Discrete Dislocation Dynamics (D^3)

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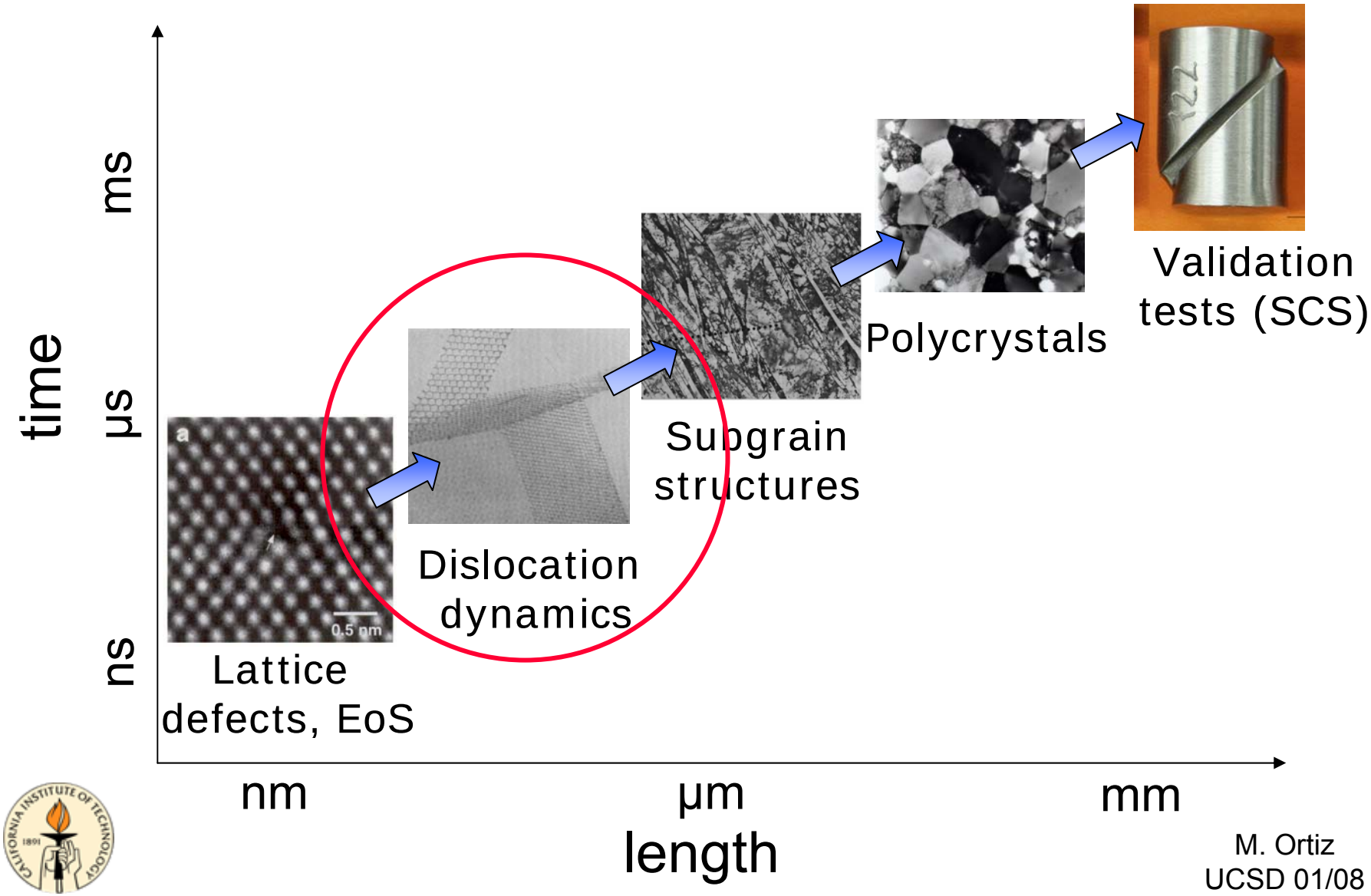
Strength – Multiscale modeling



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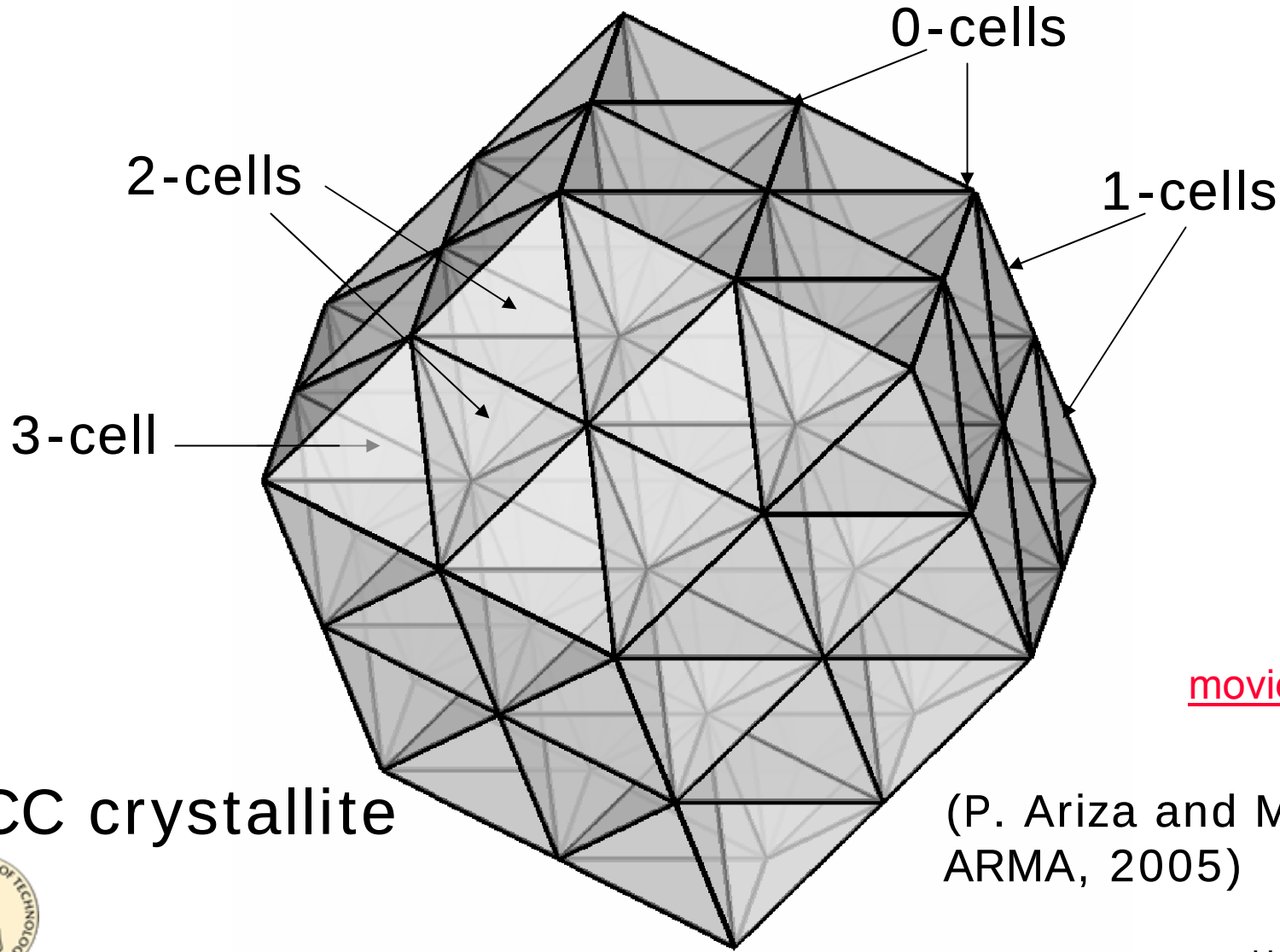
Dislocation dynamics – Limitations

- Dislocation energy/length diverges as $\sim log(R/r_0)$
- Core cut-off radius r_0 is extraneous parameter
- No natural separation between slip planes
- No dislocation core structure accounted for
- Evaluation of Peach-Koehler forces ~ $O(N^2)$
- Self-interaction of segments entails difficulty
- Finite bodies, general geometries, difficult
- Isotropic elasticity is often used in calculations
- Topological transitions (e.g., junctions, Orowan loops, annihilation...) are difficult to account for
- Dislocation nucleation is difficult to account for
- Mobility law needs to be supplied

Discrete Dislocation Dynamics (D^3)

- Discrete dislocations in discrete crystal lattice
  - *No logarithmic divergence*
  - *Dislocation lines have full core structure*
  - *Gamma-surface*
- Empirical potentials (EAM, Finis-Sinclair, …)
- 3D anisotropic dislocation interactions, reactions
- Topological transitions automatically included
- Computationally efficient:
  - *O(N logN) complexity*
  - *Nonlinear equilibrium calculations restricted to small sets (cores, junctions, …)*
- Amenable to analysis (e.g., Γ-convergence)

