



Optimal scaling laws for ductile fracture derived from strain-gradient microplasticity

Michael Ortiz

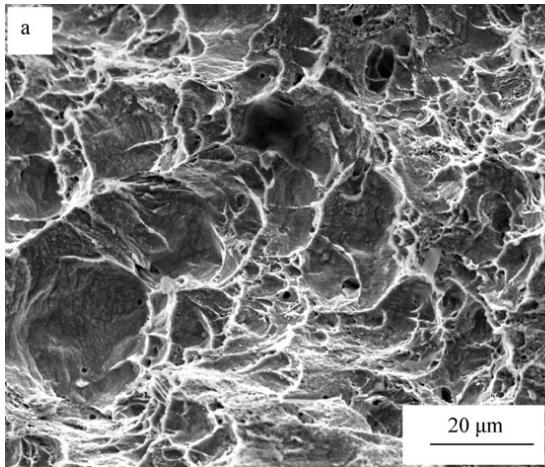
California Institute of Technology and
Rheinische Friedrich-Wilhelms Universität Bonn

With: M.P. Ariza (Universidad Sevilla),
S. Conti (Universität Bonn),
A. Pandolfi (Politecnico Milano)

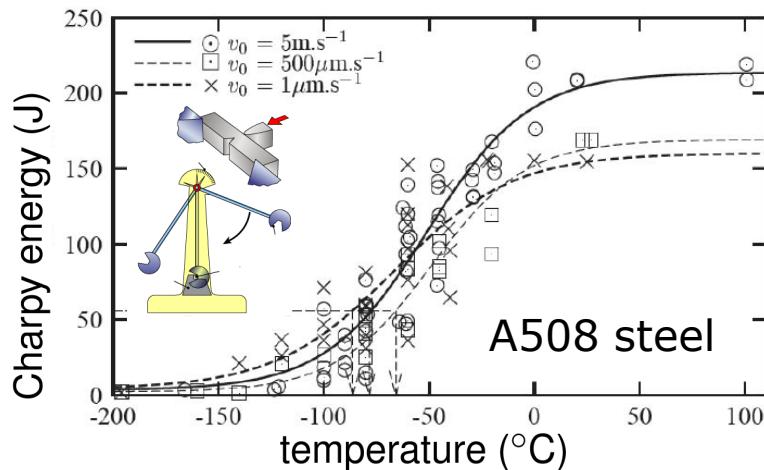
ECCOMAS-CMCS 2023
Eindhoven, The Netherlands
October 10-13, 2023

Michael Ortiz
CMCS 2023

Ductile fracture of metals



SA333 steel, T=300K, $d\varepsilon/dt = 3 \times 10^{-3} s^{-1}$
(S.V. Kamata, M. Srinivasa and P.R. Rao,
Mater. Sci. Engr. A, **528** (2011) 4141.)

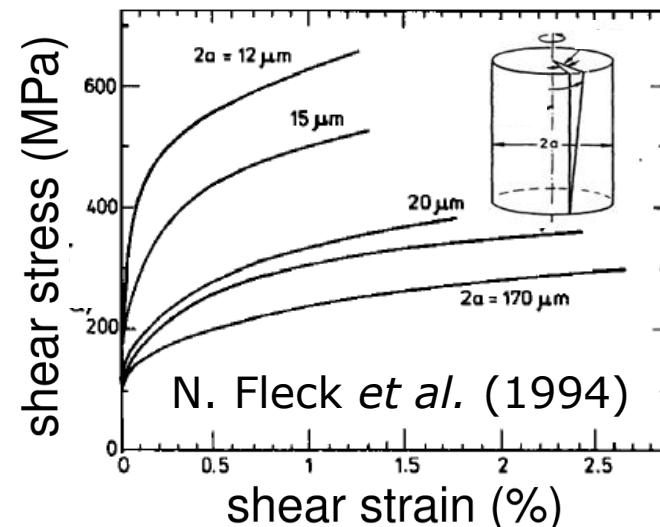
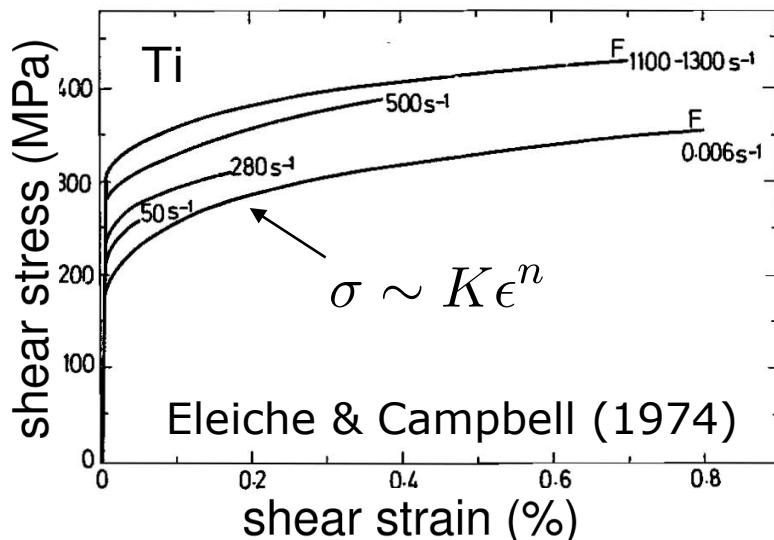


Tanguy, B., Besson, J., Piques, R. & Pineau, A.,
Eng. Frac. Mechanics, **72** (2005) 49.

- Ductile fracture in metals occurs by *void nucleation, growth and coalescence*
- Fractography of ductile fracture surfaces exhibits profuse *dimpling*, a vestige of microvoids
- Ductile fracture entails large amounts of *macroscopic plastic deformation* and dissipation above TDB transition temperature
- *Ductile fracture is the quintessential multiscale phenomenon!*

Ductile fracture – Micromechanical basis

(plane-strain)
specific fracture energy $\rightarrow J_{Ic} = \sigma_0 \ell$ ← dimensional analysis!
from J -testing (ASTM E813)



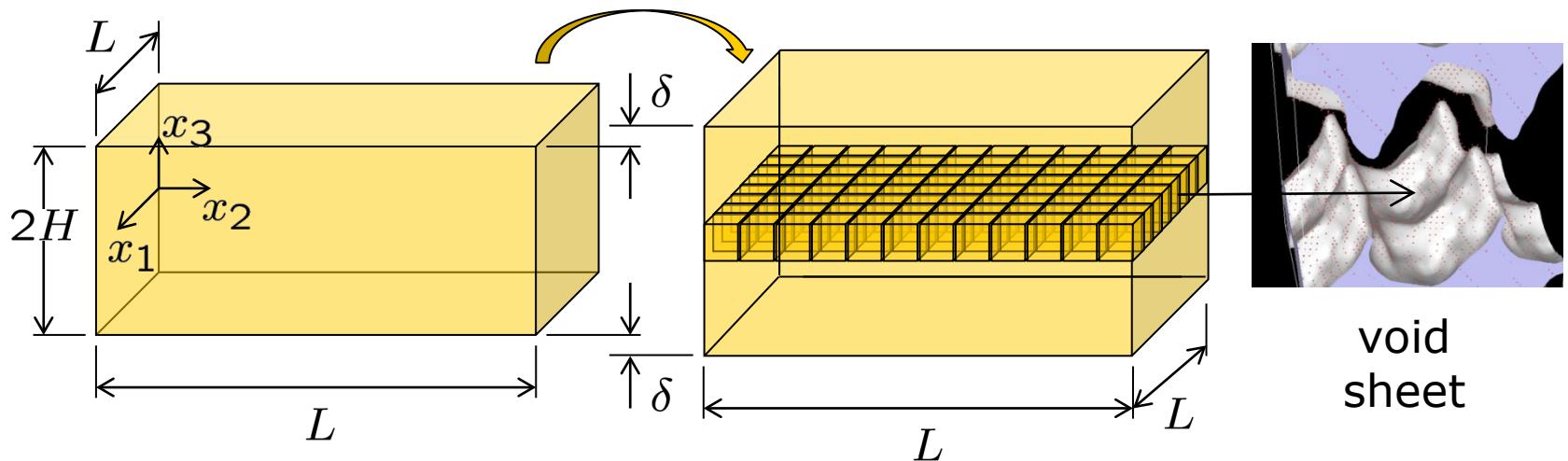
Plastic strength, material testing
ultimate strength $\sigma_0 = K/(n + 1)$

Intrinsic characteristic length ℓ ,
empirical material constant

N. A. Fleck, G.M. Muller, M.F. Ashby I and J.W. Hutchinson,
“Strain-gradient plasticity: Theory and experiment”,
Acta metall. mater., **42**(2) (1994) 475.

