Variational Methods in Dislocation Dynamics

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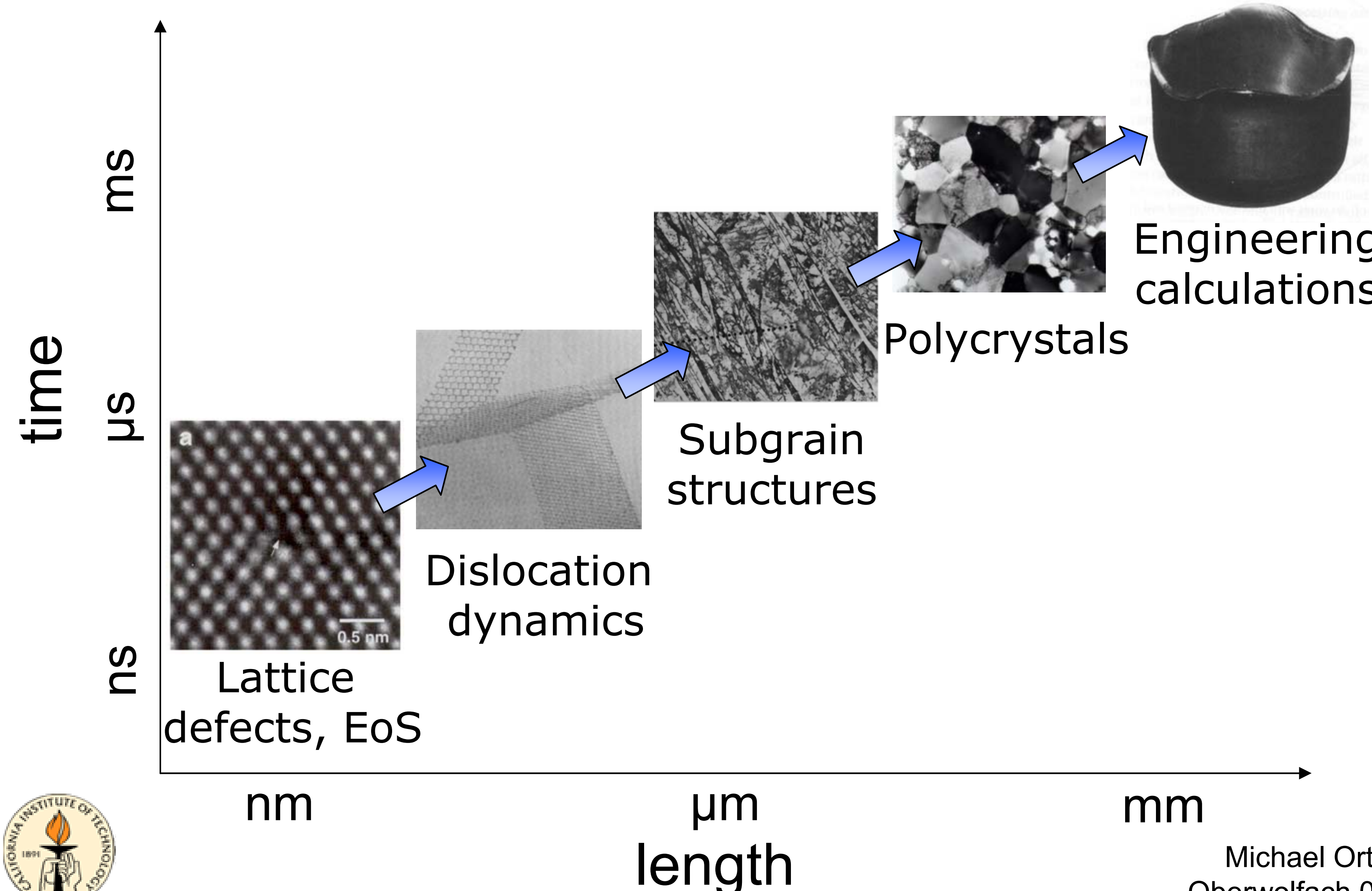
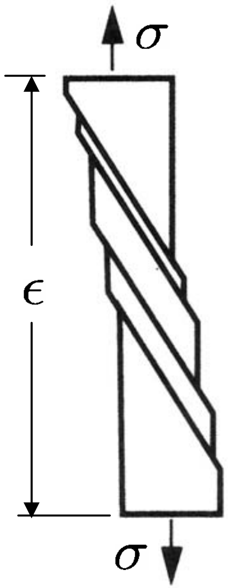
Outline

