An exactly solvable phase-field model of dislocation dynamics

Michael Ortiz

Caltech

In collaboration with: M. Koslowski and A.M. Cuitino

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Introduction

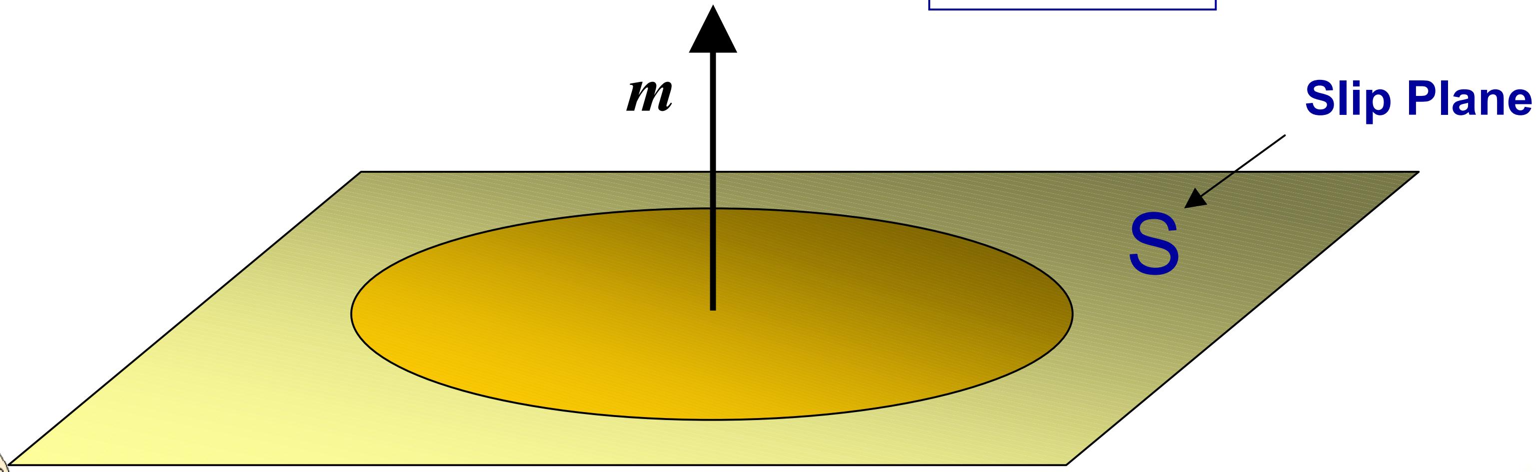
- **Objective**: Develop analytically tractable models of the cooperative behavior of large dislocation ensembles (energetics and kinetics):
  - *Yield phenomena*
  - *Hardening, hysteresis*
  - *Dislocation densities*
- **Phase field**: Representational tool for describing discrete crystallographic slip, dislocation-loop topology.
- Model is exactly solvable, implementaton is gridless, complexity governed by number of obstacles.
- Dislocation dynamics without all the dislocations

Energetics

$$E = \int_S \phi(\delta)\,dS + \int \frac{1}{2} c_{ijkl}\beta^e_{ij}\beta^e_{kl}\,d^3x - \int_S t_i\delta_i\,dS$$
$$\equiv E^{\text{core}} + E^{\text{int}} + E^{\text{ext}}$$

where: $u_{i,j} = \beta^e_{ij} + \beta^p_{ij}$, $\beta^p_{ij} = \delta_i\, m_j\, \delta_S$