From SGP to ductile fracture

- *Can ductile fracture be predicted by strain-gradient plasticity?*
- Model problem: Uniaxial extension of infinite slab



- Goals: *Bridge micro and macro scales analytically! Derive effective law that can be used in macroscale calculations!*
- Methodology and approach:
 - *Deformation theory of plasticity, finite kinematics, Lagrangian*
 - *Incompressible, rate-independent, rigid-plastic solid*
 - Micro-macro handshake: *Variational optimal scaling*

R. V. Kohn and S. Müller, Phil. Mag. A, **66**(5) (1992) 697-715.

Local deformation theory

- Deformation theory: Minimize

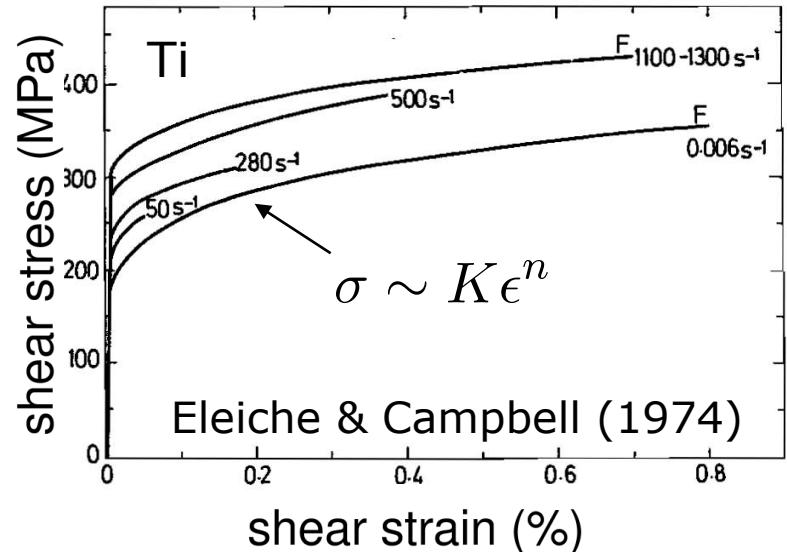
$$E(y) = \int_{\Omega} W(Dy(x)) dx,$$

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

- (Observed) growth of $W(F)$?
- Assume power-law hardening

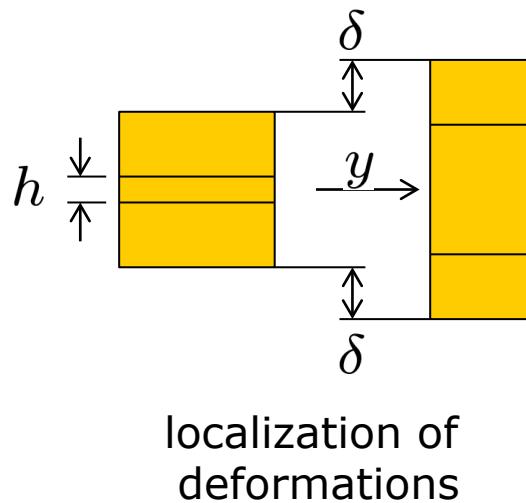
$$\sigma \sim K\epsilon^n = K(\lambda - 1)^n.$$

- Nominal stress: $\partial_{\lambda} W = \sigma/\lambda = K(\lambda - 1)^n/\lambda$.
- For large 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!* ($p < 1$).

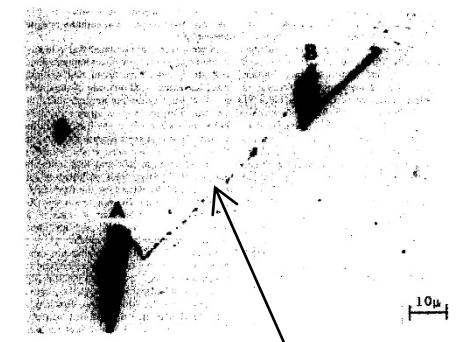


Necking of bars
Rittel et al. (2014)

Local deformation theory



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



- 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...

¹W.M. Garrison Jr. and N.R. Moody, “Ductile fracture”, *J. Phys. Chem. Solids*, 48(II) (1987) 103.

Strain-gradient deformation theory

- The yield stress of metals is observed to increase in the presence of *strain gradients*.

- Ansatz: Minimize

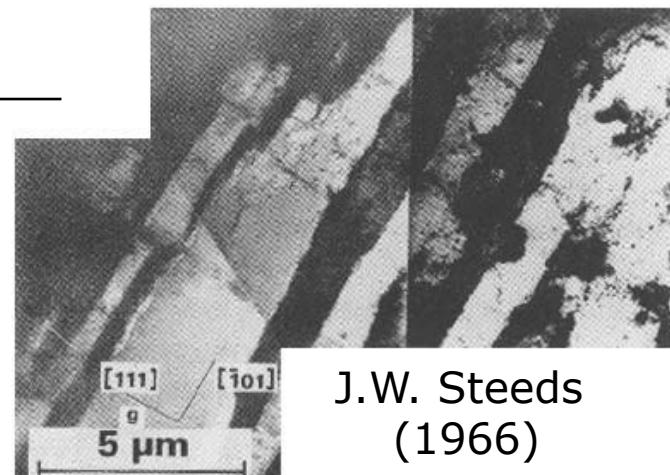
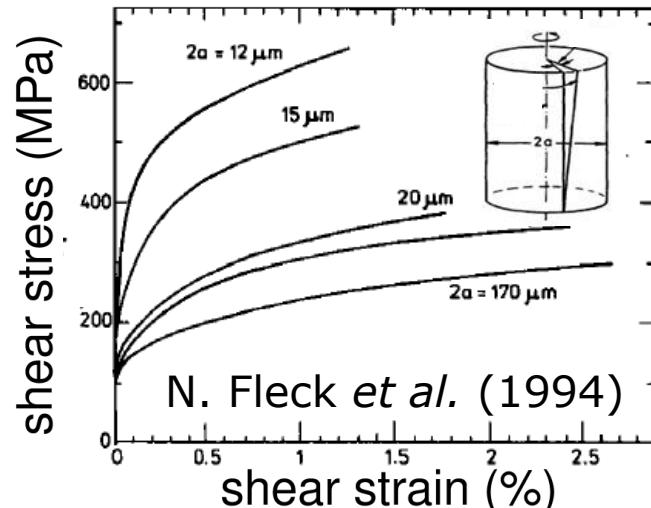
$$E(y) = \int_{\Omega} W(Dy(x), D^2y(x)) dx,$$

