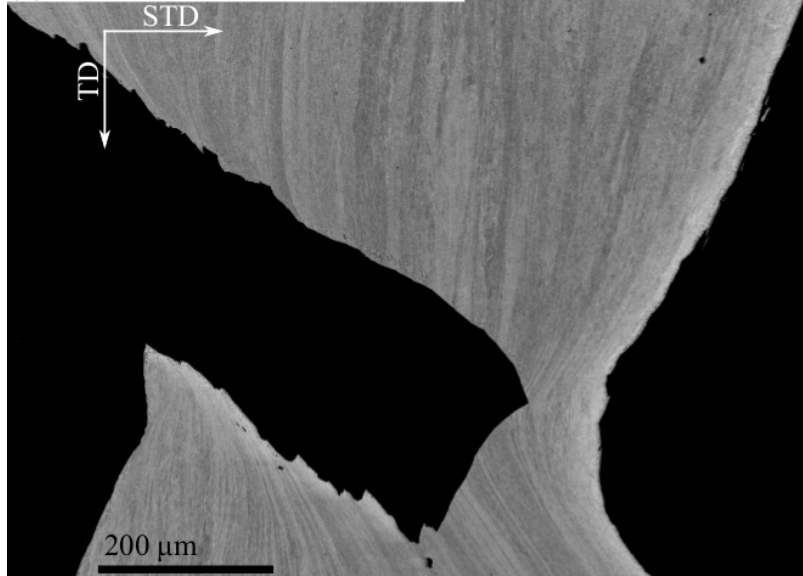
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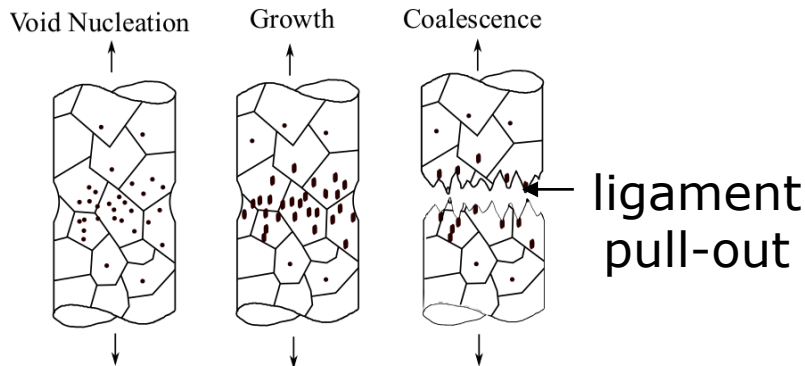
Mu, Y., Zhang, X.,  
Hutchinson, J.W., Meng, W.J.,  
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# Critique of SBP (II): Final stages of fracture