displacement jump across S: $\delta_i = [\![u_i]\!]$

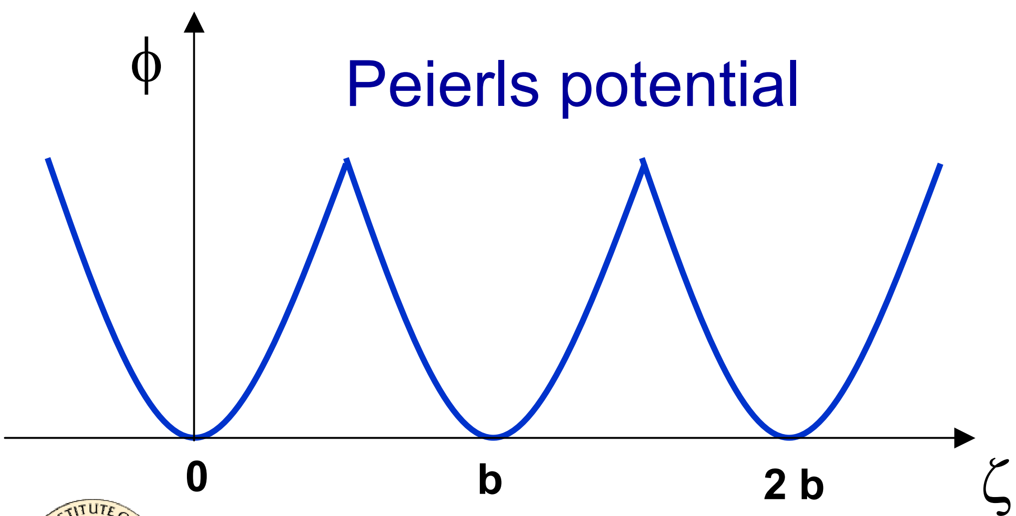


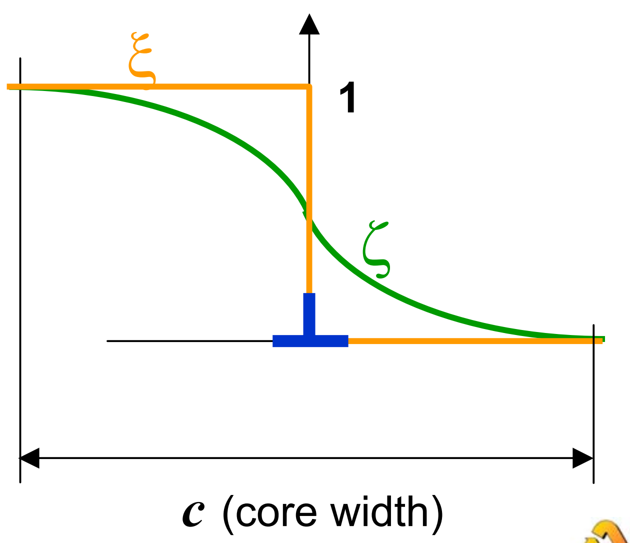
Piecewise-quadratic Peierls potential

$$\phi(\delta) = \min_{\xi \in Z} \frac{1}{2} \frac{\mu b^2}{d} |\zeta - \xi|^2$$

Constraint slip assumption: $\delta_i = \zeta b_i$, $s = t_i b_i / b$

ζ = normalized slip field





Variational problem

$$E[\zeta|\xi] = \underbrace{\int \frac{\mu b^2}{2d}|\zeta - \xi|^2 d^2x}_{\text{Core energy}} + \underbrace{\frac{1}{(2\pi)^2}\int \frac{\mu b^2}{4} K |\hat{\zeta}|^2 d^2k}_{\text{Elastic interaction}} - \underbrace{\int bs\zeta d^2x}_{\text{External field}}$$

Where: $K = \frac{k_2^2}{\sqrt{k_1^2 + k_2^2}} + \frac{1}{1-\nu}\frac{k_1^2}{\sqrt{k_1^2 + k_2^2}}$

ξ = integer-valued phase field (slip in *quanta* of Burgers vector)