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

- Growth in $D^2y(x)$ *linear*, and

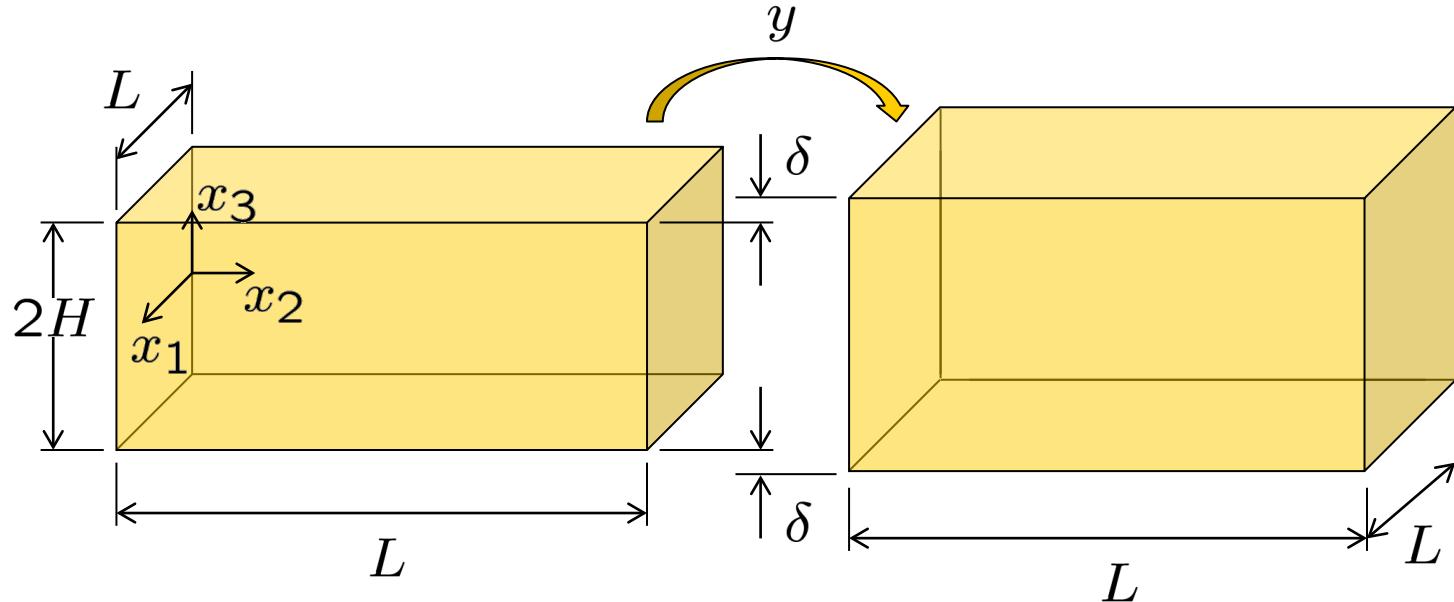
$$\ell = \frac{\mu b}{K} \quad (\text{characteristic length!})$$

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



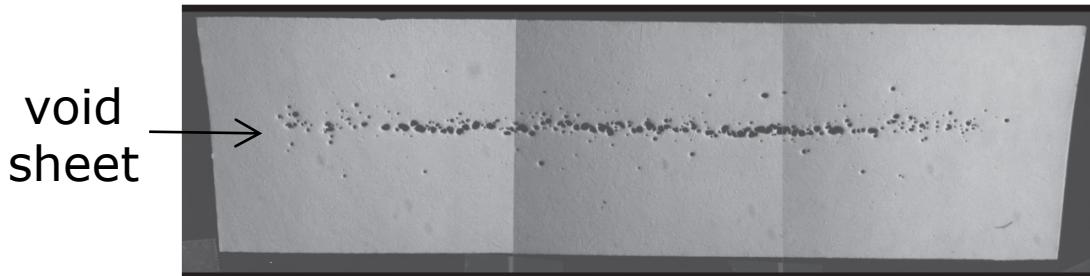
Dislocation walls in copper (fence) Michael Ortiz CMCS 2023

Ductile fracture: Optimal scaling



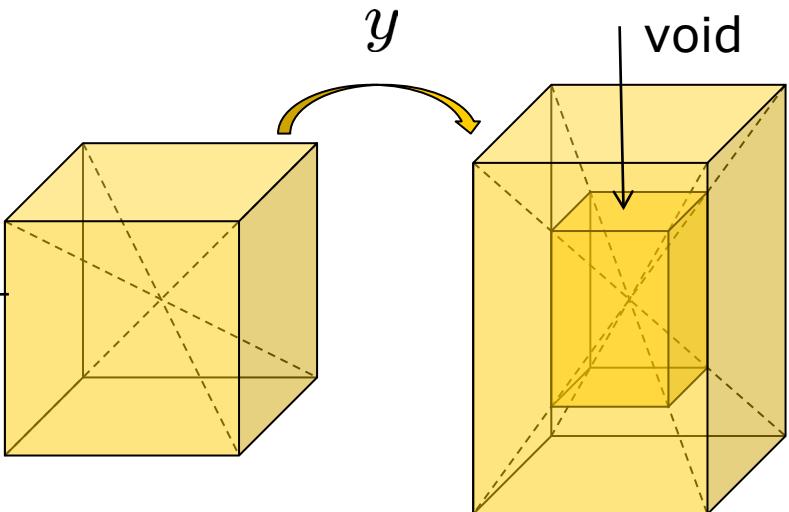
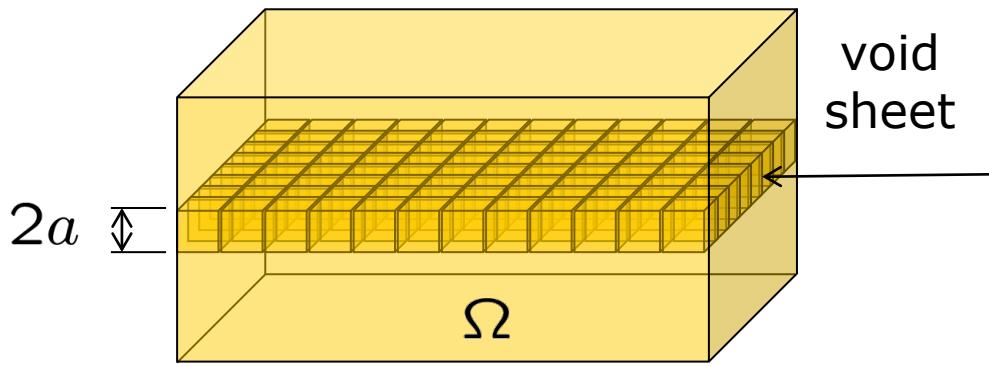
- Slab: $\Omega = [0, L]^2 \times [-H, H]$, in-plane periodic.
- Deformation $y \in W^{1,1}(\Omega; \mathbb{R}^3)$ and $Dy \in BV(\Omega; \mathbb{R}^{3 \times 3})$,
$$\det Dy(x) = 1, \quad \text{a. e. in } \Omega.$$
- Uniaxial extension: $y_3(x_1, x_2, \pm H) = \pm(H + \delta)$.
- Growth: $E(y) \sim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

