Multiscale models of metal plasticity
Part II: Crystal plasticity to subgrain microstructures

M. Ortiz
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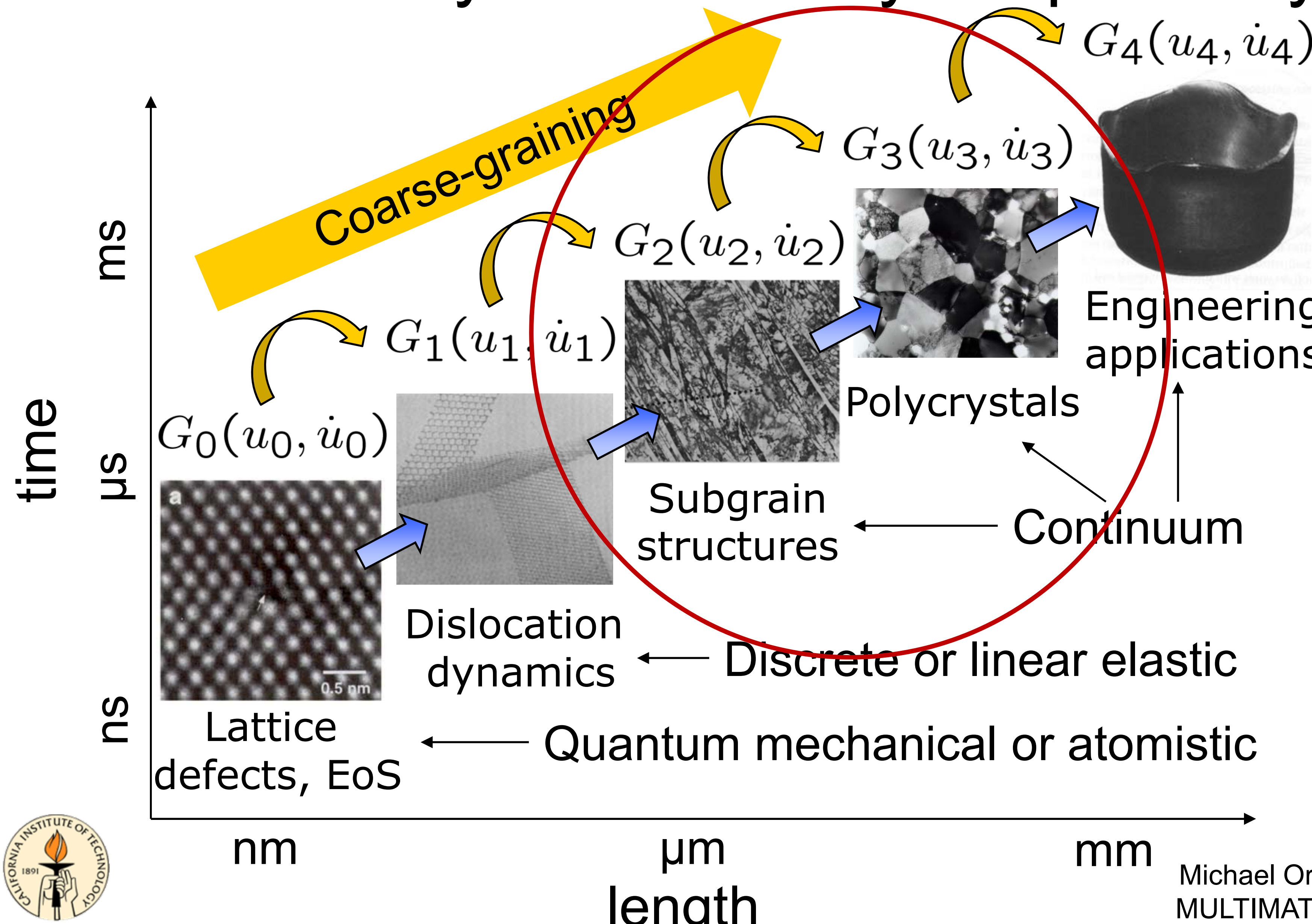
MULTIMAT closing meeting
Bonn, Germany, September 12, 2008

