Multiscale models of metal plasticity
Lecture II: Energetics of dislocations

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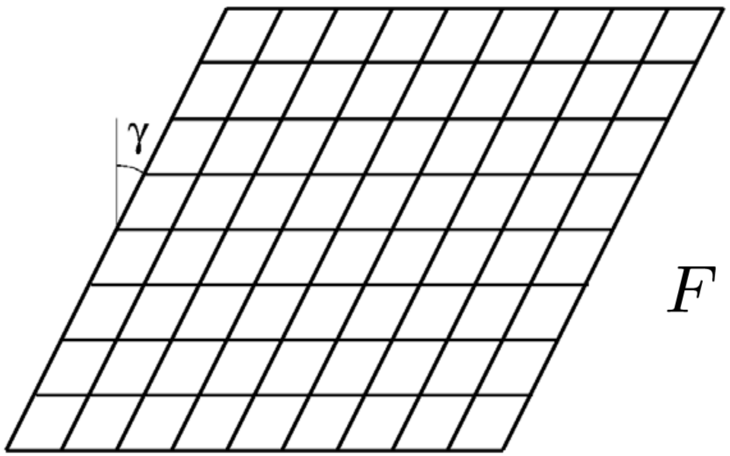
Sixth Summer School in Analysis and Applied Mathematics

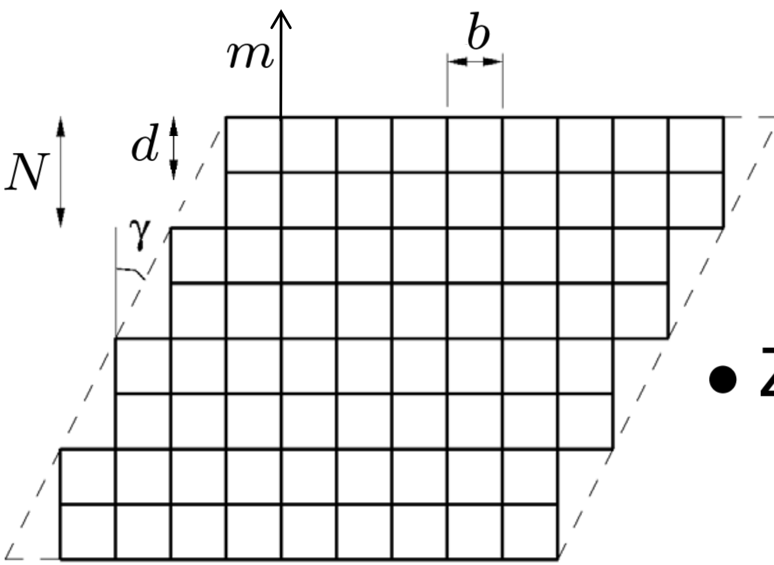
Rome, June 20-24, 2011

Outline of Lecture #2

- The necessity of dislocations
- The classical theory of linear-elastic dislocations
- The dislocation core: The Peierls-Nabarro model
- Extensions of the PN model to 3D
- Semi-discrete 2½D phase-field model
- The classical micro-macro connection
- The dilute limit and dislocation line tension

The necessity of dislocations





- Bravais lattice: $x(l) = l^i a_i, \quad l \in \mathbb{Z}^n$
  $a_i \cdot a^j = \delta_i^{\ j} \equiv$ lattice and dual bases
- Lattice-preserving affine mappings:

$$F = \mu_i^{\ j} a^i \otimes a_j \Leftrightarrow \mu_i^{\ j} \in \mathbb{Z}, \det(\mu) = \pm 1$$

- Lattice-preserving shears:

$$F = I + (b/d) \otimes m \Leftrightarrow b \cdot m = 0,$$

$m \equiv$ lattice plane unit normal

$d \equiv$ interplanar distance

$b \equiv$ lattice (Burgers) vector

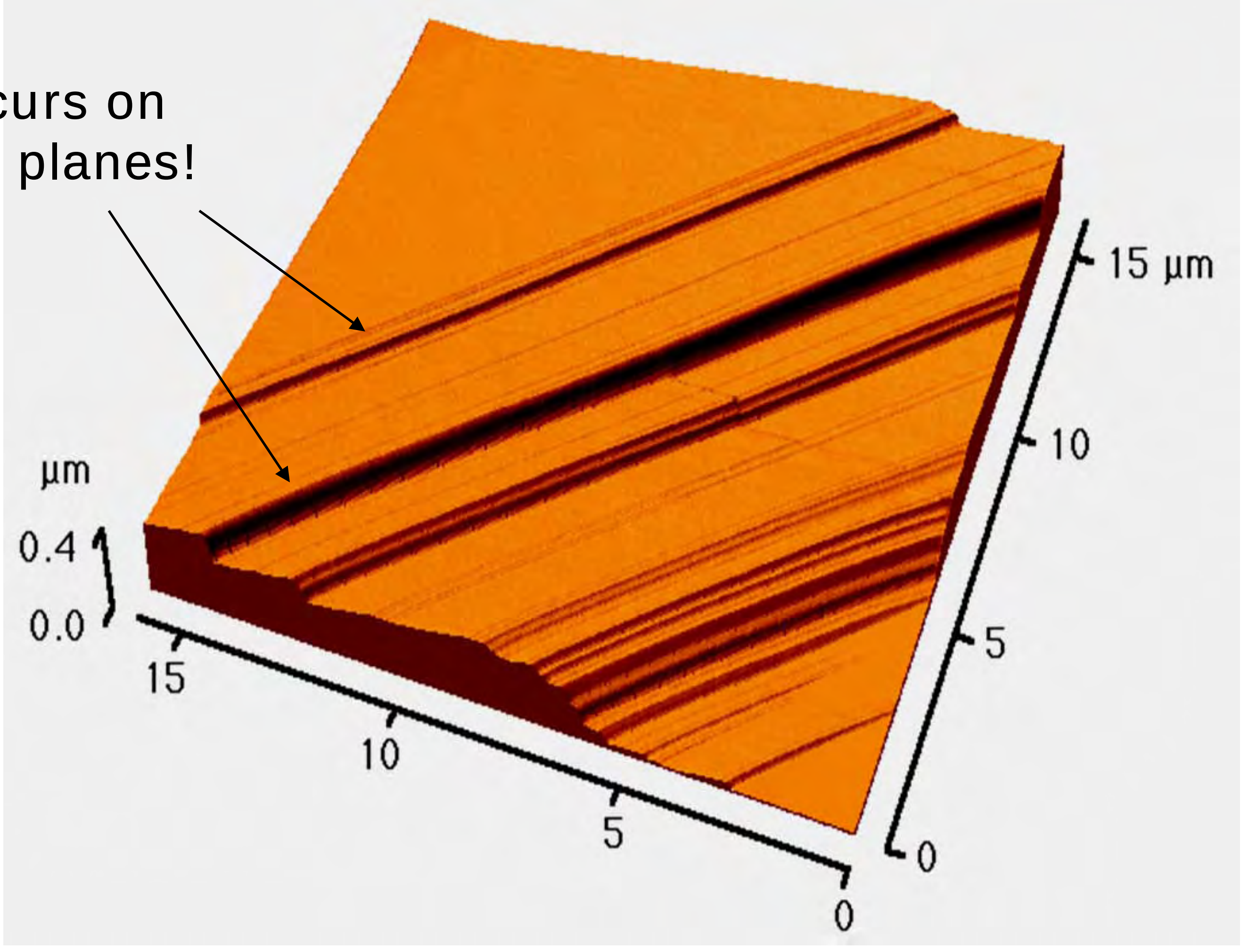
- Zero energy for any shear of the form:

$$F = \gamma s \otimes m, \; s = b/|b|, \; \gamma \in \mathbb{Q}$$

J.L. Eriksen, *ARMA,* **72** (1979) 1-13.

Discreteness of crystallographic slip

Slip occurs on discrete planes!