Discrete calculus on crystal lattices



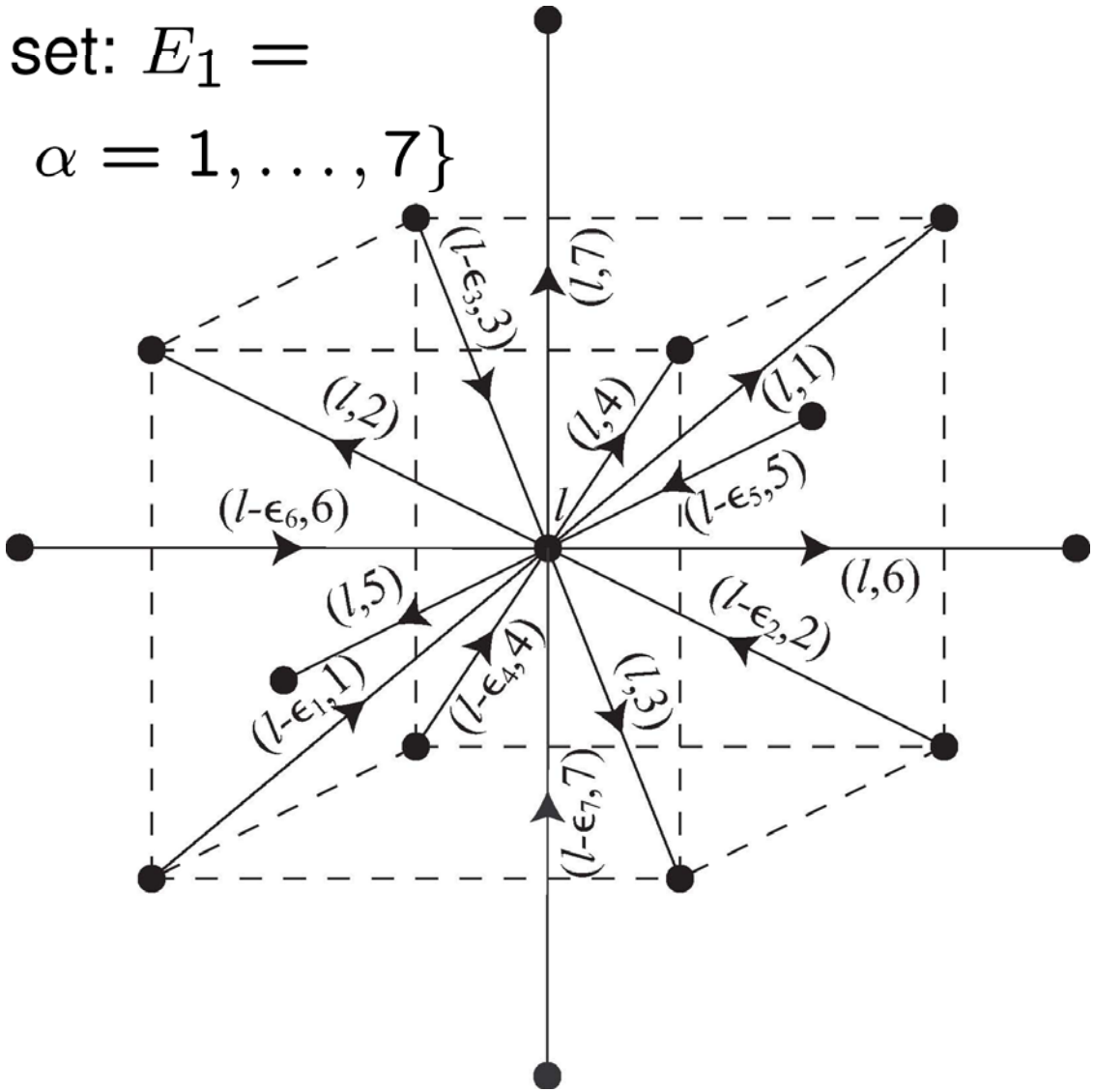
movie

BCC crystallite

(P. Ariza and M. Ortiz, ARMA, 2005)

BCC lattice complex: 1-cells

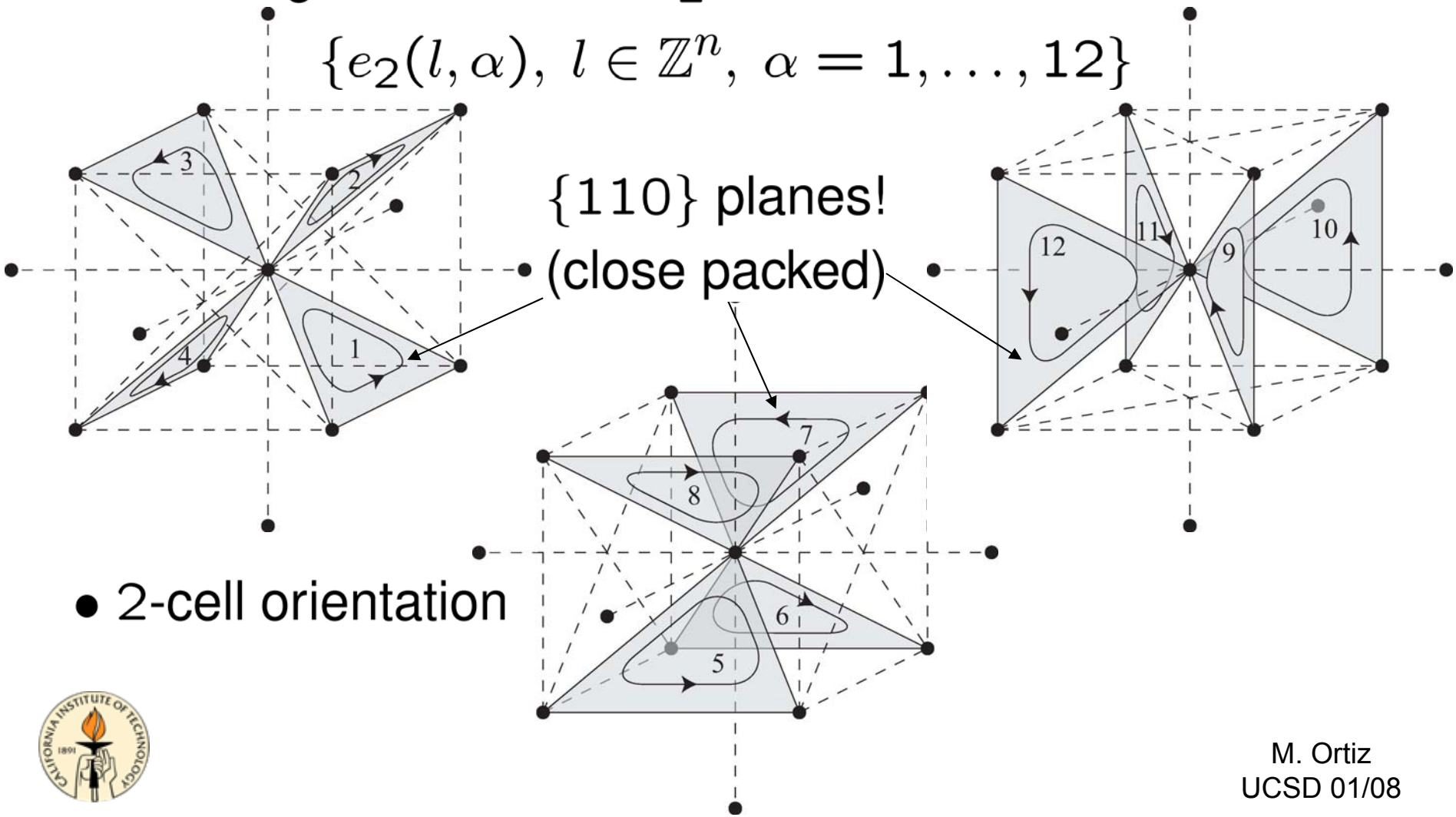
- Indexing of 1-cell set: $E_1 = \{e_1(l, \alpha),\ l \in \mathbb{Z}^n,\ \alpha = 1, \ldots, 7\}$
- 1-cell orientation



BCC lattice complex: 2-cells

- Indexing of 2-cell set: $E_2 =$

$$\{e_2(l,\alpha),\ l \in \mathbb{Z}^n,\ \alpha = 1,\ldots,12\}$$



- 2-cell orientation

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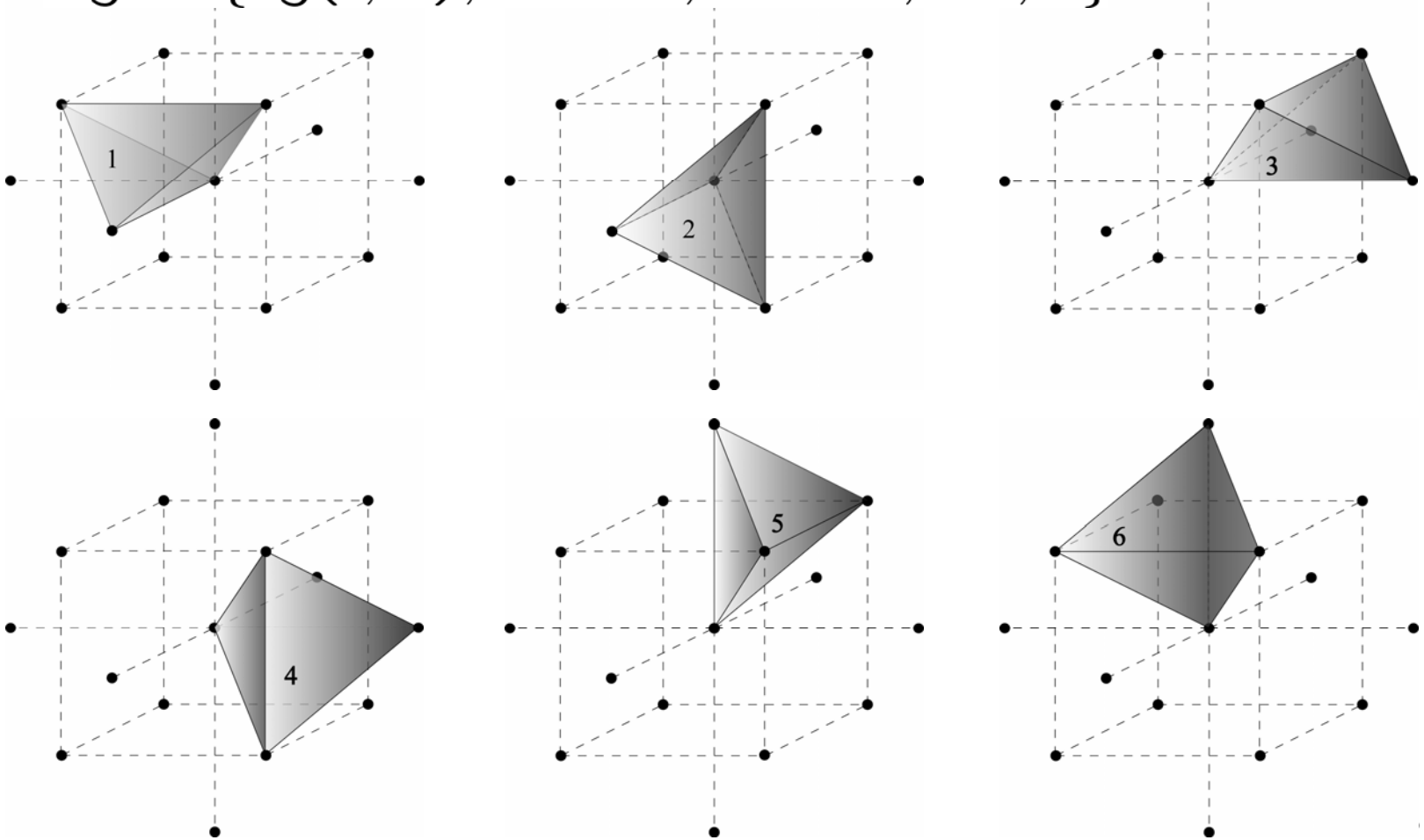
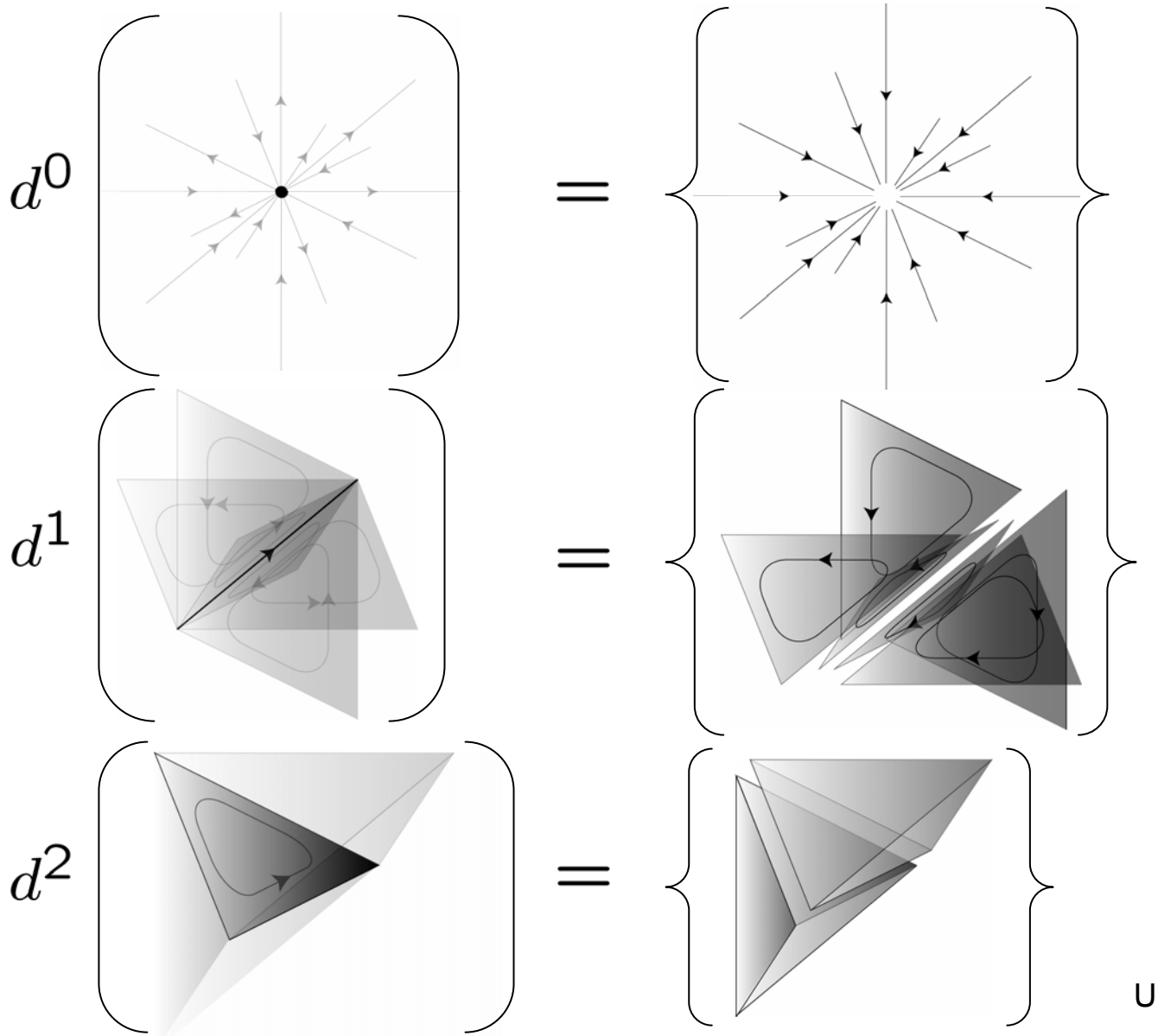
BCC lattice: Lattice complex

