Variational Methods in Dislocation Dynamics

M. Ortiz
California Institute of Technology

Acknowledgements: P. Ariza, A. Cuitiño, A. Garroni, M. Koslowski, Stefan Müller

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Outline

- Mechanistic basis of crystal plasticity.
- Theory of linear elastic dislocations.
- Special case: Activity on single slip system, single slip plane → Phase-field model.
- Numerical implementation, simulations.
- Results of rigorous analysis (Γ-convergence).
Metal plasticity - Lengthscales

- Lattice defects, EoS
- Dislocation dynamics
- Subgrain structures
- Polycrystals
- Engineering calculations

Time: ns, µs, ms
Length: nm, µm, mm
Crystal plasticity – Macroscopic behavior

Uniaxial tension test

Copper tensile test
( Franciosi and Zaoui '82)
Crystal plasticity – Relaxation

- Allow all lattice-invariant deformations as energy wells: $QW(F) \sim f(\det F)$ (Fonseca, ’87, ’88).
- Kinetics, constraints, obstructions matter!
Crystal plasticity – Energy barriers

- Estimate of peak stress: $\tau_{\text{max}} \sim \mu/30$, much higher than experimentally observed.
- Alternative mechanism: dislocation nucleation and transport (Orowan, Taylor, Polanyi, 1934).
Crystal plasticity and dislocations

- dislocation core
- slip plane

\[ \mathbf{b} \quad \mathbf{v} \]
Crystal plasticity and dislocations

Burgers vector

Burgers circuit
Example - Nanoindentation of [001] Au

- Nanoindentation of [001] Au, 2x2x1 micrometers
- Spherical indentor, R=7 and 70 nm
- Johnson EAM potential
- Total number of atoms $\sim 0.25 \times 10^{12}$
- Initial number of nodes $\sim 10,000$
- Final number of nodes $\sim 100,000$

Detail of initial computational mesh (Knap and Ortiz, 2002)
Example - Nanoindentation of [001] Au

70 nm indenter, depth = 0.75 nm
Dislocation dynamics – Numerical tools

• First-principles calculations: Dislocation cores, dipoles, quadrupoles... ~ $10^3$ atoms (T. Arias ‘00)
• Molecular dynamics: Empirical potentials... ~ $10^9$ atoms (F. Abraham ‘03)
• Linear elasticity: Dislocation dynamics, $L \sim 10^6 b$, $\varepsilon \sim 1\%$ (Bulatov et al. ‘03)

Ta quadrupole (T. Arias ‘00)  
FCC ductile fracture (F.F. Abraham ‘03)  
FCC dislocation dynamics (M. Rhee et al. ´02)
Theory of linear-elastic dislocations

- Volterra dislocation:
  \[ \nabla \cdot \mathbf{C} \nabla u = 0, \quad \text{in } \mathbb{R}^3 \]
  \[ [u] = b, \quad \text{on } S \]
  \[ [\mathbf{C} \nabla u] \cdot \mathbf{m} = 0, \quad \text{on } S \]

- Burgers circuit:
  \[ b = \oint_{\Gamma \setminus S} \nabla u \, dr \]

- Dislocation dipole:
  \[ \frac{E}{L} \sim \frac{\mu b^2}{4\pi(1-\nu^2)} \log \frac{R}{r_0} \to \infty \]

- Need to model dislocation core!
Theory of linear-elastic dislocations

- Preferred slip systems: Minimize
  - i) Burgers vector length $b$
  - ii) Interplanar distance $d$

The slip systems of fcc crystals (Schmidt and Boas nomenclature)
Theory of linear-elastic dislocations

- Peierls theory of the dislocation core (Peierls ’47):
  Let $\delta(x) = \|u_x\|(x)$, $\phi(\delta)$ periodic of period $b$,

$$E(\delta) = \int_{-\infty}^{\infty} \phi(\delta(x)) \, dx +$$

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{B}{2} \log \frac{R}{|x - y|} \delta'(x) \delta'(y) \, dx \, dy$$

- Nabarro’s potential (Nabarro ’47):

$$\phi(u) = A \left( 1 - \cos \frac{2\pi \delta}{b} \right)$$

- Nabarro’s solution: $\delta(x) = \frac{b}{2} \left( 1 - \frac{2}{\pi} \arctan \frac{x}{c} \right)$