(d) 4N-Ni Sheet Material 10 UTS

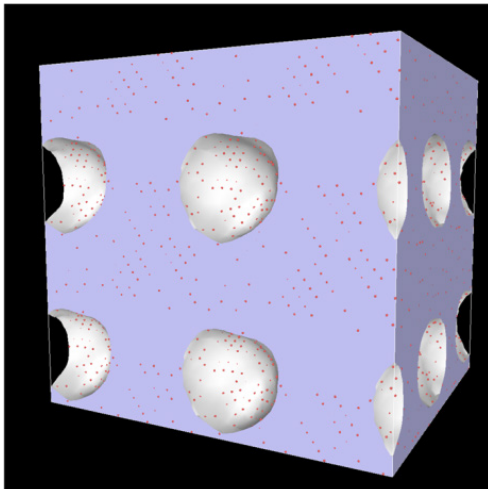


## Final fracture of high-purity Ni



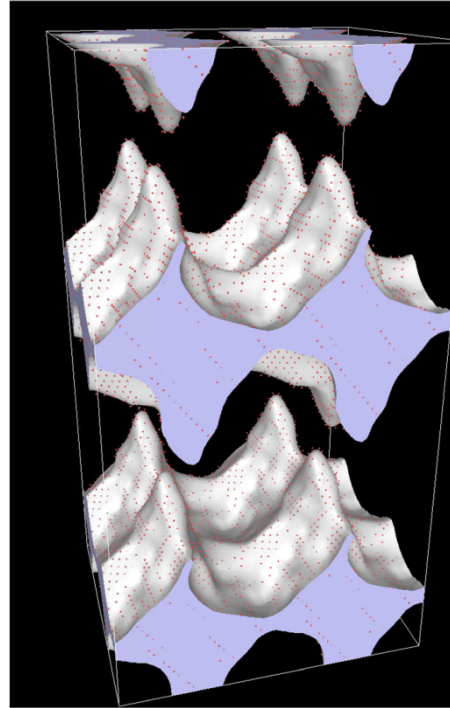


# Final stages of fracture in metals

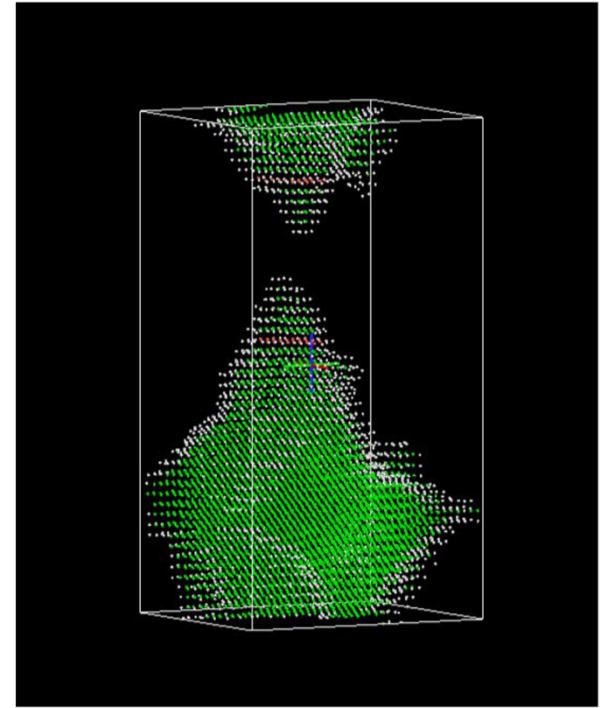


(a)

EAM Nickel,  
[111] loading,  
NPT 300K<sup>1</sup>



(b)

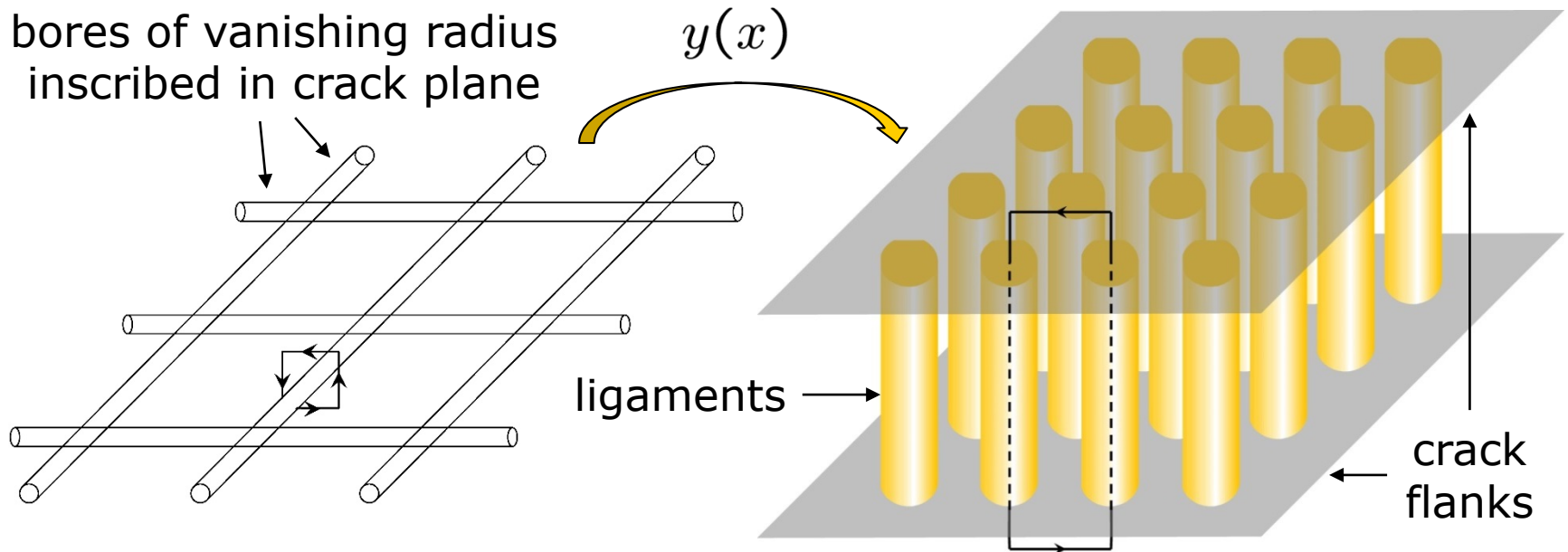


(c)

- 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.

