Multiscale modeling of materials: (1) Dislocation structures → polycrystals

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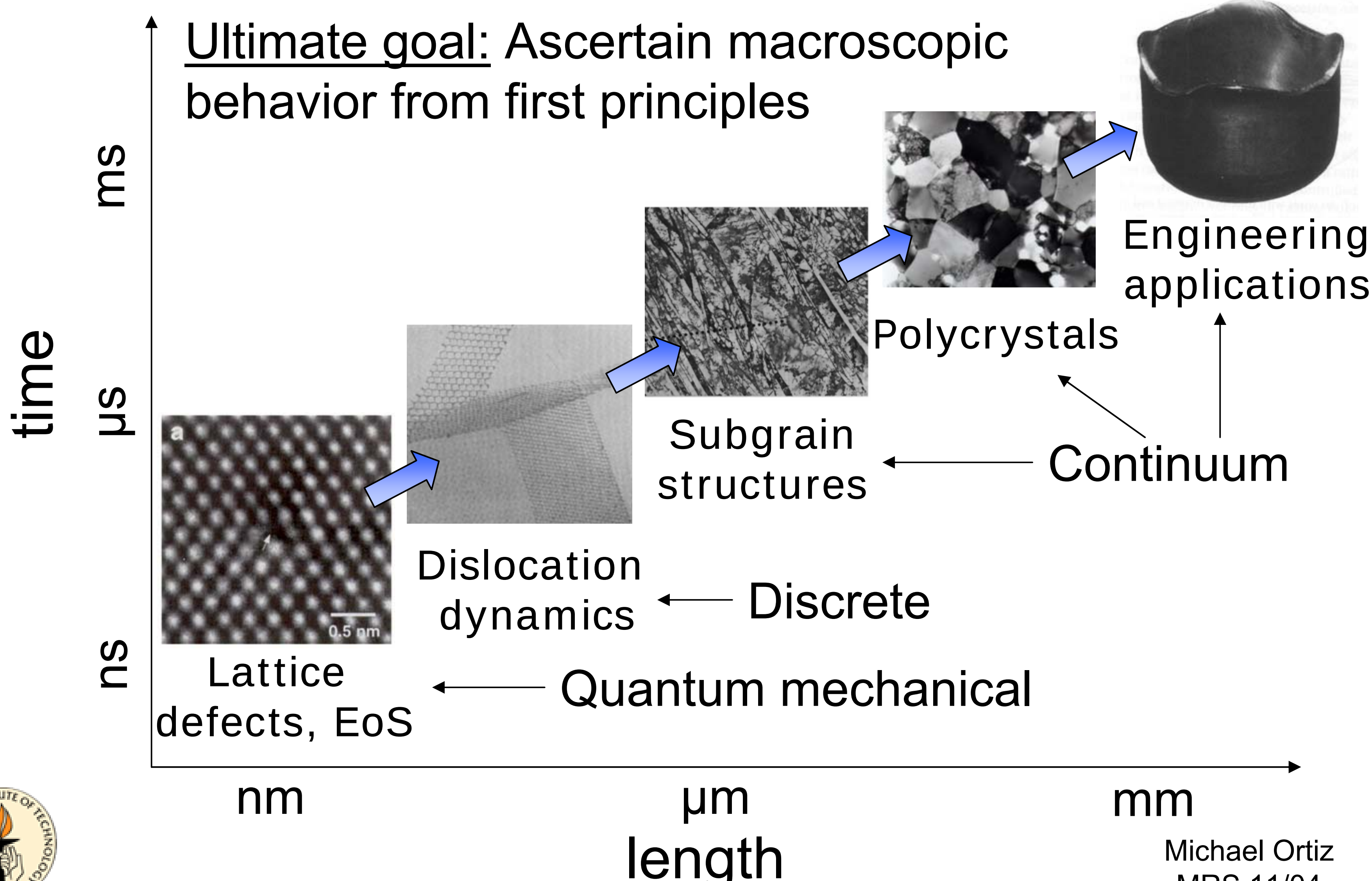
Metal plasticity – Multiscale hierarchy

Ultimate goal: Ascertain macroscopic behavior from first principles



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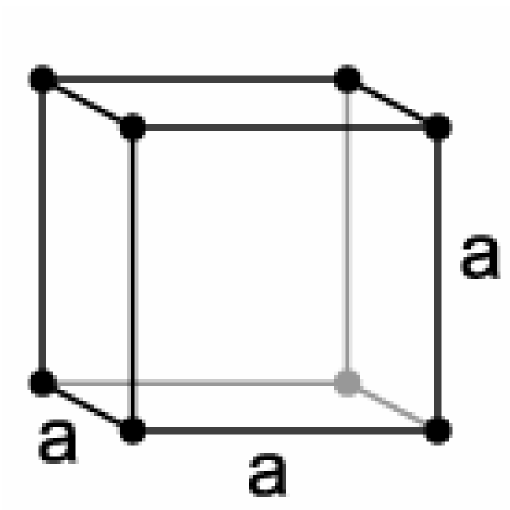
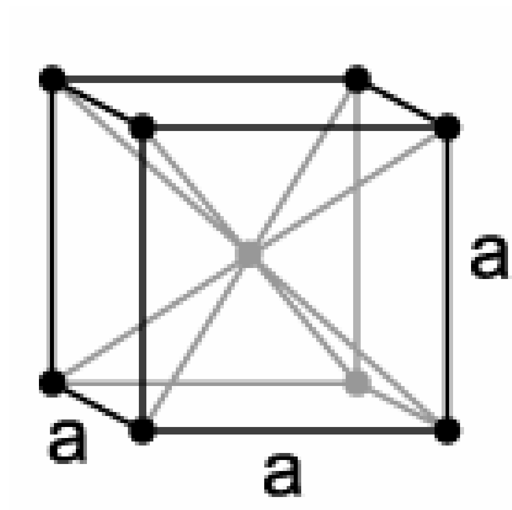
Classical view of crystal lattices

- Crystal lattice $\equiv$ discrete subgroup of $\mathbb{R}^n$,

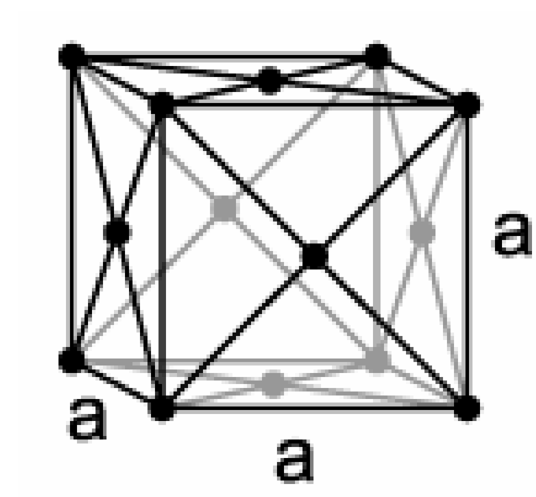
$$L = \{x(l) = l^i a_i,\ l \in \mathbb{Z}^n\}$$



Simple cubic (SC)



