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)

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Ductile fracture of metals

- 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 **macrosopic plastic deformation** and dissipation above TDB transition temperature
- **Ductile fracture is the quintessential multiscale phenomenon!**

SA333 steel, $T=300K$, $\frac{d\varepsilon}{dt}=3\times10^{-3}s^{-1}$

A508 steel

Ductile fracture – Micromechanical basis

(plane-strain) specific fracture energy
from $J$-testing (ASTM E813)

$$J_{lc} = \sigma_0 \ell$$

Dimensional analysis!

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

Intrinsic characteristic length $\ell$, empirical material constant

N. A. Fleck, G.M. Muller, M.F. Ashby I and J.W. Hutchinson,
“Strain-gradient plasticity: Theory and experiment”,
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

Local deformation theory

- Deformation theory: Minimize
  \[ E(y) = \int_{\Omega} W(Dy(x)) \, dx, \]
  \[ y : \Omega \to \mathbb{R}^d, \text{ volume preserving}. \]
- (Observed) growth of \( W(F) \)?
- Assume power-law hardening
  \[ \sigma \sim K \varepsilon^n = K(\lambda - 1)^n. \]
- 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 \( \Rightarrow \text{Sublinear growth!} \ (p < 1). \)

Armand Considère, *Annales des Ponts et Chaussées*, 9 (1885) 574-775. CMCS 2023
Local deformation theory

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...

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Strain-gradient deformation theory

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

\[ E(y) = \int_{\Omega} W\left(Dy(x), D^2 y(x)\right) \, dx, \]

\[ y : \Omega \rightarrow \mathbb{R}^d, \text{ volume preserving.} \]

- Growth in \( D^2 y(x) \) **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?**
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: \( E(y) \sim \int_{\Omega} \left( |Dy(x)|^p + \ell|D^2y(x)| \right) dx, \quad 0 < p < 1. \)

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: \( a_{\text{opt}} \sim \ell^{\frac{1}{2-p}} \delta^{\frac{1-p}{2-p}} \) (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:
  \[ C_L(p) \ell^{2-p} \delta^{1-p} \leq J \leq C_U(p) \ell^{2-p} \delta^{1-p}. \]

- Energy scales with power of opening displ (\(\delta\)): Cohesive behavior!
- Bounds degenerate when the intrinsic length \(\ell\) decreases to zero
- Theory provides a link between micro-plasticity (\(\ell\), 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 \( y \in W^{1,1}_{\text{loc}}(\mathbb{R}^3; \mathbb{R}^3) \) 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

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

The constant \( C \) depends only on \( p \) and \( \sigma \).

**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 \( \ell \) we have

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

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

\[ \sigma = \frac{\partial J}{\partial \delta} \]

**nucleation stress**
(decohesion of second phase particles)

**Optimal scaling:**
\[ \sigma \sim K (\delta / \ell)^{-\frac{1-n}{2-n}} \]

\[ \delta_c \sim \ell \left( \frac{\sigma_c}{K} \right)^{\frac{n}{2-n}} \]

\( K \equiv \) strength
\( \ell \equiv \) intrinsic length
\( n \equiv \) hardening

Spall fracture – Multiscale analysis

Ni specimen

\( D = 50 \text{ mm}, \ t = 4.95 \text{ mm} \)

A. Pandolfi & MO (unpublished)

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

Fracture effective cohesive law
cohesive elements

Bulk

\( h \gg \ell \)

back-surface loading profile

Boundary velocity / Max velocity

Time [microseconds]
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A. Pandolfi & MO (unpublished)
What have we learned?

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

G. E. BELTZ\(^1\), J. R. RICE\(^2\), C. F. SHIH\(^3\) and L. XIA\(^3\)

\(^1\)Department of Mechanical and Environmental Engineering, University of California, Santa Barbara, CA 93106-5070, \(^2\)Division of Engineering and Applied Sciences and Department of Earth and Planetary Sciences, Harvard University, Cambridge, MA 02138 and \(^3\)Division 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?


(F)SGP:

\[
\frac{J_c}{\gamma} \sim \left(\frac{\gamma}{\gamma_c}\right)^\beta
\]

\[\gamma_c \sim \mu b^2/\ell\]

\[(\gamma \sim \sigma_c b)\]

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

### Table 1

Materials 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: $K$, $n$, $\delta_c$ and $\mu$ 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); $\gamma_c$ as tabulated in Hirth and Lothe (1968).