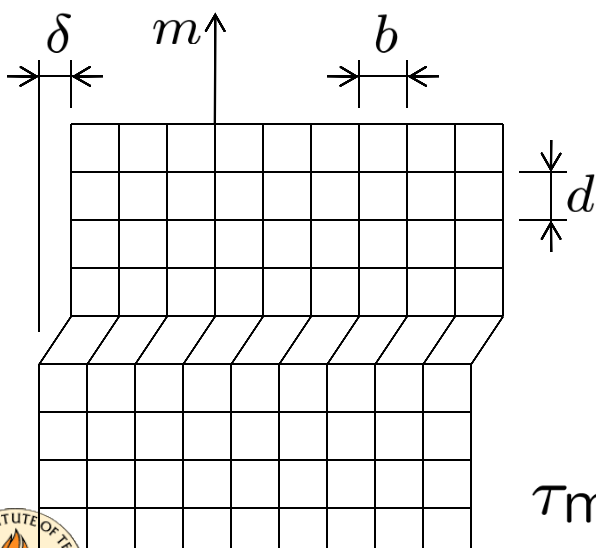


Slip traces on crystal surface
(AFM, C. Coupeau)

The necessity of dislocations

Theorem [I. Fonseca] *Let* $W : \mathbb{R}^{m\times n} \to \mathbb{R}$ *be invariant under lattice-preserving affine deformations. Then, its lower-semi-continuous envelop is of the form* $f(\det(F))$ *(compressible fluid!).*

- Need to account for energy barriers, metastability!



- Peierls-Nabarro model: $[\![u]\!] = \delta s$

$$\Gamma(\delta) = A\,(1 - \cos(2\pi\delta/b))$$

$$A = c_{ijkl} s_i m_j s_k m_l/(2\pi/b)^2 d$$

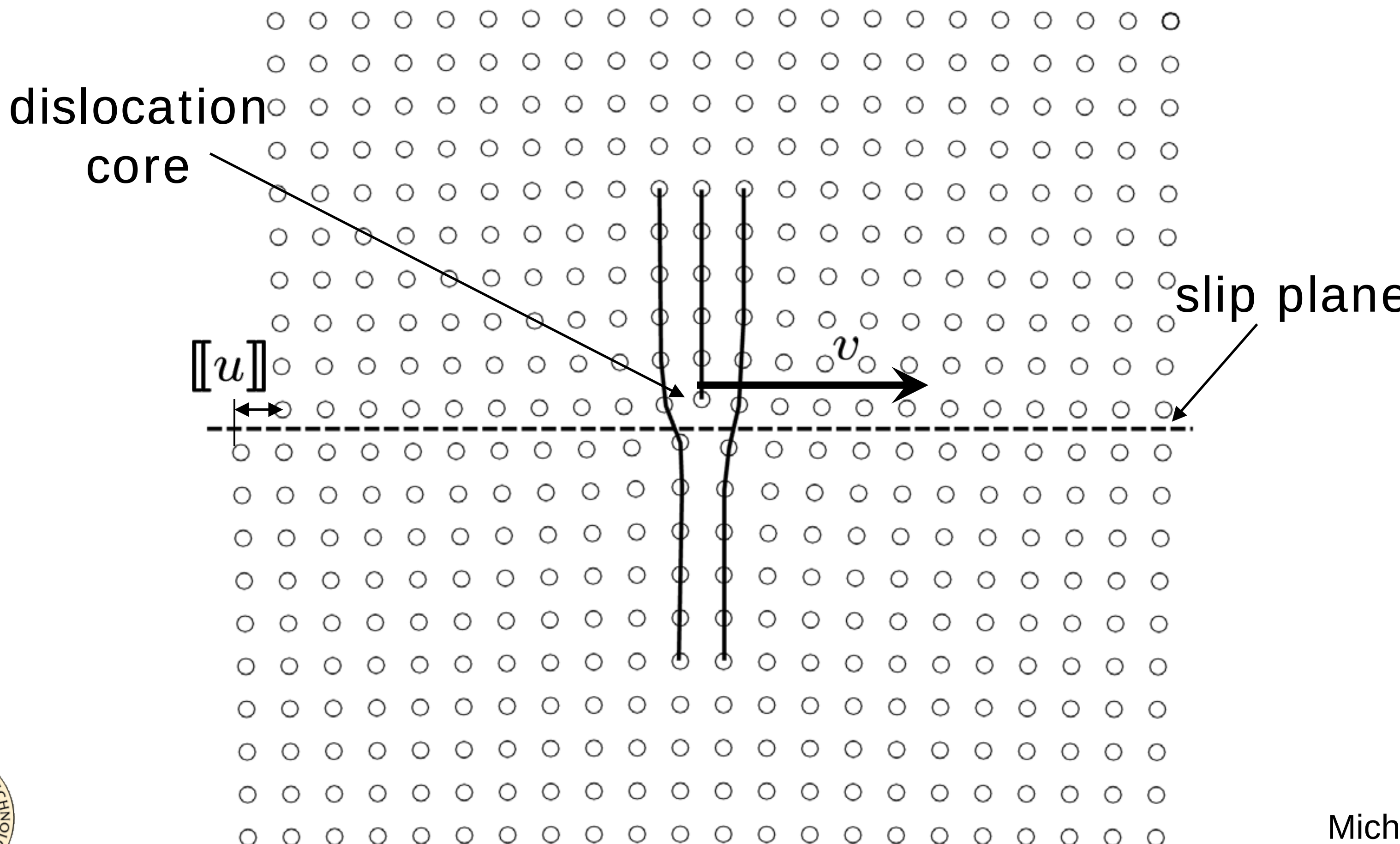
$$\tau(\delta) = D\Gamma(\delta) = A(2\pi/b)\sin(2\pi\delta/b)$$