- Logarithmic singularity is eliminated!
Theory of linear-elastic dislocations

- General theory based on Peierls concept:
  i) Assumption: \( u \in SBV(\mathbb{R}^3) \).
  ii) Assumption: \( S(u) \in S \equiv \) set of all slip planes.
  iii) Assumption: The energy is of the form
      \[
      E(u) = \int \frac{1}{2} c_{ijkl} \beta_{ij}^e \beta_{kl}^e \, dx + \int_S \phi(\|u\|) \, dS
      \]
      with \( \phi \) periodic.
Theory of linear-elastic dislocations

- Nye's dislocation-density tensor (Nye '53):
  \[ b(\Sigma) = \int_{\Sigma} \alpha n dS \]

- But also:
  \[ b(\Sigma) = \oint_{\Gamma} \beta^e d\Gamma \]

- By Stokes theorem (Kröner '55):
  \[ \alpha = \text{curl} \beta^e = -\text{curl} \beta^p \]

- For a distribution of Volterra dislocations:
  \[ \alpha = b \otimes t\delta_L \]
Theory of linear-elastic dislocations

- From general results for elastic cut surfaces:

\[ \beta_{jn}^e(x) = \int c_{kpim} G_{ij,mn}(x, x') \beta_{kp}^p(x') dx' \]

- Elastic interaction energy:

\[ E^{\text{int}}([u]) = \int_S \int_S A_{ij}(x, x') [u_i](x) [u_j](x') dS dS' \]

where: \( A_{kl} = c_{lqjn} c_{kpim} G_{ij,mn}(x, x') m_p(x) m_q(x') \)

- Total energy:

\[ E([u]) = E^{\text{int}}([u]) + \int_S \phi([u]) dS \]

\[ \text{nonlocal} \quad \text{local} \]
Single slip plane – Phase field model

- Consider the special case (Koslowski et al ’02):
  i) Activity on single slip system, single slip plane.
  iii) Constrained slip assumption (Rice and Beltz ’92):
      \[ [u](x) = b\zeta(x)s, \quad \zeta : \mathbb{R}^2 \to \mathbb{R} \text{ (‘slip field’)} \]
  iv) Peierls potential: \( \phi(\zeta) = \frac{\mu b^2}{2d} \text{dist}^2(\zeta, \mathbb{Z}) \)
Single slip plane – Phase field model

- Total energy: \[ E(\zeta) = \int_{\mathbb{R}^2} \frac{\mu b^2}{2d} \text{dist}^2(\zeta, \mathbb{Z}) \, dx + \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mu b^2}{4} K|\widehat{\zeta}|^2 \, dk - \int_{\mathbb{R}^2} bs\zeta \, dx \]

  \begin{align*}
  \text{Core energy} & \quad \text{Elastic energy} & \quad \text{External} \\
  \text{where} & \quad K = \frac{k_2^2}{\sqrt{k_1^2 + k_2^2}} + \frac{1}{1 - \nu} \frac{k_1^2}{\sqrt{k_1^2 + k_2^2}}
  \end{align*}

- Structure of the energy:

  \[ E_\varepsilon(\zeta) = \frac{1}{2\varepsilon} \int_{\mathbb{R}^2} \text{dist}^2(\zeta, \mathbb{Z}) \, dx + |\zeta|_{H^{1/2}}^2 + \text{linear term} \]

(cf Alberti, Bouchitte and Seppecher ’98)
Single slip plane – Phase field model

- Problem: $\inf_{\zeta} E(\zeta)$

- Solution strategy: Write $\phi(\zeta) = \min_{\xi \in \mathbb{Z}} \frac{\mu b^2}{2d} |\zeta - \xi|^2$

- Then: $\inf_{\zeta} \inf_{\xi} E(\zeta, \xi)$
  
  where $E(\zeta, \xi) = \int_{\mathbb{R}^2} \frac{\mu b^2}{2d} |\zeta - \xi|^2 \, dx + \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mu b^2}{4} K|\hat{\zeta}|^2 \, dk - \int_{\mathbb{R}^2} bs \zeta \, dx$

- Exchange order of minimization: $\zeta = \zeta_0 + \varphi_d * \xi$

  where $\varphi_d(k) = \frac{1}{1 + Kd/2}$ $\Rightarrow$ mollifier.
Single slip plane – Phase field model