<table>
<thead>
<tr>
<th>Material</th>
<th>$K$ (MPa)</th>
<th>$n$</th>
<th>$\delta_c$ (mm)</th>
<th>$b$ (nm)</th>
<th>$\mu$ (GPa)</th>
<th>$\gamma_c$ (J/m$^2$)</th>
<th>$\ell$ (nm)</th>
<th>$s=0.2$</th>
<th>$s=0.3$</th>
<th>$s=0.4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>OFHC Cu</td>
<td>400</td>
<td>0.29</td>
<td>6.47</td>
<td>0.255</td>
<td>44</td>
<td>1.725</td>
<td>8.14</td>
<td>0.305</td>
<td>0.180</td>
<td>0.127</td>
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<tr>
<td>Beryllium Cu</td>
<td>920</td>
<td>0.36</td>
<td>8.87</td>
<td>0.255</td>
<td>49</td>
<td>1.752</td>
<td>4.85</td>
<td>0.577</td>
<td>0.328</td>
<td>0.227</td>
</tr>
<tr>
<td>Al 1100</td>
<td>162</td>
<td>0.25</td>
<td>5.33</td>
<td>0.286</td>
<td>26</td>
<td>0.980</td>
<td>11.49</td>
<td>0.157</td>
<td>0.095</td>
<td>0.067</td>
</tr>
<tr>
<td>Al 356</td>
<td>358</td>
<td>0.10</td>
<td>1.77</td>
<td>0.286</td>
<td>27</td>
<td>0.980</td>
<td>2.18</td>
<td>0.806</td>
<td>0.519</td>
<td>0.382</td>
</tr>
<tr>
<td>Fe 310</td>
<td>1109</td>
<td>0.34</td>
<td>8.33</td>
<td>0.248</td>
<td>77</td>
<td>1.950</td>
<td>5.92</td>
<td>0.700</td>
<td>0.402</td>
<td>0.279</td>
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<tr>
<td>Fe 347</td>
<td>1343</td>
<td>0.31</td>
<td>7.35</td>
<td>0.248</td>
<td>74</td>
<td>1.950</td>
<td>4.34</td>
<td>0.915</td>
<td>0.534</td>
<td>0.374</td>
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<tr>
<td>Fe 303</td>
<td>1469</td>
<td>0.40</td>
<td>10.64</td>
<td>0.248</td>
<td>74</td>
<td>1.950</td>
<td>5.03</td>
<td>0.802</td>
<td>0.444</td>
<td>0.304</td>
</tr>
<tr>
<td>Fe 304</td>
<td>1319</td>
<td>0.39</td>
<td>10.15</td>
<td>0.248</td>
<td>74</td>
<td>1.950</td>
<td>5.44</td>
<td>0.740</td>
<td>0.413</td>
<td>0.283</td>
</tr>
<tr>
<td>Ni Annealed</td>
<td>2702</td>
<td>0.31</td>
<td>6.99</td>
<td>0.249</td>
<td>76</td>
<td>2.280</td>
<td>2.13</td>
<td>1.908</td>
<td>1.120</td>
<td>0.786</td>
</tr>
<tr>
<td>Ni Rene 41</td>
<td>2340</td>
<td>0.20</td>
<td>3.90</td>
<td>0.249</td>
<td>61</td>
<td>2.280</td>
<td>1.39</td>
<td>2.277</td>
<td>1.410</td>
<td>1.017</td>
</tr>
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<td>Ni K-Monel</td>
<td>1865</td>
<td>0.20</td>
<td>3.90</td>
<td>0.249</td>
<td>61</td>
<td>2.280</td>
<td>1.60</td>
<td>1.953</td>
<td>1.209</td>
<td>0.872</td>
</tr>
</tbody>
</table>

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 layers\(^1\).

SGP model prediction shown as dashed line.

Insert shows SEM image of experimental setup.


Optimal scaling – FE verification

- Nonlocal energy:
  \[ E_{\text{nonlocal}} = \sum_{\text{interior element faces}} K \ell | [F] | \]