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

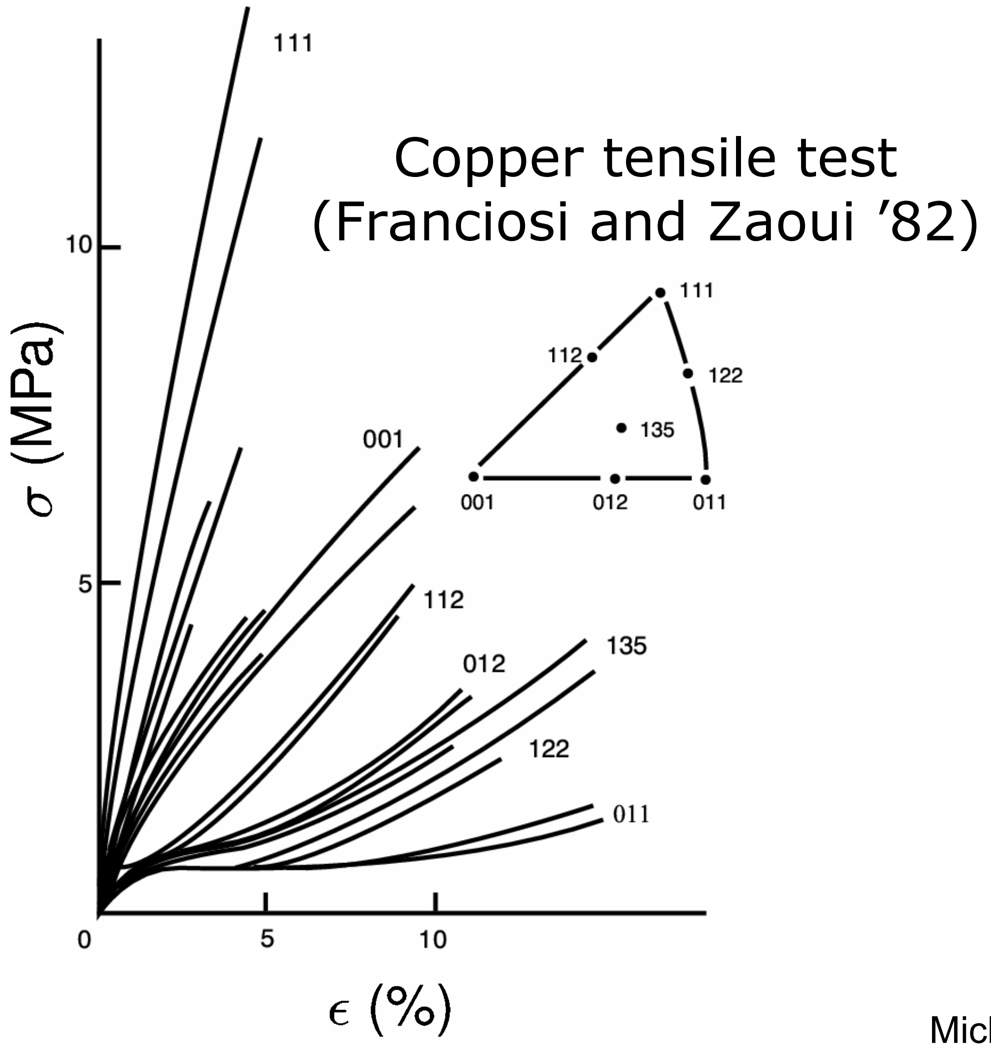
Metal plasticity - Lengthscales



Crystal plasticity – Macroscopic behavior



Uniaxial
tension test



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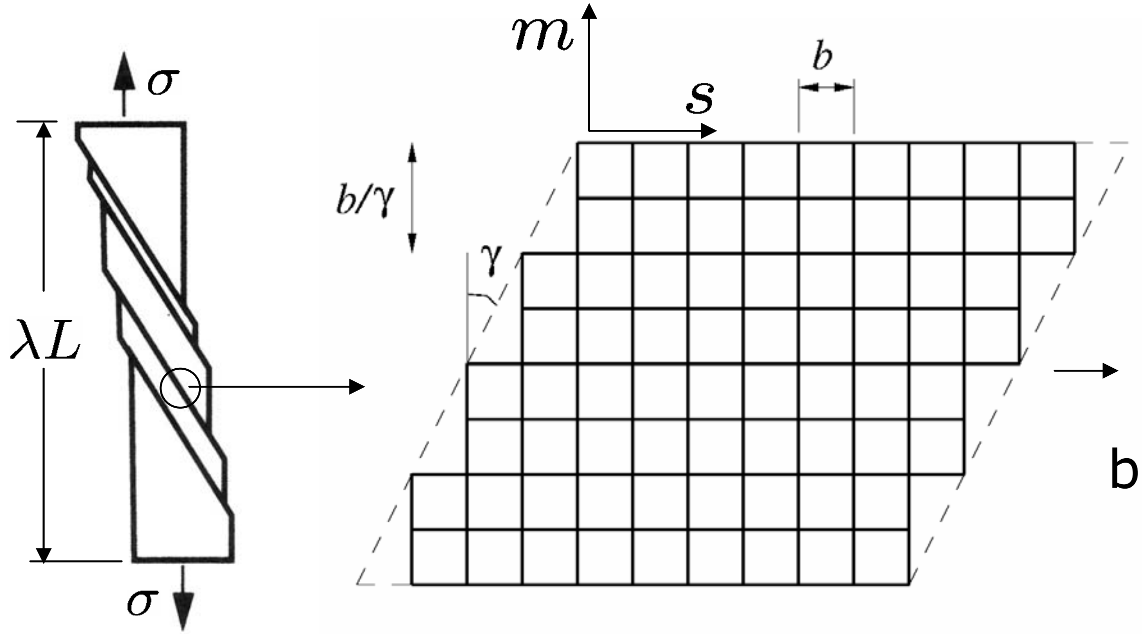
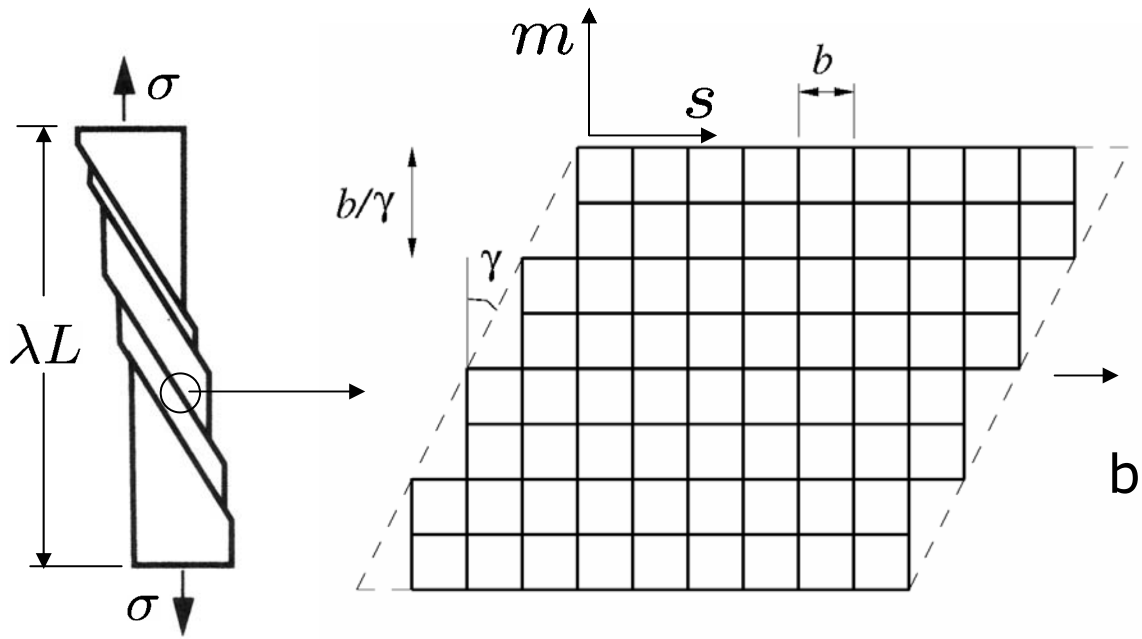
Crystal plasticity – Relaxation