Upper bound: Sketch of proof



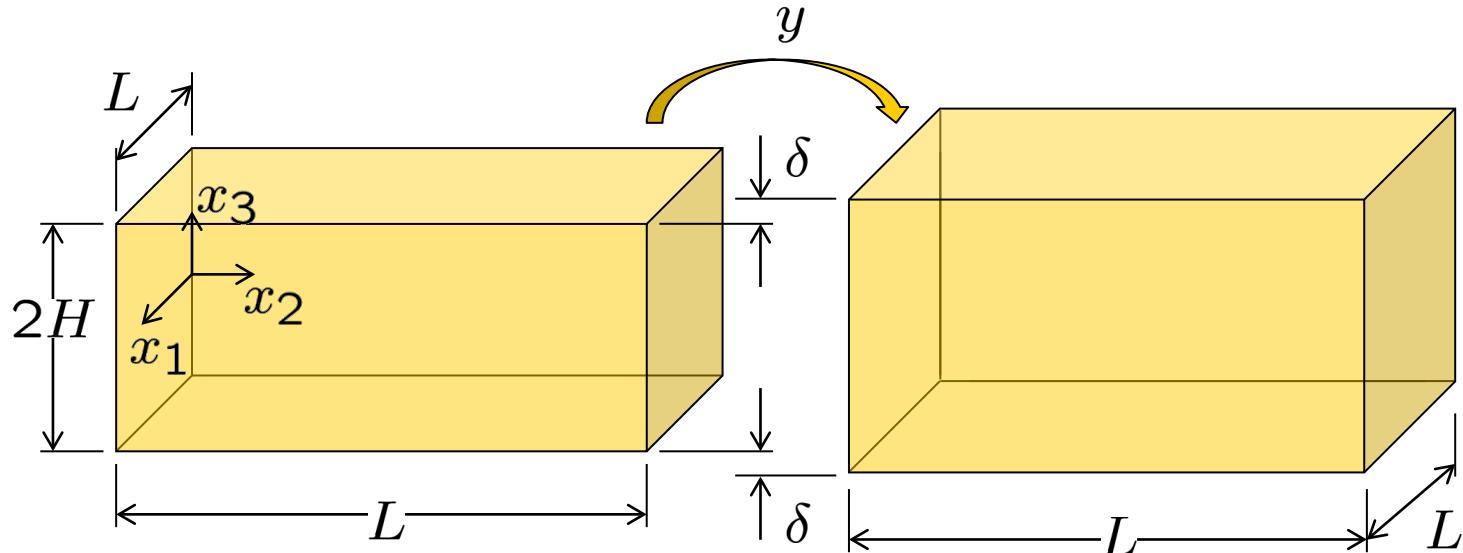
Heller, A., How Metals Fail,
Science & Technology Review
Magazine, LLNL, pp. 13-20,
July/August, 2002

- Void-sheet construction:

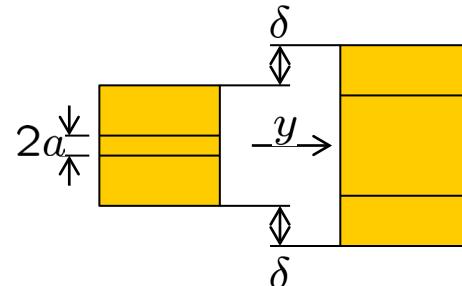


- Calculate, estimate: $E \leq CL^2 (a^{1-p} \delta^p + \ell \delta / a)$.
- Optimize thickness: $a_{\text{opt}} \sim \ell^{\frac{1}{2-p}} \delta^{\frac{1-p}{2-p}}$ (coarsening).
- Optimal bound: $E \leq CL^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$.

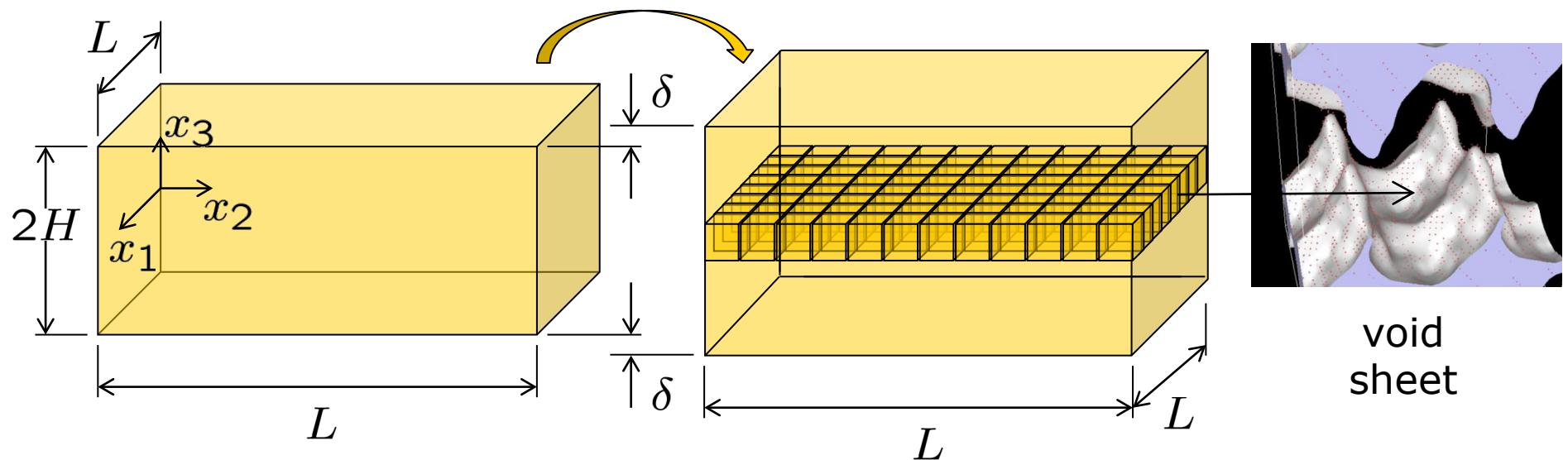
Lower bound: Heuristics



- 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.



From SGP to ductile fracture



- Bounds on specific fracture energy:

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

- Energy scales with power of opening displ (δ): Cohesive behavior!
- Bounds degenerate when the intrinsic length ℓ decreases to zero
- Theory provides a link between micro-plasticity (ℓ , constants) and macroscopic fracture (J).

From SGP to ductile fracture

Theorem (Upper bound)

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 σ .

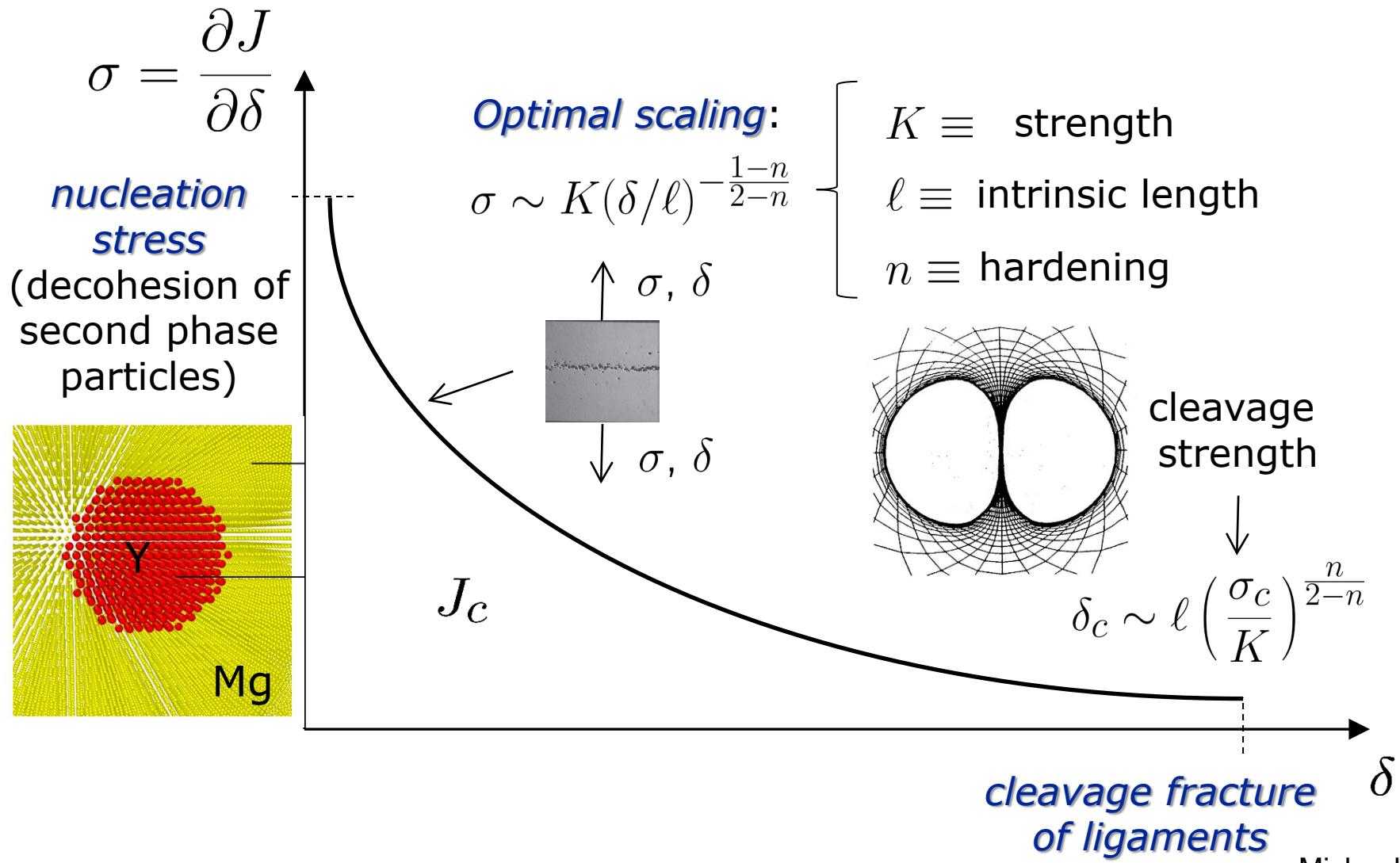
Theorem (Lower bound)