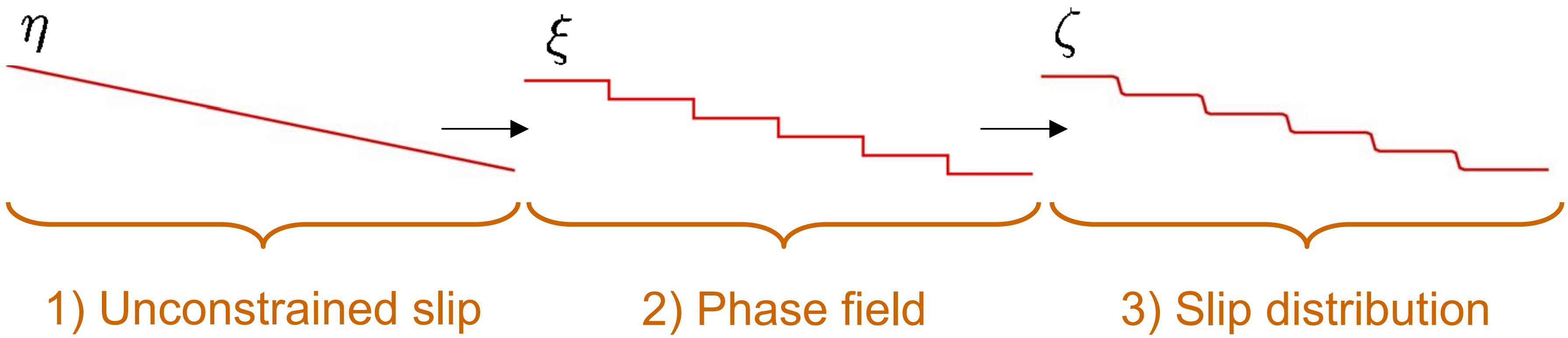
Problem (no friction, no obstacles): $\inf_{\xi} \inf_{\zeta} E[\zeta|\xi]$

Problem is:

- **Nonlocal** (due to long-range elastic interactions)
- **Nonconvex** (due to multi-well Peierls potential)
- **Nonlinear!**

General (exact) analytical solution

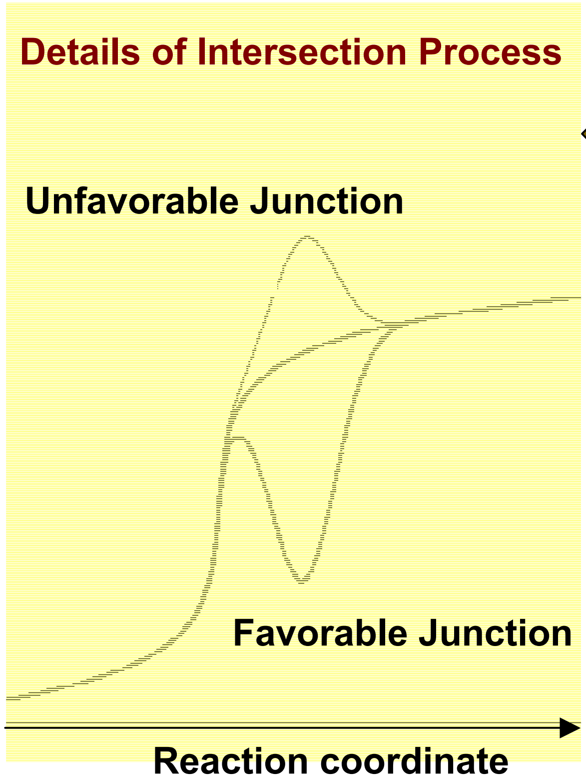
- Solution proceeds in <u>three steps</u>:

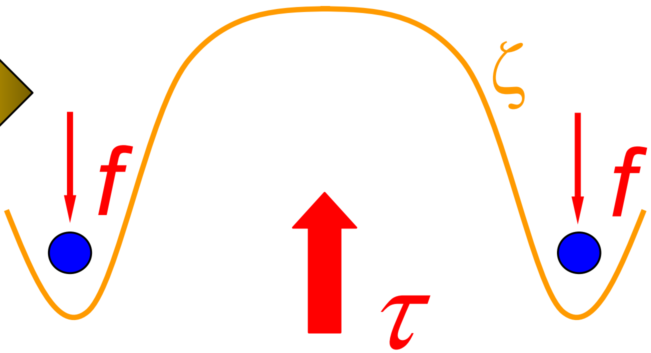


1. Unconstrained slip distribution: $\hat{\eta} = \frac{2}{Kb}\frac{\hat{s}}{\mu} + 2\pi C \delta_D$
2. Phase field (Volterra dislocations): $\xi(\mathbf{x}) = P_{\mathbb{Z}}\eta(\mathbf{x})$
3. Core-reguralized slip distribution: $\hat{\zeta} = \frac{\xi + d\hat{s}/\mu b}{1 + Kd/2}$