Irreversible accommodation of shear deformation by crystallographic slip

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

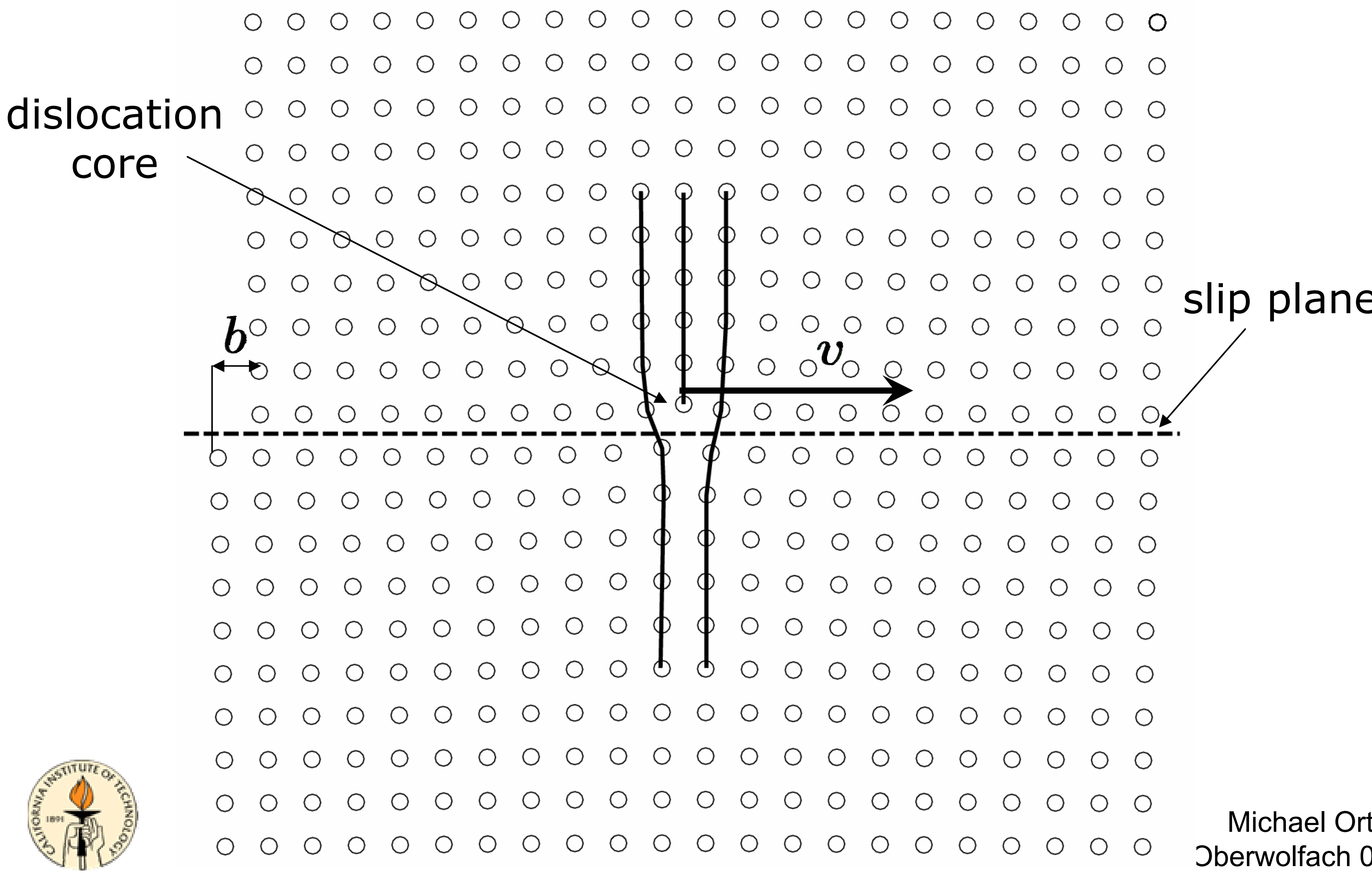
Crystal plasticity – Energy barriers



Irreversible accommodation of shear deformation by crystallographic slip

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

Crystal plasticity and dislocations



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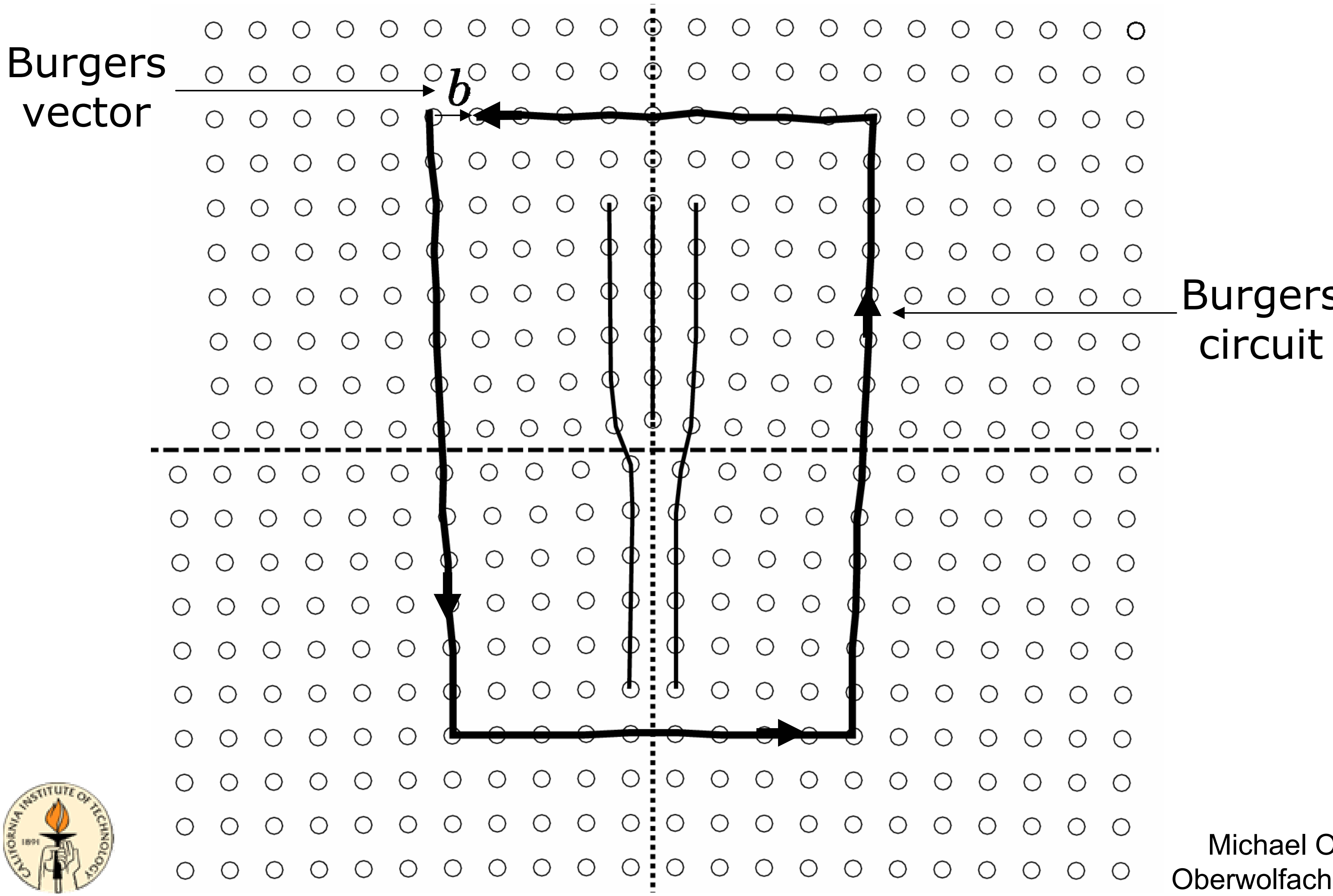
Crystal plasticity and dislocations



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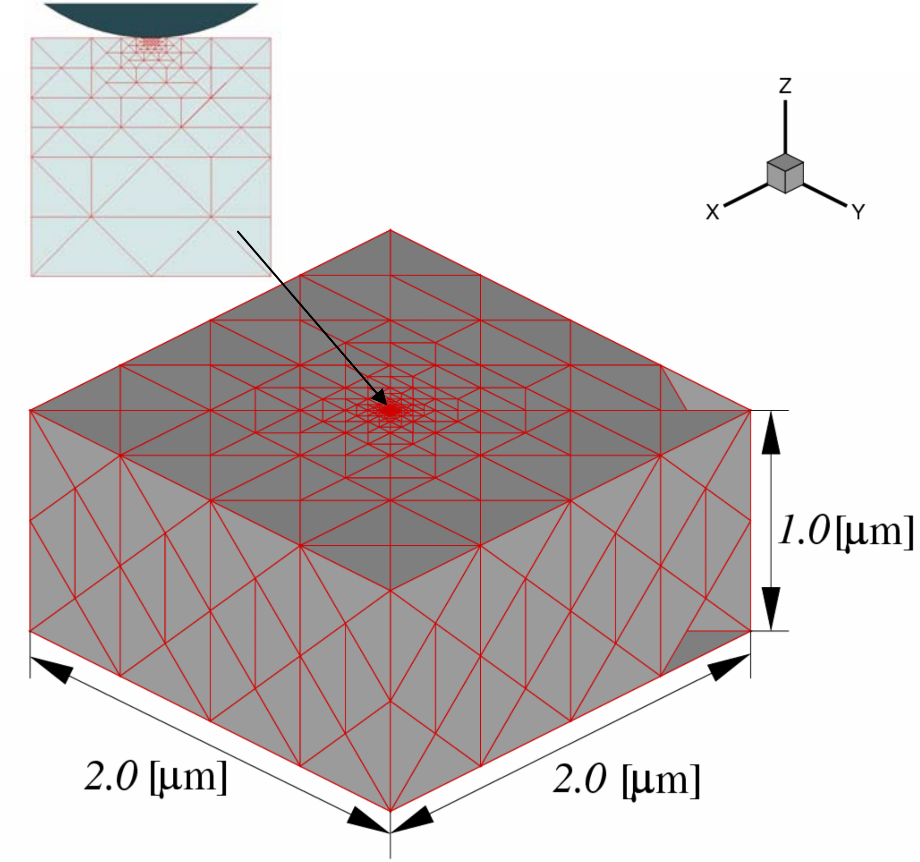
Example - Nanoindentation of [001] Au

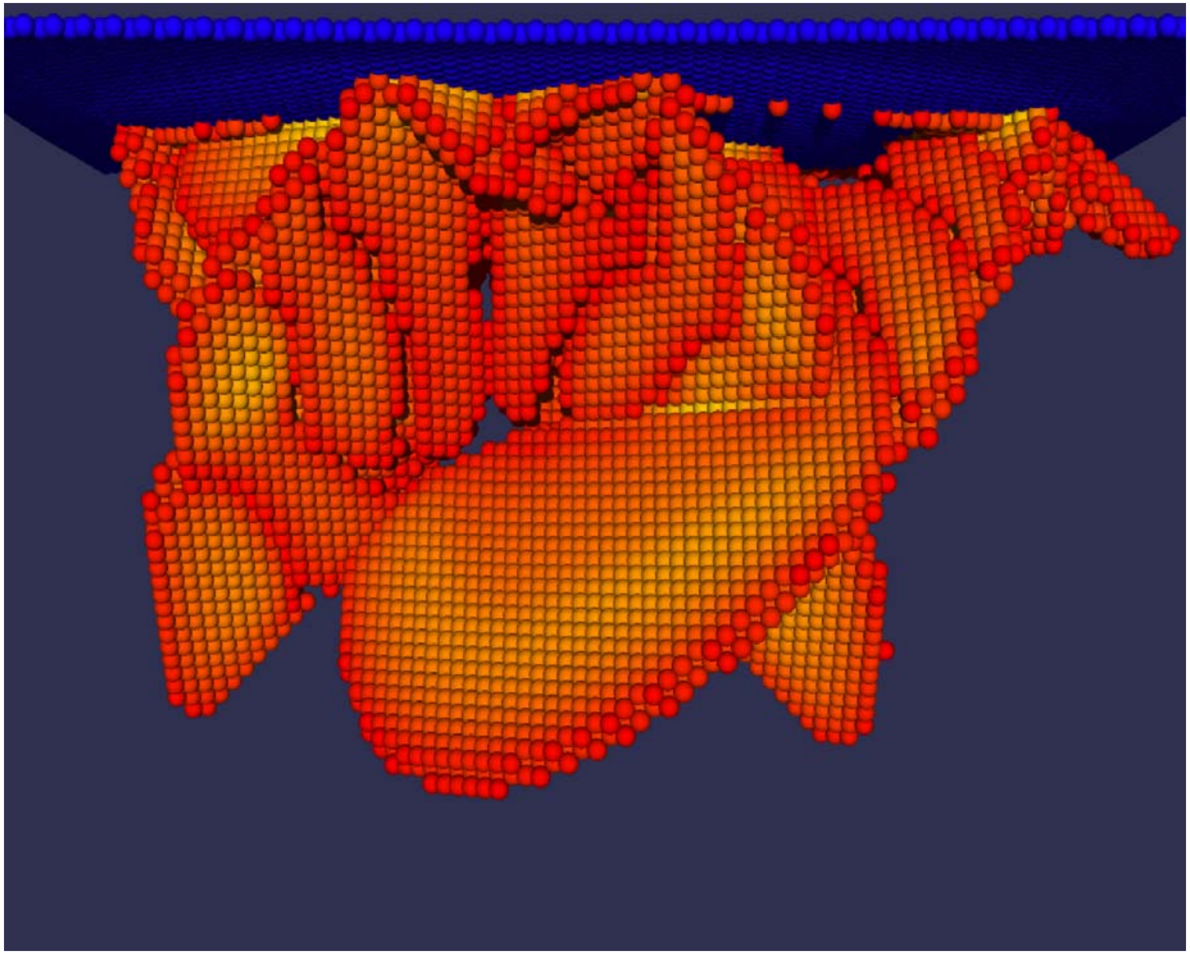


Detail of initial computational mesh (Knap and Ortiz, 2002)

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

(Movie)

Example - Nanoindentation of [001] Au



70 nm indenter, depth = 0.75 nm

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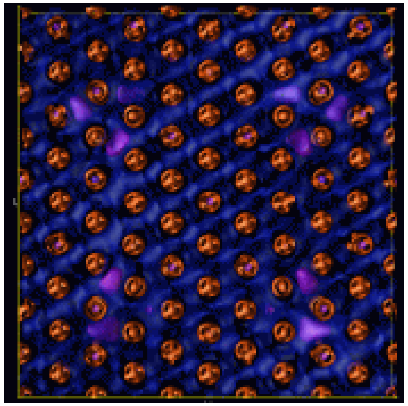
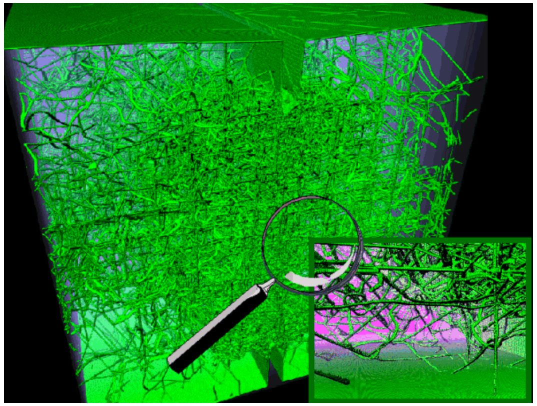
Dislocation dynamics – Numerical tools

