Multiscale modeling of materials: (2) Dislocation structures → polycrystals

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Metal plasticity – Multiscale hierarchy

Ultimate goal: Ascertain macroscopic behavior from first principles

Lattice defects, EoS

Dislocation dynamics

Subgrain structures

Polycrystals

Continuum

Engineering applications

Quantum mechanical

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Continuum models of crystal plasticity

- Aim: 'Cook up' empirical models of crystal plasticity 'inspired' in dislocation mechanics that explain observed behavior (microstructure, macroscopic stress-strain behavior, scaling laws).
- To date: 'Deformation theory of plasticity' (one incremental step from initial to final state), energy minimization, relaxation, \( \Gamma \)-convergence.
- Open question: Which continuum models (energy + kinetics) are limits of discrete (hence more fundamental) models?
- Open question: General deformation paths?
General linear elastic dislocations

- Volterra dislocation: \( u \in SBV \) such that

\[
Du = \nabla u \mathcal{L}^3 + b \otimes m \mathcal{H}^2 \subset S_u \equiv \beta^e \mathcal{L}^3 + \beta^p \mathcal{H}^2 \subset S_u
\]

- Elastic deformation
- Plastic deformation

- Dislocation density: \( \alpha = -\text{curl} \beta^e = \text{curl} \beta^p \)
General dislocations – Energy

- Stored energy:

\[ E(\alpha) = \int \int \text{tr}[\alpha^T(x) \Gamma(x, y) \alpha(y)] \, dx \, dy \]

where: \( \Gamma(x, y) = \int [\nabla G(x, z) \cdot \nabla G(y, z) I - \nabla G(x, z) \otimes \nabla G(x, z)] \, dz \)

and: \( G = \Delta^{-1} \equiv \text{Green’s function of the Laplacian.} \)
Straight dislocations – Dissipation

- Peierls stress $\tau_0$: Threshold stress for dislocation motion
- Dissipation $= \tau_0 \times$ (slipped area)
  - Lattice friction
Obstacles – Topological obstructions

- Example: Precipitates.

Impenetrable obstacles

(Humphreys and Hirsch ’70)

- Junctions:

.pinning points

\[ b_1 \rightarrow b_2 \]

\[ b_1 + b_2 \]
The standard continuum model

\[ u = \bar{\beta}x \] (affine BC)

\[ \beta^p, \alpha \] given

- Elastic energy: \( \inf_u \int_{\Omega \setminus S_u} \left( \frac{1}{2} |\epsilon(u)|^2 - \epsilon(u) \cdot \epsilon^p \right) \, dx \)

\[ = |\Omega| \left( \frac{1}{2} |\bar{\epsilon}|^2 - \bar{\epsilon} \cdot \bar{\epsilon}^p \right) + E(\alpha) \]

\[ \beta^p = \frac{1}{|\Omega|} \int_{\Omega} \beta^p \, dx \equiv \text{average plastic deformation} \]
The standard continuum model

- Average plastic deformation:

\[
\bar{\beta}^p = \frac{1}{|\Omega|} \int_{\Omega} \beta^p \, dx
\]

\[
\bar{\beta}^p = \frac{1}{|\Omega|} \int_{S_u} [u] \otimes m dH^2 \equiv \sum_{i=1}^{N} \gamma_i s_i \otimes m_i
\]

where \( \gamma_i \equiv \) slip strain on system \( i \).

\[
\gamma = \frac{3b}{L} = \frac{b3L^2}{L^3} = \frac{b \times \text{Area}}{\text{Volume}}
\]
The standard continuum model

- Standard model: \[ E(u, \gamma) = \int_{\Omega} \left( \frac{1}{2} |\varepsilon(u) - \varepsilon^p(\gamma)|^2 + W^p(\gamma) + \frac{T}{b} |\text{curl} \beta^p(\gamma)| \right) \, dx \]

  \( \text{strain energy} \quad \text{plastic work} \quad \text{core energy} \)

- Plastic work (infinite latent hardening):
  \[ W^p(\gamma) = \begin{cases} 
  \tau_i |\gamma_i| & \text{if } \gamma_j = 0, \quad \forall j \neq i \\
  \infty & \text{otherwise},
  \end{cases} \]