Global equilibrum: $\langle s \rangle = 0$

Lattice friction, obstacle interaction





Incremental variational principle:

$$\inf_{\zeta_{n+1}} W[\zeta^{n+1}|\zeta^n]$$

where: $W[\zeta^{n+1}|\zeta^n] = E[\zeta^{n+1}] - E[\zeta^n] + \sum_{i=1}^{N} f_i|\zeta_i^{n+1} - \zeta_i^n|$

Irreversibility, path dependency, hysteresis

Solution procedure

1. *Stick predictor.* Set $\tilde{\eta}_i^{n+1} = \eta_i^n$, and compute the predictor reactions:

$$\tilde{g}_j^{n+1} = \sum_{i=1}^{N} G_{ji}^{-1}(C_{n+1} - \tilde{\eta}_i^{n+1})$$

2. *Reaction projection.* Project $\tilde{g}_i^{n+1}$ onto admissible set: $|g_i| \leq f_i$.

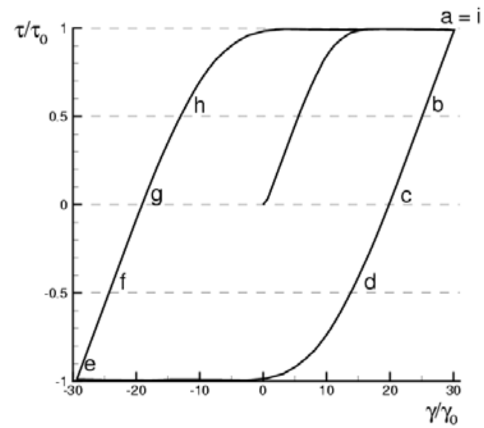
3. *Phase-field evaluation:* $\eta_i^{n+1} = \sum_{j=1}^{N} G_{ij} g_j^{n+1} + C_{n+1}$

4. *Post-processing.* Compute (analytically):

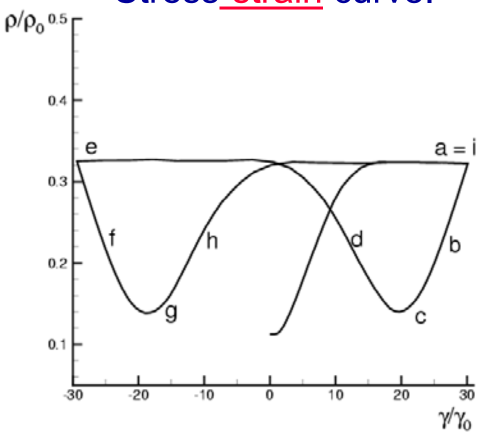
$$\gamma_{n+1} = \frac{b}{l}\langle \xi^{n+1} \rangle, \qquad \tau_{n+1} = \sum_{i=1}^{N} g_i^{n+1}, \qquad \rho_{n+1} = \frac{1}{l}\langle |\nabla \xi^{n+1}| \rangle$$