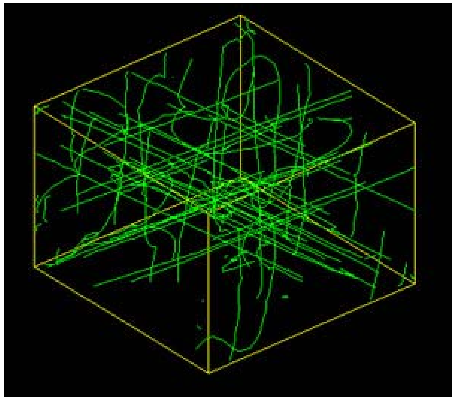
- First-principles calculations: Dislocation cores, dipoles, quadrupoles… ~ 10^3 atoms (T. Arias '00)
- Molecular dynamics: Empirical potentials… ~ 10^9 atoms (F. Abraham '03)
- Linear elasticity: Dislocation dynamics, L ~ 10^6b, ε ~ 1% (Bulatov et al. '03)



Ta quadrupole
(T. Arias ´00)

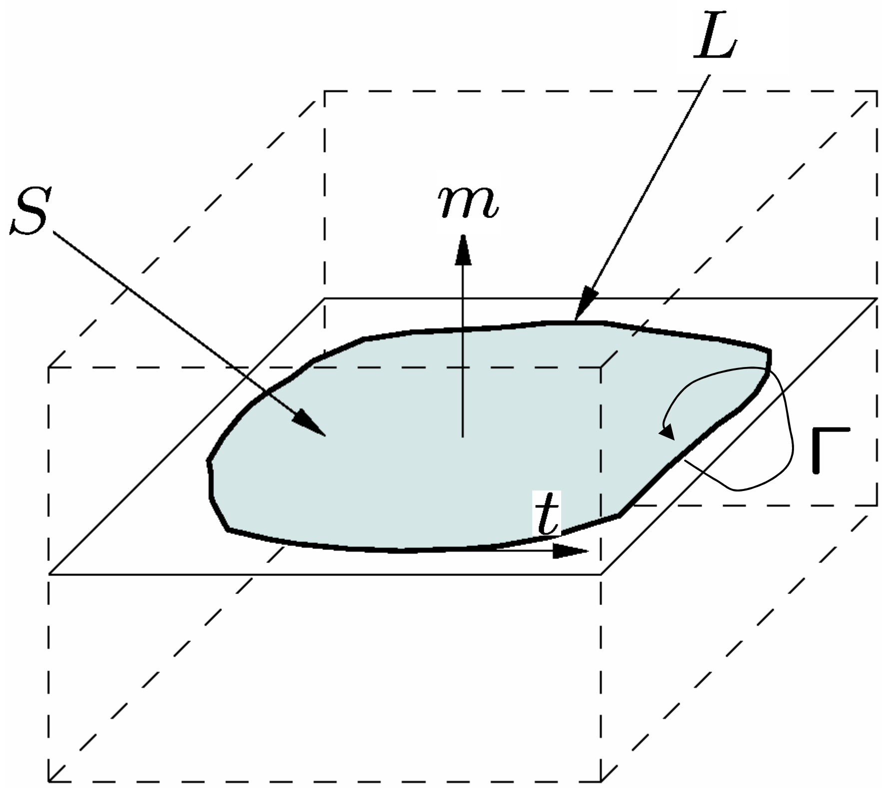


FCC ductile fracture
(F.F. Abraham ´03)



FCC dislocation dynamics
(M. Rhee et al.´02)

Theory of linear-elastic dislocations



- Volterra dislocation:

$$\mathrm{div} C \nabla u = 0, \quad \text{in } \mathbb{R}^3$$
$$[\![u]\!] = b, \quad \text{on } S$$
$$[\![C\nabla u]\!] \cdot m = 0, \quad \text{on } S$$

- Burgers circuit:

$$b = \oint_{\Gamma \setminus S} \nabla u \, dr$$

- Dislocation dipole: $\dfrac{E}{L} \sim \dfrac{\mu b^2}{4\pi(1-\nu^2)} \log \dfrac{R}{r_0} \to \infty$
- Need to model dislocation core!

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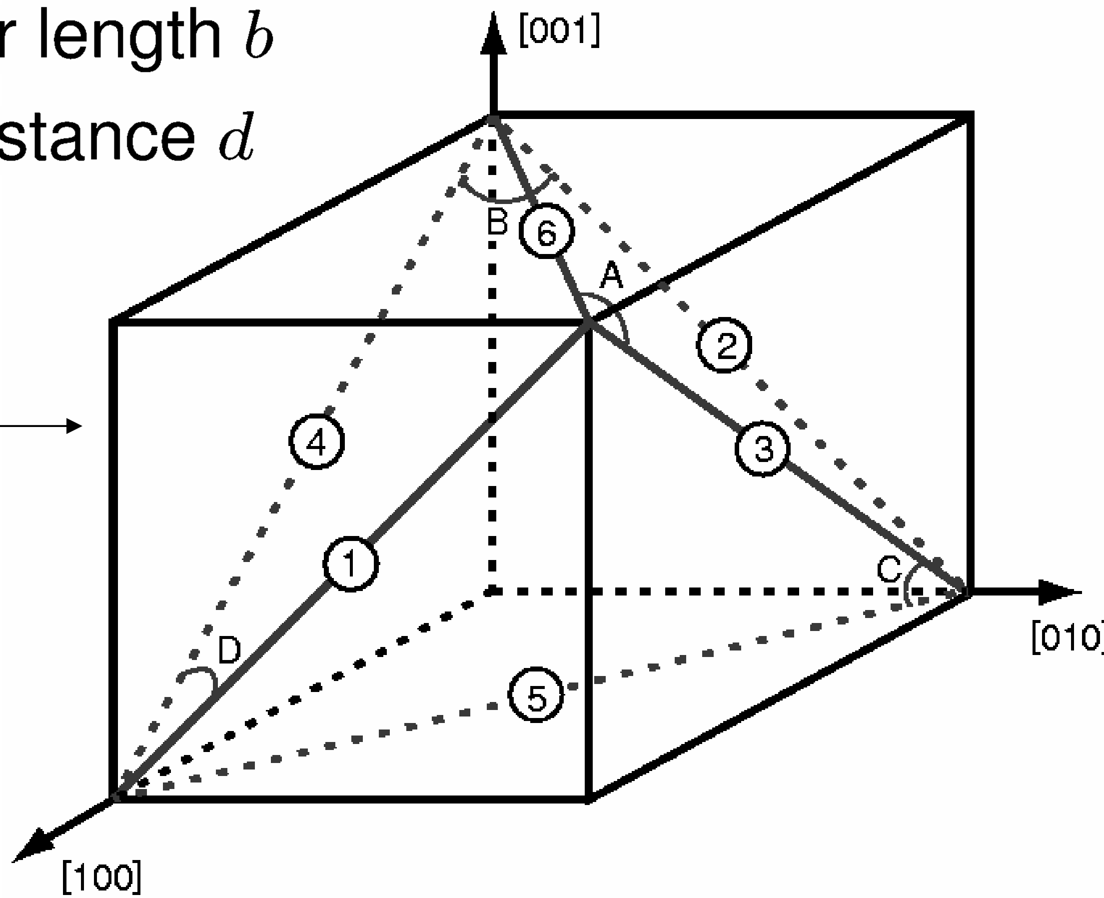
Theory of linear-elastic dislocations

- Preferred slip systems: Minimize

  i) Burgers vector length b

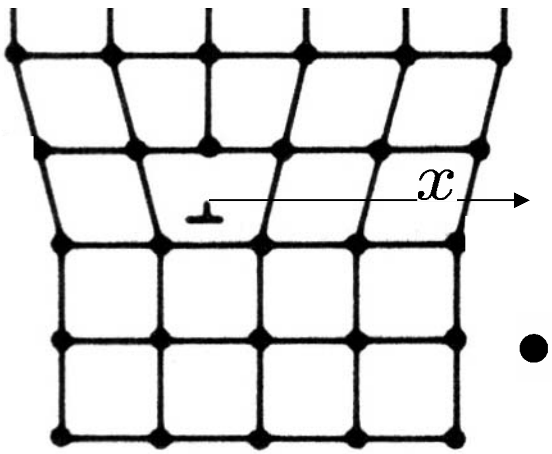
  ii) Interplanar distance d

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,



$$E(\delta) = \int_{-\infty}^{\infty} \phi(\delta(x))dx + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{B}{2} \log \frac{R}{|x-y|} \delta'(x)\delta'(y)dxdy$$

- 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: $S(u) \in \mathcal{S} \equiv$ set of all slip planes.