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

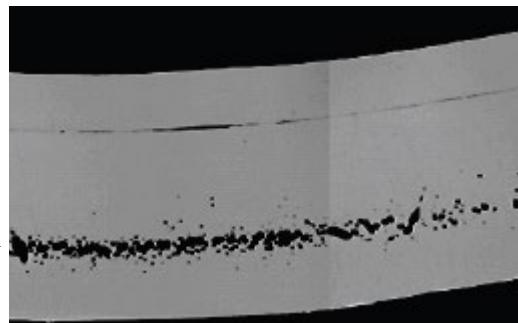
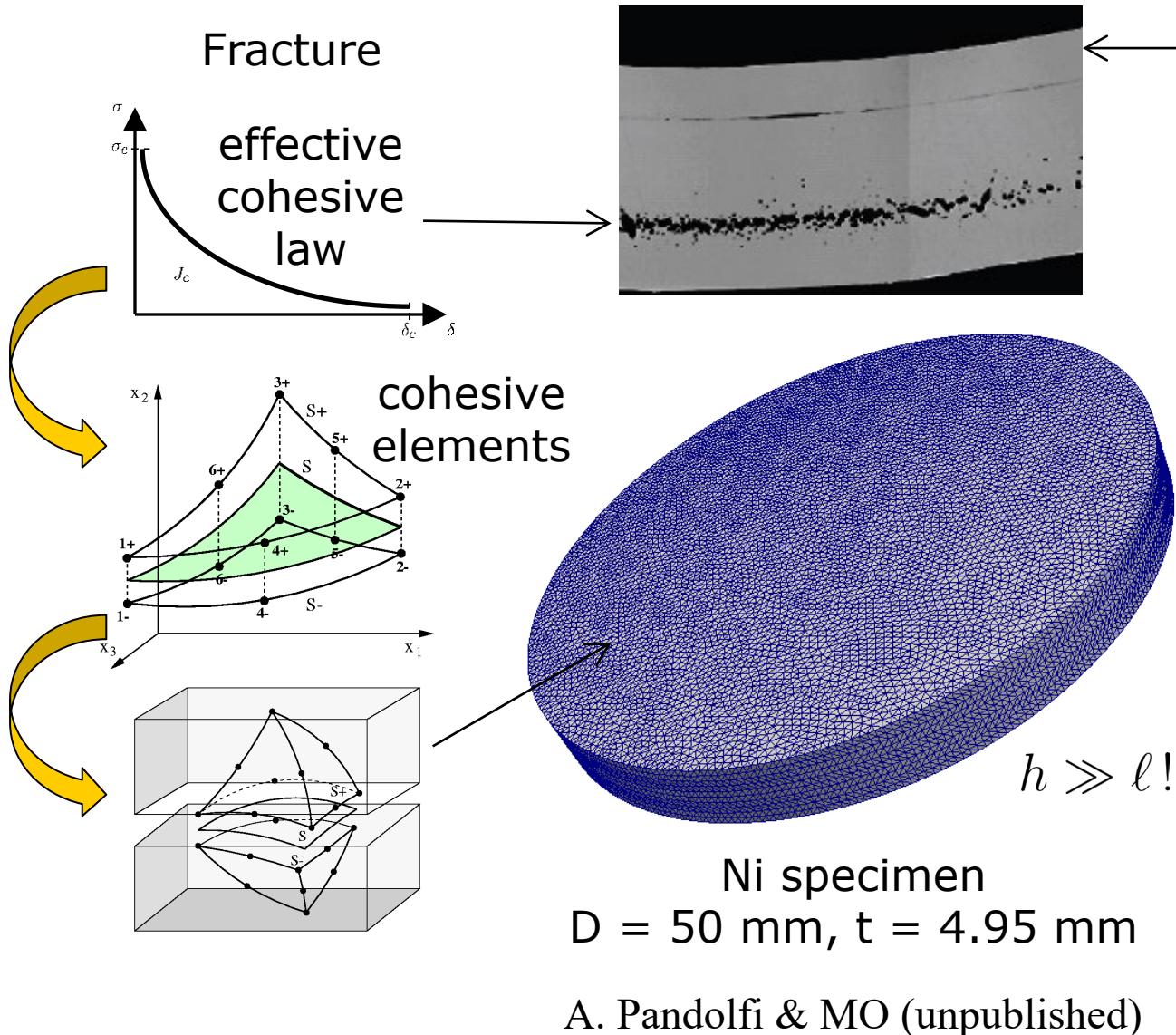
$$CL^2 \ell^{\frac{\sigma(1-p)}{1+\sigma-p}} \delta^{\frac{1-(1-\sigma)p}{1+\sigma-p}} \leq E(y),$$

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 .

Upscaling: Effective cohesive law

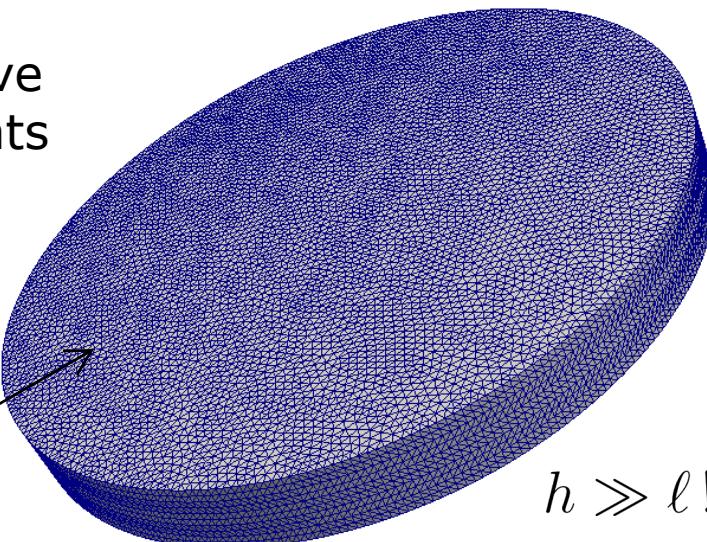


Spall fracture – Multiscale analysis



Bulk

- J2 plasticity, power-law hardening
- $h = 0.49 \text{ mm}$, 191,960 tets, 456,262 nodes