$$\tau_{\max} = c_{ijkl} s_i m_j s_k m_l/(2\pi d/b) \sim \mu/30!$$

I. Fonseca, *ARMA*, **97** (1987) 189-220.
I. Fonseca, *J. Math. Pures et Appl.*, 67 (1988) 175-195.

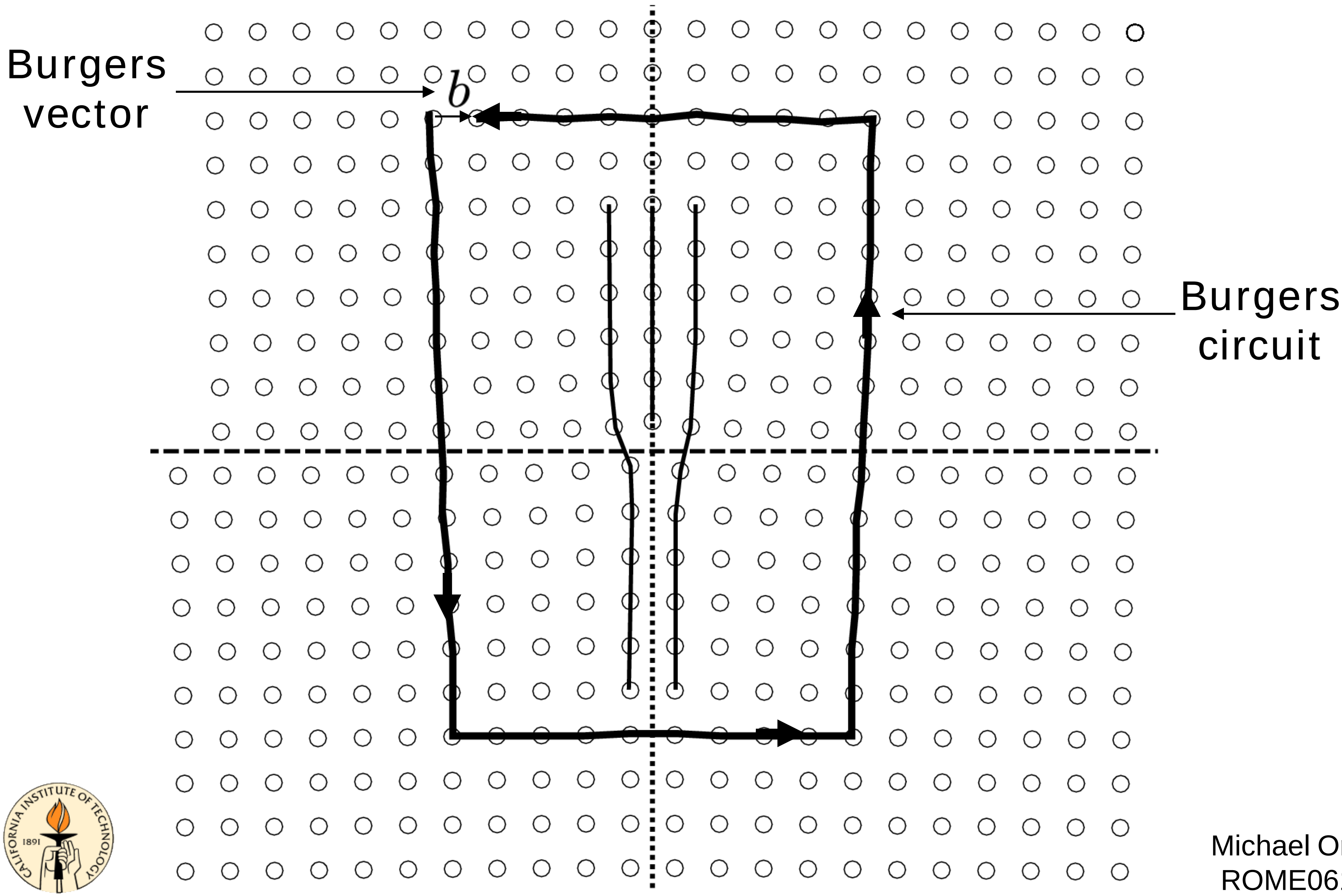
The necessity of dislocations

- Uniform crystallographic slip requires: $\tau \sim \mu/30$!
- Observed (fcc): $\tau_c \sim 10^{-5}\mu \Rightarrow$ dislocations!



(Orowan, Taylor, Polanyi, 1934)

The necessity of dislocations



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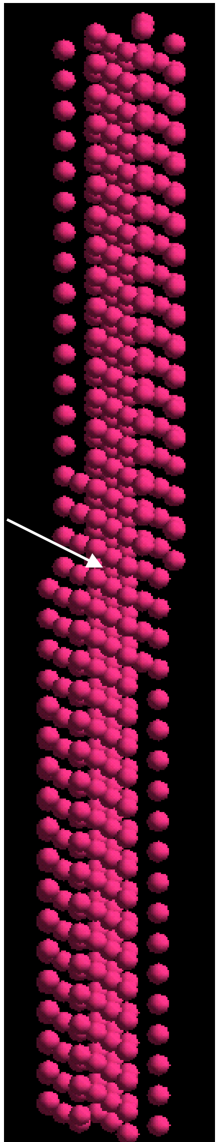
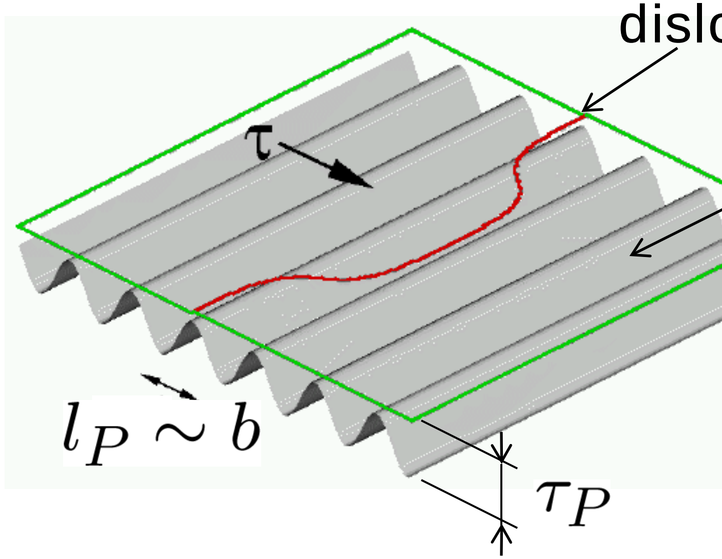
The necessity of dislocations





L. Stainier, A.M. Cuitino and M. Ortiz, *JMPS*, **50** (2002) 1511-1554.

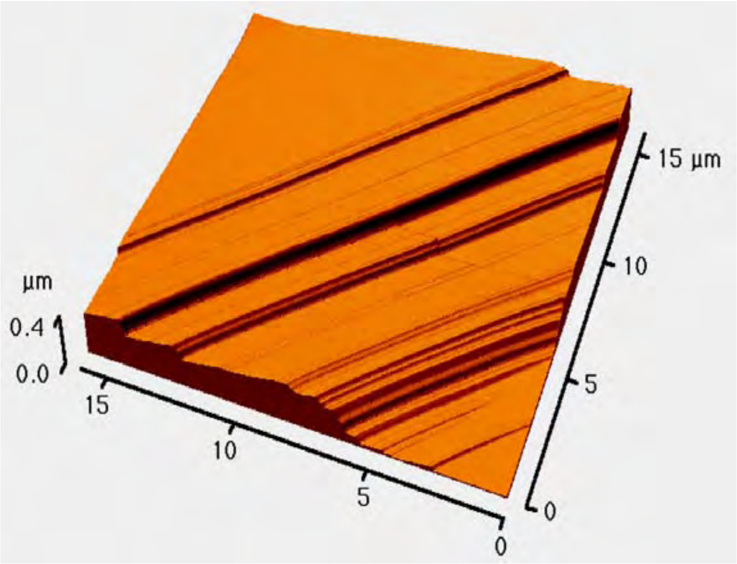
- Dislocation line experiences *Peierls potential*.
- Cottrell's estimate of Peierls stress:

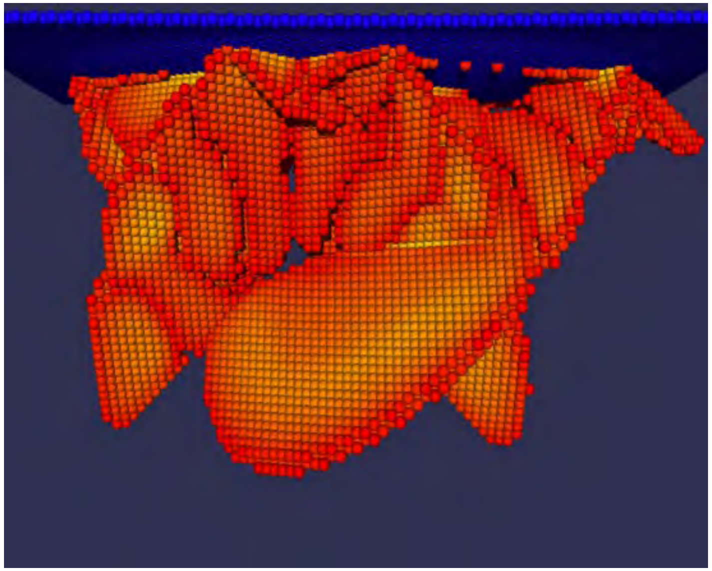
$$\tau_P = \frac{2\mu}{1-\nu} \exp\left(-\frac{2\pi d}{(1-\nu)b}\right) \sim 10^{-5}\mu$$

A.M. Cuitino *et al.*,
J. Comput.-Aided Mater., **8** (2001) 127-149.