- $u \in SBV(\mathbb{R}^3) \Rightarrow \beta = Du$ is a Borel measure,

$$\beta = \beta^e + \beta^p = \begin{cases} \beta^e \text{ absolutely continuous} \\ \beta^p = [\![u]\!] \otimes m\delta_S \end{cases}$$

  iii) Assumption: The energy is of the form

$$E(u) = \int \frac{1}{2} c_{ijkl} \beta^e_{ij} \beta^e_{kl} dx + \int_S \phi([\![u]\!]) dS$$

with ϕ periodic.

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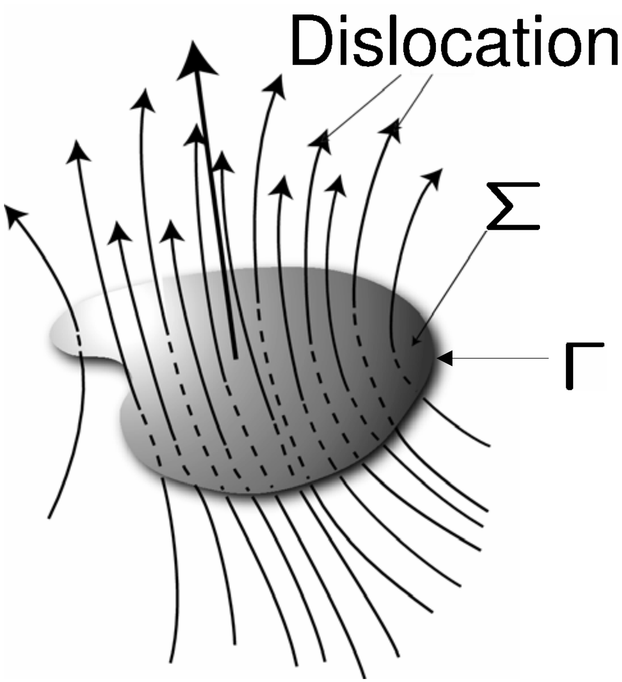
Theory of linear-elastic dislocations

- Nye's dislocation-density tensor (Nye '53):



$$b(\Sigma) = \int_{\Sigma} \alpha n dS$$

- But also:

$$b(\Sigma) = \oint_{\Gamma} \beta^e dr$$

- By Stokes theorem (Kröner '55):

$$\alpha = \text{curl}\beta^e = -\text{curl}\beta^p$$

- For a distribution of Volterra dislocations:

$$\alpha = b \otimes t\delta_L$$

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Theory of linear-elastic dislocations

- From general results for elastic cut surfaces:

$$\beta^e_{jn}(x) = \int c_{kpim} G_{ij,mn}(x, x') \beta^p_{kp}(x') dx'$$

- 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:

$$E([\![u]\!]) = \underbrace{E^{\text{int}}([\![u]\!])}_{\text{nonlocal}} + \underbrace{\int_S \phi([\![u]\!]) dS}_{\text{local}}$$

Single slip plane – Phase field model

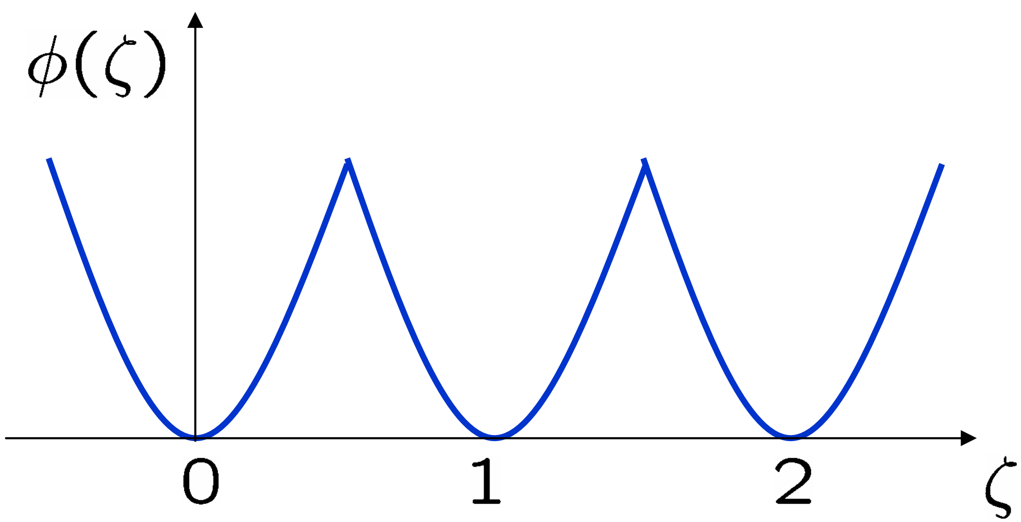
- Consider the special case (Koslowski et al '02):

  i) Activity on single slip system, single slip plane.

  iii) Constrained slip assumption (Rice and Beltz '92):

  $[\![u]\!](x) = b\zeta(x)s, \quad \zeta : \mathbb{R}^2 \to \mathbb{R}$ ('slip field')

  iv) Peierls potential: $\phi(\zeta) = \frac{\mu b^2}{2d}\text{dist}^2(\zeta, \mathbb{Z})$



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Single slip plane – Phase field model

- Total energy: $E(\zeta) =$

$$\underbrace{\int_{\mathbb{R}^2} \frac{\mu b^2}{2d} \mathrm{dist}^2(\zeta, \mathbb{Z}) dx}_{\text{Core energy}} + \underbrace{\frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mu b^2}{4} K |\hat{\zeta}|^2 dk}_{\text{Elastic energy}} - \underbrace{\int_{\mathbb{R}^2} b s \zeta dx}_{\text{External}}$$

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

- Structure of the energy:

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

(cf Alberti, Bouchitte and Seppecher ’98)

Single slip plane – Phase field model

- Problem: $\inf_{\zeta} E(\zeta)$
- Solution strategy: Write $\phi(\zeta) = \min_{\xi \in \mathbb{Z}} \frac{\mu b^2}{2d} |\zeta - \underbrace{\xi}_{\text{('phase field')}}|^2$
- 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: $\zeta = \zeta_0 + \varphi_d \star \xi$

where $\hat{\varphi}_d(\boldsymbol{k}) = \frac{1}{1 + Kd/2}$ $\Rightarrow$ mollifier.

Single slip plane – Phase field model

- Remaining problem: $\begin{cases} \inf_{\xi} E(\xi) \\ \text{subject to constraint: } \xi : \mathbb{R}^2 \to \mathbb{Z}. \end{cases}$

  where

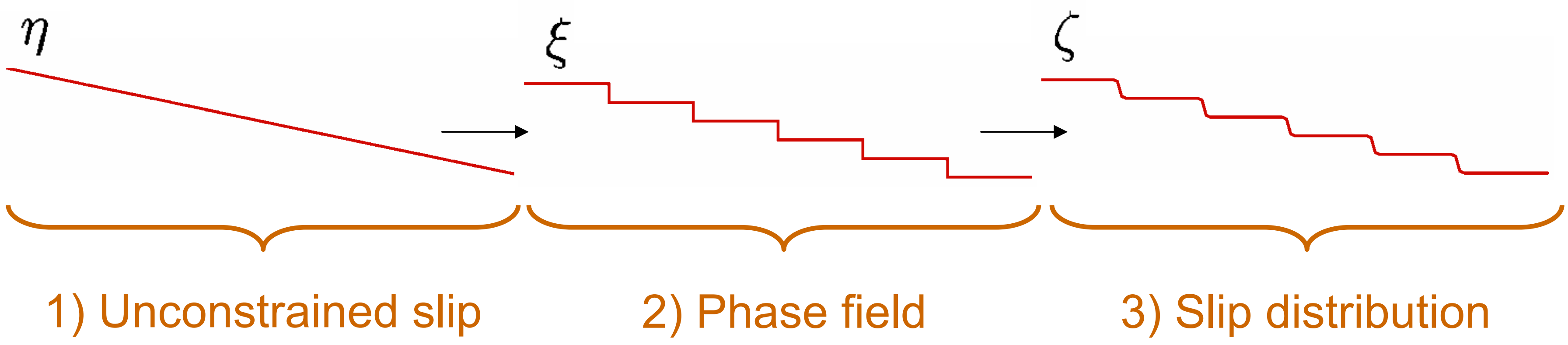
$$E(\xi) = \frac{1}{(2\pi)^2} \int_{\mathbb{R}^2} \frac{\mu b^2}{4} \frac{K}{1 + Kd/2} |\hat{\xi}|^2 dk + \dots$$

- Equivalently:

  i) Minimize E without integer contraint.

  ii) Project unconstrained minimizer η onto 'closest' integer-valued function ξ.