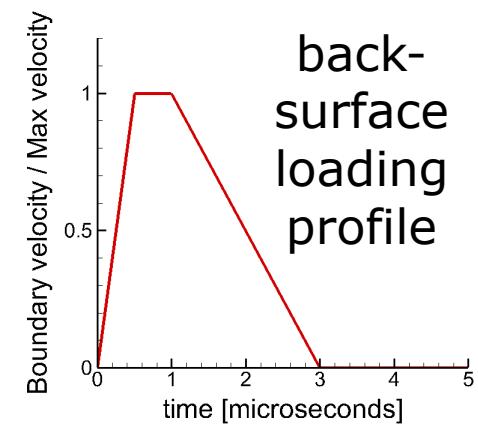


$$h \gg \ell!$$

Ni specimen

$D = 50 \text{ mm}$, $t = 4.95 \text{ mm}$

A. Pandolfi & MO (unpublished)



Spall fracture – Multiscale analysis



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

A. Pandolfi & MO (unpublished)

Michael Ortiz
CMCS 2023

Spall fracture – Multiscale analysis

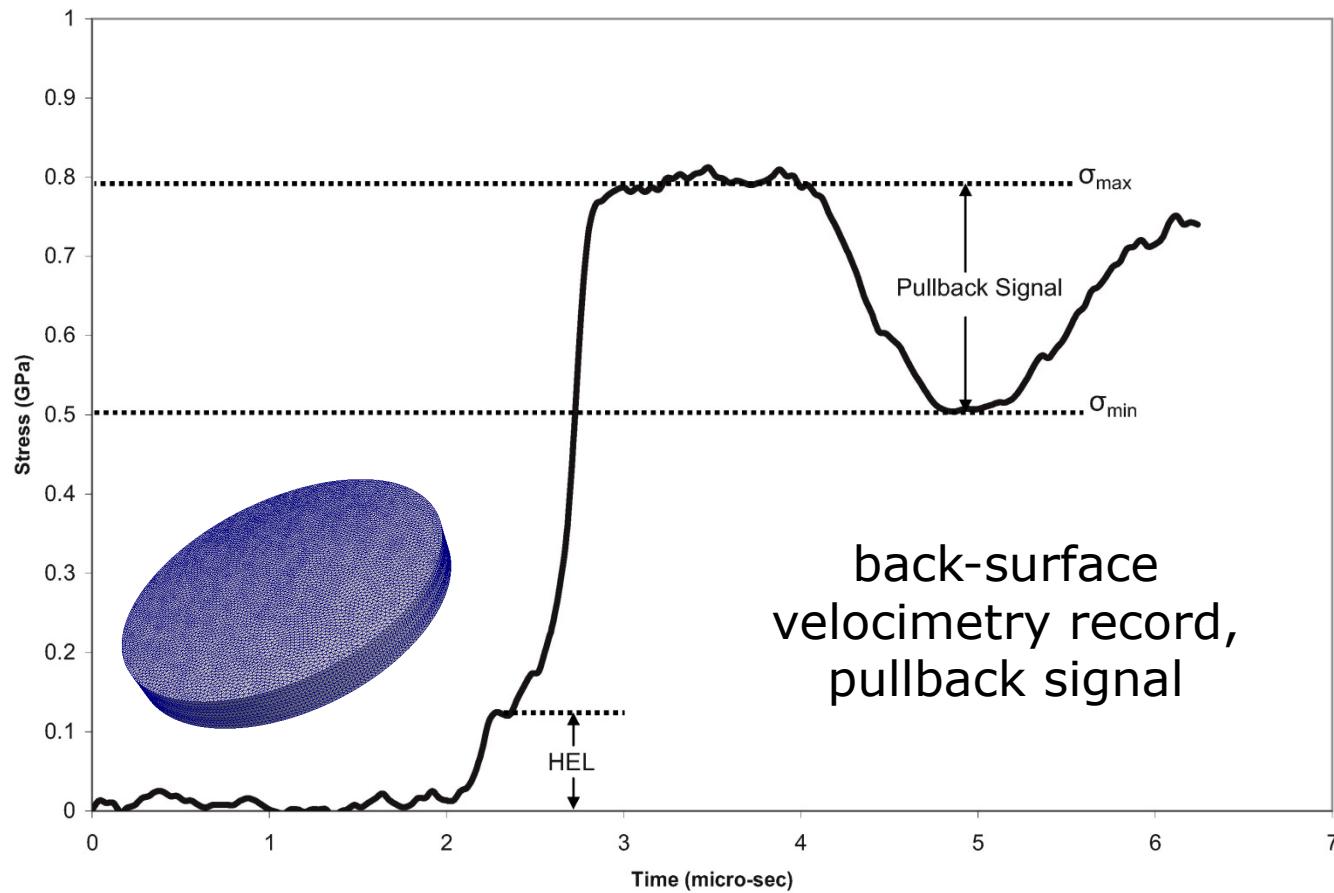


- Ni specimen, $D = 50 \text{ mm}$, $t = 4.95 \text{ mm}$
- J2 plasticity, power-law hardening
- $h = 0.49 \text{ mm}$, 191,960 tets, 456,262 nodes

A. Pandolfi & MO (unpublished)

Michael Ortiz
CMCS 2023

Spall fracture – Multiscale analysis



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

A. Pandolfi & MO (unpublished)

What have we learned?



Pergamon

PII S-1359-6454(96)00047-X

Acta mater., Vol. 44, No. 10, pp. 3943–3954, 1996

Copyright © 1996 Acta Metallurgica Inc.

Published by Elsevier Science Ltd

Printed in Great Britain. All rights reserved

1359-6454/96 \$15.00 + 0.00

A SELF-CONSISTENT MODEL FOR CLEAVAGE IN THE PRESENCE OF PLASTIC FLOW

G. E. BELTZ¹, J. R. RICE², C. F. SHIH³ and L. XIA³

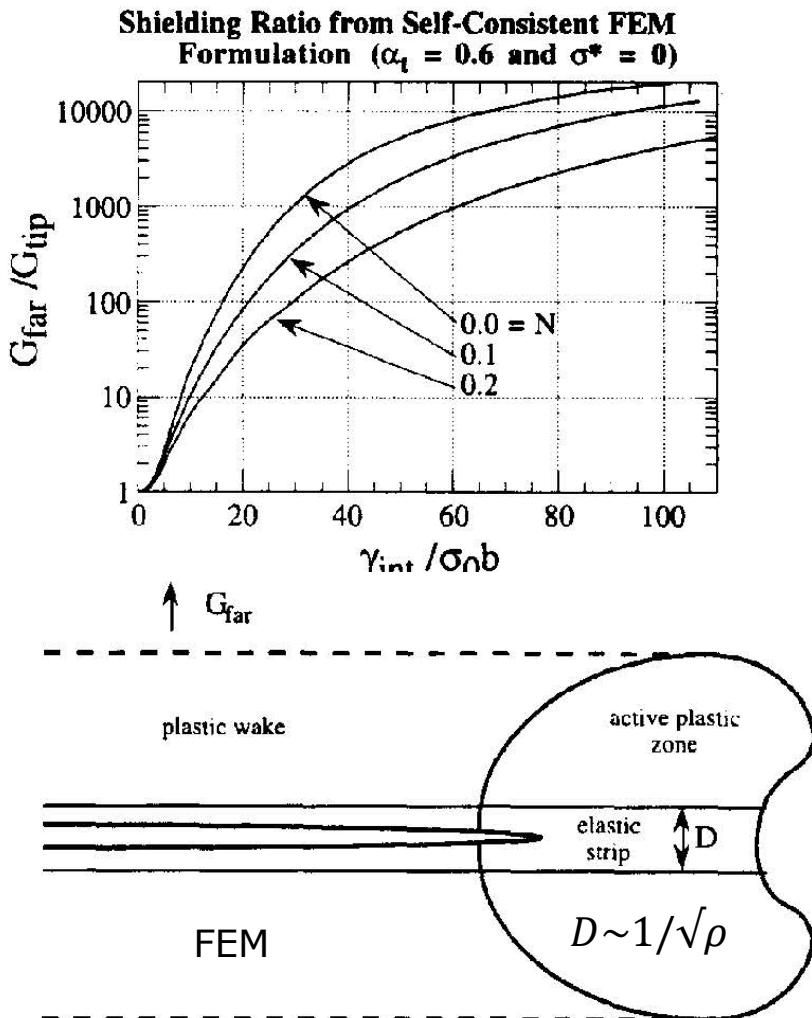
¹Department of Mechanical and Environmental Engineering, University of California, Santa Barbara, CA 93106-5070. ²Division of Engineering and Applied Sciences and Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA 02138 and ³Division of Engineering, Brown University, Providence, RI 02912, U.S.A.