<sup>1</sup>M.I. Baskes and M. Ortiz, *JAM*, **82**: 071003-1-071003-5, 2015

# Ligament formation as topological transition

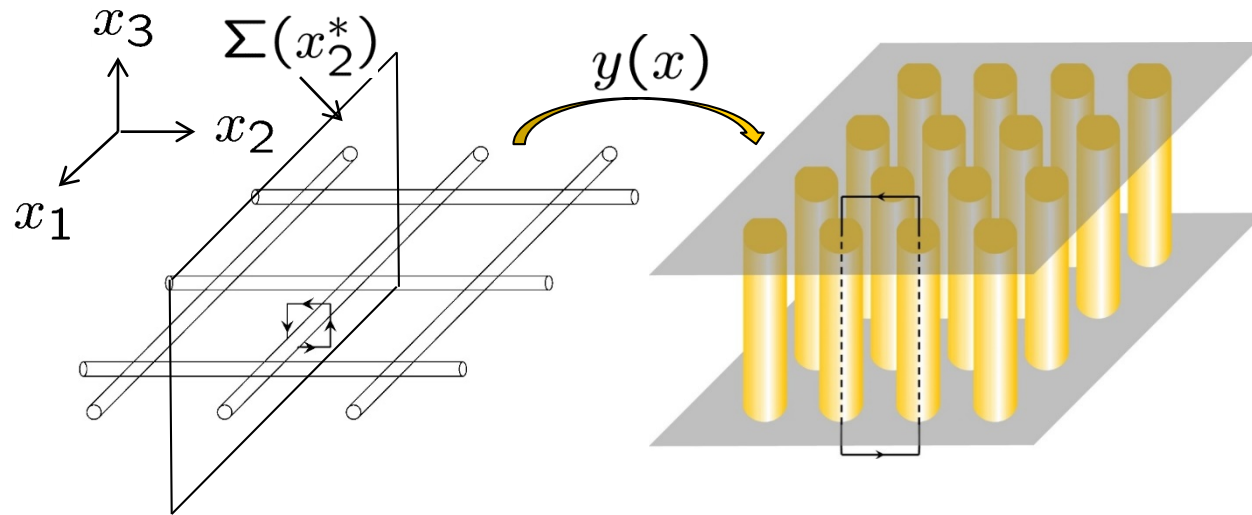


Topology of ligament formation

- Circuit can be shrunk homotopically to a point before deformation.
- Circuit cannot be shrunk homotopically to a point after deformation, evincing *topological transition*.



# Strain-gradient plasticity misses final stages of fracture!



- Suppose  $\Omega = (0, L)^2 \times (-H, H)$ ,  $y \in W^{1,1}(\Omega)$ ,  $|D^2 y|(\Omega) < +\infty$ .
- Let  $x_2^* \in (0, L)$ ,  $\Sigma(x_2^*) = \Omega \cap \{x_2 = x_2^*\}$ ,  $u(\cdot, \cdot) = y(\cdot, x_2^*, \cdot)$ .  
Then,  $u \in W^{1,1}(\Sigma(x_2^*))$ ,  $|D^2 u|(\Sigma(x_2^*)) < +\infty$ .

## Lemma (S. Conti & MO'2016)

Let  $u \in W^{1,1}(\mathbb{R}^2)$  with  $Du \in BV(\mathbb{R}^2; \mathbb{R}^2)$ . Then,  $u$  has a continuous representative.