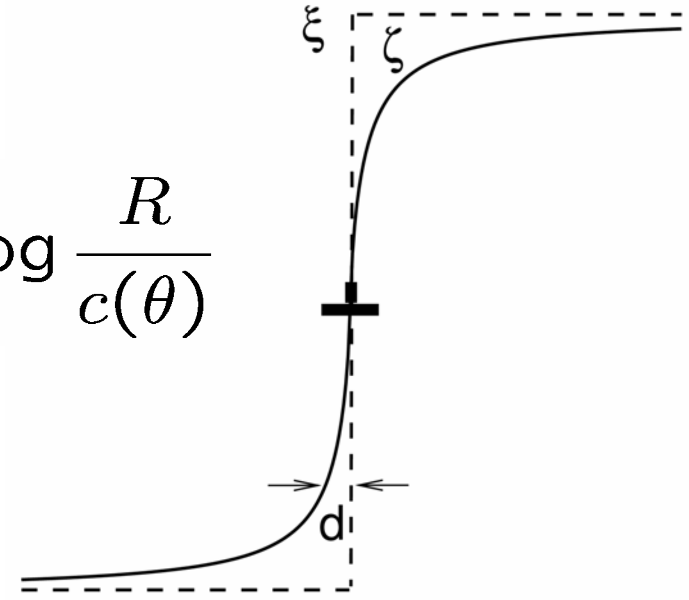
Single slip plane – Phase field model



- Example: Straight dislocation.

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

$$c(\theta) = \left(\sin^2\theta + \frac{\cos^2\theta}{1-\nu}\right)\frac{d}{2}$$



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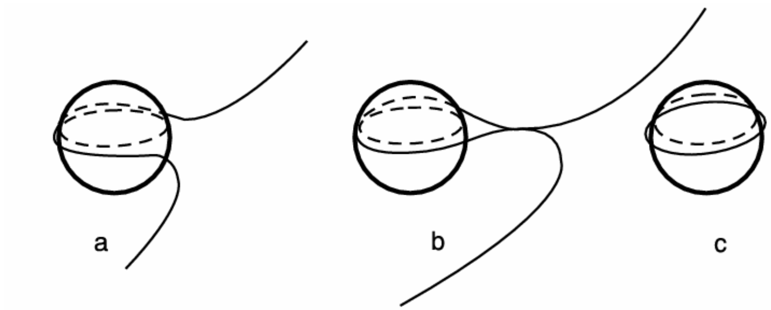
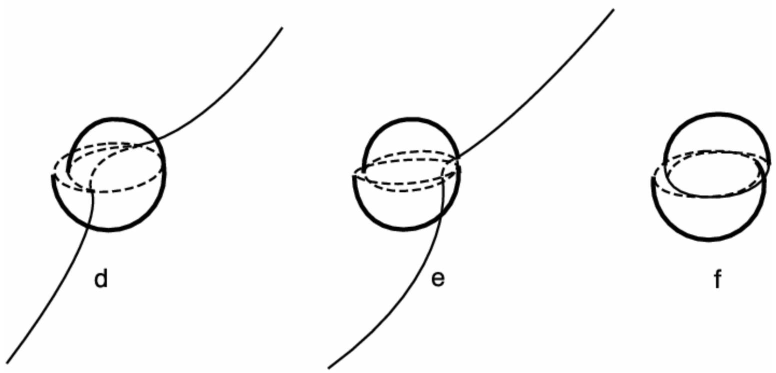
Dislocation-obstacle interaction

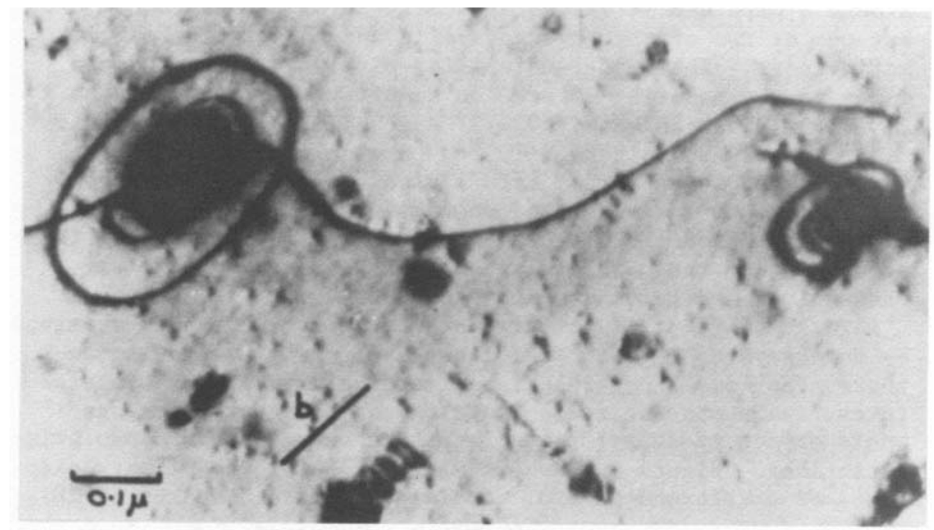
- Example: Precipitation hardening.



Impenetrable obstacles

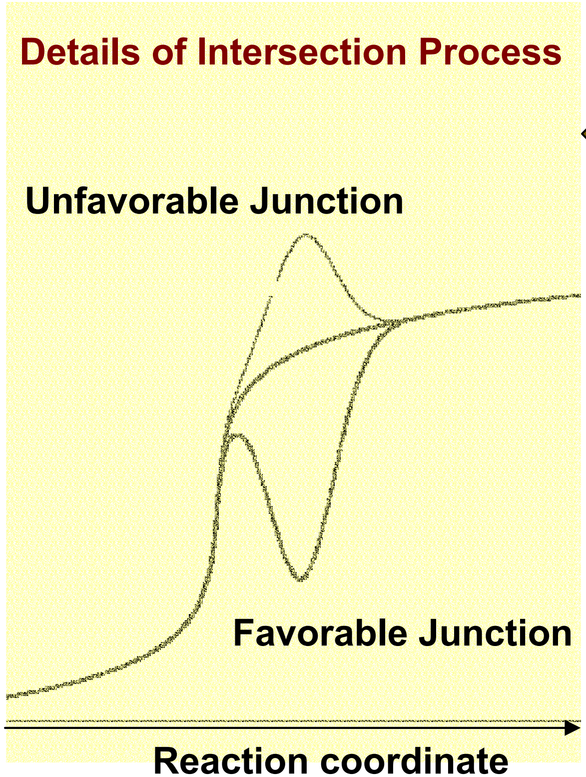


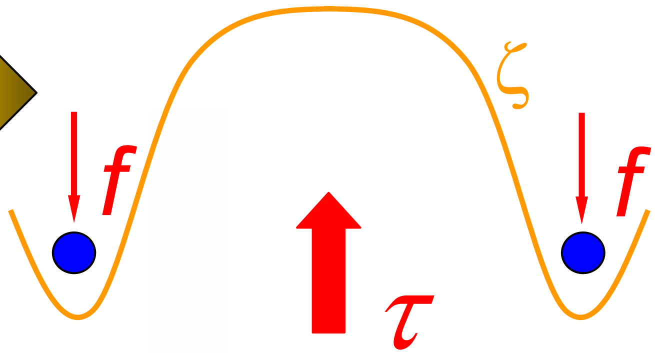
Obstacles of finite strength



(Humphreys and Hirsch ’70)

Dislocation obstacle interaction





- 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

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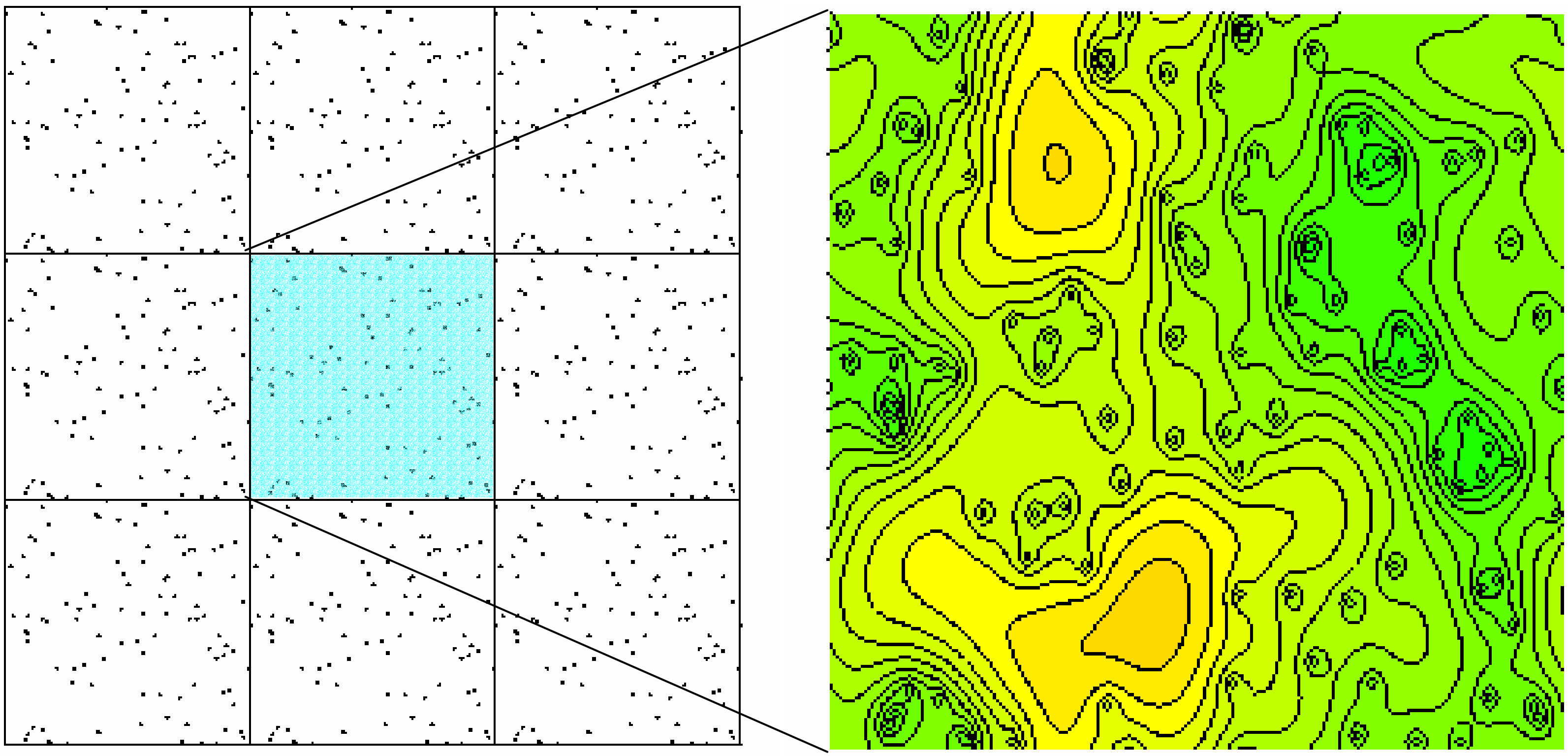
Dislocation-obstacle interaction