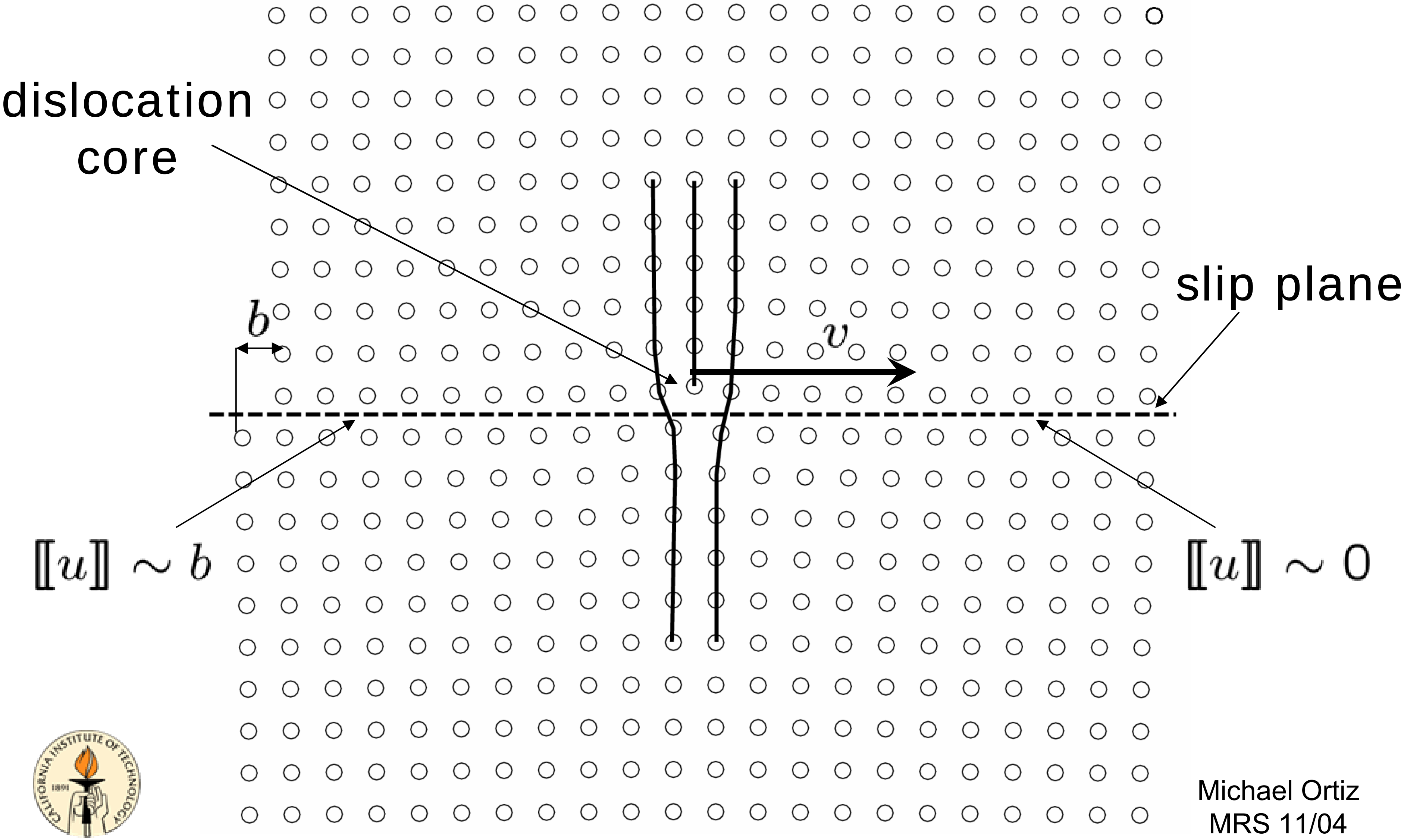
Body-centered cubic (BCC)



Face-centered cubic (FCC)

- Energy invariant under the action of $gl(3)$: massive lack of convexity!

Straight dislocations: 2D view



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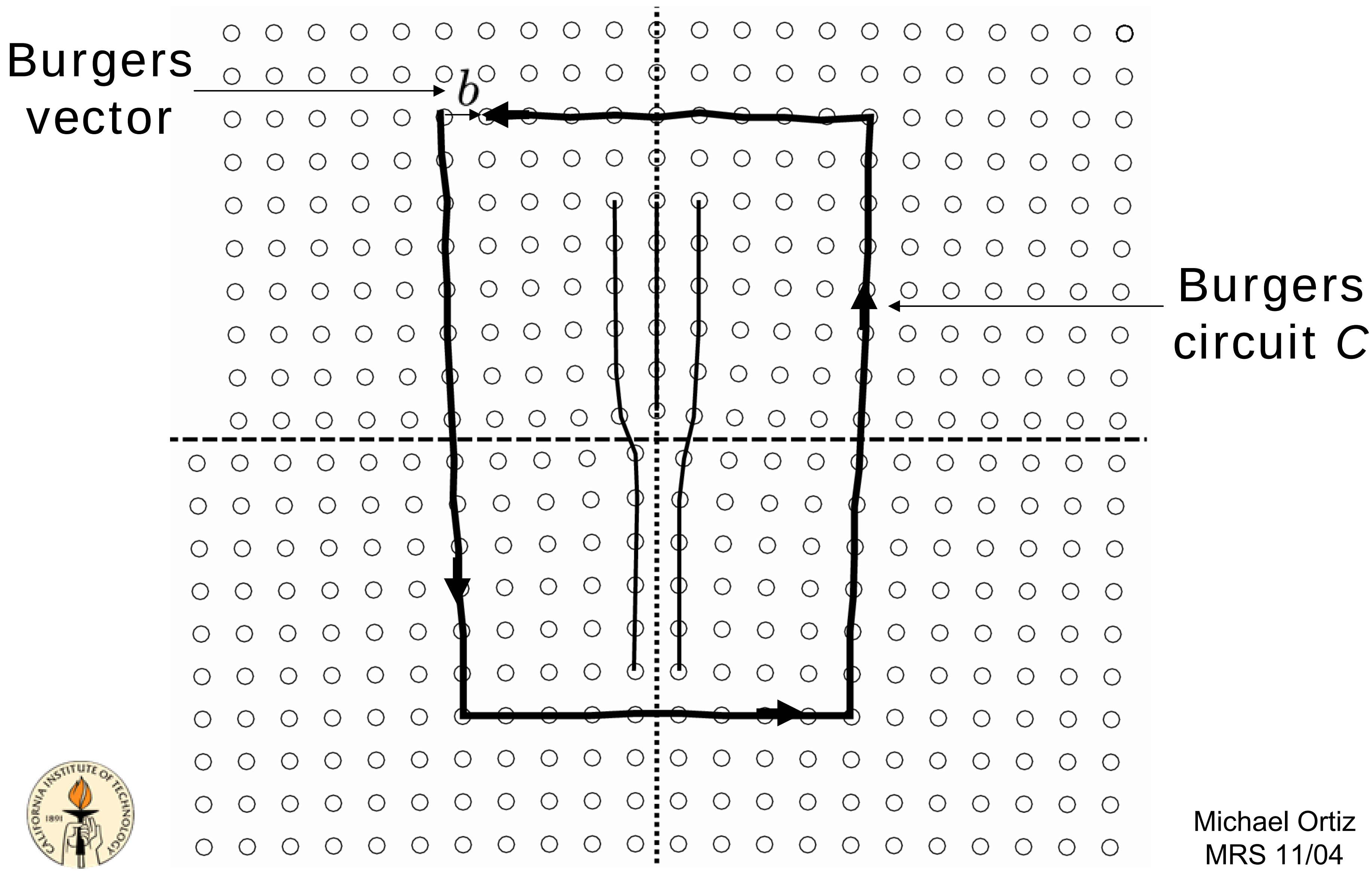
Straight dislocations: 2D view



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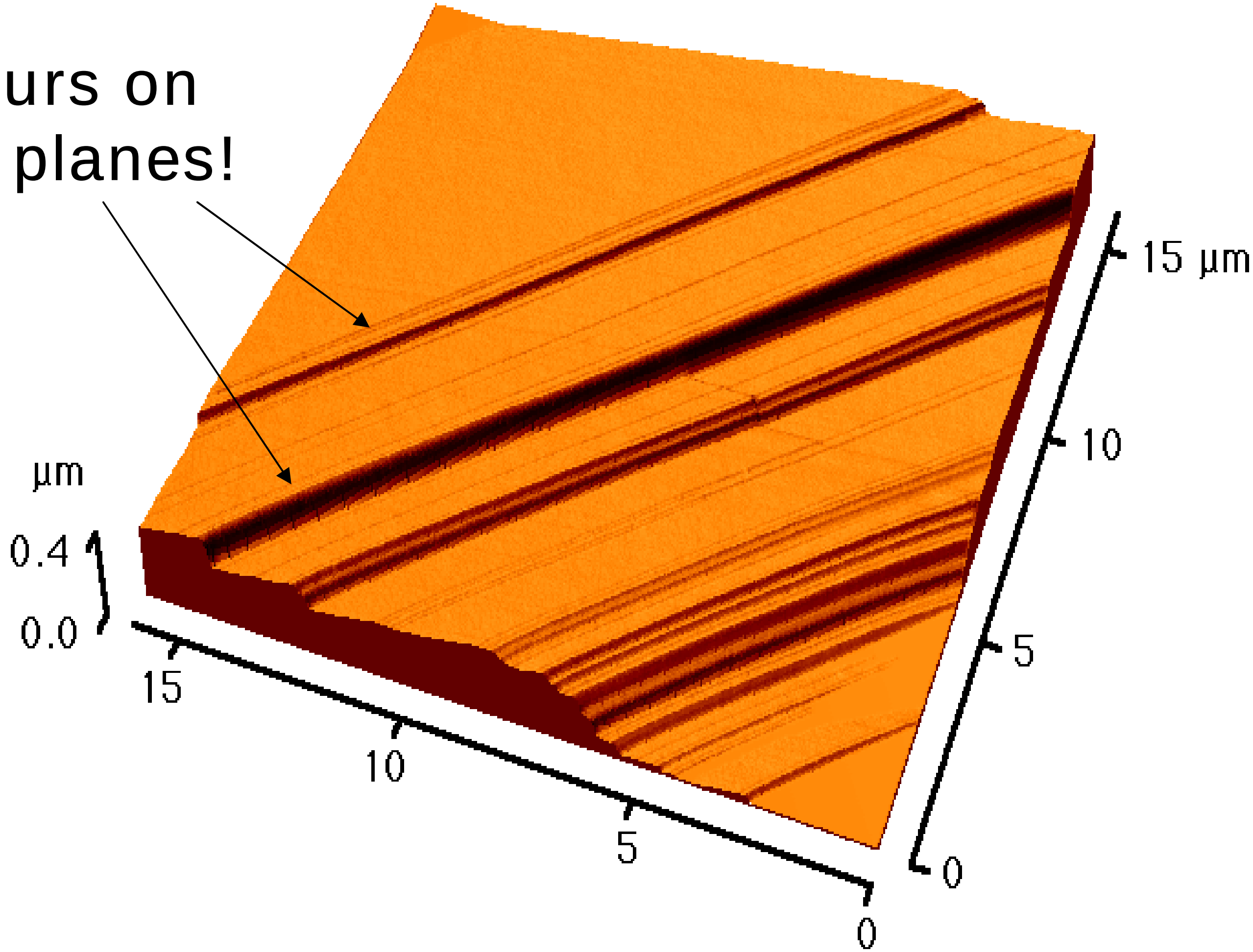
Discreteness of crystallographic slip

Slip occurs on discrete planes!