- Indexing of 3-cell set (+ outward orientation):

$$E_3 = \{e_3(l, \alpha),\ l \in \mathbb{Z}^n,\ \alpha = 1, \ldots, 6\}$$



BCC lattice – Differential operators



The discrete differential complex

- Wedge product bilinear, associative,

$$d^{p+q}(\alpha^p \wedge \beta^q) = d^p\alpha^p \wedge \beta^q + (-1)^p\, \alpha^p \wedge d^q\beta^q$$

- Discrete Stoke's theorem:

$$\langle d\omega, \chi_A\rangle = \langle \omega, \partial\chi_A\rangle \Longleftrightarrow \int_A d\omega = \int_{\partial A} \omega$$

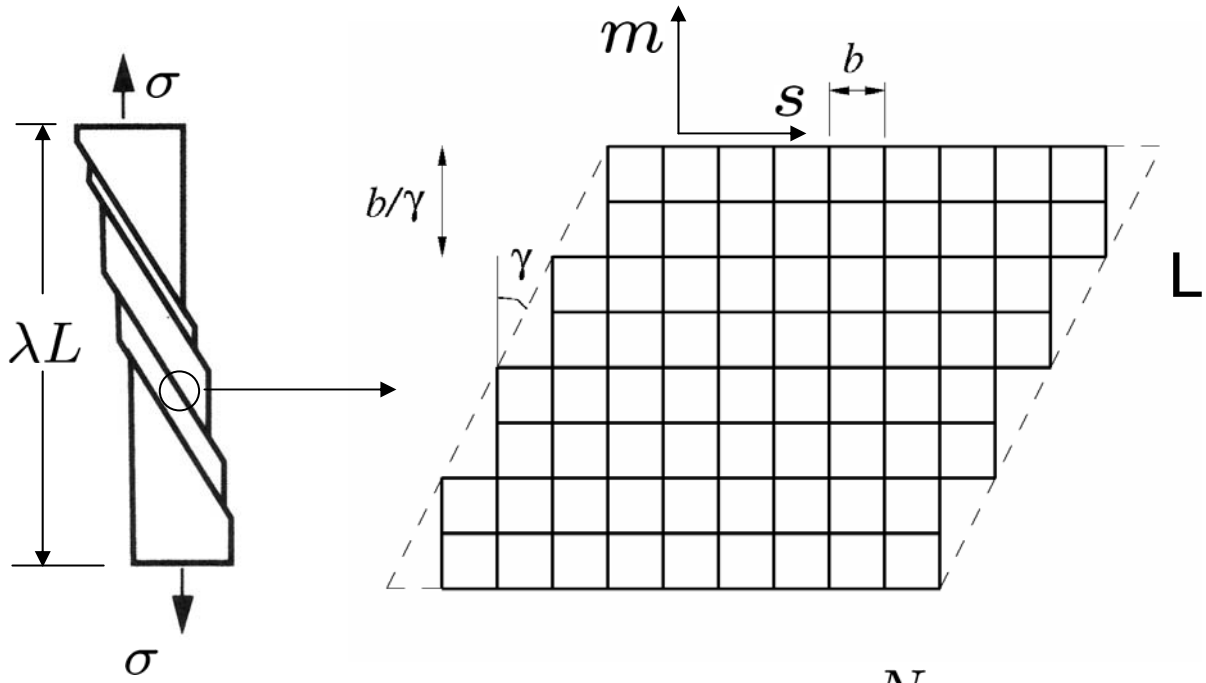
- Integration-by-parts formula:

$$\int_{\partial A} \alpha \wedge \beta = \int_A (d\alpha) \wedge \beta + \int_A (-1)^p \alpha \wedge (d\beta)$$

- Perfect lattice: $H^* = 0$, same as de Rham cohomology of $\mathbb{R}^n$ (Poincare's Lemma)

Corollary. *Perfect lattice,* $\Omega^* \ni \omega = d\alpha + \delta\beta$ (discrete Helmholtz-Hodge decomposition)

Continuum crystal plasticity

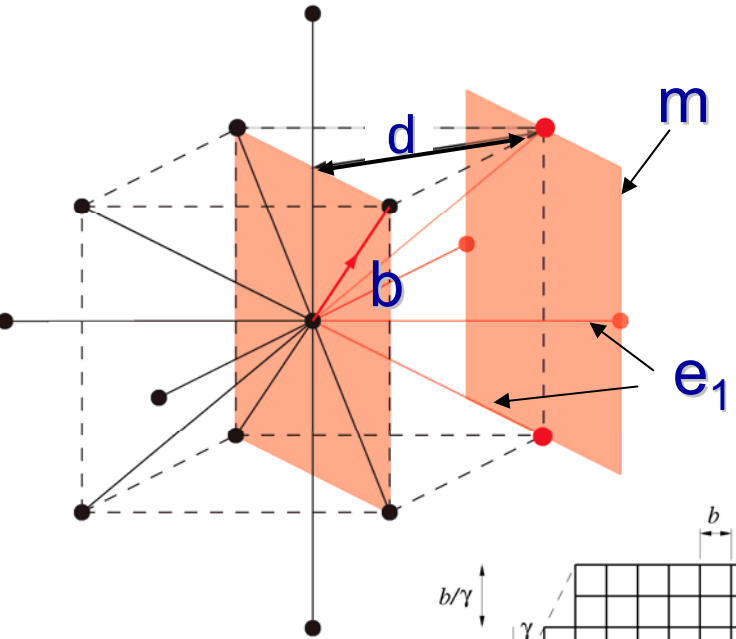


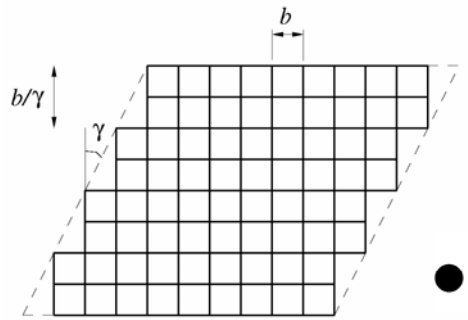
Lattice-invariant deformations (no elastic energy cost!)

- Elastic energy: $\beta_{ij} = \sum_{s=1}^{N} \gamma^s s_i^s m_j^s \,,$

$$E(u,\beta) = \int_{\mathbb{R}^3} \frac{1}{2} c_{ijkl}(u_{i,j} - \beta_{ij})(u_{k,l} - \beta_{kl})\, dx$$

Discrete crystal plasticity





- Displacements: $u : E_0 \to \mathbb{R}^3$
- Eigendeformations:

$$\beta(e_1) = \sum_{s=1}^{N} \xi^s(e_1)\, \underbrace{b^s \frac{dx(e_1)\cdot m^s}{d}}$$

lattice-invariant shears

- Slip fields: $\underbrace{\xi : E_1 \to \mathbb{Z}^N}$

integer-valued!

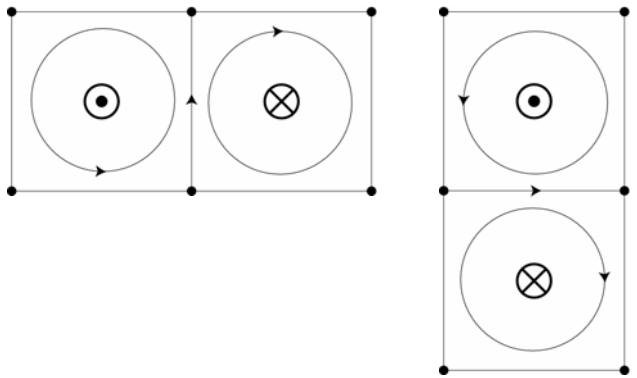
- Elastic energy:

$$E(u,\xi) = \frac{1}{2}\langle \Psi * (du-\beta), (du-\beta)\rangle$$

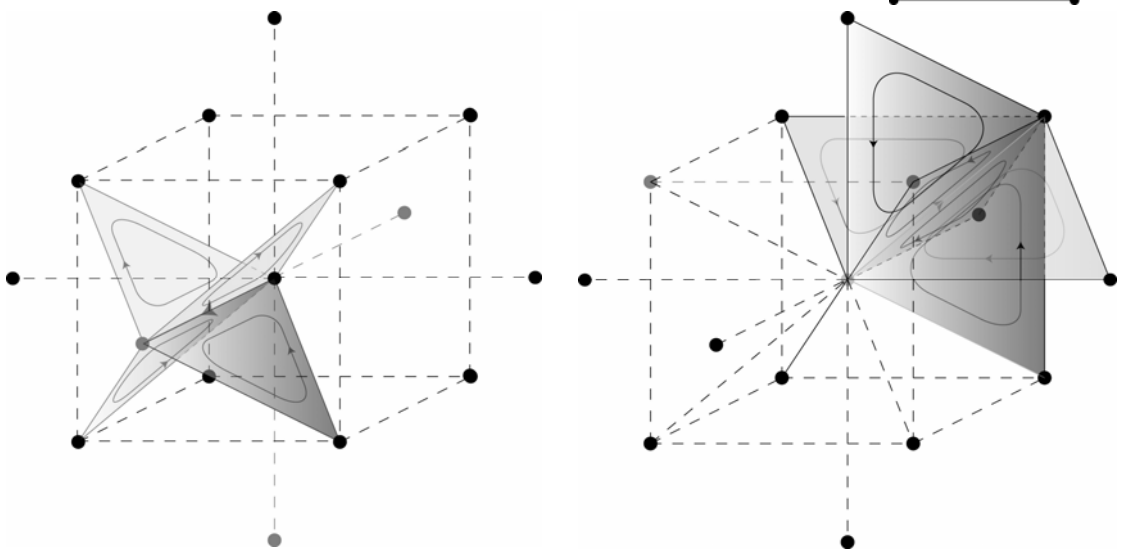
force constants

Discrete dislocations

- Discrete dislocation density: $Z^2 = B^2 \ni \alpha = d\beta$
- Conservation of Burgers vector: $d\alpha = 0$
- Square lattice:



- BCC lattice:



Elementary dislocation "loopons" and Burgers circuits

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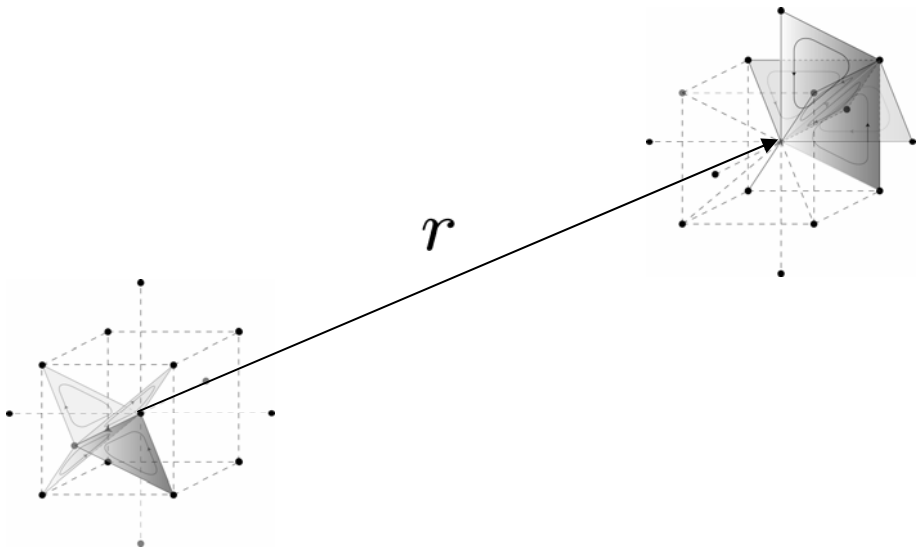
Discrete crystal plasticity – Stored energy

- Stored energy: $\inf_u E(u,\xi) \equiv E(\xi) = \frac{1}{2}\langle \Upsilon * \xi, \xi \rangle$

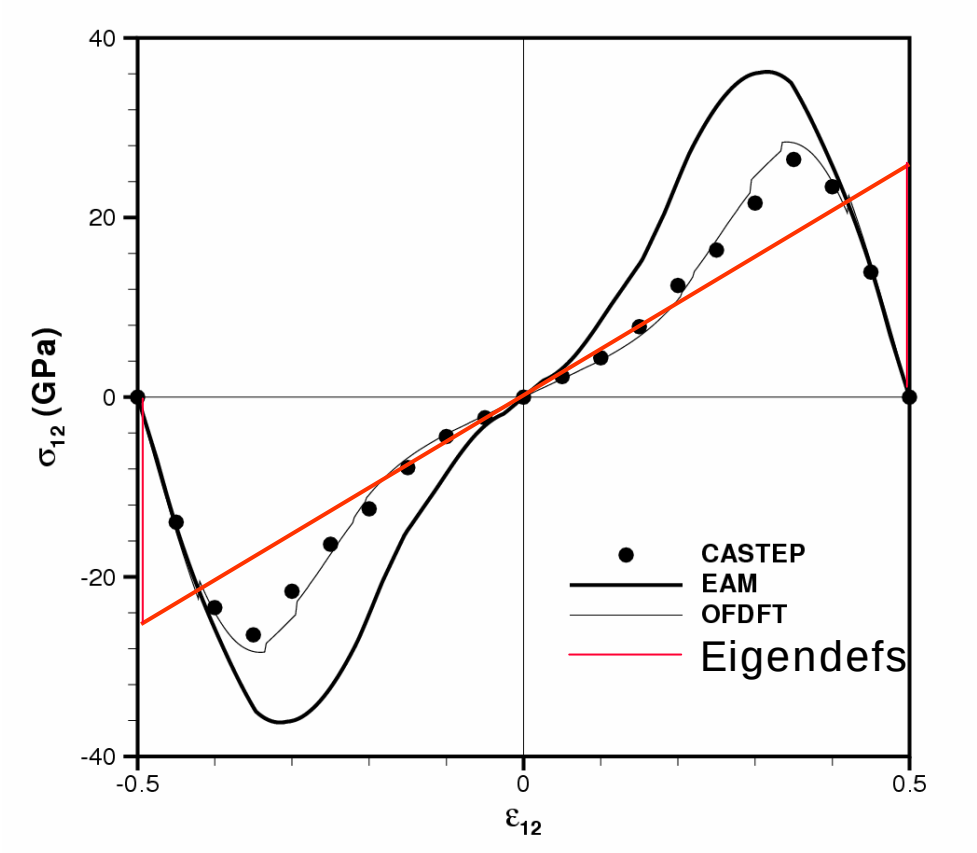
$$\Upsilon(r) \equiv \left\{ \quad \right\}$$



Interaction energy between elementary dislocation loops

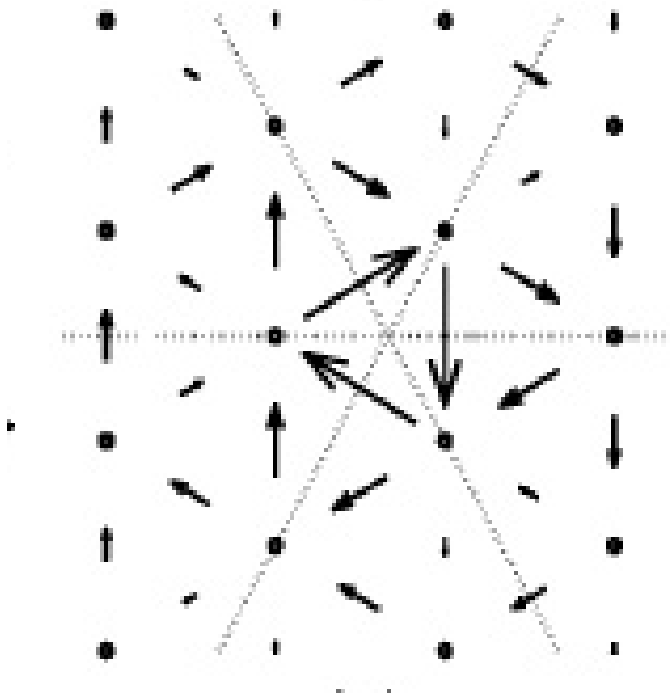
- $\Upsilon * \xi \equiv$ discrete Peach-Koehler forces
- Υ known explicity in terms of force constants Ψ

γ-energy – Comparison to first principles

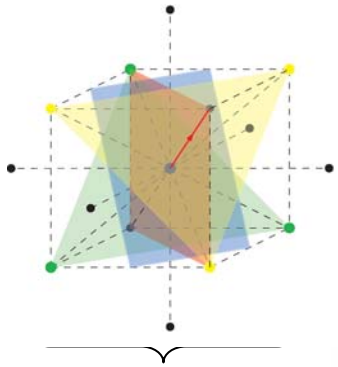


Shear stress-strain curves in FCC Al computed from EAM, OFDFT and CASTEP Kohn-Sham DFT (Fago, Hayes, Carter and Ortiz, *SIAM Multiscale Model. Simul.*, **4** (2005) p. 359)

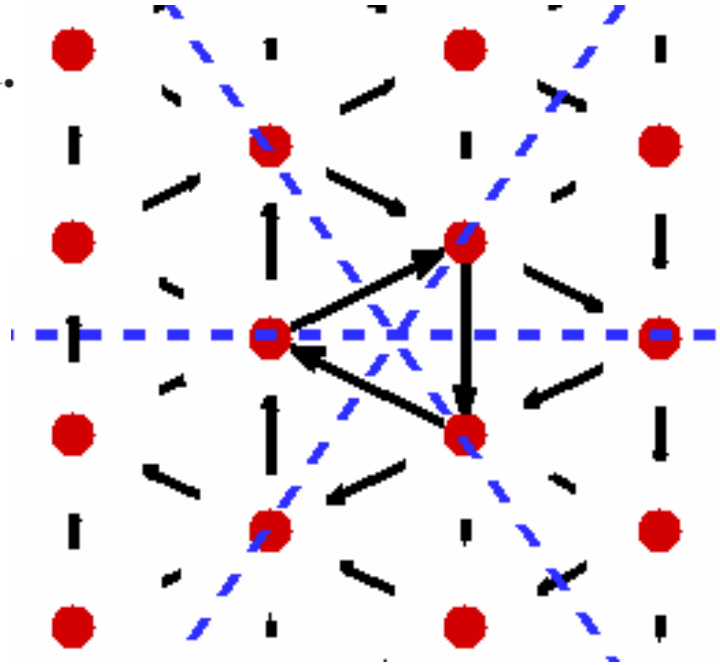
Discrete dislocations – Core structure



Ab initio Mo screw easy core
(S. Ismail-Beigi and T. Arias,
PRL, 84:1499, 2000)