- Problem geometry: i) Periodic square cell.

  ii) Random array of obstacles.



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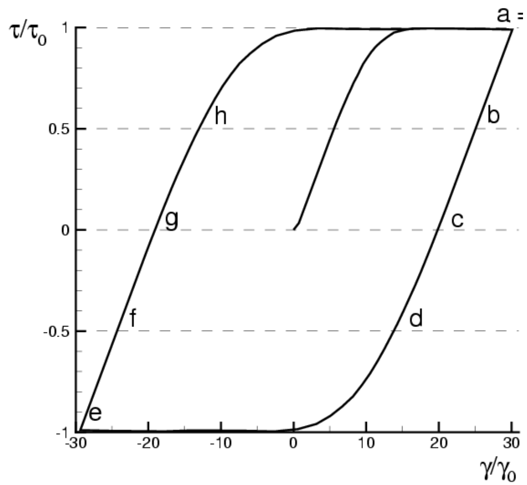
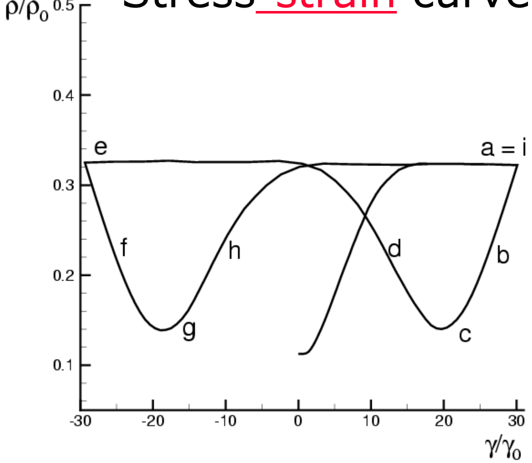
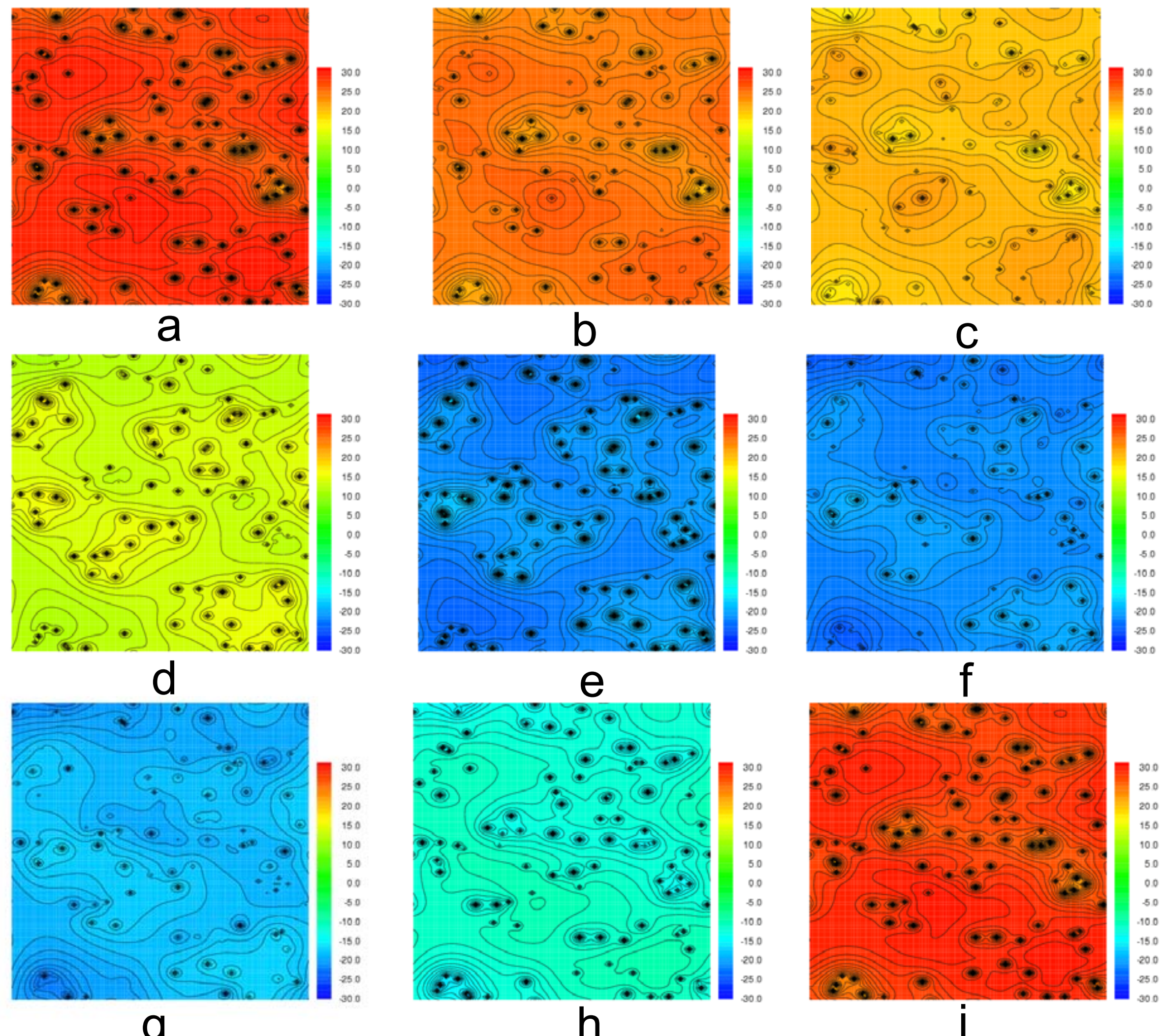
Dislocation-obstacle interaction



Stress-strain curve



Dislocation density



(Movie)