Calculations are gridless
and scale with the number of obstacles

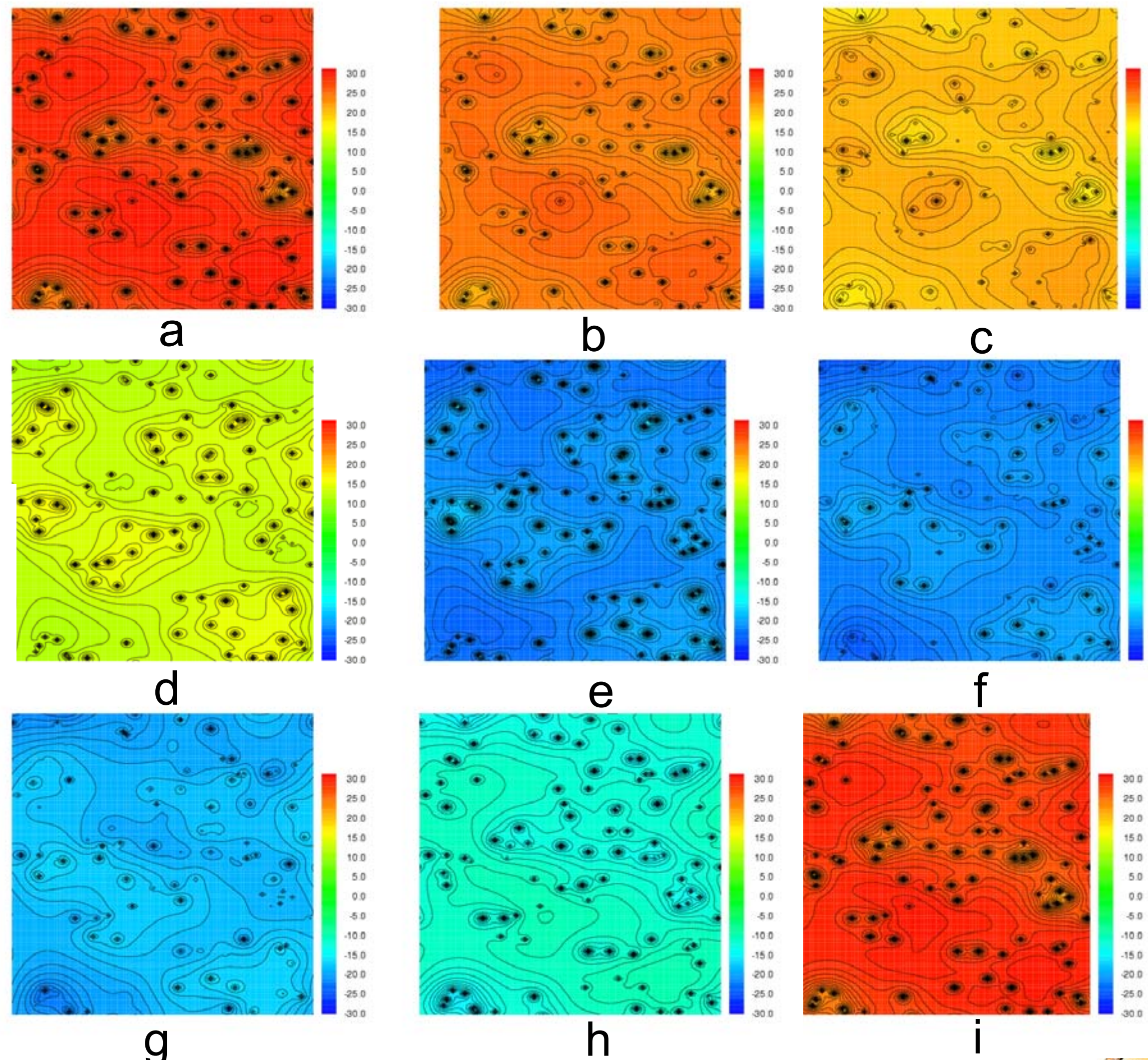
Cyclic loading