Abstract—A theory is proposed for cleavage in the presence of plastic flow, in circumstances which do not involve strong viscoplastic retardation of dislocation motion. We build upon recent notions that recognize the large disparity between relevant length scales involved in plastic flow processes around cracks in metals and on metal-ceramic interfaces.

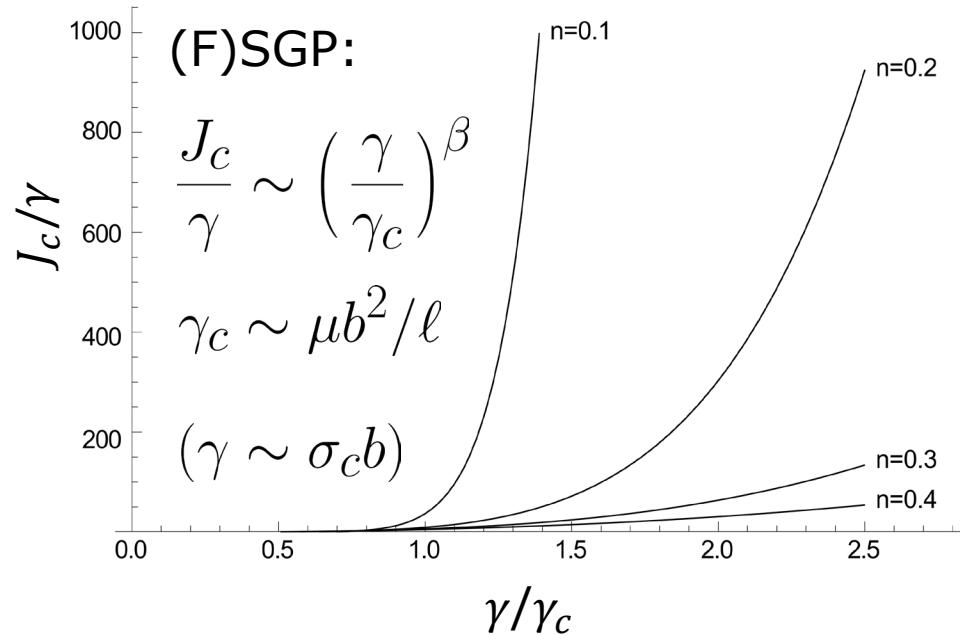
...

For steady-state crack growth to occur, it is found that the applied energy release rate G must generally be several orders of magnitude larger than the ideal work necessary to separate the interface, at least when D is taken as dislocation spacing. Furthermore, this “shielding” ratio is found to be strongly sensitive to the ideal work of fracture itself, as well as other material properties. Copyright © 1996 *Acta Metallurgica Inc.*

What have we learned?



Beltz, G., Rice, J.R., Shih, C.F. & Xia, L.,
Acta Mater., **44**(10) (1996) 3943-3954.



- J_c rises sharply above γ , provided $\gamma > \gamma_c$ (threshold)
- γ has **gating effect** on J_c
- (F)SGP + work hardening exponents < 1 , explain ductile fracture, scaling

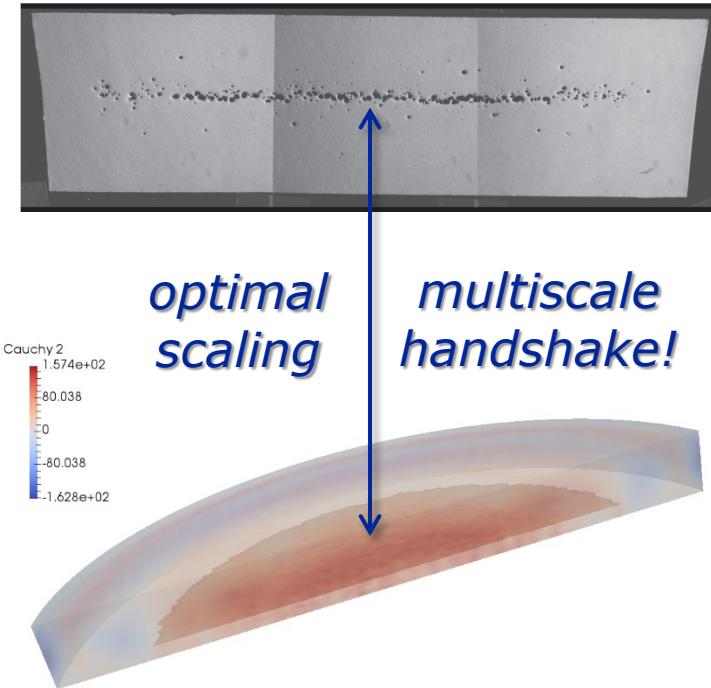
Ductile vs. brittle fracture

Material	K (MPa)	n	δ_c (mm)	b (nm)	μ (GPa)	γ (J/m ²)	ℓ (nm)	γ_c (J/m ²)	$s=0.4$
								$s=0.2$	
OFHC Cu	400	0.29	6.47	0.255	44	1.725	8.14	0.305	0.180
Beryllium Cu	920	0.36	8.87	0.255	49	1.752	4.85	0.577	0.328
Al 1100	162	0.25	5.33	0.286	26	0.980	11.49	0.157	0.095
Al 356	358	0.10	1.77	0.286	27	0.980	2.18	0.806	0.519
Fe 310	1109	0.34	8.33	0.248	77	1.950	5.92	0.700	0.402
Fe 347	1343	0.31	7.35	0.248	74	1.950	4.34	0.915	0.534
Fe 303	1469	0.40	10.64	0.248	74	1.950	5.03	0.802	0.444
Fe 304	1319	0.39	10.15	0.248	74	1.950	5.44	0.740	0.413
Ni Annealed	2702	0.31	6.99	0.249	76	2.280	2.13	1.908	1.120
Ni Rene 41	2340	0.20	3.90	0.249	61	2.280	1.39	2.277	1.410
Ni K-Monel	1865	0.20	3.90	0.249	61	2.280	1.60	1.953	1.209

Table 1

Material constants for OFHC Cu, Beryllium Cu, Al 1100, Al 365, Fe 310, Fe 347, Fe 303, Fe 304, Ni, Ni Rene 41 and Ni K-Monel at room temperature. Sources: K , n , δ_c and μ from Warren and Reed (1963); b from Simon et al. (1992); $s = 0.2$ inferred for copper from Mu et al. (2014, 2016, 2017) by Dahlberg and Ortiz (2019); γ as tabulated in Hirth and Lothe (1968).