# 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*.

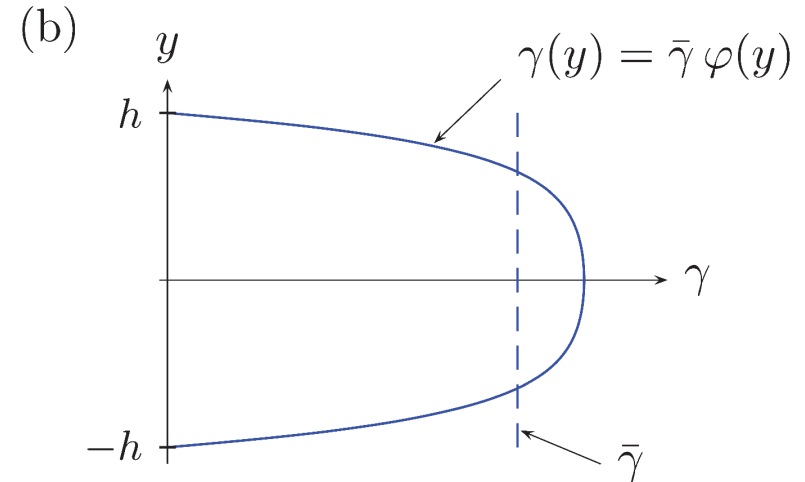
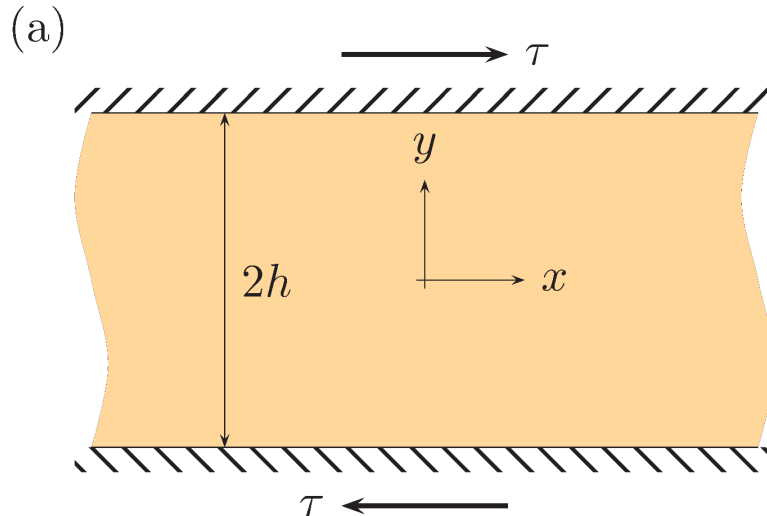
- *Fractional strain-gradient plasticity* (FSGP): Assume energy growth

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

- Recall:  $W^{\sigma,1}(\Omega, \mathbb{R}^m)$  interpolation space  $(L^1, W^{1,1})_{\sigma,1}$  with norm

$$\|u\|_{\sigma,1} = \inf \left\{ (1-\sigma) \int_{[0,\infty) \times \Omega} t^{-\sigma} (|D_x f| + |D_t f|) : \right. \\ \left. f(0, \cdot) = u, f \in BV_{\text{loc}}((0, \infty) \times \Omega) \right\}$$

# Confined layer under prescribed simple shear



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

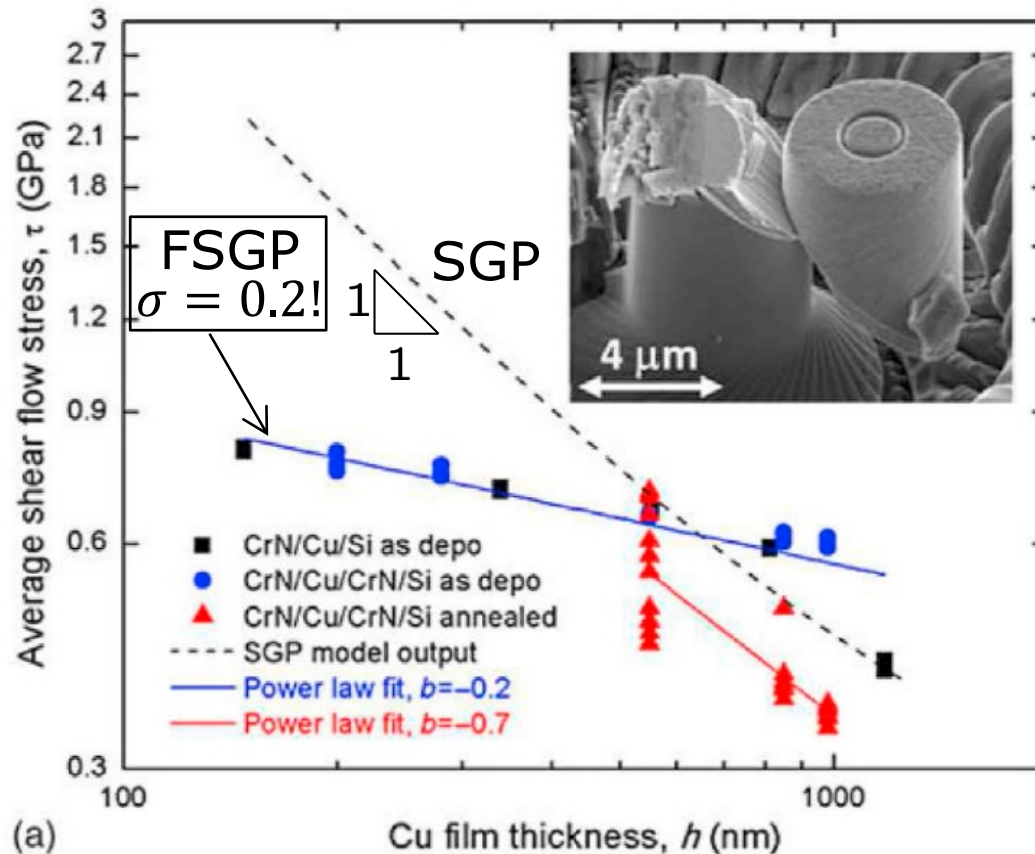
$$\Psi_g(\varepsilon) = \int_{\Omega} \int_{\Omega} B \frac{\ell^\sigma}{\varepsilon_0} \frac{|\varepsilon(x') - \varepsilon(x'')|}{|x' - x''|^{d+\sigma}} dx' dx''.$$