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

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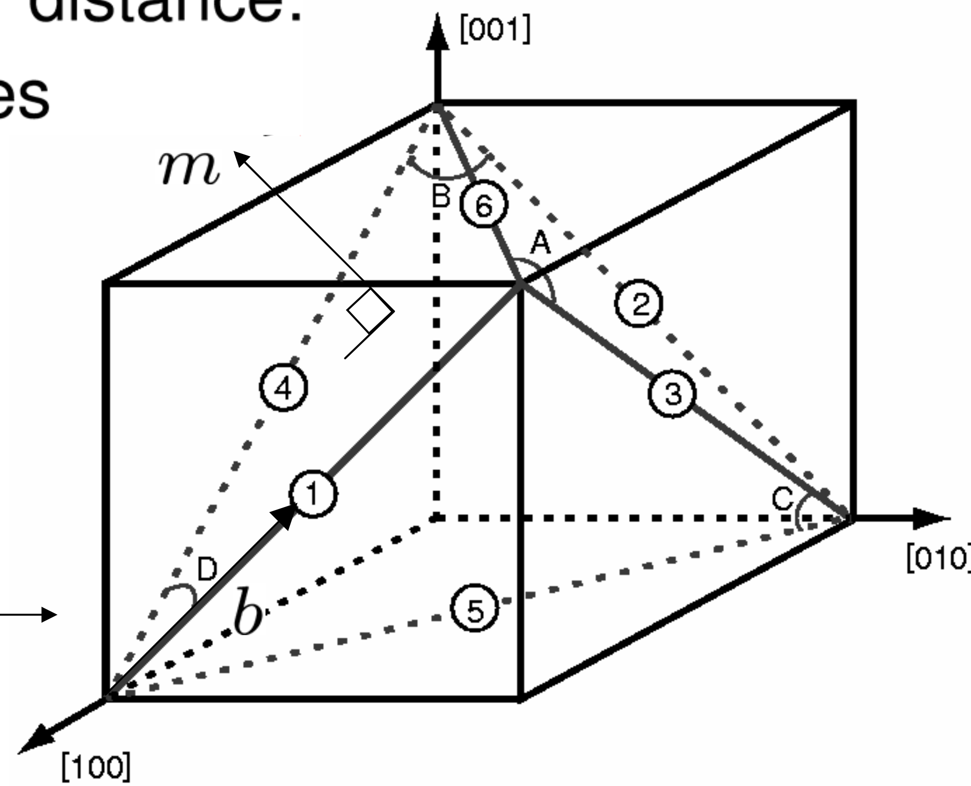
Dislocations and crystallography

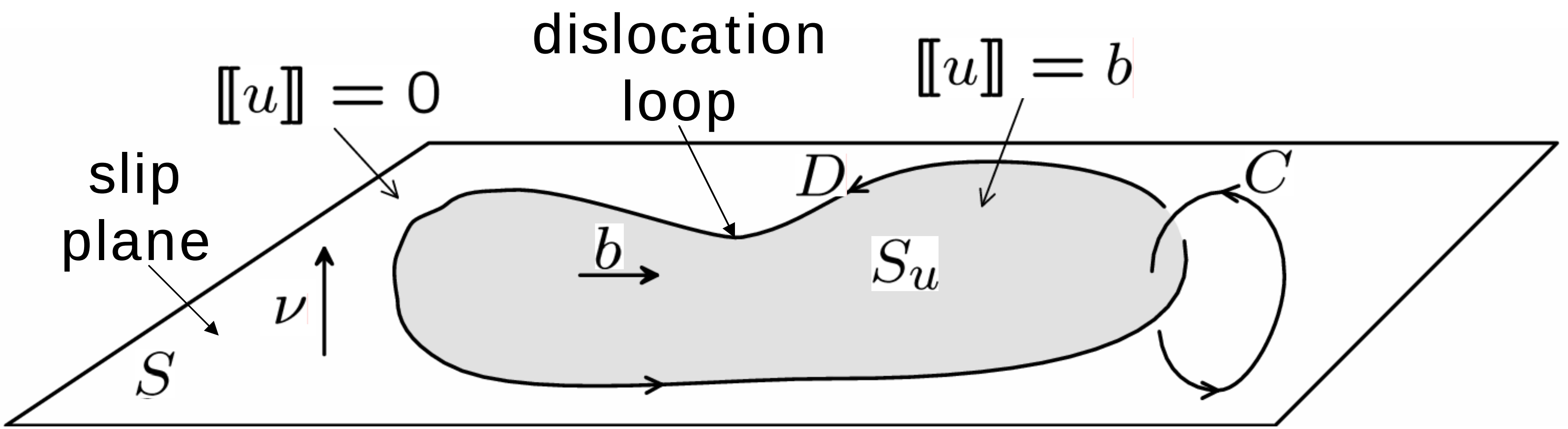
- Preferred slip systems:
  - i) Minimize Burgers vector: Smallest translation vector of lattice
  - ii) Maximize interplanar distance: Closed-packed planes

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

$$\left.\begin{array}{l} b \in \mathcal{S}(1,1,0) \\ m \in \mathcal{S}(1,1,1) \end{array}\right\} \longrightarrow$$



General linear elastic dislocations



- Volterra dislocation: $u \in SBV$ such that

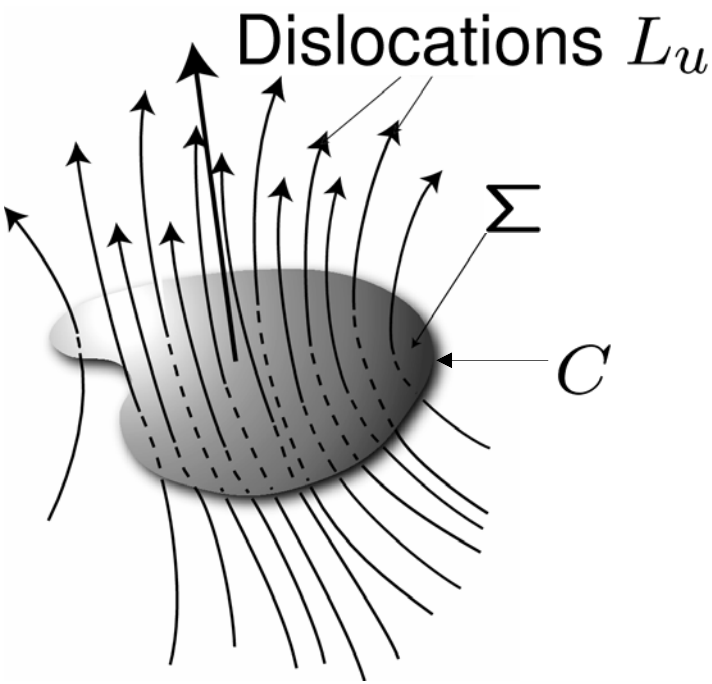
$$Du = \nabla u \, \mathcal{L}^3 + b \otimes \nu \, \mathcal{H}^2 \llcorner S_u \equiv \beta^e \, \mathcal{L}^3 + \beta^p \, \mathcal{H}^2 \llcorner S_u$$

elastic deformation (β^e)

plastic deformation (β^p)

- Burgers circuit test: $\int_C \beta^e \, dx = -\text{Link}(C, D) \, b$

Dislocation field theory



- Total Burgers vector across Σ:

$$b(\Sigma) = \oint_C \beta^e \, dx$$

- Dislocation density (Nye 1953):

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

- Kröner's (1958) formula: $\alpha = -\mathsf{curl}\beta^e = \mathsf{curl}\beta^p$
- Conservation of Burgers vector: $\mathsf{div}\alpha = 0$
- Dislocation measure: $\mu = \alpha \, \mathcal{H}^1 \llcorner L_u$