- Core energy: \( T \sim Gb^2 \equiv \text{dislocation line tension} \),
  \( T/b \sim Gb \sim O(\epsilon) \)
Standard model – Local

- Minimize slip strains pointwise:

\[ \inf_{\gamma} E(u, \gamma) = I(u) = \int_{\Omega} W(c(u)) \, dx \]

where:

\[ W(\epsilon) = \min_{\gamma} \left( \frac{1}{2} |\epsilon - \bar{\epsilon}^{p}(\gamma)|^2 + W^{p}(\gamma) \right) \]

- Properties of \( W(\epsilon) \):
  - Linear growth along orbits of \( s_i \otimes m_i, i = 1, \ldots, N \).
  - Quadratic growth in all other directions.

- Question: Relaxation of \( I(u) \)?
Standard model – Local

- Example: FCC crystal deforming on (1\bar{1}0)-plane

\[ \beta^p \in \gamma s \otimes m + so(3) \]
(Single slip)

- \( W(\nabla u) \) non-convex!

\( W(\nabla u) \) non-convex!

(Ortiz and Repetto, *JMPS*, 47(2) 1999, p. 397)
Standard model – Relaxation

- Convex envelop: \( W^{**}(\beta) = \inf \left\{ \sum_i \lambda_i W(\beta_i) : \lambda_i \geq 0, \sum_i \lambda_i = 1, \beta_i \in \mathbb{R}^{3 \times 3} \right\} \).

- Linear growth on traceless symmetric matrices
- Quadratic growth on the trace

- Regression function: \( W^\infty(\beta) = \lim_{t \to \infty} \frac{1}{t} W^{**}(t/\beta) \).

**Definition.** A set of slip systems \( S = \{ s_i \otimes m_i \} \) is complete if the symmetric lamination convex hull of \( \{ \pm (s_i \otimes m_i)^{\text{sym}} \} \) contains a neighbourhood of the origin in the space of symmetric traceless matrices.
Standard model – Relaxation

- Let: \( U(\Omega) = \left\{ u \in BD(\Omega, \mathbb{R}^3) : \text{div}u \in L^2(\Omega) \right\} \)

**Theorem** (Conti and Ortiz, ARMA ’05) *Suppose that the set of slip systems is complete. Then, the relaxation of \( I(u) \) with respect to the strong \( L^1 \) topology is*

\[
J(u) = \begin{cases} \\
\int_{\Omega} W^{**}(c(u)) \, dx + \int_{\Omega} W^{\infty} \left( \frac{E_s u}{|E_s u|} \right) \, d|E_s u|, & \text{if } u \in U(\Omega) \\
+\infty, & \text{otherwise.}
\end{cases}
\]
Standard model – Relaxation

- Proof: Match upper & lower bounds, $W^{qc} = W^{**}$.
- Lower bound: $J(u)$ convex functional of measure $Eu$, $J(u) \leq I(u)$.

**Lemma** Let $S$ be a complete set of slip systems. For any $\beta \in \mathbb{R}^{3 \times 3}$ and any $\epsilon > 0$ there is a laminate $\nu$ (of finite order) such that

$$\langle \nu, \text{Id} \rangle = \beta \quad \text{and} \quad \langle \nu, W \rangle \leq W^{**}(\beta) + \epsilon.$$

- Some of the deformations in the laminate may become unbounded as $\epsilon \to 0$ and become slip lines in the limit.
Standard model – Relaxation

\[ J(u) = \int_{\Omega} W^{**}(\varepsilon(u)) dx + \int_{\Omega} W^{\infty} \left( \frac{E_s u}{|E_s u|} \right) d|E_s u| \]

Ideal plasticity

Slip-line energy

(Rice, Mech. Mat., 1987)