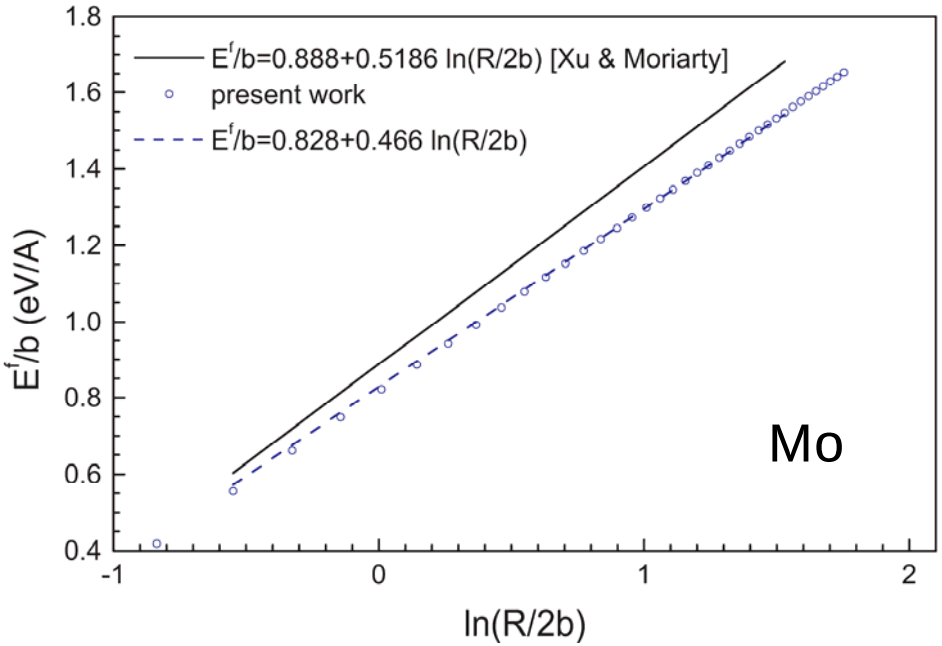
Bcc screw
disocation



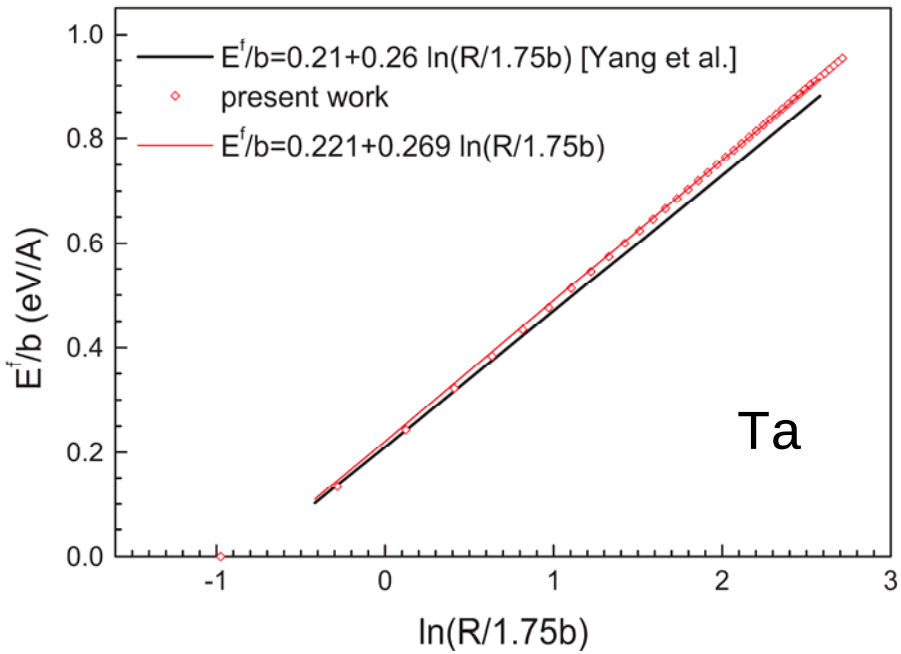
Discrete Mo screw core
(Ramasubramanian,
Ariza and Ortiz' 05)

Displacement-difference maps

Discrete dislocations – Core energy



Energy of Mo screw core
(Xu & Moriarty, *Phys. Rev. B* **54**, 1996)



Energy of Ta screw core
(Yang et al. *Phil.Mag. A* **81**, 2001)

Energy per unit length of screw dislocation in concentric cylinder of radius R

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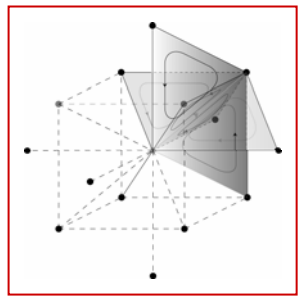
Discrete dislocation dynamics – D^3

- Incremental potential:

$$F(\xi) = \underbrace{E(\xi)}_{\text{stored energy}} + \underbrace{\Delta t\, \phi\left(\frac{\xi - \xi_0}{\Delta t}\right)}_{\text{mobility law}} - \underbrace{\langle \tau, \xi \rangle}_{\text{applied forcing}}$$

- Equilibrium configurations:

$$F(\xi - s) \leq F(\xi) \leq F(\xi + s)$$

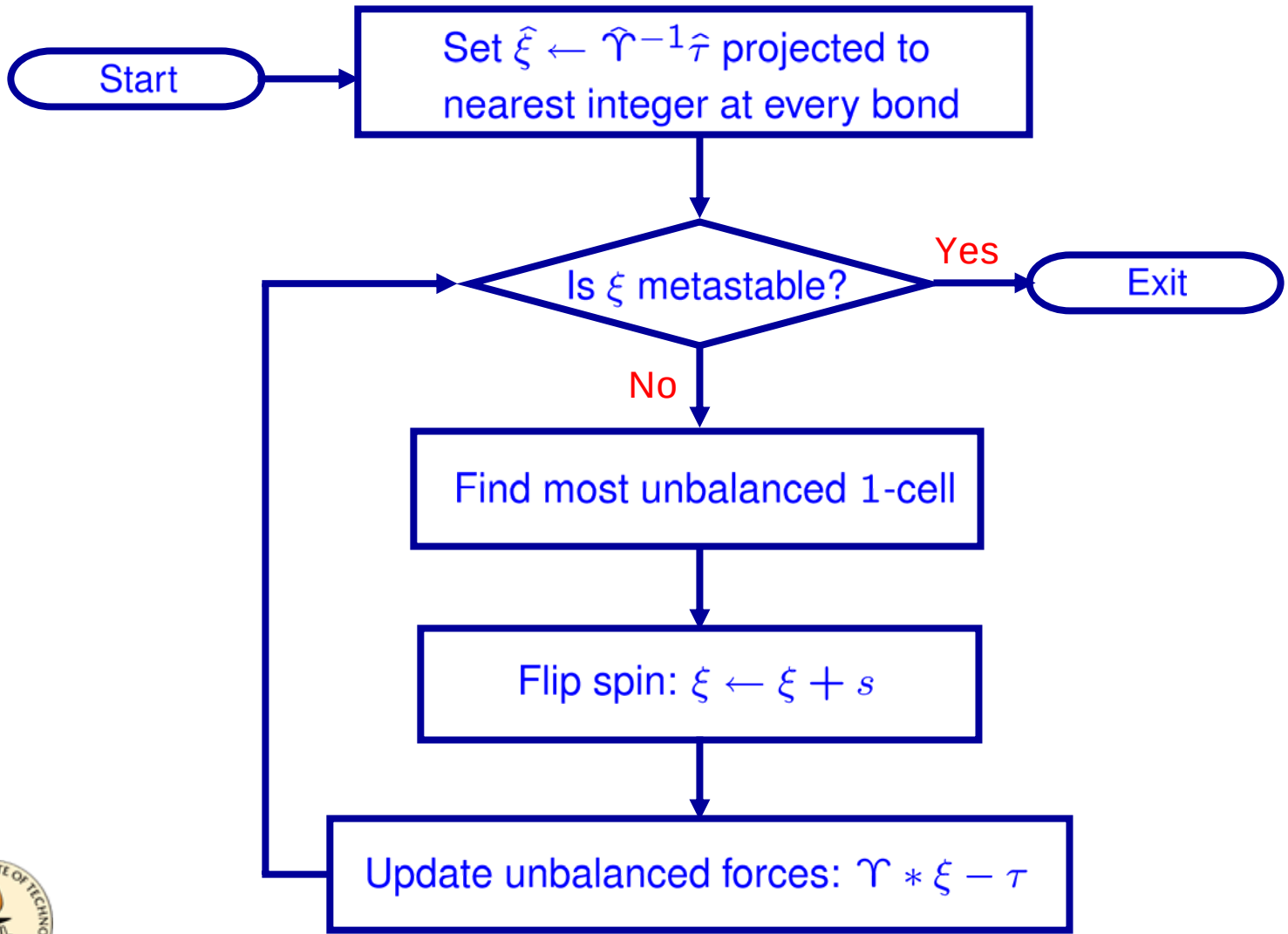


- System of inequalities:

$$|\Upsilon * \xi - \tau| \leq \tau_c, \qquad \text{for all bonds}$$

- ξ integer valued $\Rightarrow$ problem NP complete!

D^3 – Solution procedure



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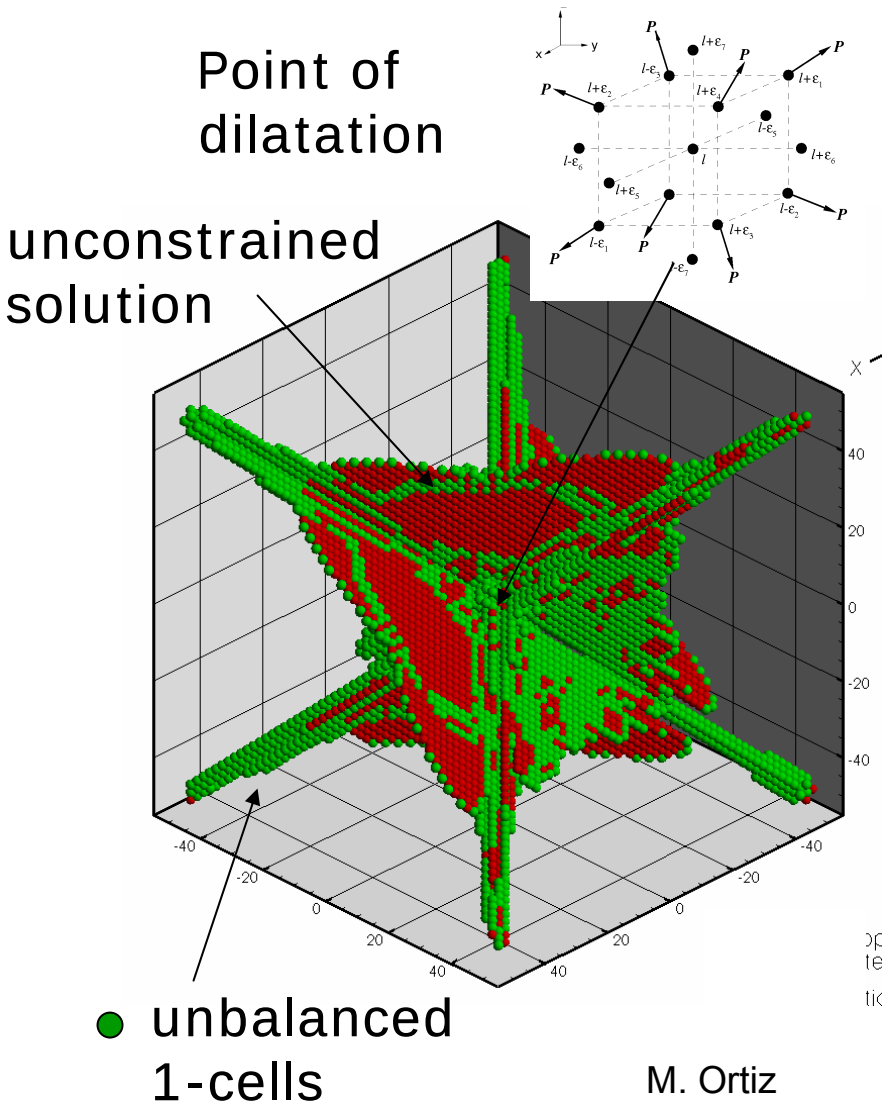
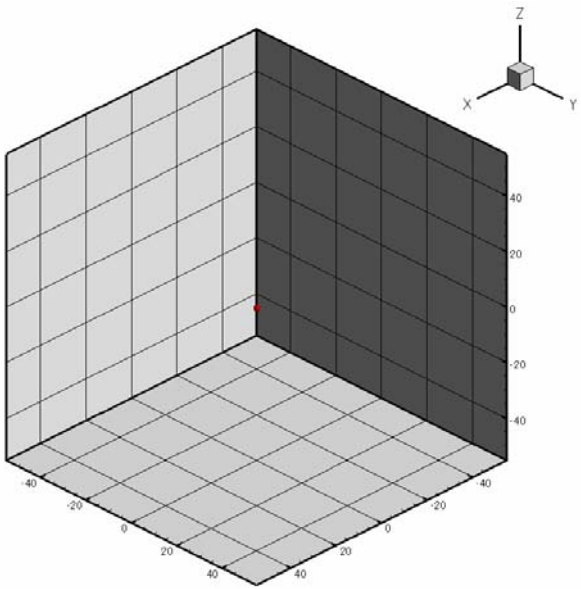
D^3 – Solution procedure