Dislocation dynamics to crystal plasticity



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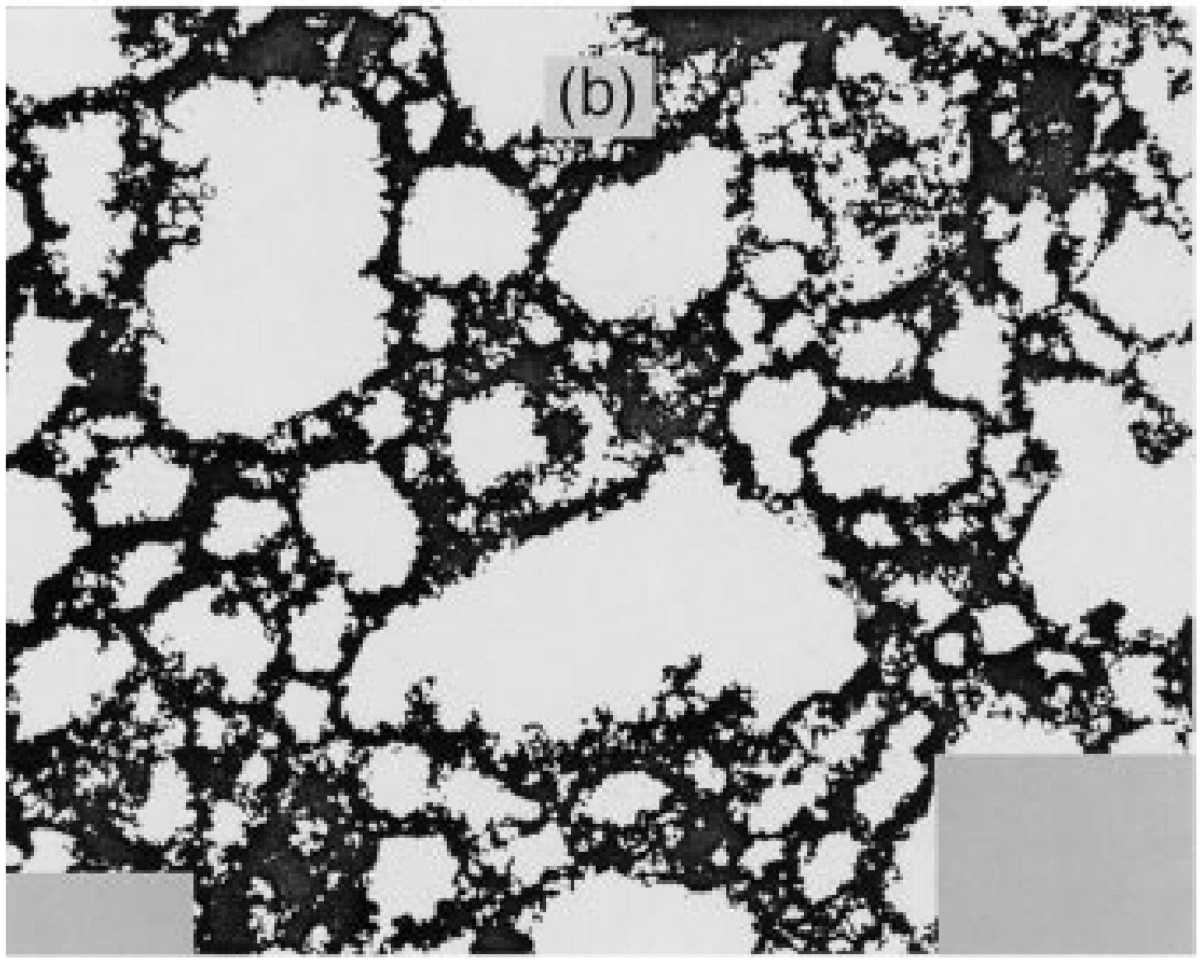
Dislocation structures – Cells



Cell structures in copper
(Mughrabi, H., *Phil. Mag.*, **23** (1971) 869)