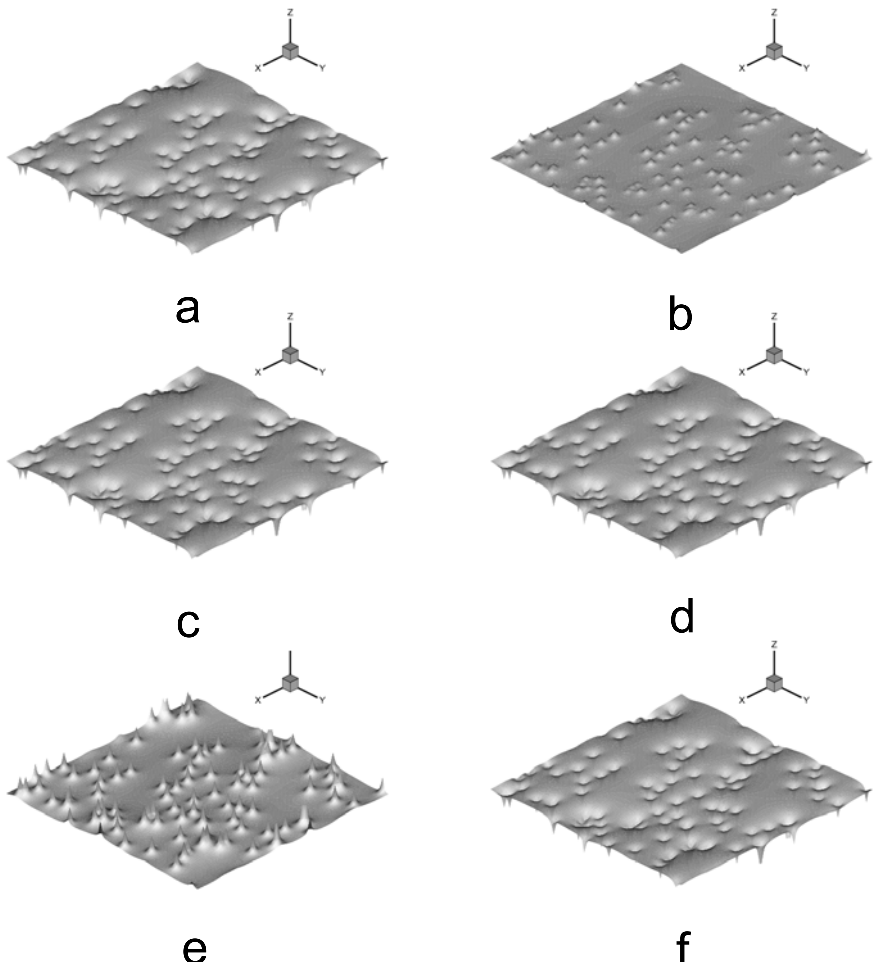
Stress-strain curve.

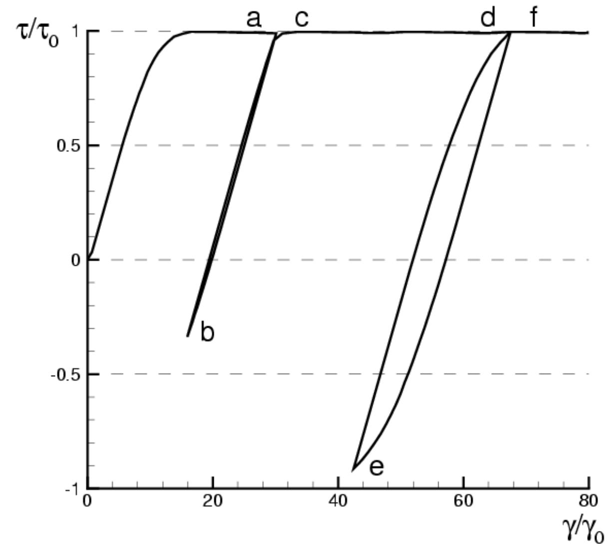


Evolution of dislocation density with strain.