Micromechanics of plastic deformation: Dislocation theory

- Kinematics of crystallographic slip
- The cut-surface problem of linear elasticity
- The Peierls-Nabarro model of the core
- Extensions of the PN model to 3D





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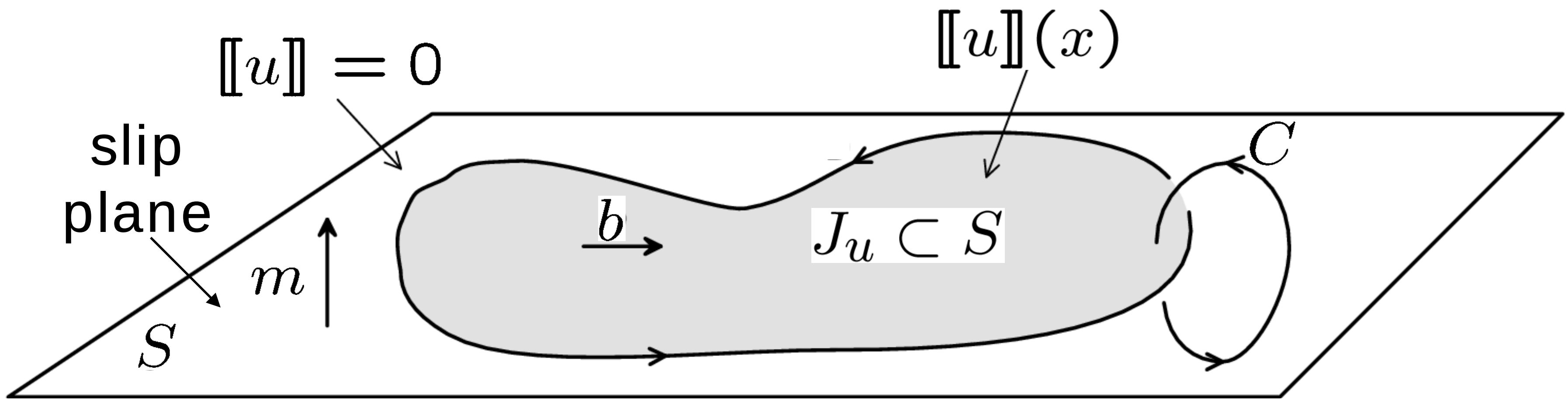
Dislocation theory - Kinematics

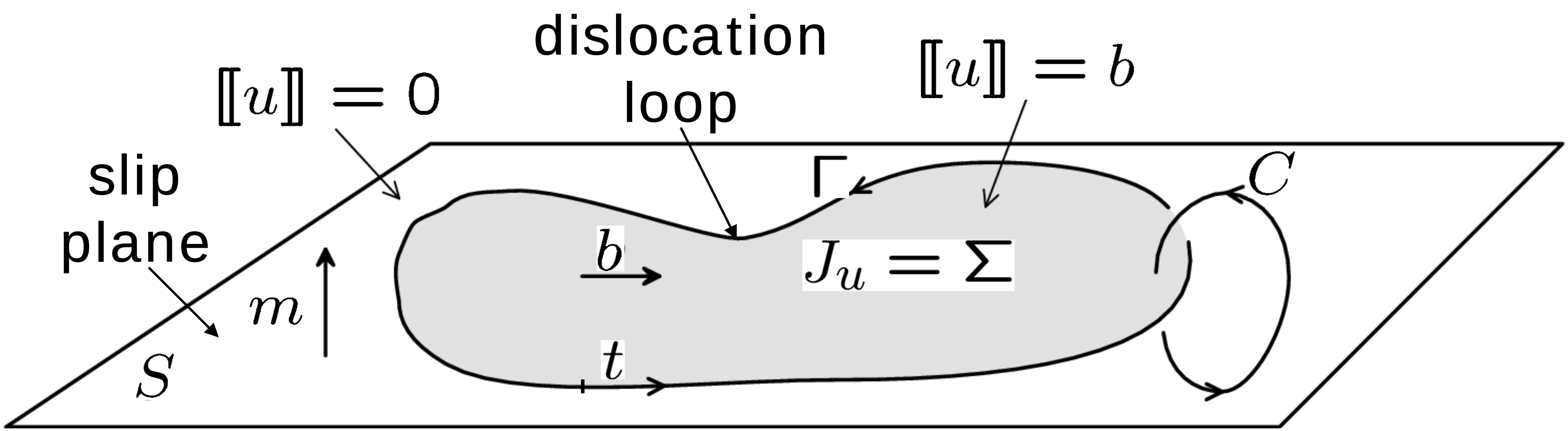


- Crystallographic slip: $u : \mathbb{R}^3 \to \mathbb{R}^3$ such that

$$Du = \underbrace{\nabla u \mathcal{L}^3}_{\text{elastic deformation}} + \underbrace{[\![u]\!] \otimes m \, \mathcal{H}^2 \lfloor J_u}_{\text{plastic deformation (currents)}} \equiv \beta^e + \beta^p$$

- Dislocation density: $\alpha = d\beta^p$ (coboundary, curl)
- Conservation of Burgers vector: $d\alpha = d^2\beta^p = 0$ $(\mathrm{div} \circ \mathrm{curl} = 0)$

Dislocation theory - Kinematics



- Volterra dislocation: $[\![u]\!] \in \{0, b\}$,

$$Du = \nabla u \mathcal{L}^3 + b \otimes m\, \mathcal{H}^2 \lfloor \Sigma \equiv \beta^e + \beta^p$$

  - Dislocation density: $\alpha = d\beta^p = b \otimes t\, \mathcal{H}^1 \lfloor \Gamma$

- Dislocation line: $\Gamma = \partial \Sigma$

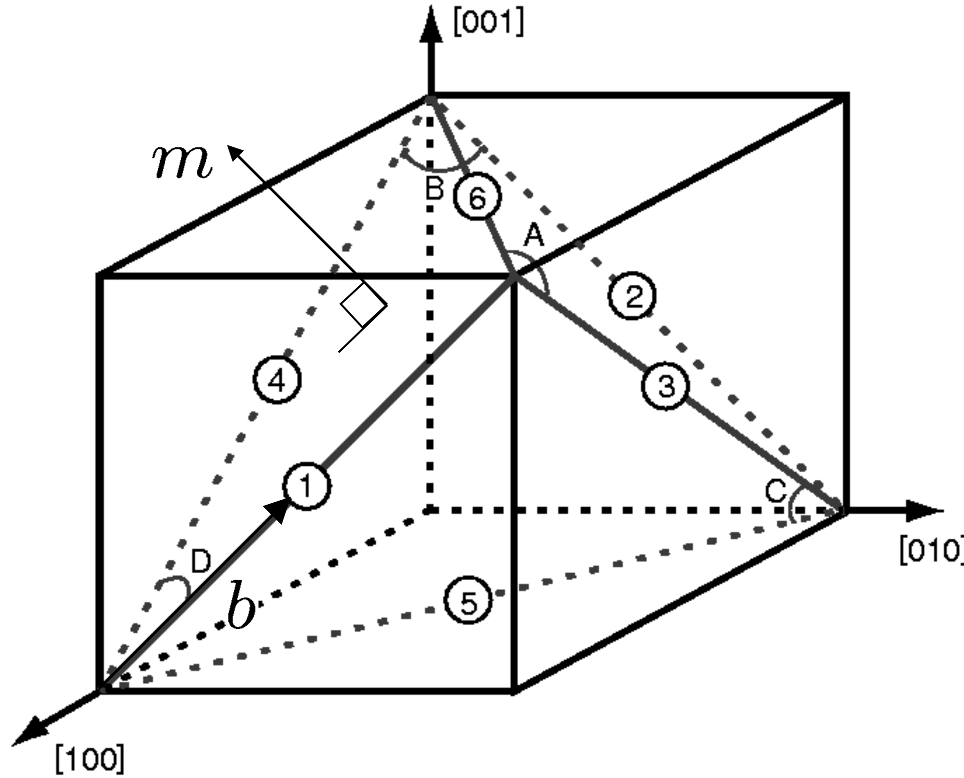
- Multiple Volterra dislocations: $[\![u]\!] \in b\mathbb{Z}$

V. Volterra, *Ann. École Normale Supérieure*, **24** (1907), 401

Dislocation theory – Constrained

- Mobility: $J_u \subset$ {closed-packed planes of lattice}
- Energy: β^p/d = lattice-preserving deformation
- Energy: $[\![u]\!]$ in $\text{span}_{\mathbb{Z}}$({shortest translation vectors of lattice}) $\underbrace{*\varphi_\epsilon}$