(Crone and Shield, JMPS, 2002)
Relaxation and computation

Indentation of [001] surface of FCC crystal
(Hauret and Ortiz, 2005)
Relaxation and computation

rank 2/2, $|γ|_∞ = 0.0025$

rank 4/14, $|γ|_∞ = 0.43$

rank 4/12, $|γ|_∞ = 0.02$

rank 4/6, $|γ|_∞ = 0.026$

rank 4/16, $|γ|_∞ = 0.21$
Relaxation and computation

Indentation of [001] FCC surface

- Elastic
- Unrelaxed
- Relaxed
- Bubble enrichment

(Hauret and Ortiz, 2005)
Relaxation and computation

Microstructures generated at quadrature points on the fly

average deformation

local deformation

average stress

local stress
Model boundary-value problem

- Standard model: \( E(u, \gamma) = \)
  \[
  \int_\Omega \left( \frac{1}{2} |\varepsilon(u) - \bar{\varepsilon}^p(\gamma)|^2 + W^p(\gamma) + \left( \frac{T}{b} \right) |\text{curl} \bar{\beta}^p(\gamma)| \right) \, dx \\
  + \mu \|u - \gamma x\|^2_{H^{1/2}(\partial \Omega)}
  \]

- Assumptions:
  * \( \Omega = [0, d]^3 \), \( d \equiv \) grain size.
  * Collinear double slip at \( 90^\circ \).
  * Scalar displacement \( u_3 \).
  * Shear strain \( \gamma \) prescribed at infinity.
Optimal scaling laws

**Theorem** (Conti and Ortiz, ARMA ’05) *There are constants* $c, c'$ *such that*

$$cE_0(T, \gamma, \tau_0, \mu, d) \leq \inf E \leq c'E_0(T, \gamma, \tau_0, \mu, d)$$

*where*

$$E_0(T, \gamma, \tau_0, \mu, d) \big/ G \gamma^2 d^3 =$$

$$\min \left\{ 1, \frac{\mu}{G}, \frac{\tau_0}{G \gamma} + \left( \frac{\mu}{G} \right)^{1/2} \left( \frac{T}{G \gamma bd} \right)^{1/2}, \frac{\tau_0}{G \gamma} + \left( \frac{T}{G \gamma bd} \right)^{2/3} \right\}$$

- Upper bounds determined by construction
- Lower bounds: Rigidity estimates, ansatz-free lower bound inequalities (Kohn and Müller ’92, ’94; Conti ’00)
Optimal scaling – Laminate construction

- Energy:
  $$W \equiv \frac{E'_{0}}{d^3} \sim \tau_0 \gamma + \left( \frac{\mu' T' \gamma}{b d} \right)^{1/2}$$

- Yield stress:
  $$\tau \equiv \frac{\partial W}{\partial \gamma} \sim \tau_0 + \frac{1}{2} \left( \frac{\mu T \gamma}{b d} \right)^{1/2}$$

- Lamellar width:
  $$l \sim \left( \frac{\mu T d}{\mu \gamma b} \right)^{1/2}$$
Optimal scaling – Branching construction

- Energy:
  \[ W \sim \tau_0 \gamma + G \left( \frac{T \gamma^2}{Gb_d} \right)^{2/3} \]

- Yield stress:
  \[ \tau \sim \tau_0 + \left( \frac{T}{bd} \right)^{2/3} (G \gamma)^{1/3} \]

- Microstructure size:
  \[ l \sim \left( \frac{T d^2}{G \gamma b} \right)^{1/3} \]
Optimal scaling – Microstructures

Dislocation structures corresponding to the lamination and branching constructions

\[ \tau \sim d^{-1/2} \]

\[ \tau \sim d^{-2/3} \]

- Shocked Ta (Meyers et al '95)
- Laminate
- Branching
- LiF impact (Meir and Clifton '86)
Optimal scaling – Phase diagram

\[ \left( \frac{T}{G \gamma bd} \right) \]

- Rigid
- Elastic

\[ \gamma \uparrow, \gamma \uparrow, \gamma \uparrow \mu \downarrow, d \uparrow, d \uparrow, d \uparrow \mu \downarrow, \mu \downarrow \]

- Lamellar
- Branching

\[ \left( \frac{\mu}{G} \right) \]

- $T = \text{dislocation energy}$
- $G = \text{shear modulus}$
- $\gamma = \text{deformation}$
- $b = \text{Burgers vector}$
- $d = \text{grain size}$
- $\mu = \text{GB strength}$
Non-locality and computation

- Effective behavior of each grain: $E(u|_{\partial \Omega}, \Omega)$, not a functional a gradient type.

- Need ’whole grain’ elements! (open at present).