Return-point and fading memory

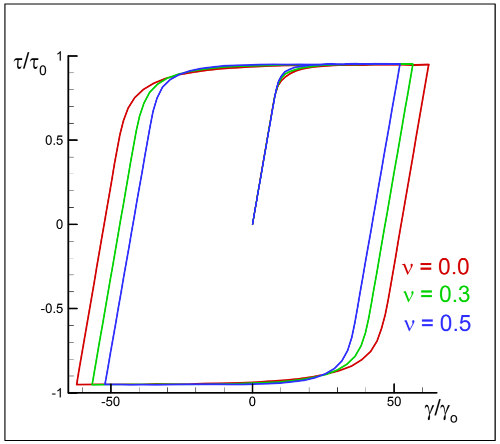




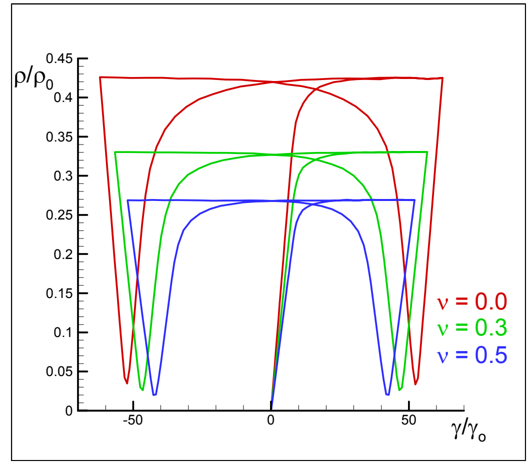
Stress-strain curve.

Three dimensional view of the evolution of the slip-field, showing the the switching of the cusps.

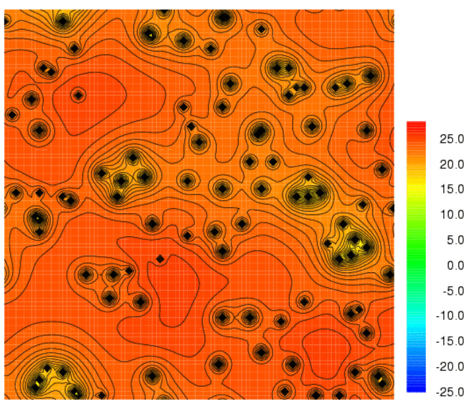
Line-tension anisotropy



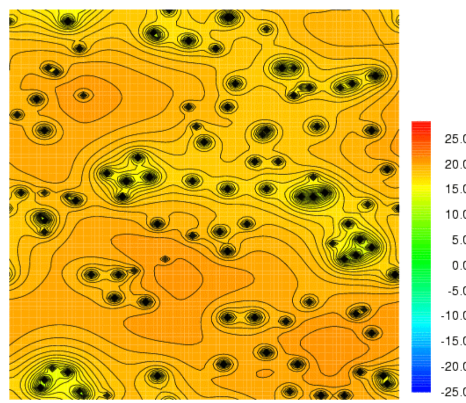
Stress-strain curve.