- 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:  $\bar{\gamma} \neq 0 \Rightarrow |\tau| \geq \tau_0 + \frac{B\ell^\sigma}{\gamma_0 h^\sigma}$  can match size scaling exactly!

# Fractional strain-gradient plasticity can match size scaling

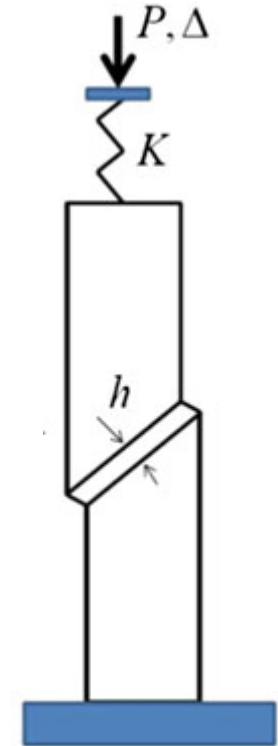


Shear flow stress as a function of thickness for Cu layers<sup>1</sup>.

SGP model prediction shown as dashed line.

Insert shows SEM image of experimental setup.

<sup>1</sup>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.

# 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  $y \in W_{\text{loc}}^{1,1}(\mathbb{R}^3; \mathbb{R}^3)$  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

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

The constant  $C$  depends only on  $p$  and  $\sigma$ .

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

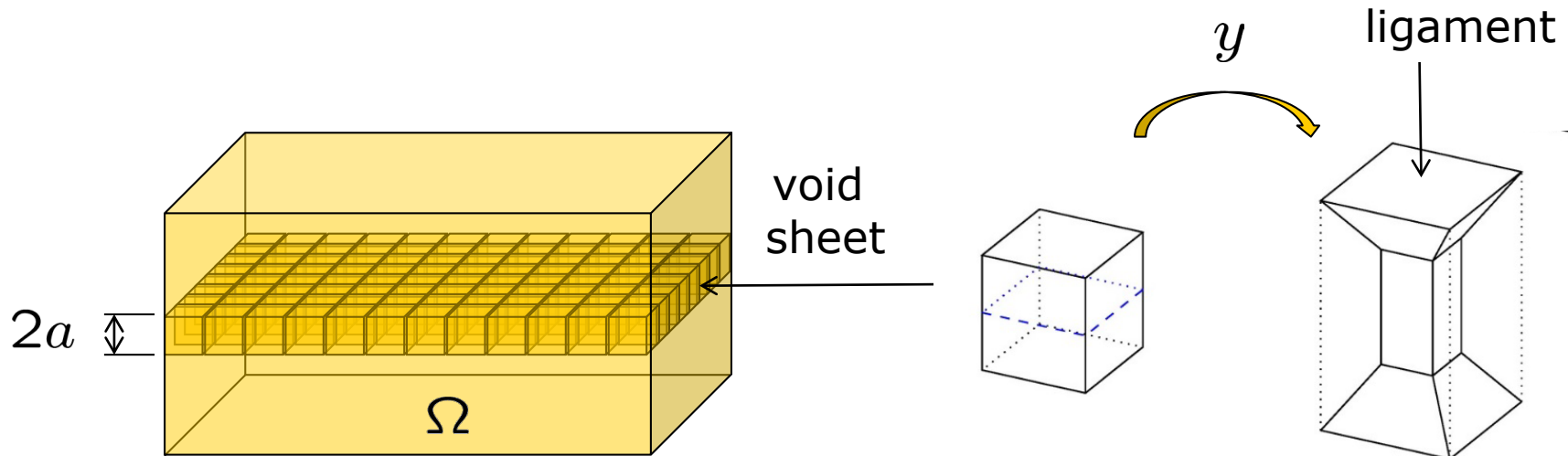
Let  $p \in [0, 1)$ ,  $\sigma \in (0, 1)$ ,  $H, L, \delta > 0$ , let  $\Omega = (0, L)^2 \times (-H, H)$ . Then for sufficiently small  $\ell$  we have