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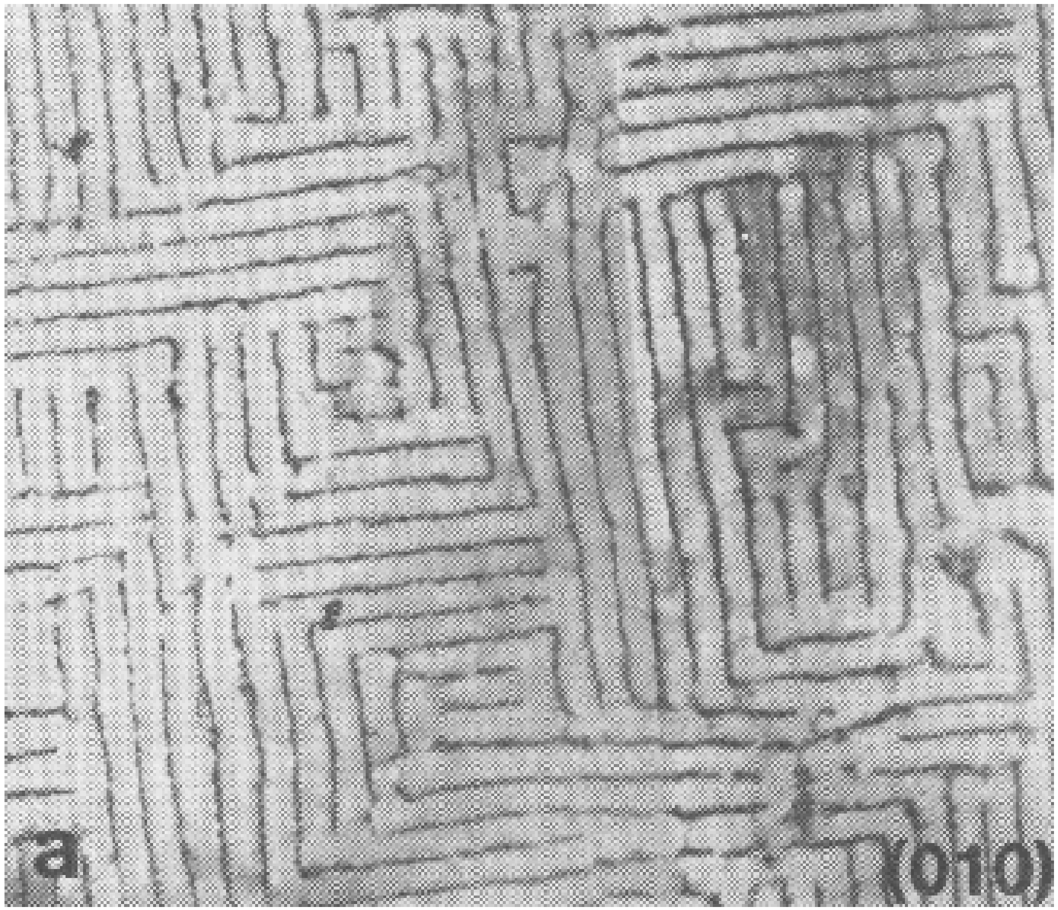
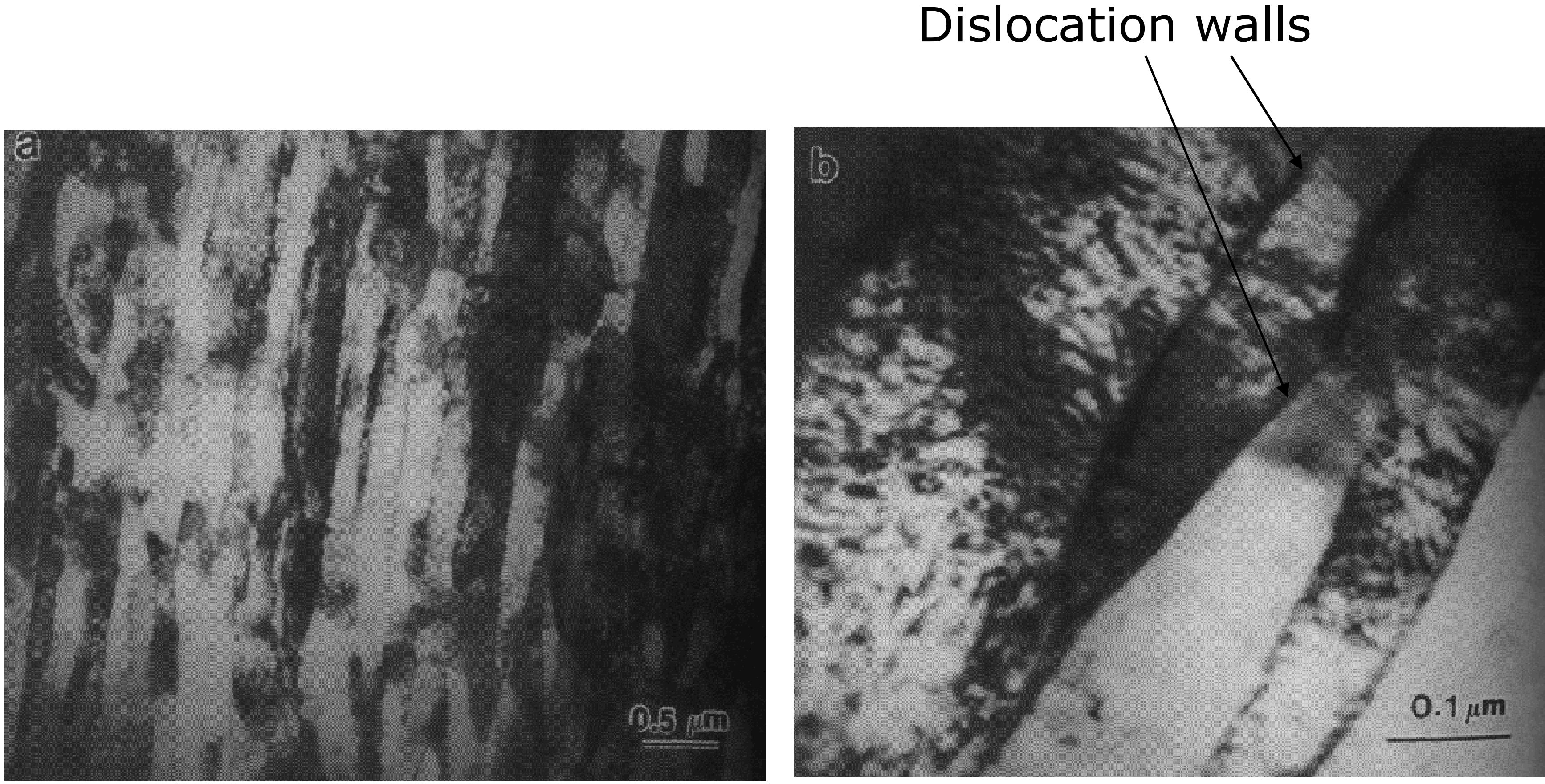
Dislocation structures – Fatigue