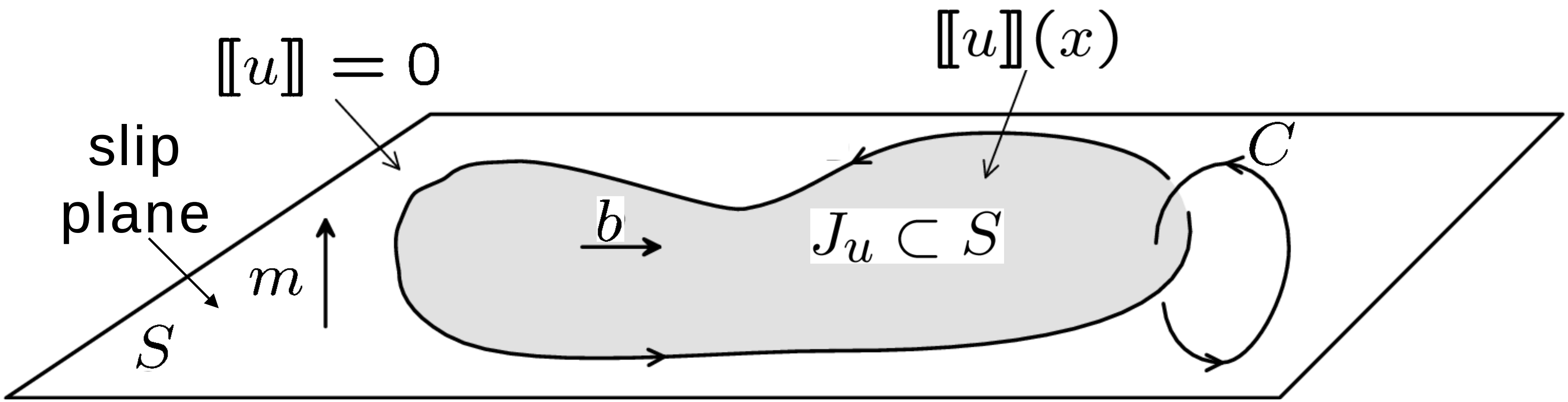
core-cutoff mollifier



The 12 slip systems of fcc crystals (Schmidt and Boas nomenclature)

$$b \in \mathcal{S}(1,1,0), \quad m \in \mathcal{S}(1,1,1)$$

Dislocation theory – Linear elasticity



- Crystallographic slip: $u : \mathbb{R}^3 \to \mathbb{R}^3$ such that

$$Du = \nabla u \mathcal{L}^3 + [\![u]\!] \otimes m \, \mathcal{H}^2 \lfloor J_u \equiv \beta^e + \beta^p$$

- Energy: $E(u) = \int_{\mathbb{R}^3 \setminus J_u} \frac{1}{2} c_{ijkl} \, \epsilon_{ij}(u(x)) \epsilon_{kl}(u(x)) \, dx,$

where: $\epsilon(u) = \frac{1}{2}(\nabla u + \nabla u^T) \equiv$ lattice strain

$c_{ijkl} \equiv$ elastic moduli

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The elastic field of cut surfaces

- **Problem** (*The elastic field of a distribution of cut surfaces*): Let $[\![\boldsymbol{u}]\!]$ be given over S. The problem then is to characterize the elastic field in $\Omega - S$.

- Integral identity: $u_j(\boldsymbol{x}) = \int_\Omega G_{kj}(\boldsymbol{x}, \boldsymbol{x}') f_k(\boldsymbol{x}') dV +$

$$\int_{\partial\Omega} G_{kj}(\boldsymbol{x}, \boldsymbol{x}') t_k(\boldsymbol{x}') dS' + \int_{\partial\Omega} c_{kpim} G_{ij,m}(\boldsymbol{x}, \boldsymbol{x}') u_k(\boldsymbol{x}') n'_p dS'$$

- Consider S as an internal boundary in equilibrium, $[\![t_k]\!] = 0$; recall that $\boldsymbol{\beta}^p = [\![\boldsymbol{u}]\!] \otimes \boldsymbol{m} \delta_S$. Then:

$$u_j(\boldsymbol{x}) = \int_S c_{kpim} G_{ij,m}(\boldsymbol{x}, \boldsymbol{x}') [\![u_k]\!](\boldsymbol{x}') m'_p dS' \Rightarrow$$

$$\boxed{u_j(\boldsymbol{x}) = \int_\Omega c_{kpim} G_{ij,m}(\boldsymbol{x}, \boldsymbol{x}') \beta^p_{kp}(\boldsymbol{x}') dV',} \quad \boldsymbol{x} \in \Omega - S$$

D.J. Bacon, D.M. Barnett and R.O. Scattergood, , *Progress in Materials Science*, **23** (1979), 51-262

The elastic field of cut surfaces

- Elastic distortions:

$$\beta^e_{jn}(\boldsymbol{x}) = \int_\Omega c_{kpim} G_{ij,mn}(\boldsymbol{x}, \boldsymbol{x}') \beta^p_{kp}(\boldsymbol{x}') dV' \quad \boldsymbol{x} \in \Omega - S$$

- Elastic (long-range) stresses: $\sigma_{im}(\boldsymbol{x}) = c_{imjn}\beta^e_{jn}(\boldsymbol{x})$, $\boldsymbol{x} \in \Omega - S$.

- Tractions on S: $t_i = \sigma_{ij} m_j$

- Work/energy identity: $E^{\text{int}} = \frac{1}{2}\int_S t_i [\![u_i]\!] dS \Rightarrow$

$$E^{\text{int}} = \frac{1}{2}\int_S \int_S c_{lqjn} c_{kpim} G_{ij,mn}(\boldsymbol{x}, \boldsymbol{x}') [\![u_k]\!](\boldsymbol{x}) m_p [\![u_l]\!](\boldsymbol{x}') m'_q dS dS'$$

$$\Rightarrow \boxed{E^{\text{int}} = \frac{1}{2}\int_\Omega \int_\Omega c_{lqjn} c_{kpim} G_{ij,mn}(\boldsymbol{x}, \boldsymbol{x}') \beta^p_{kp}(\boldsymbol{x}) \beta^p_{lq}(\boldsymbol{x}') dV dV'}$$

V. Volterra, *Ann. École Normale Supérieure*, **24** (1907), 401

The elastic field of dislocations

- **Problem** (*The elastic field of a distribution of cut surfaces*): Let $[\![\boldsymbol{u}]\!]$ be given over S. The problem then is to determine the elastic distortion field $\boldsymbol{\beta}^e$.

- Mura's formula: Apply Stoke's thm, recall $\boldsymbol{\alpha} = -\boldsymbol{\beta}^p \times \nabla$:

  Then: $$\beta^e_{in}(\boldsymbol{x}) = -e_{npl} c_{lkim} \int_\Omega G_{ij,m}(\boldsymbol{x}, \boldsymbol{x}') \alpha_{kp}(\boldsymbol{x}') dV'$$

  (Mura, 1963); $G(\boldsymbol{x}, \boldsymbol{x}') \equiv$ elastic Green's function.

- Interaction elastic energy: $E^{\text{int}} = \int_\Omega \frac{1}{2} c_{ijkl} \beta^e_{ij} \beta^e_{kl} dV \Rightarrow$

  $$\boxed{E^{\text{int}} = \int_\Omega \int_\Omega \frac{1}{2} A_{marb}(\boldsymbol{x}, \boldsymbol{x}') \alpha_{ma}(\boldsymbol{x}) \alpha_{rb}(\boldsymbol{x}') \, dV \, dV'}$$

  where: $A_{marb}(\boldsymbol{x}, \boldsymbol{x}') =$

  $$\int_\Omega e_{ina} e_{ksb} c_{ijkl} c_{pqmn} c_{uvrs} G_{ip,q}(\boldsymbol{x}, \boldsymbol{x}'') G_{lu,v}(\boldsymbol{x}'', \boldsymbol{x}') dV''$$

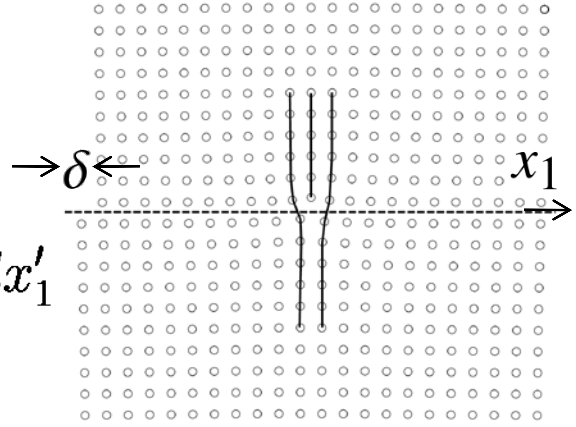
T. Mura, *Phil. Mag.*, **3** (1963) 625

The elastic field of dislocations

- **Problem**: *The core of a straight dislocation.* Single cut-surface spanning the half-plane: $x_3 = 0$, $x_1 < 0$. The dislocation line coincides with the x_2-axis. Burgers vector of the perfect dislocation is $\boldsymbol{b} = b\boldsymbol{s}$, $|\boldsymbol{s}| = 1$.