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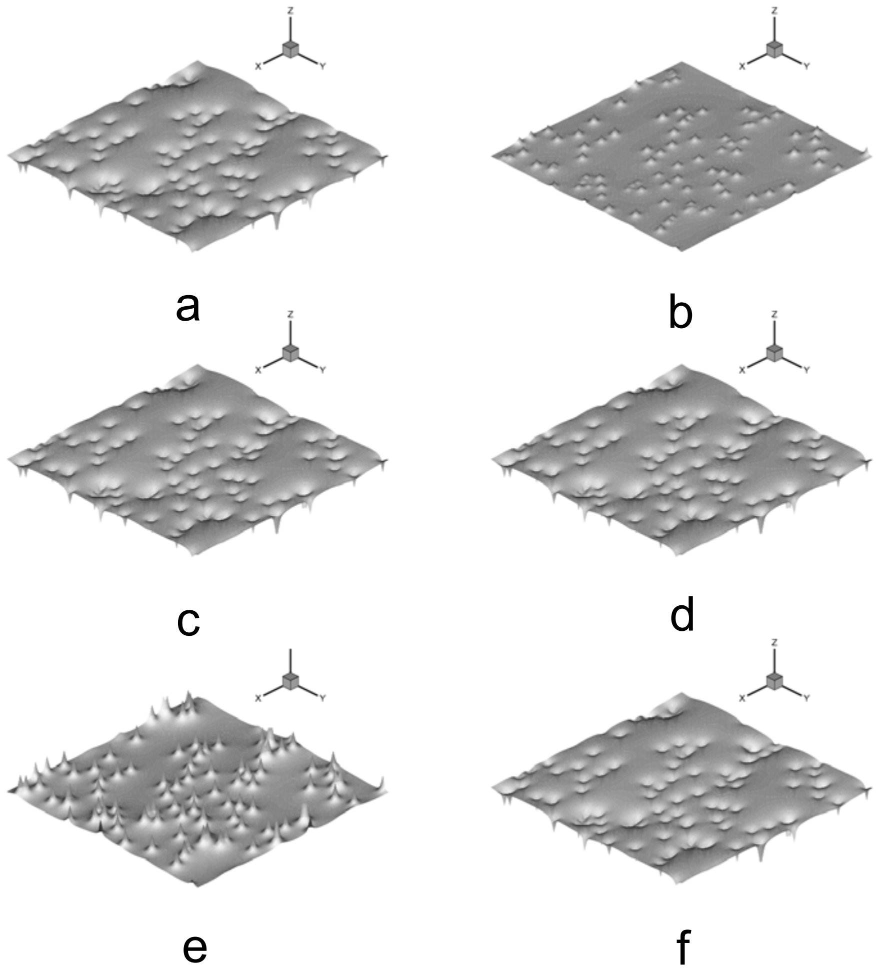
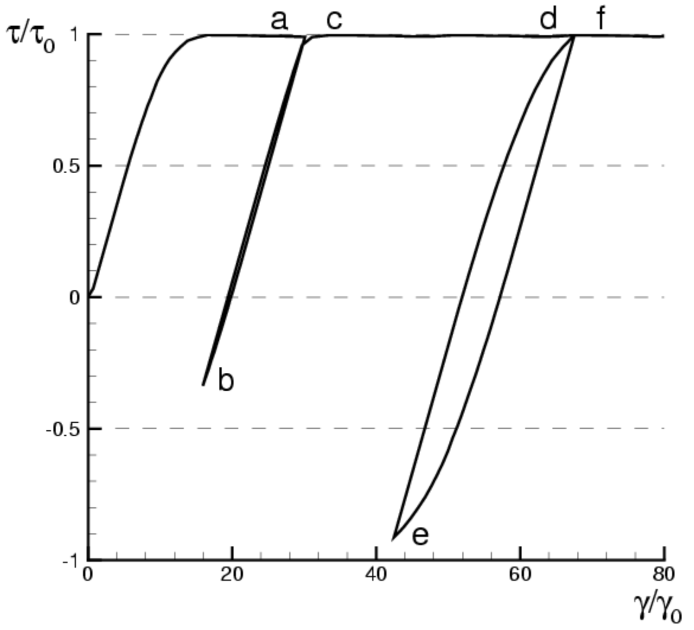
Dislocation-obstacle interaction



3D view of slip field showing switching of pinning cusps



Stress-strain curve showing return-point memory effect

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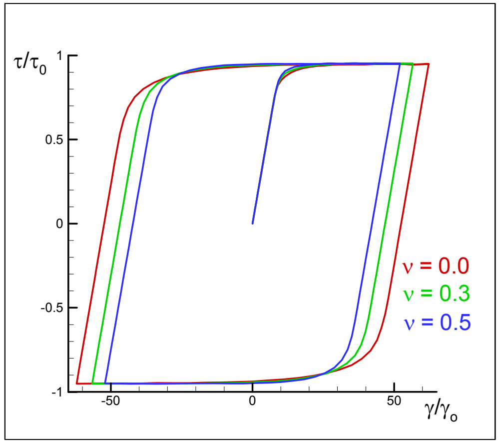
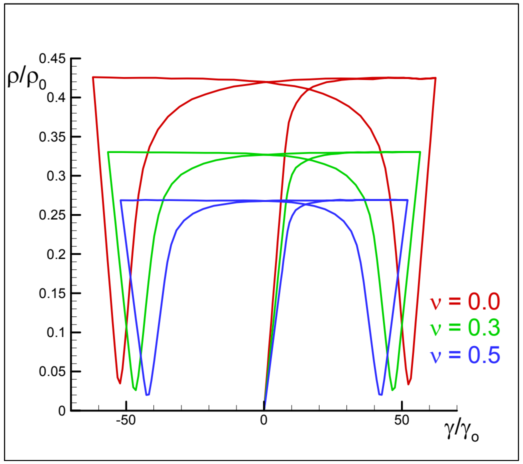
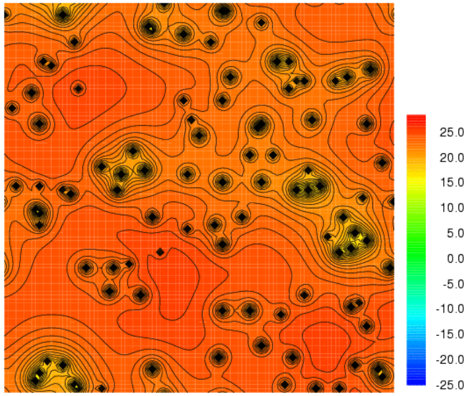
Line-tension anisotropy



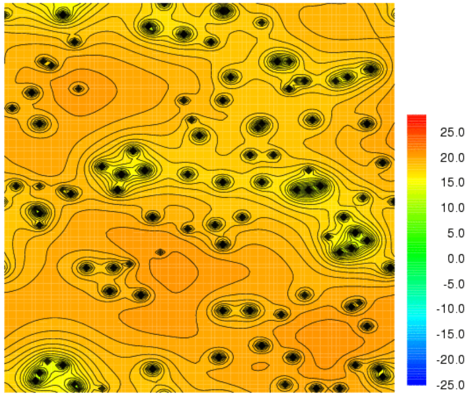
Stress-strain curve



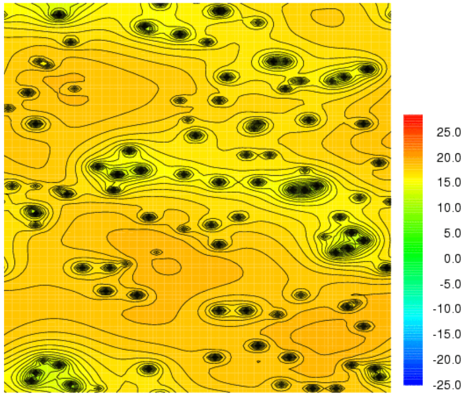
Dislocation density



$\nu = 0.0$



$\nu = 0.3$



$\nu = 0.5$

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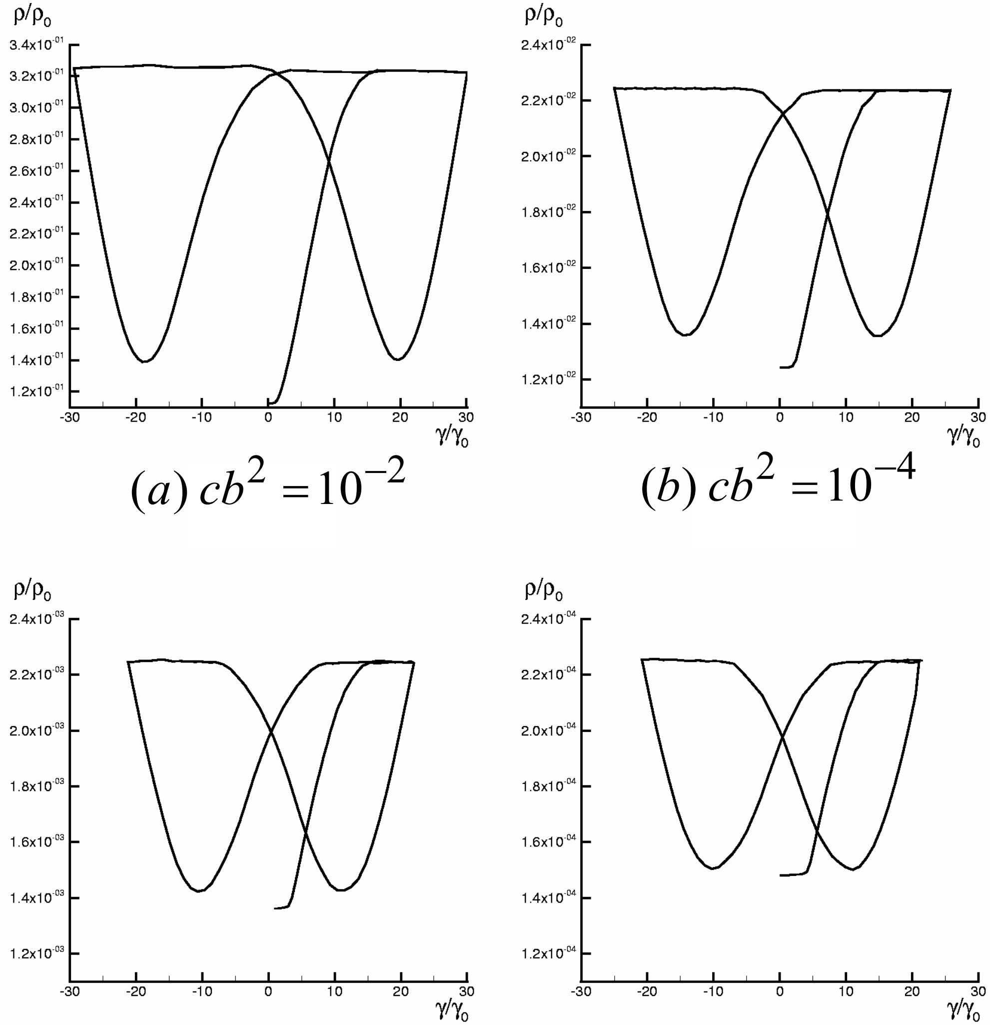
Obstacle density, sample size



(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
J MECH PHYS SOLIDS 50 (12): 2597-2635 DEC 2002