General dislocations − Energy

- Mura's theorem: $E = E(\alpha)$
- Stored energy:

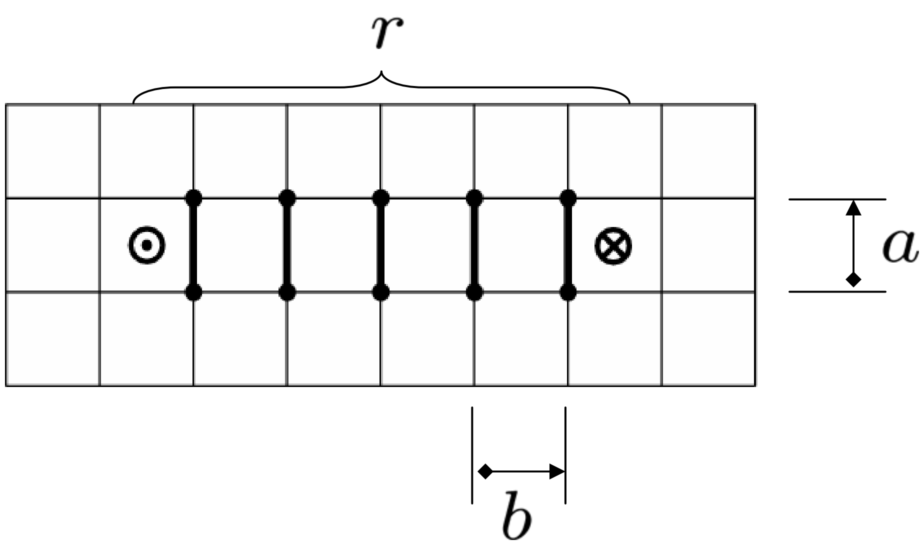
$$E(\alpha) = \int\int \mathrm{tr}[\alpha^T(x)\Gamma(x,y)\alpha(y)]\,dx\,dy$$

where: $\Gamma(x,y) =$

$$\int [\nabla G(x,z) \cdot \nabla G(y,z)\, I - \nabla G(x,z) \otimes \nabla G(x,z)]\, dz$$

and: $G = \Delta^{-1} \equiv$ Green's function of the Laplacian.

Straight dislocations – Energy



Screw dipole of size *r* in square lattice, applied stress τ

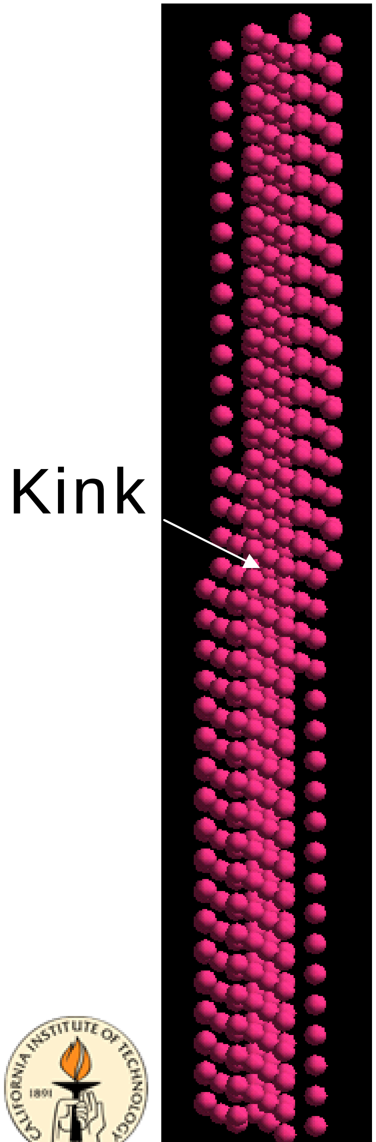
- Dipole energy, continuum limit:

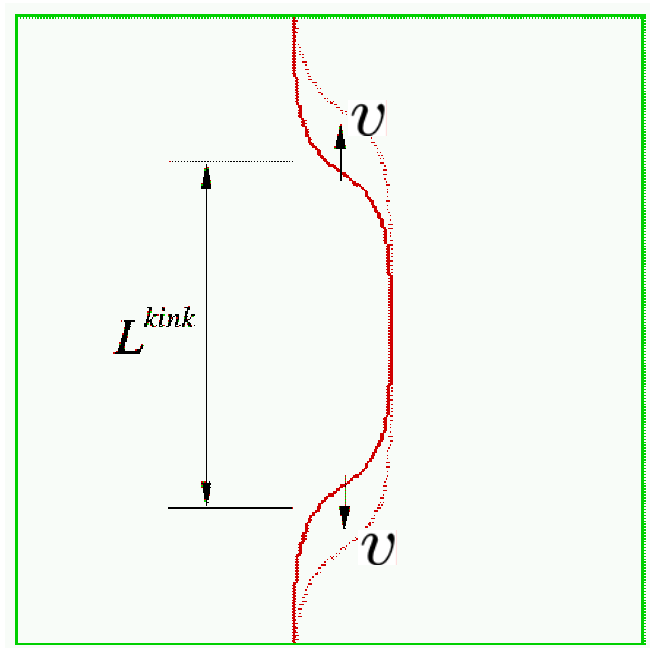
$$\frac{E}{L} \sim \frac{Gb^2}{2\pi} \log \frac{r}{r_0} + b\tau r$$

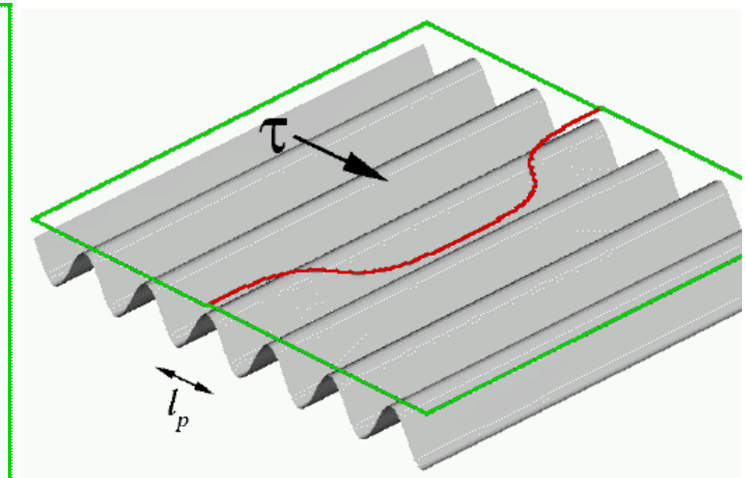
logarithmic divergence!

- Core cutoff radius: $r_0 = \frac{a}{\sqrt{8}e^{\gamma}} \approx 0.198506\, a$

Straight dislocations – Mobility







- Peierls stress τ_0: Threshold stress for dislocation motion
- Dissipation $= \tau_0 \times$ (slipped area)

lattice friction

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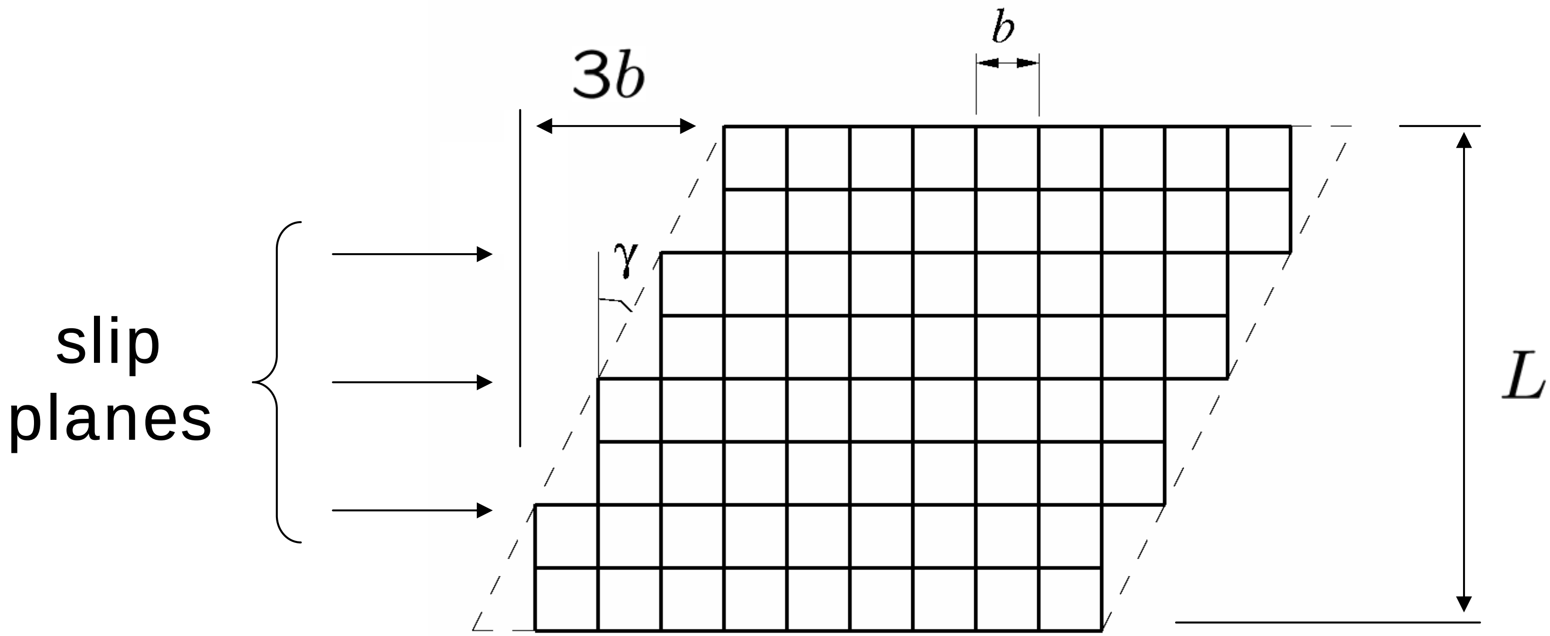
Dislocation transport and plasticity