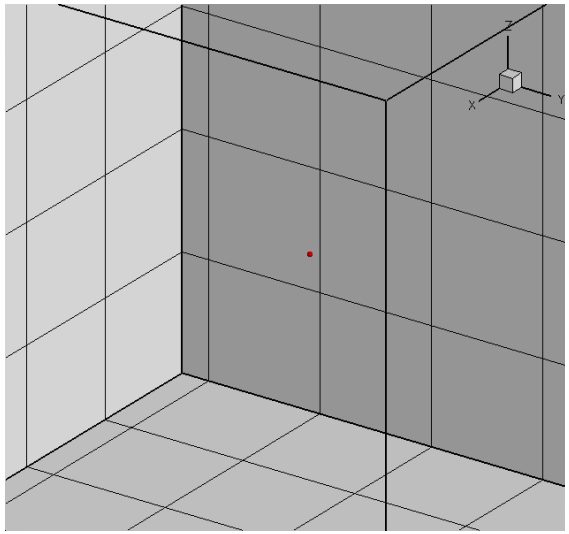
- Unconstrained problem local in Fourier space
- FFT algorithm FFTW (Johnson & Frigo)
- Force update: tabulate stress field of spin
- Easy decomposition over processors
- Minimal inter-processor communication
- Nonlinear equilibration restricted to dislocation cores and junctions: small set!



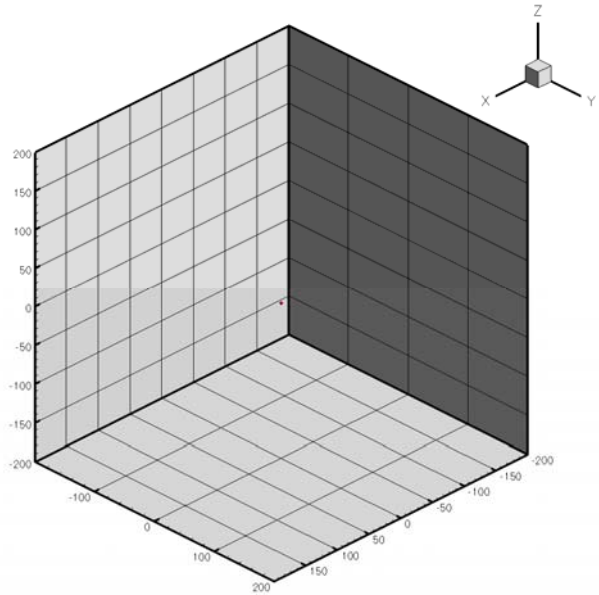
D^3 – Dilatation point – BCC vanadium



1 million atoms
in unit cell



27 million atoms
in unit cell

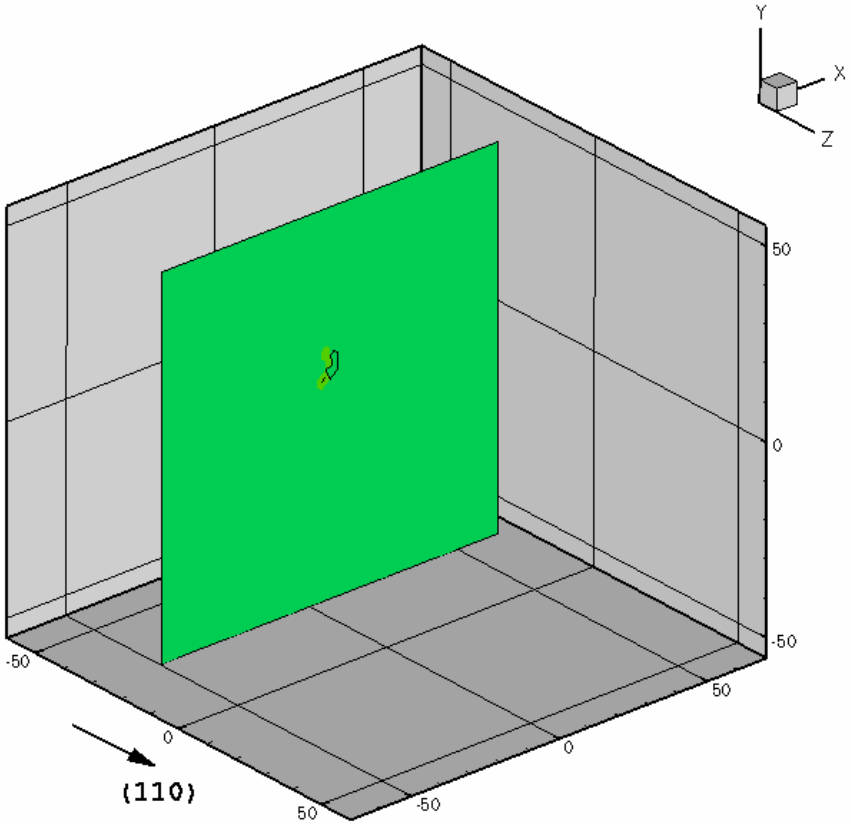


64 million atoms
in unit cell

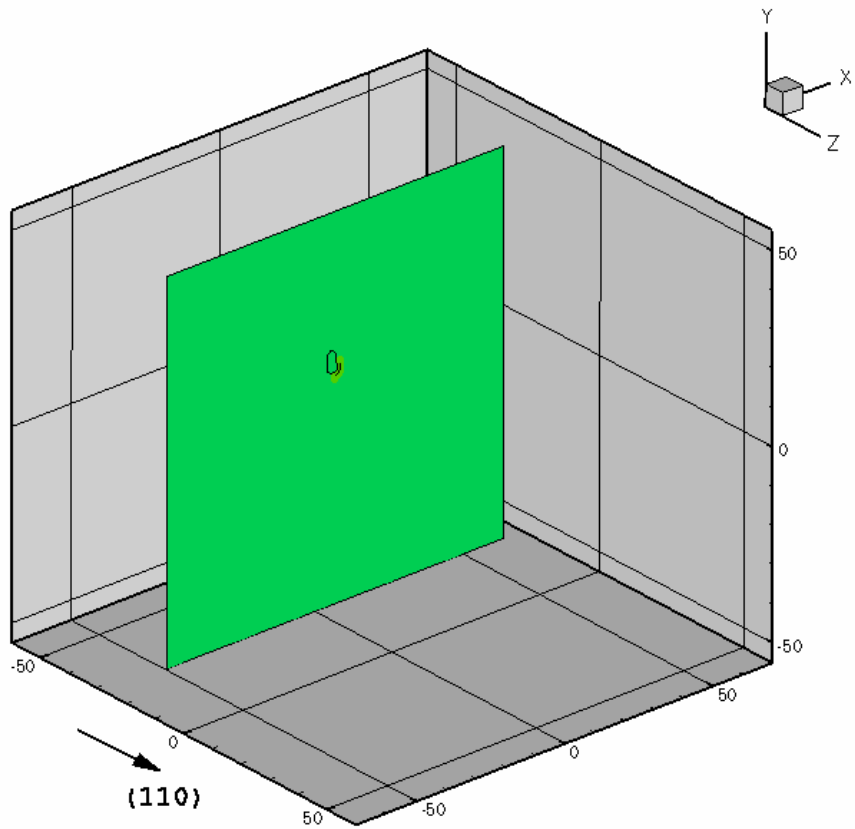
Periodic array of dilatation points in vanadium

(Ramasubramanian, Ariza and Ortiz ’05)

D^3 – Dilatation point – BCC vanadium



ξ_{D6}

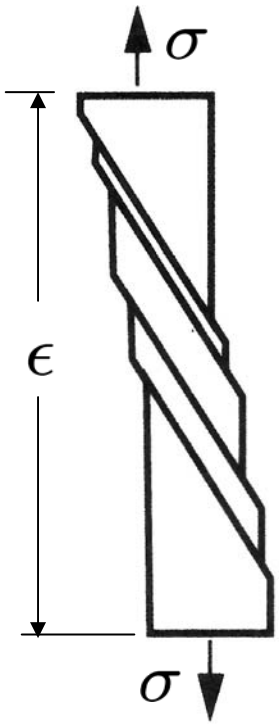


ξ_{A6}

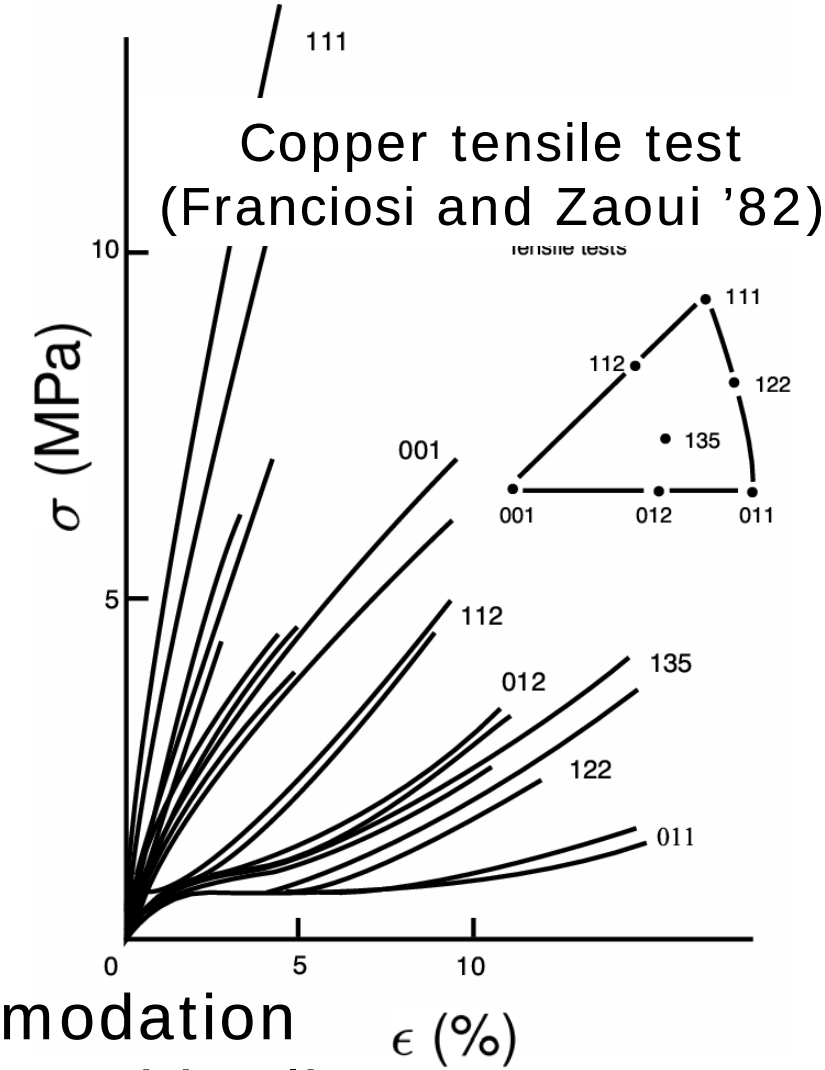
Slip system D6:
plane (1 1 0)
direction [1 1 $\bar{1}$]