- Constrained displacement jump: $[\![\boldsymbol{u}]\!] = \delta(x_1)\boldsymbol{s}$. Dislocation density tensor: $\boldsymbol{\alpha} = \delta'(x_1)\boldsymbol{s} \otimes \boldsymbol{e}_3\delta(x_3)$.

- Energy per unit length: $E^{\text{int}} =$

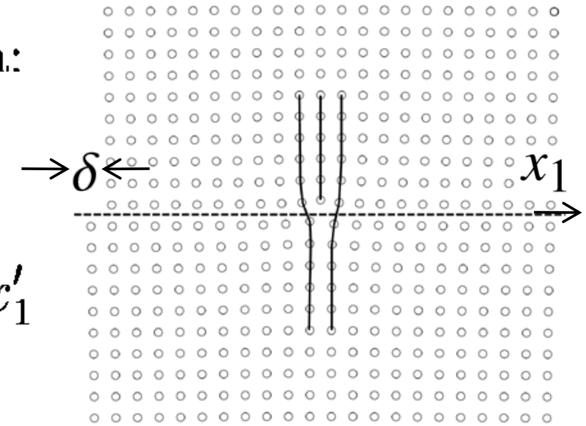


$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{B}{2} \log \frac{R}{|x_1 - x_1'|} \frac{d\delta}{dx_1}(x_1) \frac{d\delta}{dx_1}(x_1') dx_1 dx_1'$$

  where $B = 2K_{kl}s_k s_l$; $\boldsymbol{K}(\boldsymbol{t}, \boldsymbol{m}, \boldsymbol{c}) \equiv$ prelogarithmic tensor of anisotropic elasticity; $R \equiv$ screening length, e. g., dipole distance.

- Volterra dipole: $\delta(x_1) = b$, $x_1 \in (-a, a) \Rightarrow E^{\text{int}} \uparrow +\infty$. Need to model the dislocation core!

The Peierls-Nabarro dislocation core



- Energy per unit length: By Mura's formula:

$$U[\delta] = \int_{-\infty}^{\infty} \Gamma(\delta) dx_1 + \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{B}{2} \log \frac{R}{|x_1 - x_1'|} \frac{d\delta}{dx_1}(x_1) \frac{d\delta}{dx_1}(x_1') dx_1 dx_1'$$

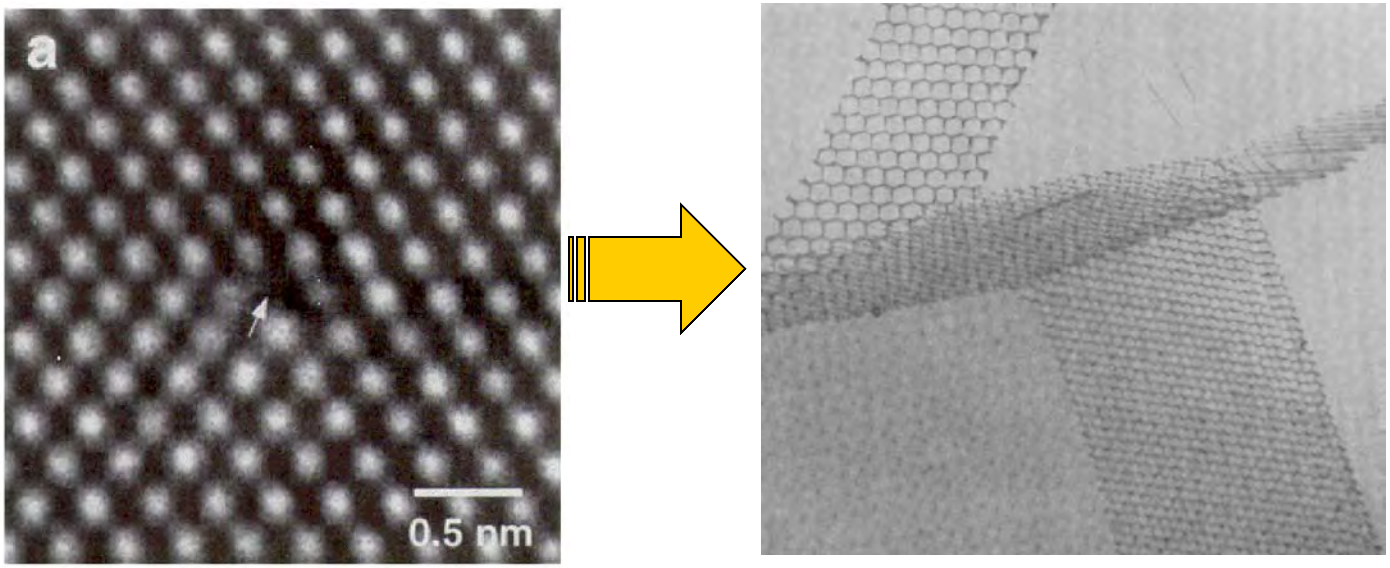
- Nabarro's solution (Nabarro, F. R. N., *Proc. Phys. Soc.*, **59** (1947) p. 256) for Nabarro's sinusoidal potential:

$$\delta(x_1) = \frac{b}{2}\left[1 - \frac{2}{\pi}\arctan\left(\frac{x_1}{c}\right)\right], \quad c = \frac{B}{A}\frac{b^2}{4\pi}$$

- Shear stress: $\tau(x_1) = Bbx_1/(x_1^2 + c^2) \sim 1/x_1$ as $|x_1| \to \infty$.
- $U = U^{\text{int}} + U^{\text{core}} = K_{kl} b_k b_l \log\left(\frac{R}{r_0}\right) + K_{kl} b_k b_l, \quad r_0 = 2c$
- Perfect-dislocation fields approached pointwise as $b/x_1 \to 0$, but U diverges logarithmically in this limit.

