Optimal scaling laws in ductile fracture

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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

Scope

- Micro-macro relations for ductile fracture
- (Universal) scaling relations in ductile fracture?
- Application of optimal scaling to ductile fracture
- Results for metals and polymers
Background on ductile fracture

- 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., $\frac{d\varepsilon}{dt}=3\times10^{-3}\text{s}^{-1}$
Background on ductile fracture

- A number of ASTM engineering standards are in place to characterize ductile fracture properties (J-testing, Charpy test)
- The Charpy test data reveals a brittle-to-ductile transition temperature
- In general, the specific fracture energy for ductile fracture is greatly in excess of that required for brittle fracture...

Charpy energy of A508 steel
(Tanguy et al., Eng. Frac. Mechanics, 2005)
Micromechanics of ductile fracture

- Objective: Elucidate microstructure/property relations (voids to specific fracture energy)

- Traditional ‘micromechanics’ approach:
  - Select a specific microscale model (crystal plasticity, porous plasticity, strain-gradient plasticity...)
  - Select a ‘representative microstructure’ (void in periodic cell, shear/damage localization band...)
  - Perform ‘unit-cell’ calculations, parametric studies...

- Critique:
  - Pros: Calculations ‘exact’ (within numerical precision)
  - Cons: Model-specific results, non-optimal static microstructures, numerical (vs. epistemic) results...

- Alternative: Analysis (e.g., optimal scaling)
Scaling laws in science

- A broad variety of physical phenomena obey power laws over wide ranges of parameters
- Scale invariance: If \( y = C x^\alpha \), then \((x,y)\) iff \((\lambda x, \lambda^\alpha y)\), law of corresponding states
- Universality:
  - Exponents are material-independent (‘universal’)
  - Systems displaying identical scaling behavior are likely to obey the same fundamental dynamics
- Experimental master curves, data collapse
- Examples:
  - Critical phenomena (second-order transitions)
  - Materials science (Taylor, Hall-Petch, creep laws...)
  - Continuum mechanics (hydrodynamic, fracture...)
Optimal scaling

- Suppose: Energy $= E(u, \epsilon_1, \ldots, \epsilon_N)$
- Optimal (matching) upper and lower bounds:

$$C_L\epsilon_1^{\alpha_1} \ldots \epsilon_N^{\alpha_N} \leq \inf E(\cdot, \epsilon_1, \ldots, \epsilon_N) \leq C_U\epsilon_1^{\alpha_1} \ldots \epsilon_N^{\alpha_N}$$

- The exponents $\alpha_1, \ldots, \alpha_N$ are sharp, universal
- The constants $C_L$ and $C_U$ are often lax, imprecise...
- Upper bound by construction, ansatz-free lower bound
- Originally applied to branched microstructures in martensite (Kohn-Müller 92, 94; Conti 00)
- Applications to micromagnetics (Choksi-Kohn-Otto 99), thin films (Belgacem et al 00)
Naïve model: Local plasticity

- Deformation theory: Minimize
  \[ E(y) = \int_{\Omega} W(Dy(x)) \, dx \]
- 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 \( \lambda \): \( \partial_\lambda W \sim K \lambda^{n-1} \Rightarrow W \sim K \lambda^n \)
- In general: \( W(F) \sim |F|^p, \quad p = n \in (0, 1) \)

\( \Rightarrow \) Sublinear growth!
Naïve model: Local plasticity

- 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...

\[ E_h \sim h \left( \frac{2\delta}{h} \right)^p \]

\[ \lim_{h \to 0} E_h = 0 \]
Strain-gradient plasticity

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

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

\( y : \Omega \rightarrow \mathbb{R}^n, \) volume preserving

- Strain-gradient effects may be expected to oppose localization
- Growth of \( W \) with respect to the second deformation gradient?
Strain-gradient plasticity

- 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:
  \[ E = \frac{T}{b} 2 \sin \theta = \frac{T}{b} |\| F \|| \]
  \[ \Rightarrow W(F, \cdot) \text{ has linear growth!} \]
Strain-gradient plasticity & fracture