- Plastic deformation resulting from the motion of three straight edge dislocations across crystal:

$$\gamma = \frac{3b}{L} = \frac{b3L}{L^2}L = |\alpha|\, L$$

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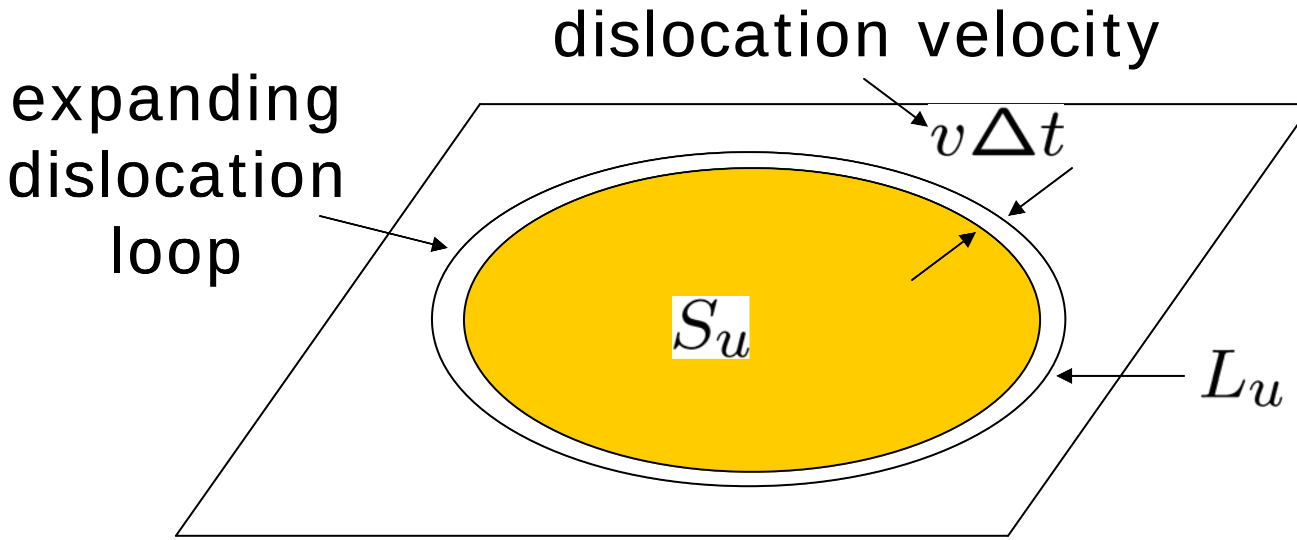
Dislocation transport and plasticity



- Dislocation transport and plastic deformation rate:

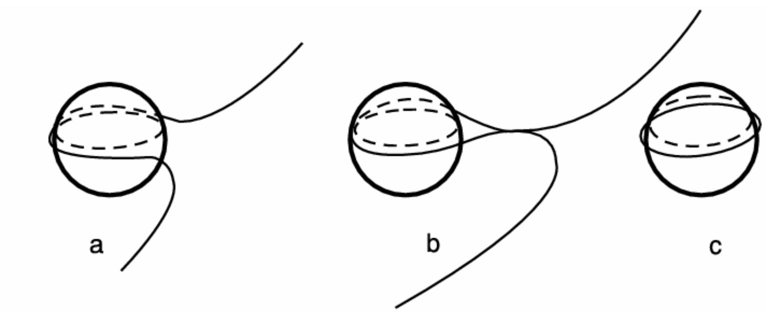
$$\frac{d}{dt}\beta^p\,\mathcal{H}^2 \llcorner S_u = v\,\alpha\,\mathcal{H}^1 \llcorner L_u$$

- Incremental transport problem: For $n = 0, 1, \ldots,$

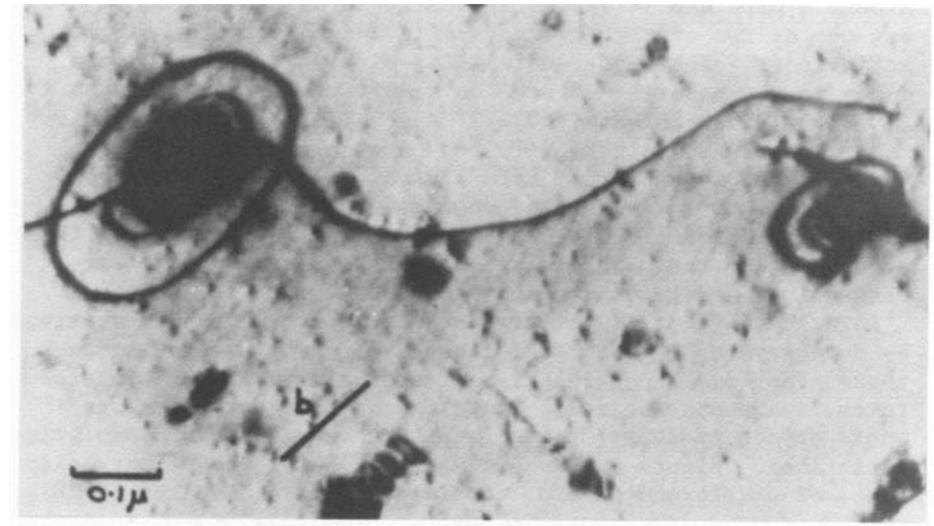
$$\inf_{\mu_{n+1}} \{\, ||\mu_{n+1} - \mu_n|| + E(\mu_{n+1}, t_{n+1})\,\}$$

Obstacles – Topological obstructions

- Example: Precipitates.

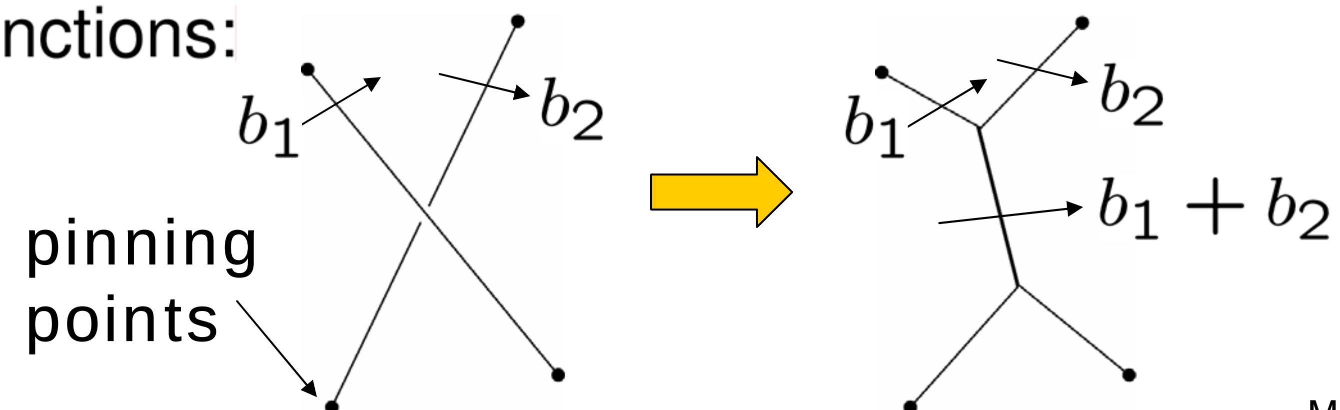


Impenetrable obstacles



(Humphreys and Hirsch ’70)

- Junctions:



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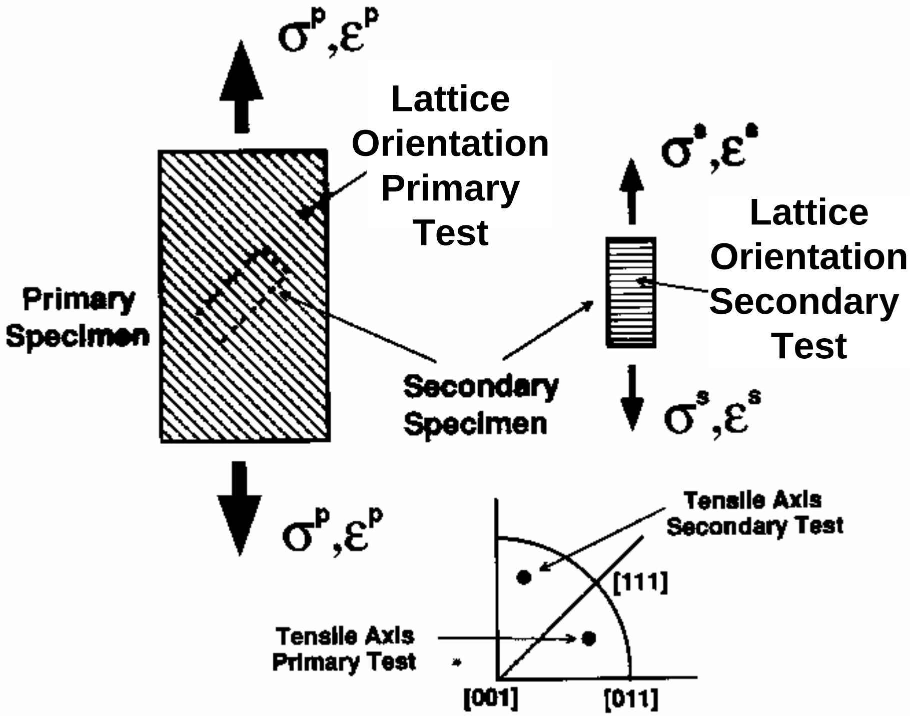
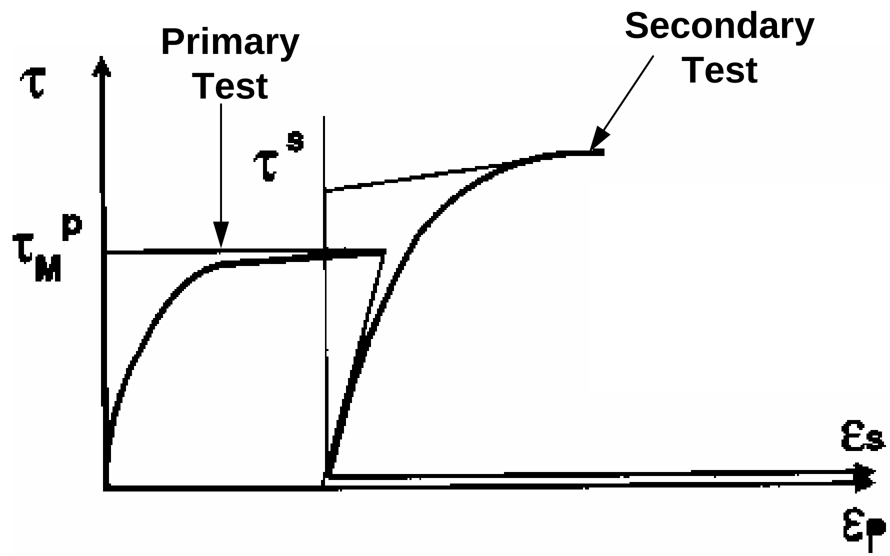
Junctions − Strong latent hardening

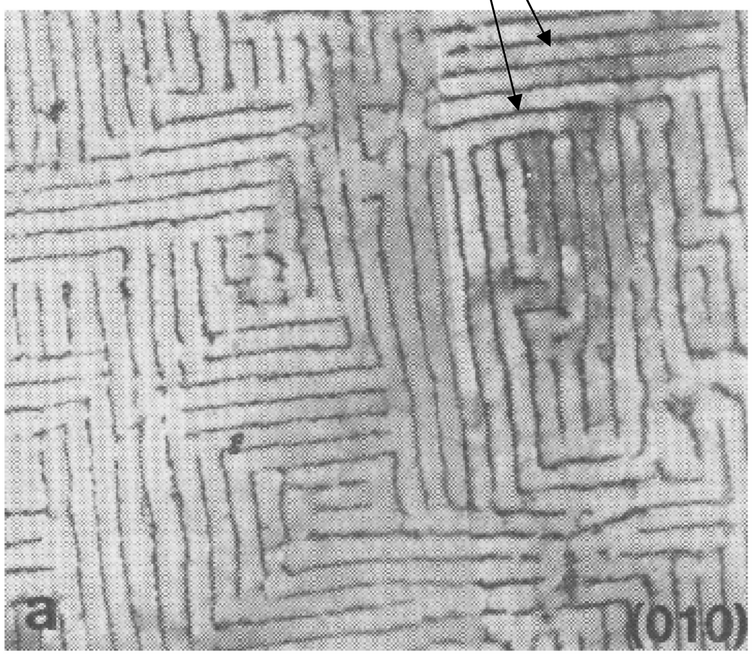




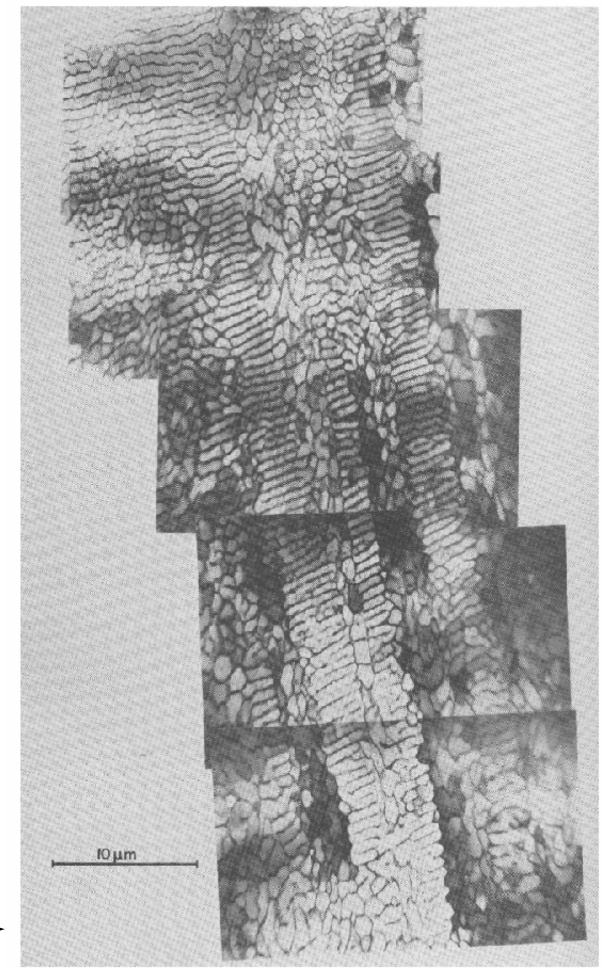
- Latent hardening: Metals much 'prefer' to activate a single slip system at each material point, though the active system may vary from point to point.

Dislocation structures - Fatigue

Dipolar dislocation walls



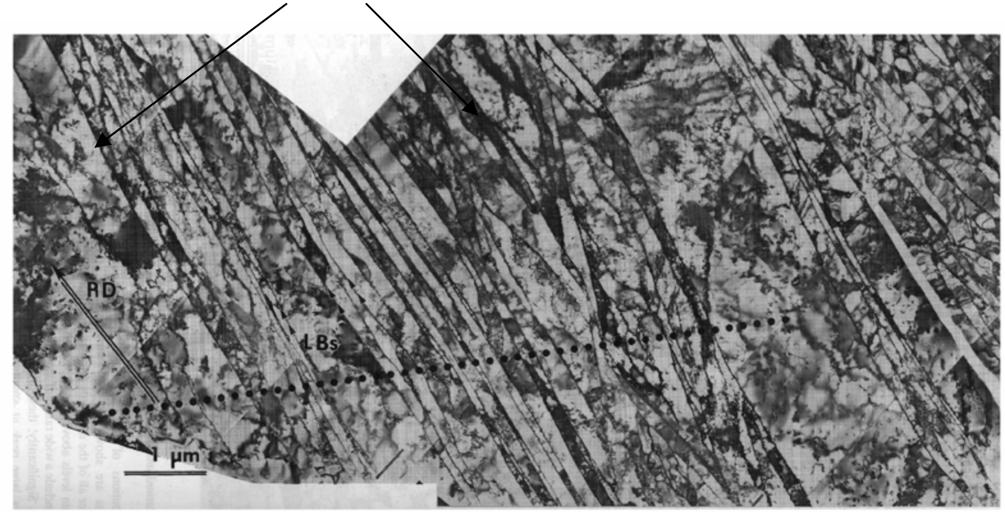
Labyrinth structure in fatigued copper single crystal
(Jin and Winter ´84)