The Micro-to-Macro transition

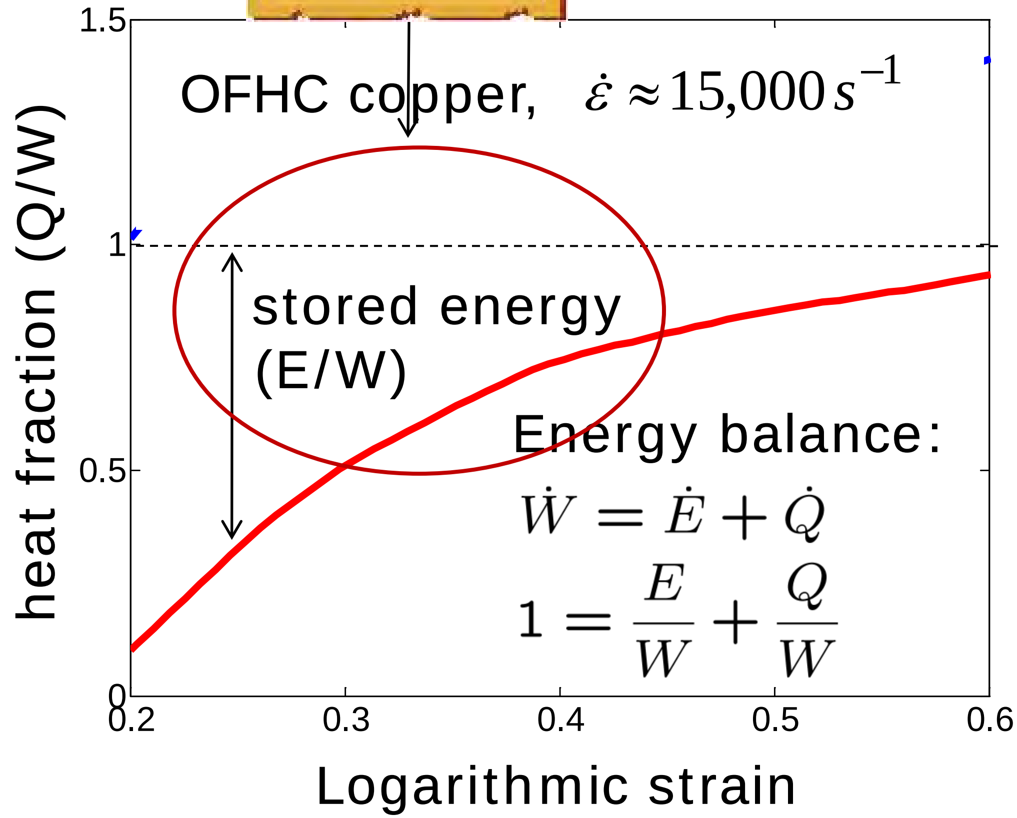
- Formal methods
- Macroscopic plastic deformation
- Macroscopic elastic energy
- Stored energy of plastic work



The Micro-to-Macro transition

- The classical micro-macro ... on
- The dilute limit and disloc... tension

Kolsky pressure bar



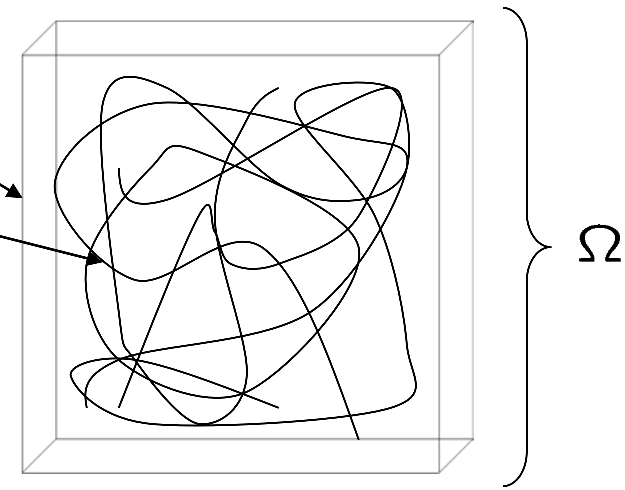
D. Rittel, G. Ravichandran and S. Lee, *Mechanics of Materials*, **34** (2002) 627-642.

The Micro-to-Macro transition

- **Problem**: Consider a crystal occupying a domain Ω. The microscopic plastic distortion field $\boldsymbol{\beta}^p$ is given. The crystal is subjected to affine displacement boundary conditions: $u_i = \bar{\beta}_{ij} x_j$, on $\partial\Omega$. We wish to determine the effective macroscopic behavior of the crystal.

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

β^p, α given!



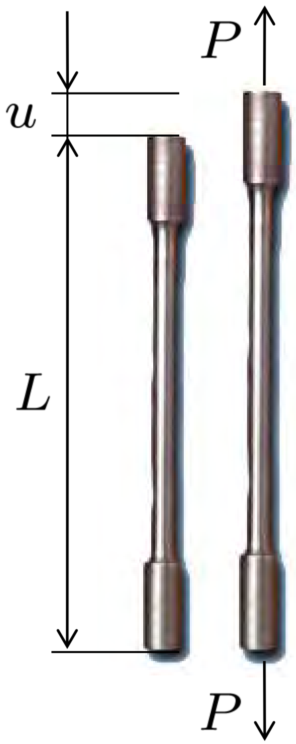
- Total energy of the crystal:

$$E[\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}^p] = \int_\Omega \frac{1}{2} c_{ijkl} \beta^e_{ij} \beta^e_{kl} dV + E^{\rm core}$$

- Let $\bar{\boldsymbol{\beta}}^p \equiv$ macroscopic plastic distortion, be the affine deformation of least energy:

$$E[\bar{\boldsymbol{\beta}}^p, \boldsymbol{\beta}^p] = \min_{\bar{\boldsymbol{\beta}}} E[\bar{\boldsymbol{\beta}}, \boldsymbol{\beta}^p]$$

The Micro-to-Macro transition



- Euler-Lagrange equations

$$\bar{\sigma}_{ij} = \frac{1}{V}\int_\Omega \sigma_{ij} dV \equiv \langle \sigma_{ij} \rangle$$

- This is turn requires:

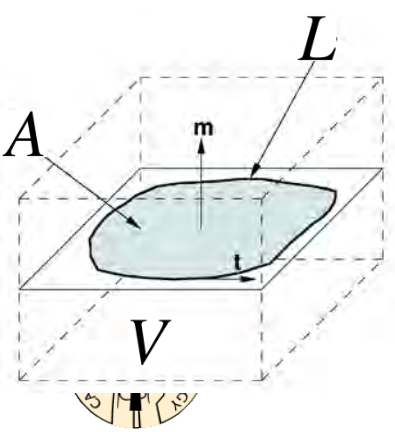
$$\bar{\beta}^p_{ij} = \frac{1}{V}\int_\Omega \beta^p_{ij} dV = \langle \beta^p_{ij} \rangle$$

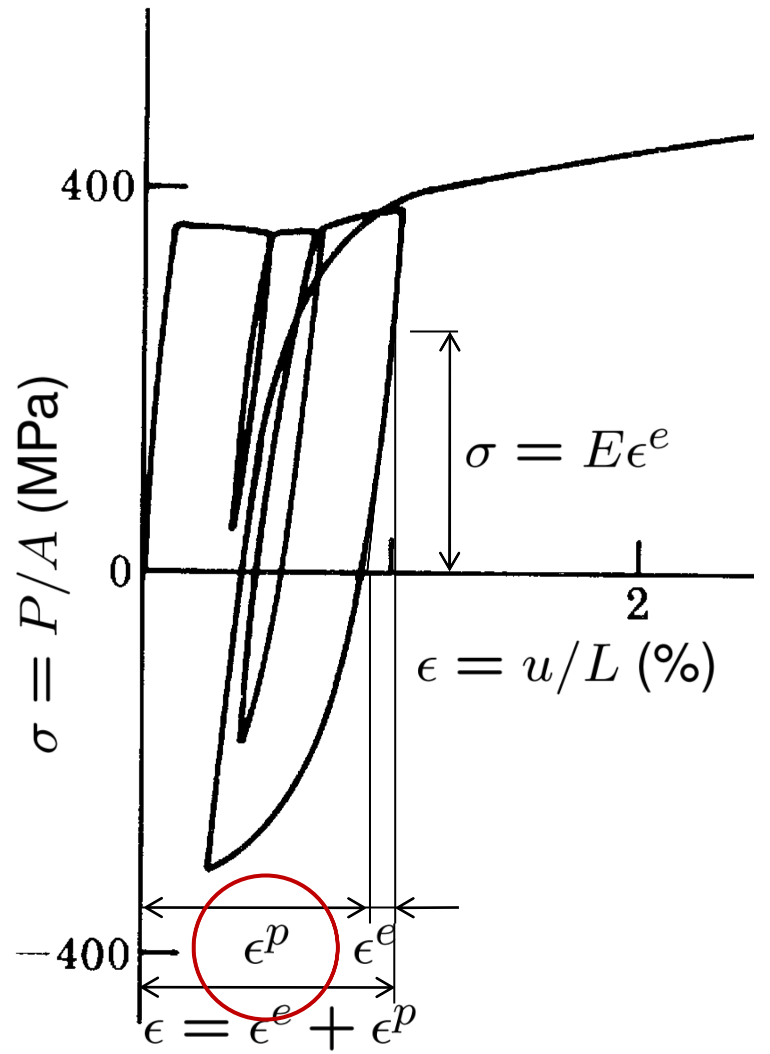
$\equiv$ average plastic distortion

- For Volterra dislocations:

$$\bar{\beta}^p = \frac{bA}{V}$$

$A \equiv$ Total dislocation area





M. Ortiz and E.P. Popov,
Proc. Roy. Soc. Lond. A **379**, 439-458 (1982)

The Micro-to-Macro transition

- Let $\boldsymbol{u}^*$ be the solution corresponding to $\bar{\boldsymbol{\beta}} = \bar{\boldsymbol{\beta}}^p$, i. e., $u_i^* = \bar{\beta}_{ij}^p x_j$ on $\partial\Omega$.