Labyrinth structure in fatigued copper single crystal
(Jin, N.Y. and Winter, A.T., *Acta Met.*, **32** (1984) 1173-1176)

Dislocation structures – Lamellar



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

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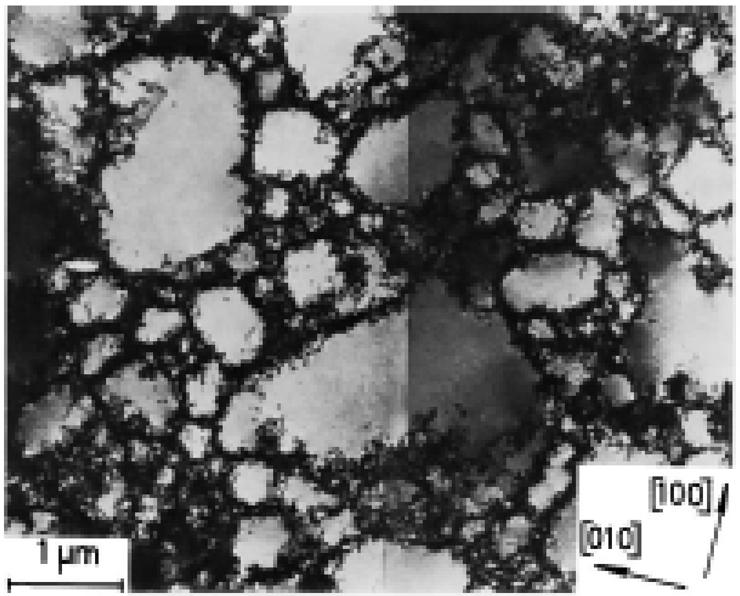
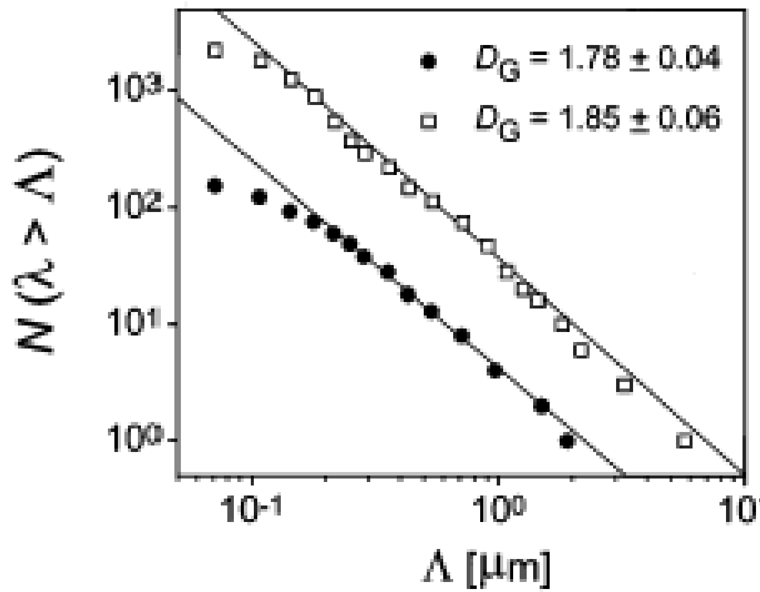
Dislocation structures – Fractality