- Remaining problem:
  \[
  \inf_{\xi} E(\xi) \\
  \text{subject to constraint: } \xi : \mathbb{R}^2 \to \mathbb{Z}.
  \]
  where
  \[
  E(\xi) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mu b^2}{4 \left( 1 + K d/2 \right)} |\hat{\xi}|^2 dk + \ldots
  \]

- Equivalently:
  i) Minimize \( E \) without integer constraint.
  ii) Project unconstrained minimizer \( \eta \) onto ‘closest’ integer-valued function \( \xi \).
Single slip plane – Phase field model

1) Unconstrained slip  
2) Phase field  
3) Slip distribution

- Example: Straight dislocation.

\[
\frac{E}{L} \equiv \gamma = \frac{\mu b^2}{4\pi} \left( \sin^2 \theta + \frac{\cos^2 \theta}{1 - \nu} \right) \log \frac{R}{c(\theta)}
\]

\[
c(\theta) = \left( \sin^2 \theta + \frac{\cos^2 \theta}{1 - \nu} \right) \frac{d}{2}
\]
Dislocation-obstacle interaction

- Example: Precipitation hardening.

Impenetrable obstacles

Obstacles of finite strength

(Humphreys and Hirsch ’70)
Dislocation obstacle interaction

Details of Intersection Process

Unfavorable Junction

Favorable Junction

Reaction coordinate

Incremental problem:

$$\inf_{\zeta^{n+1}} W(\zeta^{n+1}, \zeta^n)$$

where

$$W = E(\zeta^{n+1}) - E(\zeta^n) + \sum_{i=1}^{N} f_i |\zeta_i^{n+1} - \zeta_i^n|$$

Irreversibility, path dependency, hysteresis
Dislocation-obstacle interaction

- Problem geometry: i) Periodic square cell.
  ii) Random array of obstacles.
Dislocation-obstacle interaction

Stress-strain curve

Dislocation density

(Movie)
Dislocation-obstacle interaction

3D view of slip field showing switching of pinning cusps

Stress-strain curve showing return-point memory effect
Line-tension anisotropy

Stress-strain curve

Dislocation density

\( \tau / \tau_0 \)

\( \gamma / \gamma_0 \)

\( \nu = 0.0 \)

\( \nu = 0.3 \)

\( \nu = 0.5 \)

Michael Ortiz
Oberwolfach 09/03
Obstacle density, sample size

\[ \frac{\rho}{\rho_0} = \begin{cases} 3.0 \times 10^{-11} & \text{if } 20 < \gamma \gamma_0 < 30 \\ 2.8 \times 10^{-11} & \text{otherwise} \end{cases} \]

\[ \frac{c b^2}{\rho_0} = \begin{cases} 3.2 \times 10^{-13} & \text{if } 20 < \gamma \gamma_0 < 30 \\ 2.6 \times 10^{-13} & \text{otherwise} \end{cases} \]

\[ \frac{c b^2}{\rho_0} = \begin{cases} 3.2 \times 10^{-13} & \text{if } 20 < \gamma \gamma_0 < 30 \\ 2.6 \times 10^{-13} & \text{otherwise} \end{cases} \]

\[ \frac{c b^2}{\rho_0} = \begin{cases} 3.2 \times 10^{-13} & \text{if } 20 < \gamma \gamma_0 < 30 \\ 2.6 \times 10^{-13} & \text{otherwise} \end{cases} \]

(a) \( cb^2 = 10^{-2} \)

(b) \( cb^2 = 10^{-4} \)

(c) \( cb^2 = 10^{-6} \)

(d) \( cb^2 = 10^{-8} \)
Concluding remarks

- Phase-field model provides a variational characterization of dislocation dynamics
- Phase-field model offers computational advantages (gridless implementation), and is amenable to rigorous analysis.
- Extensions:
  - Full 3D theory, multiple slip
  - Lattice statics theory
  - Anharmonic effects in dislocation cores
- Reference:
  http://www.solids.caltech.edu/~ortiz/publications.html
  Koslowski M, Cuitino AM, Ortiz M
  A phase-field theory of dislocation dynamics, strain hardening and hysteresis in ductile single crystals
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