- For arbitrary $\bar{\boldsymbol{\beta}}$ the solution is: $u_i = u_i^* + (\bar{\beta}_{ij} - \bar{\beta}_{ij}^p)x_j$, and the elastic energy follows as:

$$\begin{aligned}
&\int_\Omega \frac{1}{2} c_{ijkl}(u_{i,j} - \beta_{ij}^p)(u_{k,l} - \beta_{kl}^p)dV \\
= &\int_\Omega \frac{1}{2} c_{ijkl}(\beta_{ij}^* + \bar{\beta}_{ij} - \bar{\beta}_{ij}^p - \beta_{ij}^p)(\beta_{kl}^* + \bar{\beta}_{kl} - \bar{\beta}_{kl}^p - \beta_{kl}^p)dV \\
= &\int_\Omega \frac{1}{2} c_{ijkl}(\bar{\beta}_{ij} - \bar{\beta}_{ij}^p)(\bar{\beta}_{kl} - \bar{\beta}_{kl}^p)dV \\
+ &\int_\Omega c_{ijkl}(\bar{\beta}_{ij} - \bar{\beta}_{ij}^p)(\beta_{kl}^* - \beta_{kl}^p)dV \\
+ &\int_\Omega \frac{1}{2} c_{ijkl}(\beta_{ij}^* - \beta_{ij}^p)(\beta_{kl}^* - \beta_{kl}^p)dV
\end{aligned}$$

The Micro-to-Macro transition

- Let $\bar{\boldsymbol{\beta}}^e \equiv \bar{\boldsymbol{\beta}} - \bar{\boldsymbol{\beta}}^p \equiv$ macroscopic elastic distortion. Then:

$$E = \frac{V}{2} c_{ijkl} \bar{\beta}^e_{ij} \bar{\beta}^e_{kl} + \int_\Omega \frac{1}{2} c_{ijkl} (\beta^*_{ij} - \beta^p_{ij})(\beta^*_{kl} - \beta^p_{kl}) dV + E^{\text{core}}$$

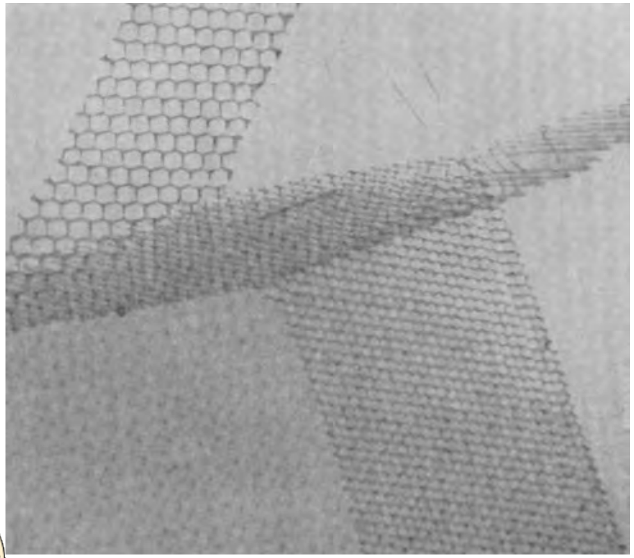
- Strain-energy density: $\bar{W} \equiv E/V$. Then $\boxed{\bar{W} = \bar{W}^e + \bar{W}^p}$,

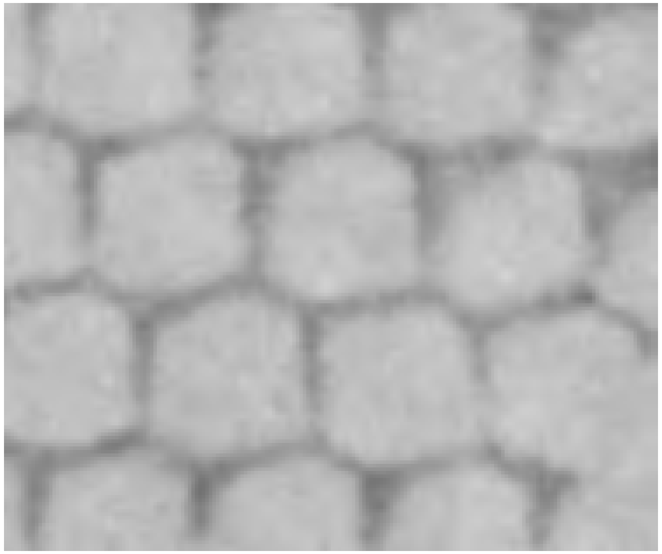
$$\begin{aligned}
\bar{W}^e &= \bar{W}^e(\bar{\boldsymbol{\beta}}^e) = \frac{1}{2} c_{ijkl} \bar{\beta}^e_{ij} \bar{\beta}^e_{kl} \quad \equiv \text{elastic energy density} \\
\bar{W}^p &= \bar{W}^p[\boldsymbol{\beta}^p] = \bar{W}^p[\boldsymbol{\alpha}] \\
&= \frac{1}{V} \left\{ \int_\Omega \frac{1}{2} c_{ijkl} (\beta^*_{ij} - \beta^p_{ij})(\beta^*_{kl} - \beta^p_{kl}) dV + E^{\text{core}} \right\} \\
&\equiv \text{stored energy density, } \underline{\text{independent of } \bar{\boldsymbol{\beta}}}
\end{aligned}$$

- $\bar{W}^p$ cannot be expressed in closed form for general distributions of disocations $\Rightarrow$ Need to *model* $\bar{W}^p$ at the macroscopic level.

Summary – Outlook

- A number of useful identities can be obtained from linear elasticity and formal methods:
  - *Elastic-plastic decomposition of macroscopic strain*
  - *Relation between macro and micro plastic strains*
  - *Additive decomposition of macroscopic energy*
  - *Dependence of stored energy on dislocation density*
- Beyond formal methods? The dilute limit!





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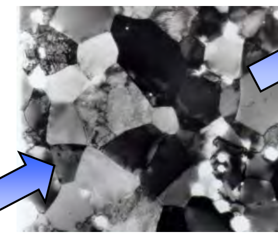
Metal plasticity – Multiscale analysis

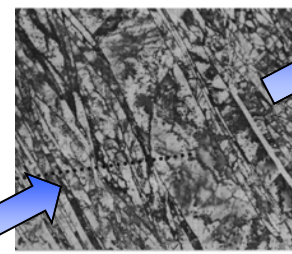
Objective: Derive *ansatz*-free, physics-based, predictive models of macroscopic behavior

time: ns, μs, ms

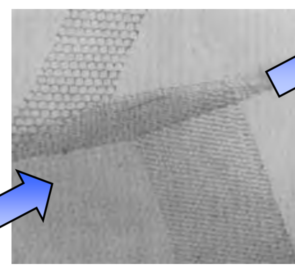
Engineering applications



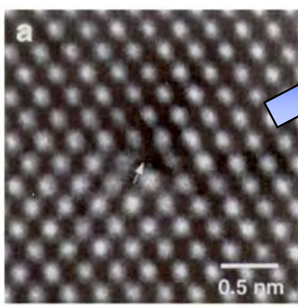
Polycrystals



Subgrain structures ← **Lecture #4**: Subgrain dislocation structures



Dislocation dynamics ← **Lecture #3**: Dislocation kinetics, the forest-hardening model



Lattice defects, EoS ← **Lecture #2**: Dislocation energies, the line-tension approximation

length: nm, μm, mm

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