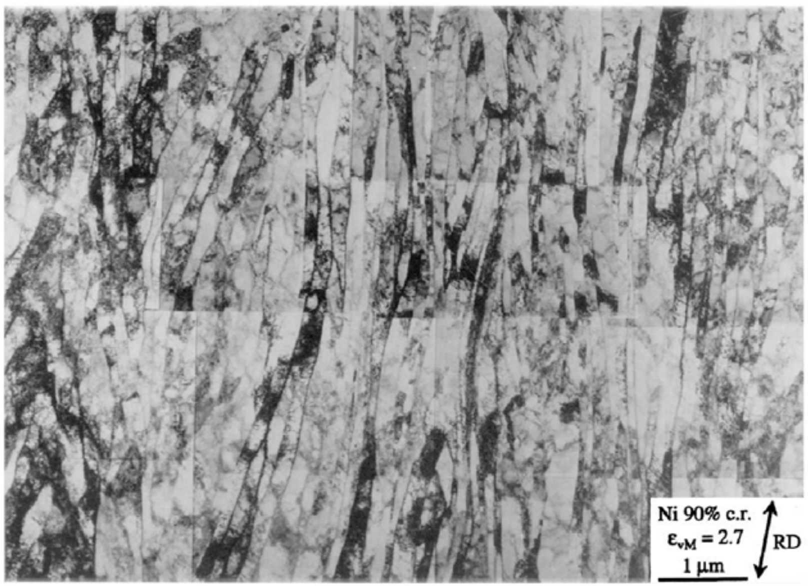
TEM micrograph of dislocation cells of single copper deformed at 75.6MPa
(Mughrabi *et al.*, 1986)



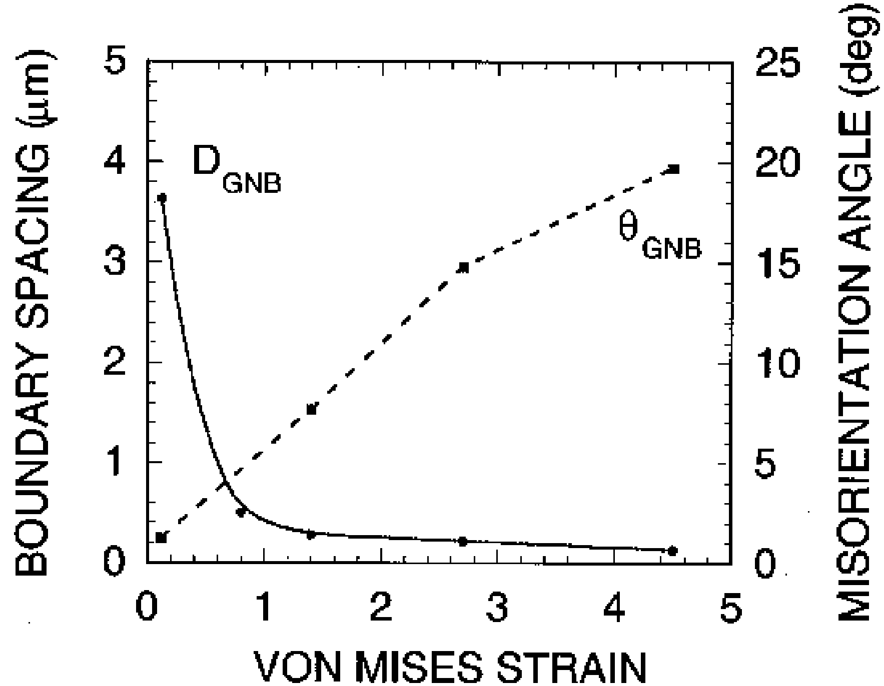
Cell distribution for deformed single crystal of copper and determination of the fractal dimension
(Haehner *et al.*, 1998).