Concluding remarks

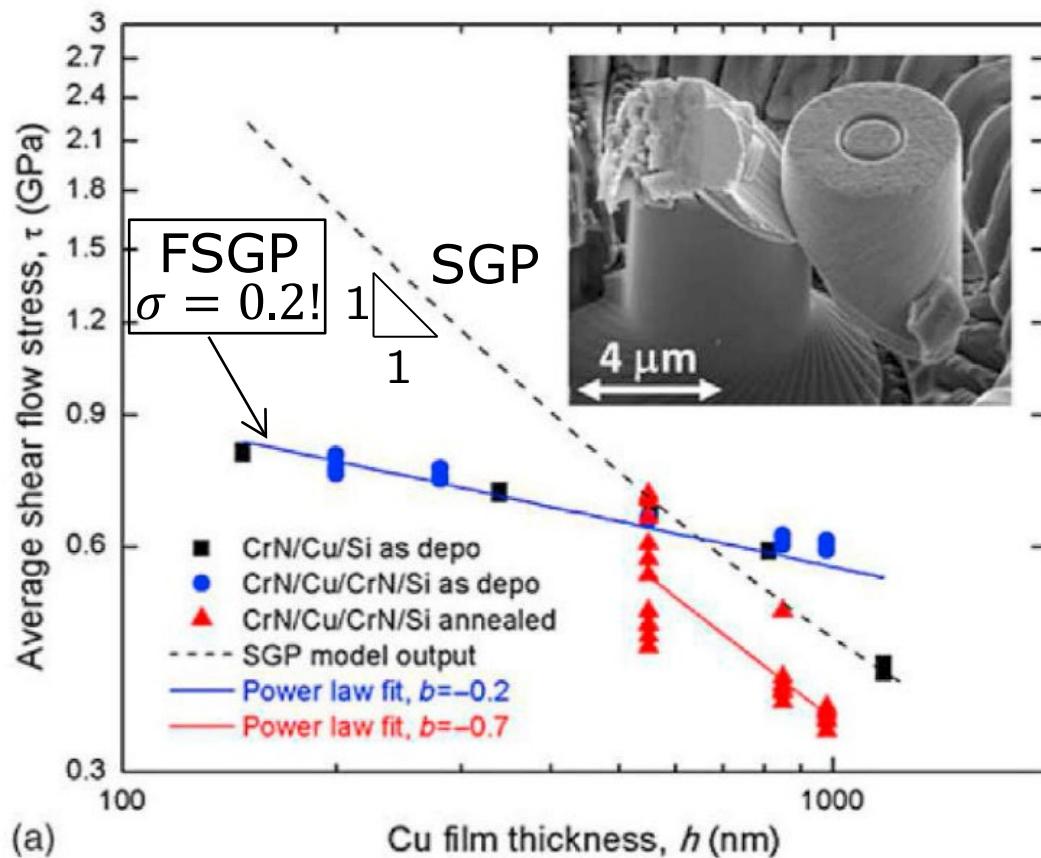


- *Strain-gradient plasticity* predicts *ductile fracture* as the result of a *competition* between *geometrical softening and strain-gradients*.
- *Optimal scaling* supplies an effective *analytical tool* for characterizing effective behavior at the macroscale (upscaling)
- Average normal stress vs opening displacement are found to *obey a power-law cohesive law*
- Exponents depend solely on the *growth properties* of the strain-gradient model, other details get 'buried' into constant factors
- *Effective cohesive law* represents *microscale mechanisms* (e.g., void sheets) in an effective sense at the *subgrid level*
- Can be embedded into standard *macroscale FE calculations*, e.g., as cohesive elements, in a *mesh-size insensitive* way

Concluding remarks

Thank you!

Fractional strain-gradient plasticity

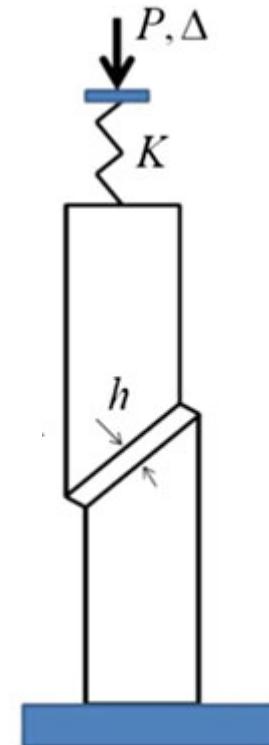


Shear flow stress as a function of thickness for Cu layers¹.

SGP model prediction shown as dashed line.

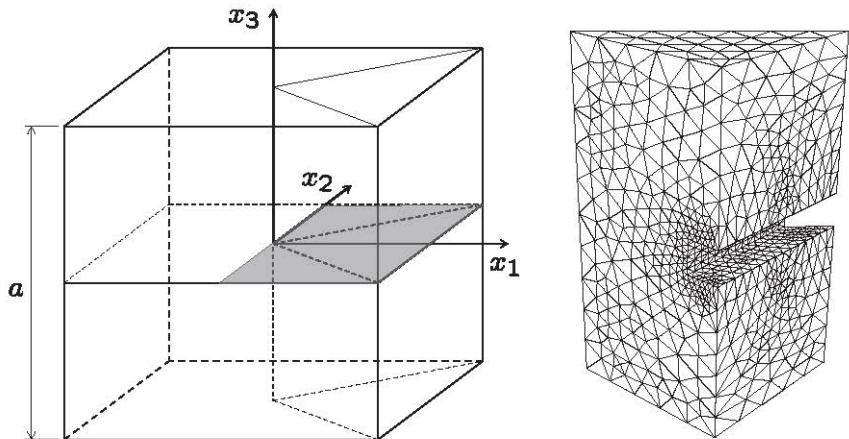
Insert shows SEM image of experimental setup.

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



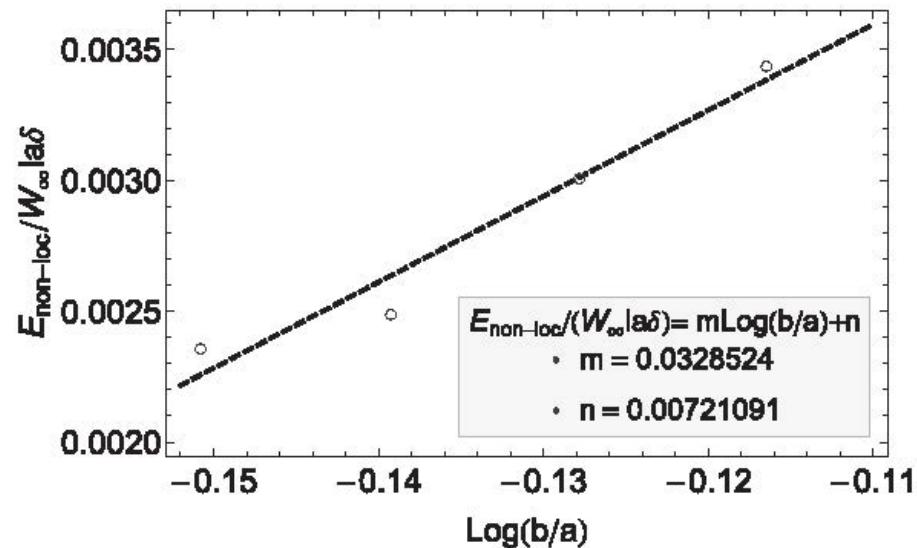
Mu, Y., Zhang, X.,
Hutchinson, J.W., Meng, W.J.,
2017. J. Mater. Res.
32 (8), 1421–1431.

Optimal scaling – FE verification



- Nonlocal energy:

$$E_{\text{nonlocal}} = \sum_{\text{interior element faces}} K \ell |[F]|$$



S. Heyden, S. Conti and M. Ortiz,
Mechanics of Materials, 90 (2015) 131-139.

Michael Ortiz
CMCS 2023