Slip system C3:
plane (1 0 1)
direction [1 1 $\bar{1}$]

Crystal plasticity – Hardening



Uniaxial tension test



Irreversible accommodation of shear by crystallographic slip

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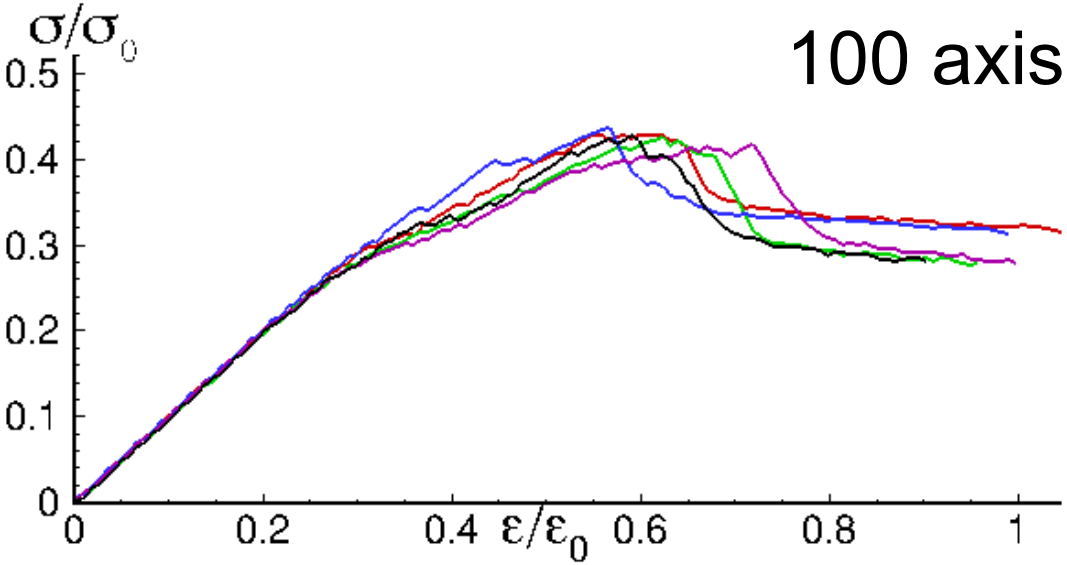
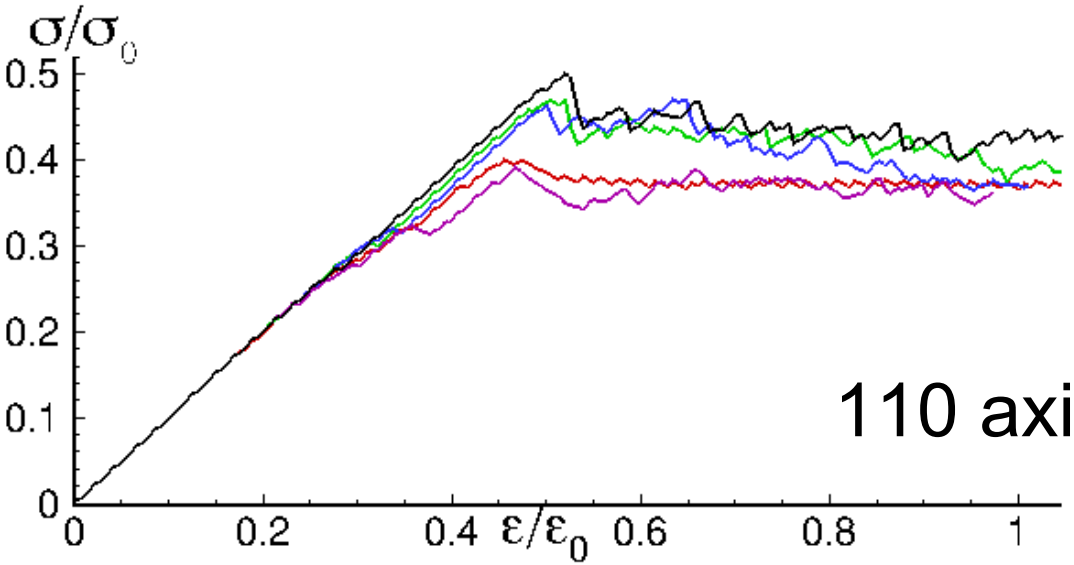
Uniaxial tension test - Vanadium



100 axis



110 axis

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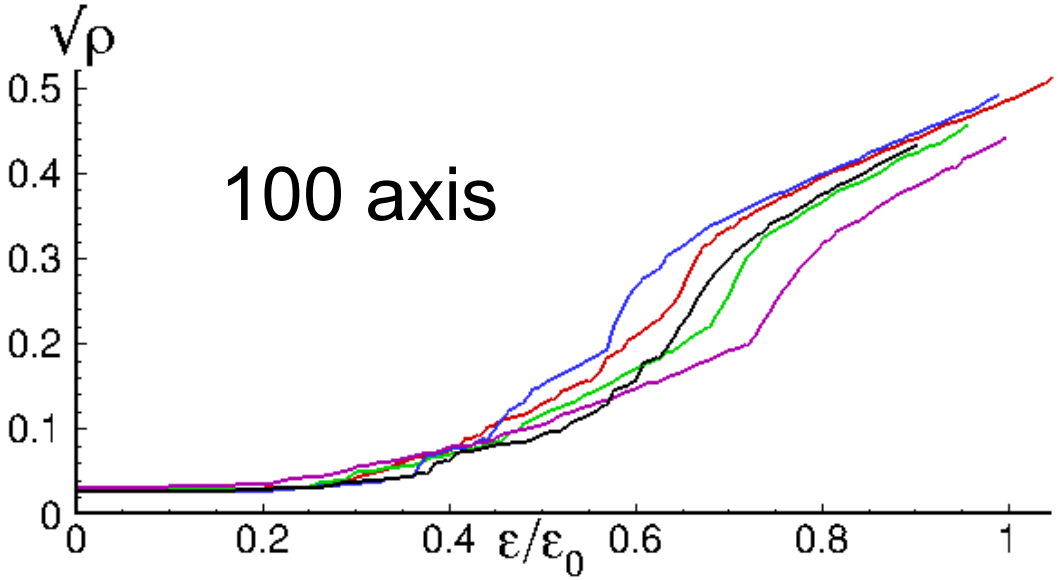
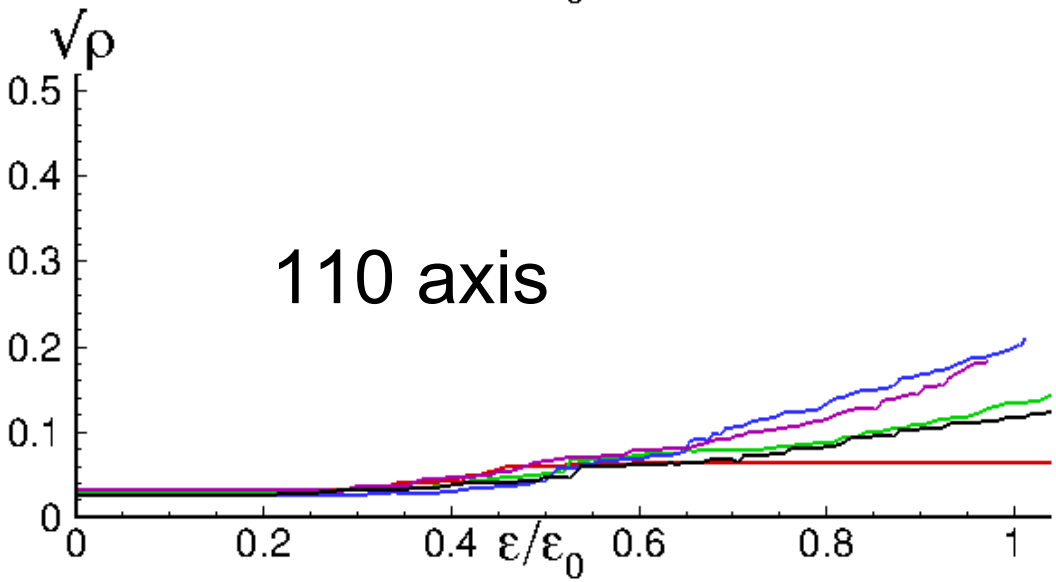
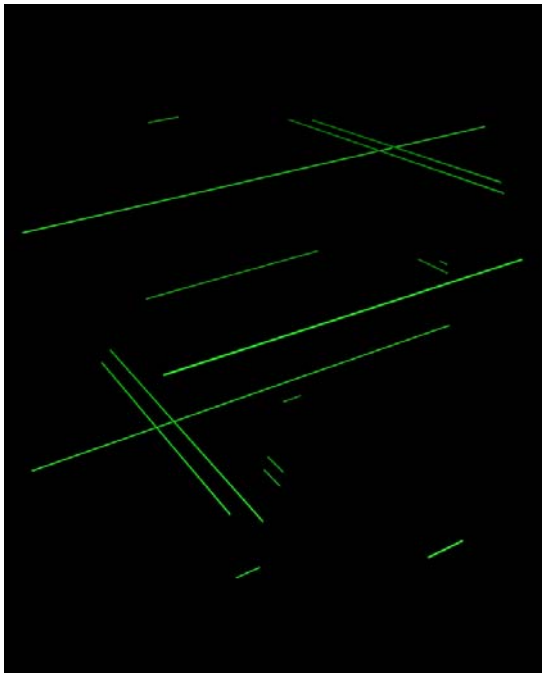
Uniaxial tension test - Vanadium