Nested bands in copper single crystal fatigued to saturation
(Ramussen and Pedersen ´80)

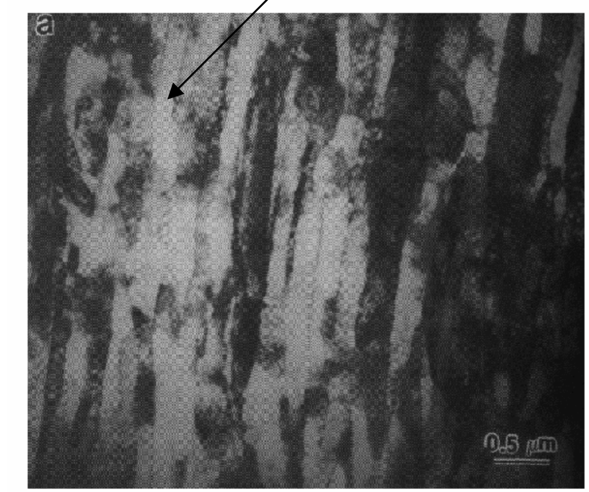
Dislocation lamellar structures

Dislocation walls



Lamellar dislocation structure
in 90% cold-rolled Ta
(DA Hughes and N Hansen, Acta Materialia,
44 (1) 1997, pp. 105-112)

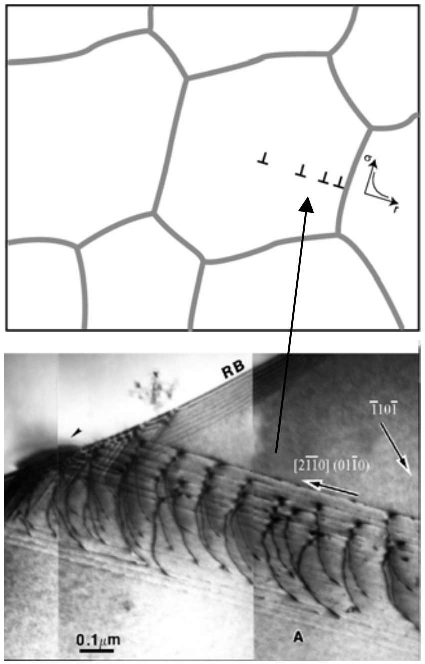
Dislocation walls



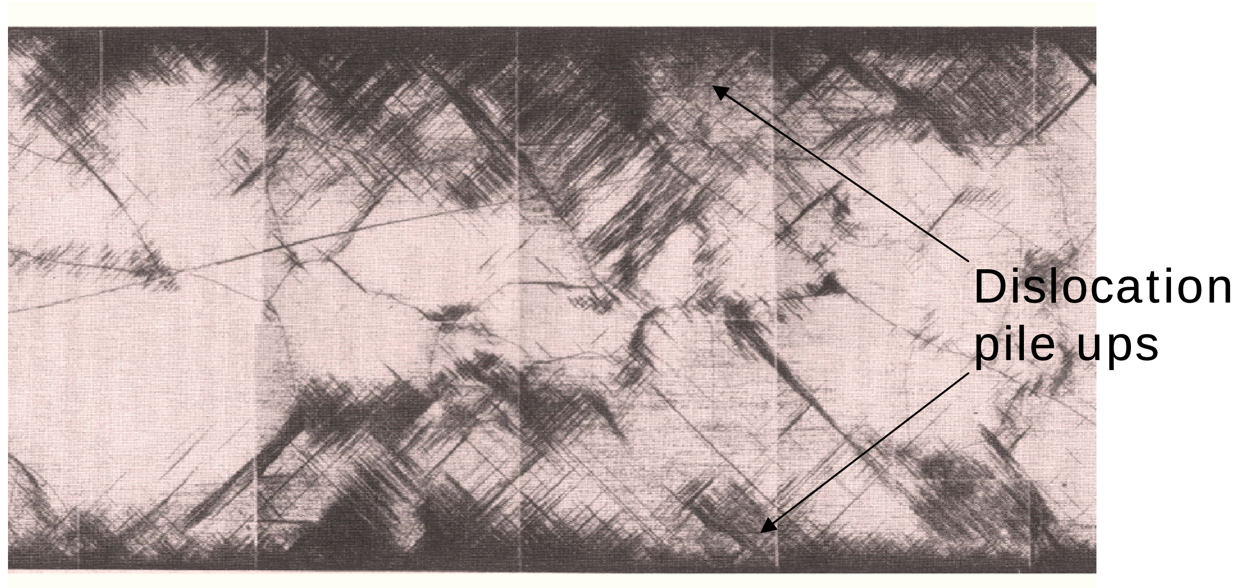
Lamellar structure
in shocked Ta
(MA Meyers et al.,
Metall. Mater. Trans.,
26 (10) 1995, pp. 2493-2501)

Lamellar dislocation structures at large strains

Dislocation structures – Pile-ups



Dislocation pile-up
at Ti grain boundary
(I. Robertson)



LiF plate impact experiment.
Dislocation pile-ups at surfaces
and grain boundaries
(G Meir and RJ Clifton, J. Appl. Phys.,
59 (1) 1986, pp. 124-148)

Effect of grain boundaries, surfaces

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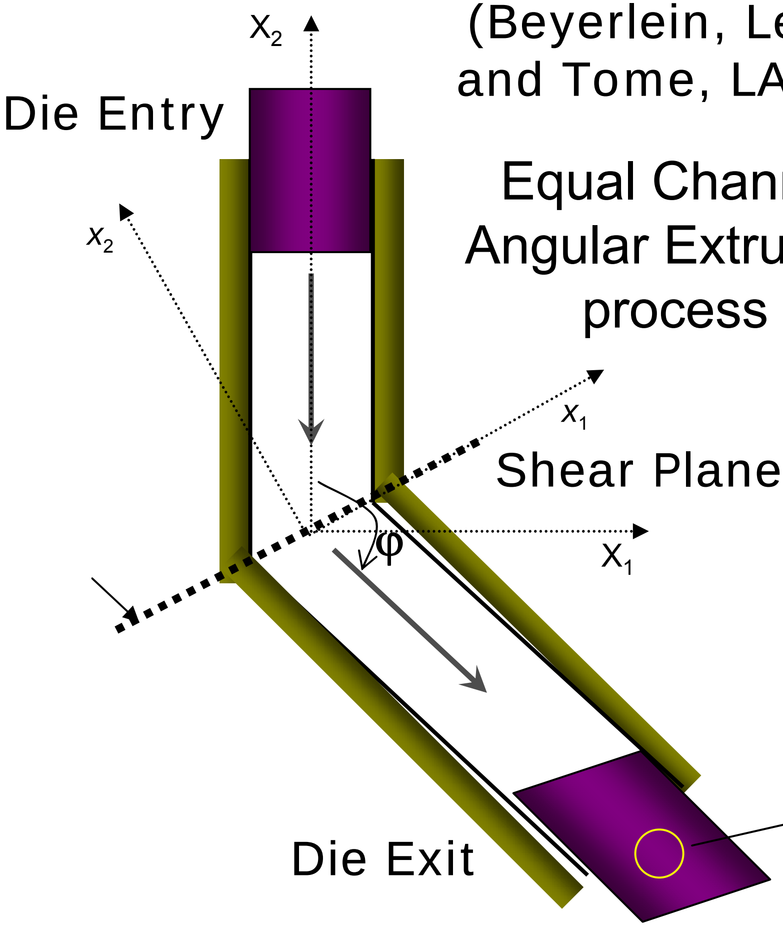
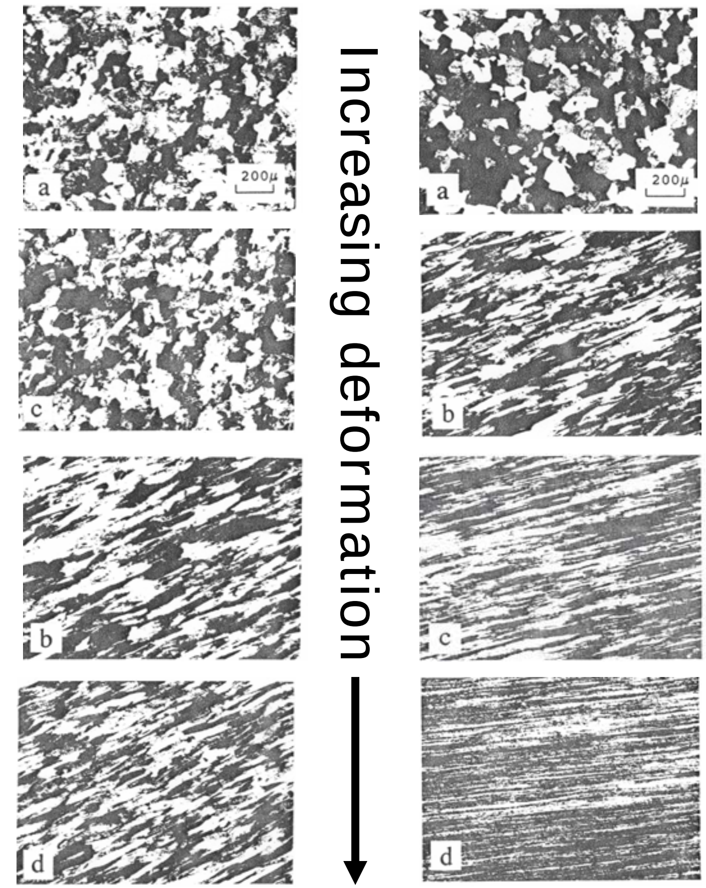
Dislocation structures – Effect of strain