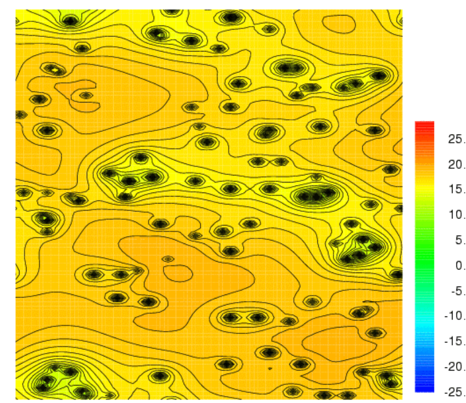
Dislocation density



$\nu = 0.0$



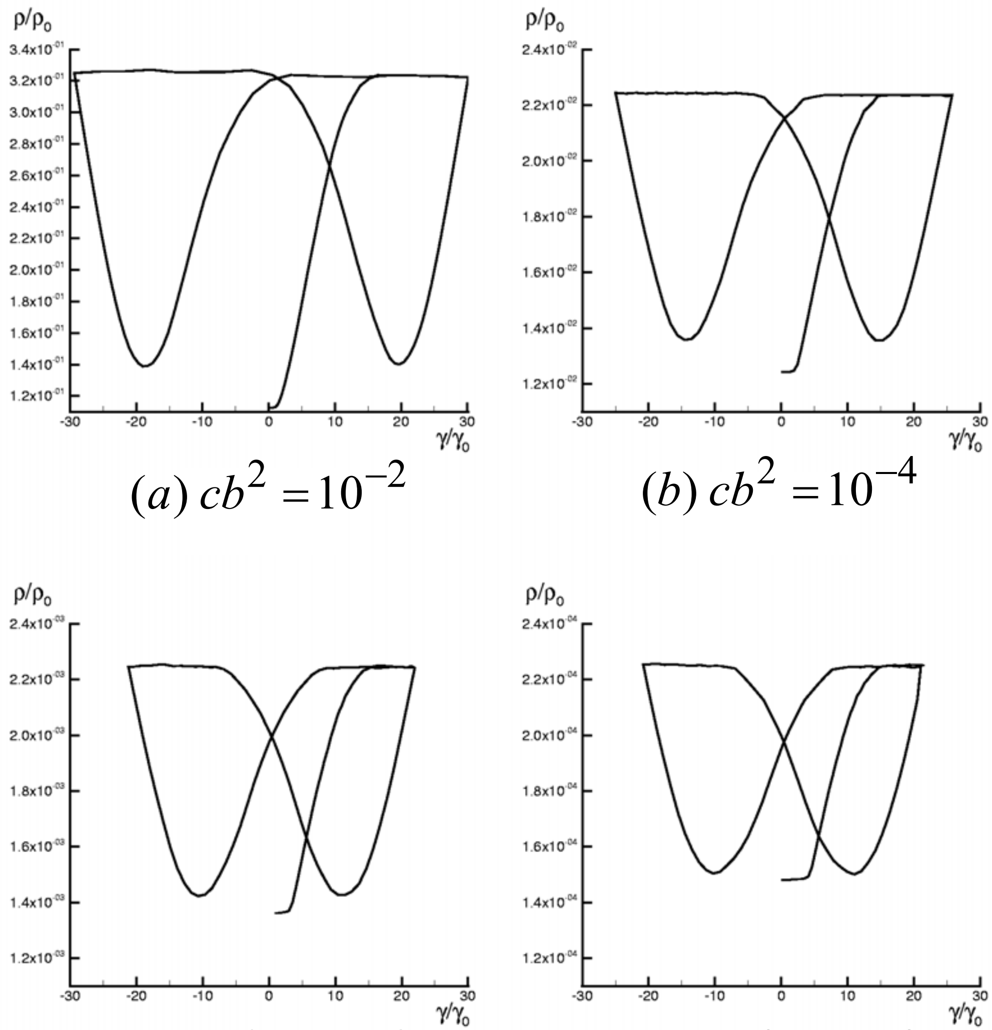
$\nu = 0.3$



$\nu = 0.5$

b

Obstacle density, sample size



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

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

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

(d) $cb^2 = 10^{-8}$

Summary

- Phase-field representation provides an effective analytical tool for describing the behavior of large dislocation ensembles
- Present model accounts for:
  - *Core structure, anisotropic line tension*
  - *Long-range elastic interactions*
  - *Interaction with applied field*
  - *Lattice friction and irreversible interactions with obstacles*
- Theory predicts:
  - *Dislocation pattern evolution, Orowan loops*
  - *Cyclic stress-strain curve, Bauschinger effect*
  - *Evolution of dislocation density*
- Theory is exactly solvable, implementation is gridless, complexity governed by number of obstacles

Future directions, challenges

- Full 3D implementation:
  - *Parallel array of slip planes per slip system*
  - *Multiple slip, coupling between slip systems*
  - *Cross slip*
- General (e.g., nonlocal) Peierls potentials
- Anisotropic Peierls stresses
- General dislocation mobility laws, finite temperature
- Statistics of obstacle distribution, strength
- Implementation as constitutive model in FE code
- Preprint: www.solids.caltech.edu/~ortiz