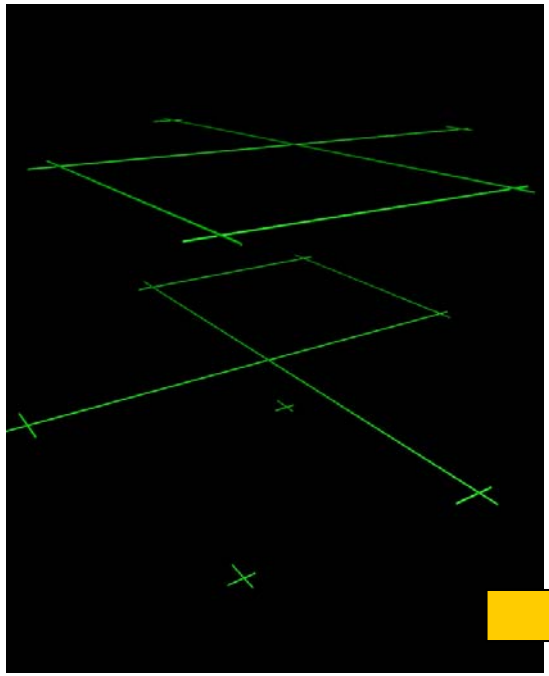




Uniaxial tension test - Vanadium



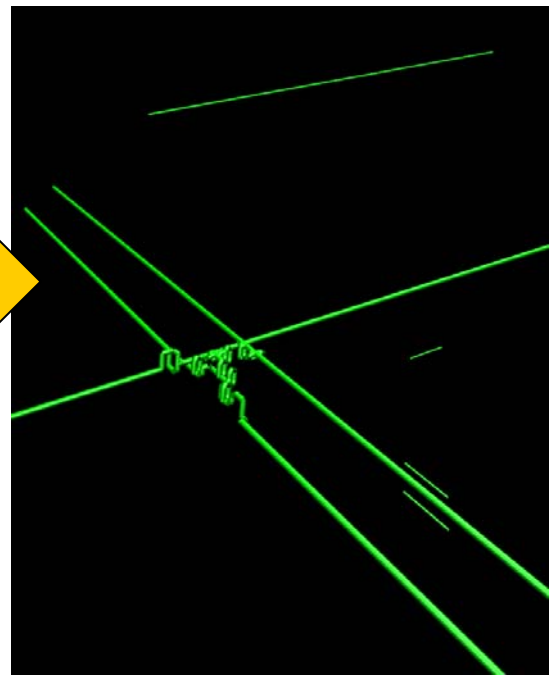
initial



deformed

Molybdenum

Systems C5 & A6



Junction formation

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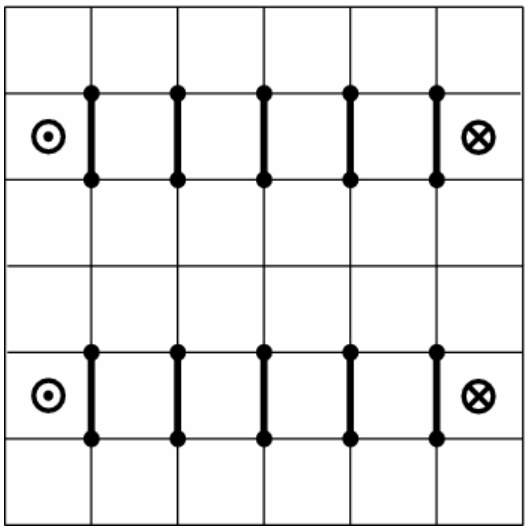
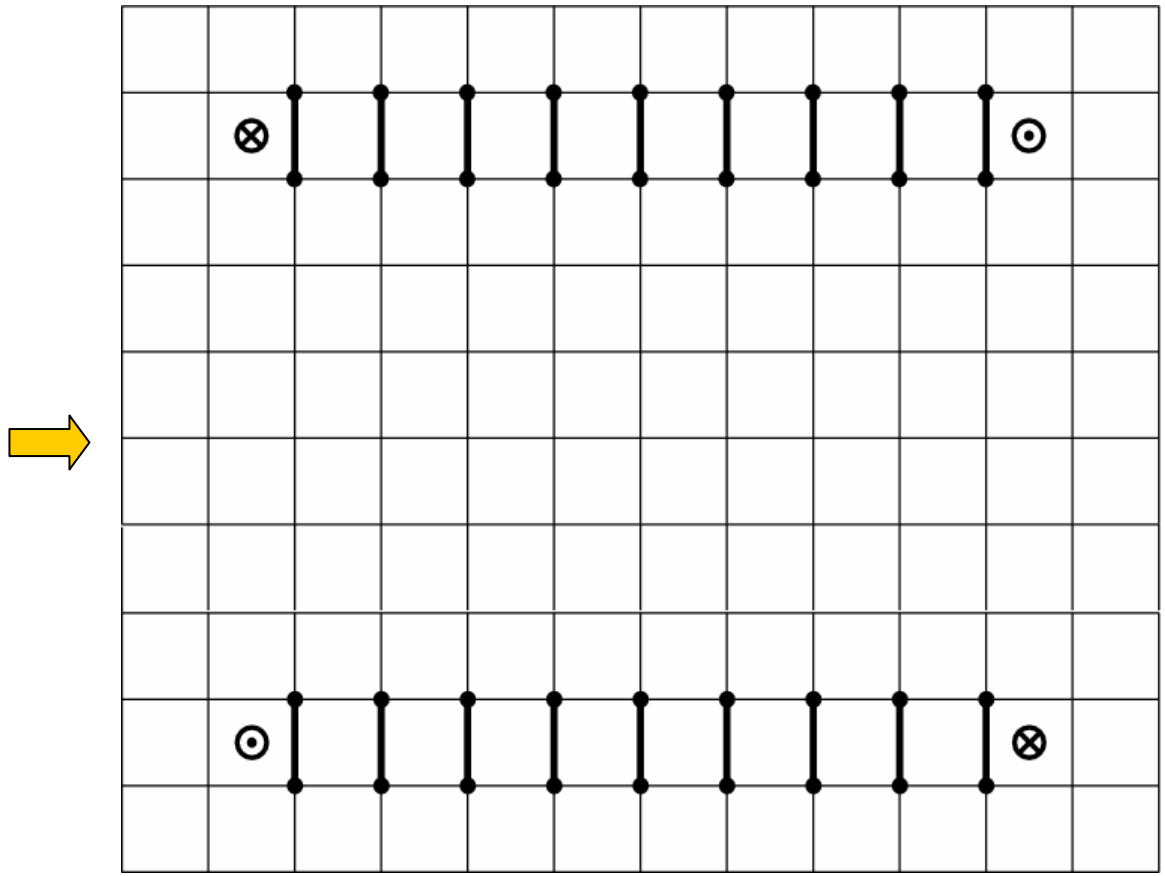
Stored energy - Dilute limit

- Uniform expansion of dislocation distribution:

$\equiv \xi = 1$





- Question: $\Gamma - \lim_{h \to \infty} E_h$?

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Stored energy – Continuum limit

phys. stat. sol. (b) 48, 419 (1971)

The Elastic Energy of a Straight Dislocation in an Infinite Anisotropic Elastic Medium

By

D. M. BARNETT and L. A. SWANGER

Finally, we obtain

$$E = K_{mg}\, b_m\, b_g \ln \frac{R}{r_0}, \tag{34}$$

where

$$K_{mg} = (K^*_{mg} + K^*_{gm}) = K_{gm} \tag{35}$$

and

$$K^*_{mg} = \frac{1}{16\,\pi^2}\, \varepsilon_{pjm}\, t_j\, C_{ngip}\, C_{wmrs} \left\{ \varepsilon_{vsn}\, t_v \int_0^\pi M^*_{ir}\, \mathrm{d}\psi + \right.$$

$$\left. + (\alpha_s\, \beta_n + \beta_s\, \alpha_n) \int_0^\pi M^*_{ir} \cos 2\,\psi\, \mathrm{d}\psi + (\beta_n\, \beta_s - \alpha_n\, \alpha_s) \int_0^\pi M^*_{ir} \sin 2\,\psi\, \mathrm{d}\psi \right\}. \tag{36}$$

Stored energy – Dilute limit

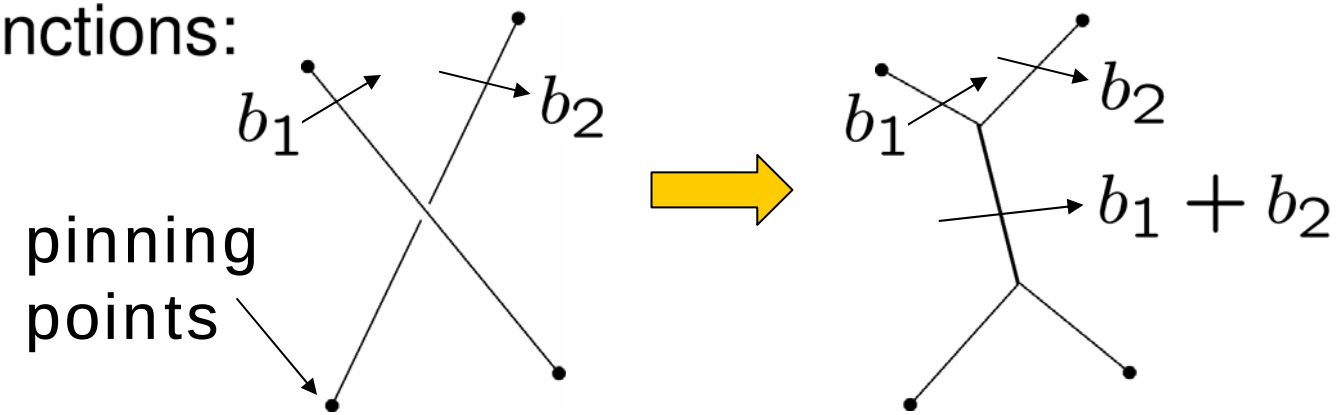
- Γ-limit of stored energy: $F_h(\xi) \sim F_0(\xi) \log h$

  $F_0(\xi) \sim \int \langle Kb, b \rangle |\rho| \equiv$ *line-tension approximation*!

  $\alpha = b\rho, \quad \rho \equiv$ discrete dislocation line density

  $K \equiv$ discrete prelogarithmic factor

- Junctions:



- The macroscopic behavior predicted by the discrete line-tension approximation is *exact* in the dilute limit!

D^3 – Outlook

- D^3 combines realism of discrete models:
  - *Discrete dislocations on crystal lattices*
  - *Dislocation cores, reactions, topological transitions…*

  with convenience of continuum models
  - *Analytical interaction law*
  - *Dimensional reduction (dislocation lines, junctions…)*
  - *Analytical tractability (continuum limit, dilute limit…)*
- Extensions in progress:
  - *Implementation of dilute limit (discrete line tension)*
  - *Application to forest hardening…*
- Future extensions:
  - *Fully anharmonic treatment* (Gallego R and Ortiz M, "A Harmonic-Anharmonic Energy Partition Method for Lattice Statics Computations" *Model. Simul. Mater. Sci. Engr.,* **1** (4): 417-436, 1993)