(Beyerlein, Lebensohn and Tome, LANL, 2003)

Equal Channel Angular Extrusion process

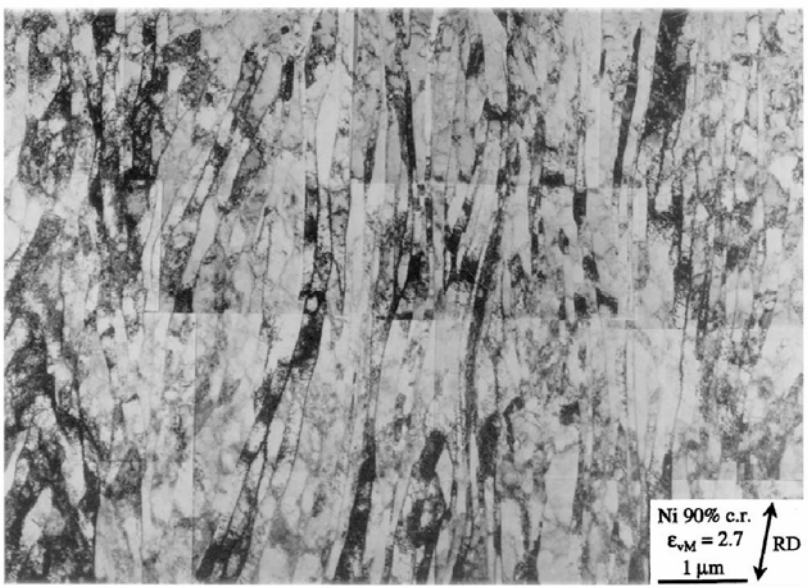




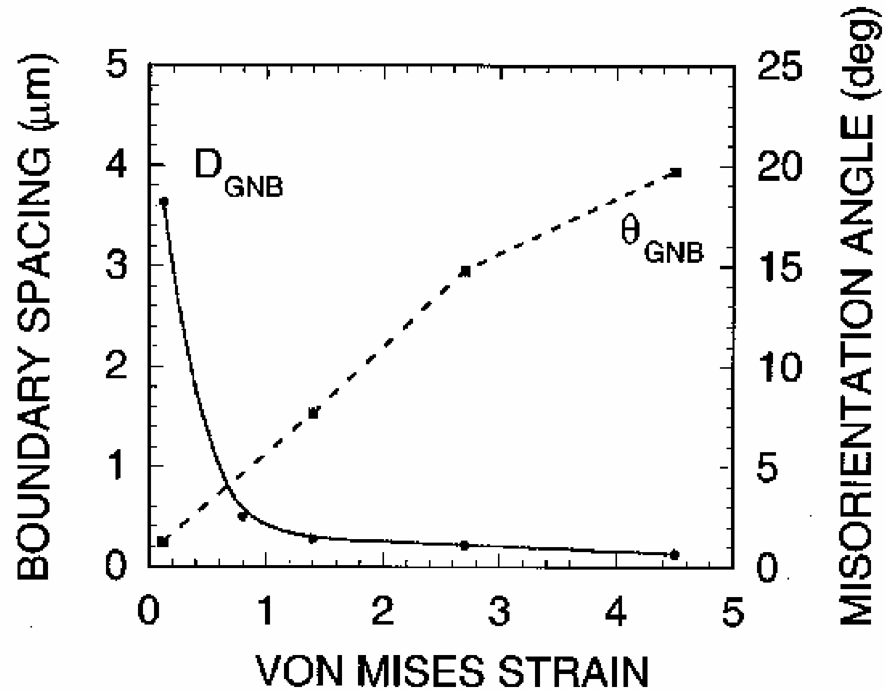
Route C   Route A

Evolution of dislocation structures in Cu specimen. Lamellar width: $l \sim \gamma^{-0.65}$

Dislocation structures – Scaling laws



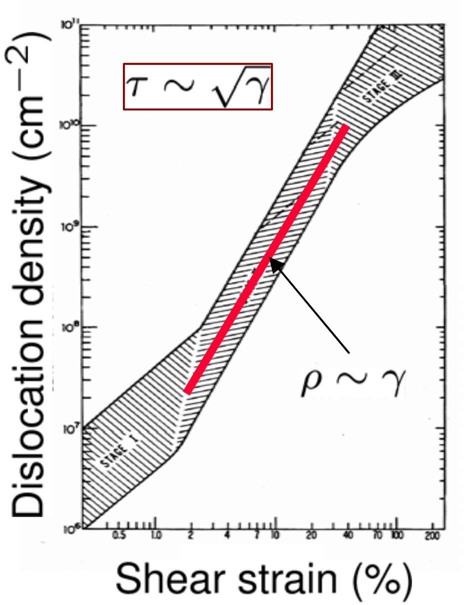
Pure nickel cold rolled to 90%
Hansen *et al.* Mat. Sci. Engin. A317 (2001).



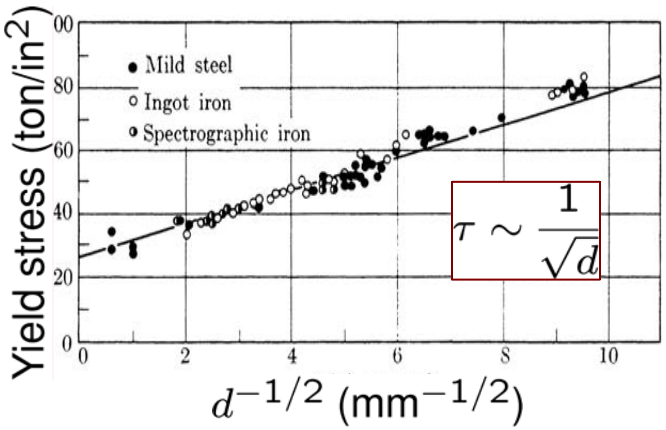
Lamellar width and misorientation angle as a function of deformatation
Hansen *et al.* Mat. Sci. Engin. A317 (2001).

Scaling of lamellar width and misorientation angle with deformation

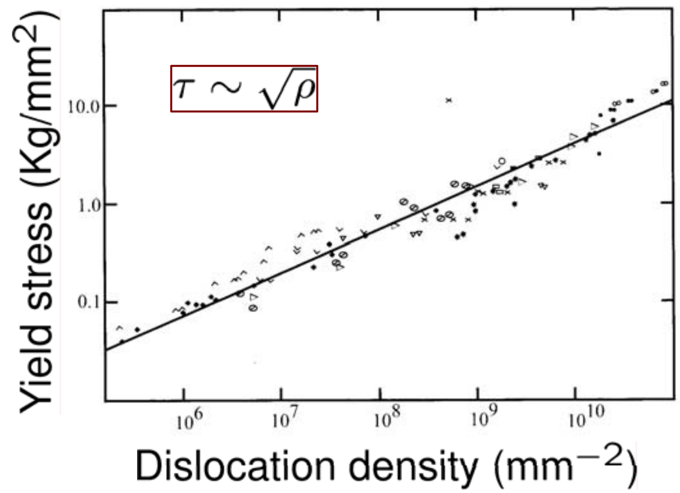
Dislocation structures – Scaling laws



Taylor hardening
(RJ Asaro,
Adv. Appl. Mech.,
23, 1983, p. 1.)



Hall-Petch scaling
(NJ Petch,
J. Iron and Steel Inst.,
174, 1953, pp. 25-28.)



Taylor scaling
(SJ Basinski and ZS Basinski,
Dislocations in Solids,
FRN Nabarro (ed.)
North-Holland, 1979.)

Classical scaling laws of crystal plasticity

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