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

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

# Upper bound: Sketch of proof

- Void-sheet construction:



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

# Micro-plasticity to ductile fracture revisited

- Optimal (matching) upper and lower bounds:

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

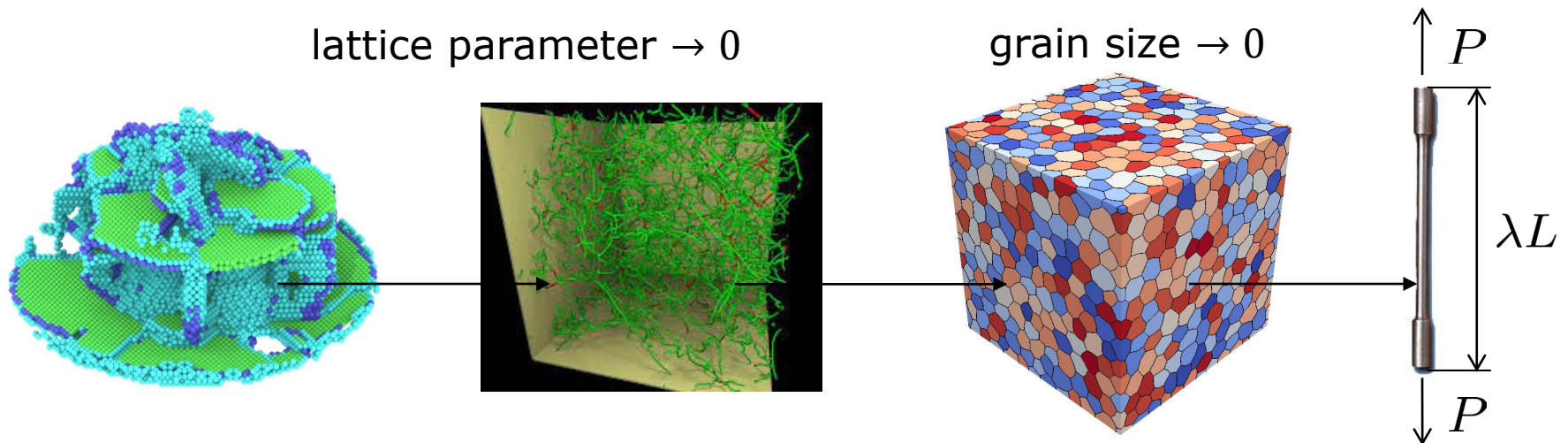
- Bounds apply to classes of materials having the same growth, fractional differentiation order.
- Energy scales with area ( $L^2$ ): Fracture scaling!
- Energy scales with power of opening displ ( $\delta$ ): Cohesive behavior!
- Bounds degenerate when the intrinsic length  $\ell$  decreases to zero.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



# Concluding remarks



- (Optimal) *bounds* are often sufficient for *engineering design*
- *Optimal scaling provides a practical avenue for traversing length scales*: Exact form of effective behavior (e.g., from a Gamma-expansion) need not be known, only suitable *bounding functionals* are required.
- The *precise form* of such bounding functionals remains the *subject of conjecture* (Integral? Differential order? Growth exponents? Multiplicative constants?)
- Can *multiscale analysis* aid in the determination of *rigorous bounding functionals* from micromechanics?



Concluding remarks

Thank you!