The observed cell size distribution is of the form:
$N(d) \sim d^{-D}$, with fractal dimension $D \sim 1.78—1.85$

Dislocation structures – Scaling



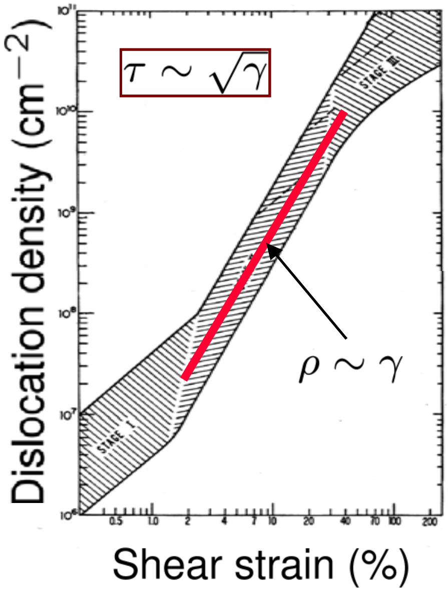
Pure nickel cold rolled to 90%
Hansen *et al., Mat. Sci. Engin*. A**317** (2001).



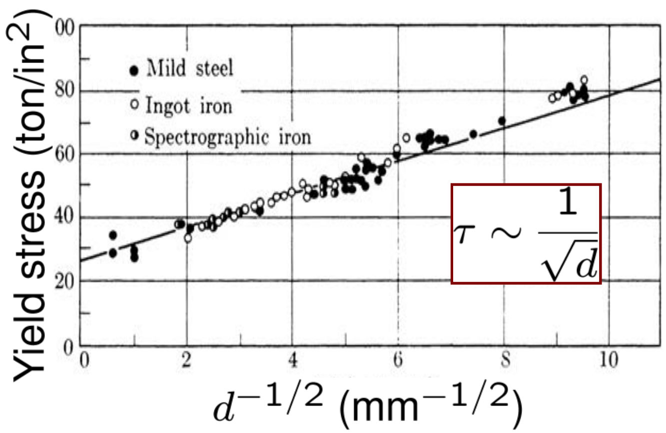
Lamellar width and misorientation angle as a function of deformatation
Hansen *et al., Mat. Sci. Engin*. A**317** (2001).

Scaling of lamellar width and misorientation angle with deformation

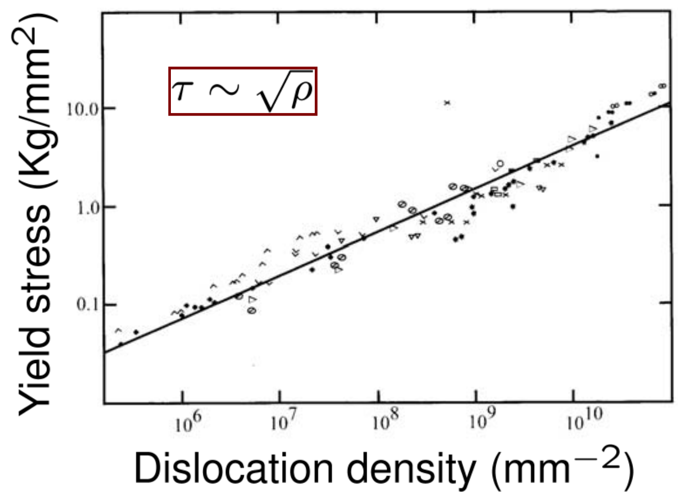
Dislocation structures – Scaling



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.)