• For metals, local plasticity exhibits sub-linear growth, strain-gradient plasticity linear growth

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

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

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

Optimal scaling – Ductile fracture

- Approach: Deformation theory SG-plasticity
- Slab, $[0, L]^2$-periodic, volume-preserving
- Uniaxial extension + voids
Optimal scaling – Ductile fracture

- $E(y) \equiv$ general deformation-theoretical energy

- Growth: For $0 < K_L < K_U$, intrinsic length $\ell > 0$,
  \[
  E(y) \geq K_L \left( \int_\Omega (|Dy|^p - 3^{p/2}) \, dx + \ell \int_\Omega |D^2y| \, dx \right)
  \]
  \[
  E(y) \leq K_U \left( \int_\Omega (|Dy|^p - 3^{p/2}) \, dx + \ell \int_\Omega |D^2y| \, dx \right)
  \]

Theorem [Fokoua et al., ARMA, 2013]. For $\ell$ sufficiently small, $p \in (0, 1)$, $0 < C_L(p) < C_U(p)$,

\[
C_L(p)L^2\ell^{2-p}\delta^{2-p} \leq \inf E \leq C_U(p)L^2\ell^{2-p}\delta^{2-p}
\]
Sketch of proof – Upper bound


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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: \[ a = (\ell \delta^{1-p})^{1/(2-p)} \Rightarrow E \leq C_U L^2 \ell^{2-p} \delta^{2-p} \]

\[ \uparrow \text{void growth!} \]
Optimal scaling – Ductile fracture

• Optimal (matching) upper and lower bounds:
\[ C_L(p) L^2 \ell^{2-p} \delta^{2-p} \leq \inf E \leq C_U(p) L^2 \ell^{2-p} \delta^{2-p} \]

• 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* \((\delta)\): Cohesive behavior!

• Lower bound degenerates to 0 when the intrinsic length \((\ell)\) decreases to zero...

• Bounds on specific fracture energy:
\[ C_L(p) \ell^{2-p} \delta_c^{2-p} \leq G_c \leq C_U(p) \ell^{2-p} \delta_c^{2-p} \]
Fracture of polymers

- 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...


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

- Suppose: For $K_U > 0$, intrinsic length $\ell > 0$, 
  $$E(y) \leq K_U \left( \int_{\Omega} (|Dy|^p - 3^{p/2}) \, dx + \ell \int_{\Omega} |D^2y| \, dx \right)$$
- If $E(y) < +\infty \Rightarrow y$ continuous on a.e. plane!
- Crazing is precluded by the continuity of $y$!
- Instead, fractional SG elasticity: For $\sigma \in (0, 1)$, 
  $$E(y) \leq K_U \left( \int_{\Omega} (|Dy|^p - 3^{p/2}) \, dx + \ell^\sigma |y|_{W^{1+\sigma,1}(\Omega)} \right)$$

**Theorem** [Conti *et al.*, ARMA, 2014] For $\ell$ 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

Crazing in 800 nm polystyrene thin film (C. K. Desai et al., 2011)
Sketch of proof – Upper bound

- In every cube:
Optimal scaling – Crazing

• Optimal (matching) upper and lower bounds:

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

• *Fractional* strain-gradient elasticity supplies bounded energies for crazing mechanism.

• Energy scales with *area* \((L^2)\): *Fracture scaling*!

• Energy scales with power of opening displacement \((\delta)\): *Cohesive behavior*!

• Lower bound degenerates to 0 when the intrinsic length \((\ell)\) decreases to zero...

• Bounds on specific fracture energy:

\[ C_L \ell^{1+\sigma} \delta_c^{1+\sigma} \frac{1}{\ell^{1+\sigma}} \leq G_c \leq C_U \ell^{1+\sigma} \delta_c^{1+\sigma} \frac{1}{\ell^{1+\sigma}} \]
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...)
- Ductile fracture can be efficiently implemented through material-point erosion schemes...
Concluding remarks

Thanks!