The classical scaling laws of single crystal plasticity

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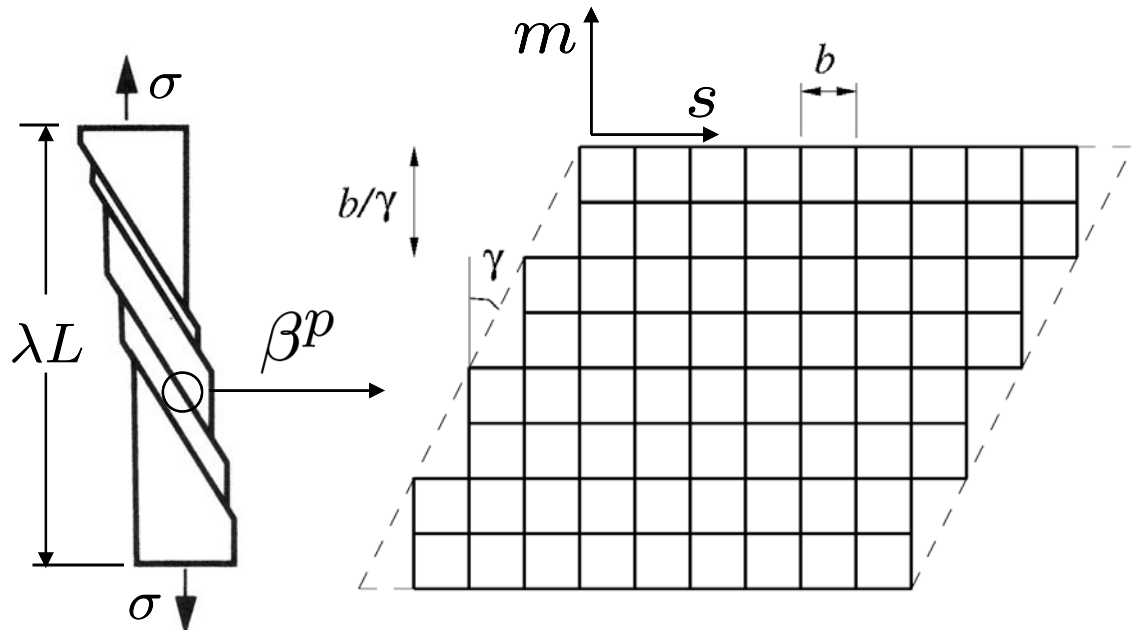
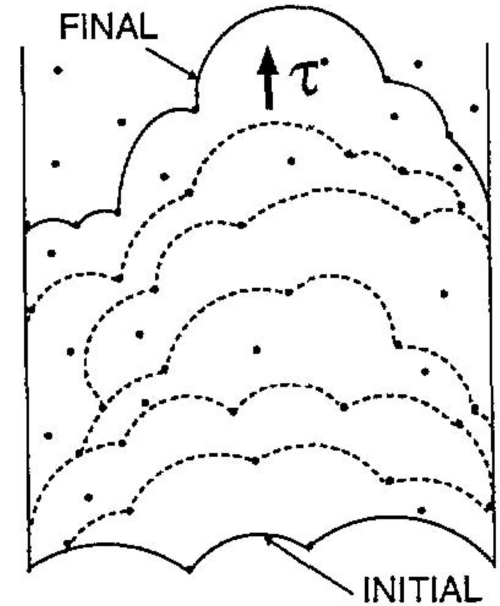
Subgrain dislocation structures

- What gives rise to observed subgrain dislocation structures, microstructural evolution?
- What gives rise to observed scaling relations?
- What is the effective macroscopic behavior that results from microstructure formation, evolution?
- What are the microstructures that give rise to a given macroscopic behavior?

Crystal plasticity – Linearized kinematics





- Kinematics: $\epsilon^p(\gamma) = \frac{1}{|\Omega|}\int_{J_u} [\![u]\!]\odot m \, d\mathcal{H}^2 \equiv \sum \gamma s \odot m$
- Energy: $E(u,\gamma) = \int_\Omega [\, W^e(\nabla u - \epsilon^p(\gamma)) + T \cancel{|\nabla\gamma\times m|} \,]\, dx$
- Dissipation: $\psi(\dot\gamma) = \begin{cases} \tau_c|\dot\gamma|, & \text{if single slip,} \\ +\infty, & \text{otherwise.} \end{cases}$

Crystal plasticity – Deformation theory

- Energy-dissipation functional:

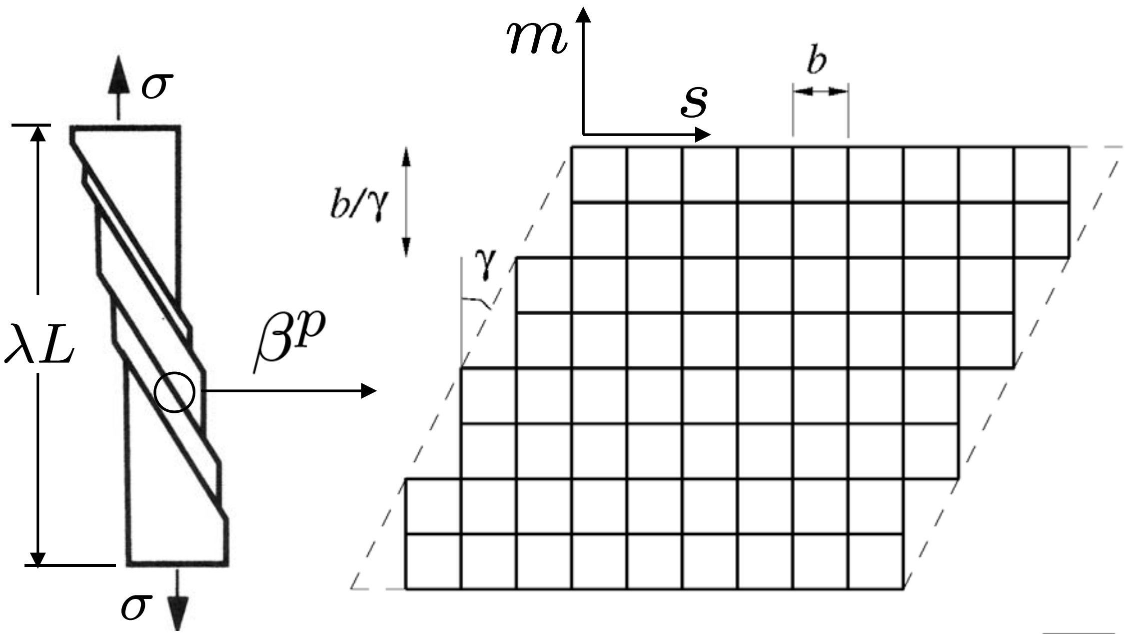
$$F_\epsilon(u,\gamma) = \int_0^T \mathrm{e}^{-t/\epsilon}[\Psi(\dot\gamma) + \frac{1}{\epsilon}E(u,\gamma)]\,dt$$

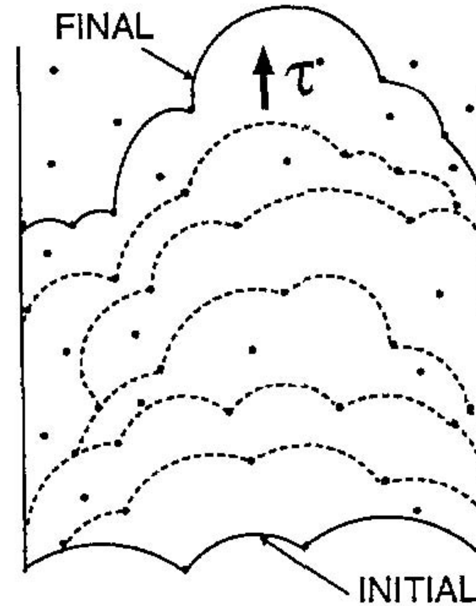
- Constraint set: $\mathbb{K} = \{\gamma :$ monotonic, single slip$\}$
- Plastic work: $W^p(\gamma) = \sum \tau_c \gamma$
- Then: $F_\epsilon(u,\gamma) = \begin{cases} \int_0^T \mathrm{e}^{-t/\epsilon} E(u,\gamma)\,\frac{dt}{\epsilon}, & \text{if } \gamma \in \mathbb{K}\,, \\ +\infty, & \text{otherwise}\,. \end{cases}$
- Pseudo-energy:

$$F(u,\gamma) = \int_\Omega [\,W^e(\nabla u - \epsilon^p(\gamma)) + W^p(\gamma) + T|\nabla\gamma\times m|\,]\,dx$$

- Single loading step: $\boxed{F(u,\gamma) + I_{\mathbb{K}}(\gamma) \to \inf!}$

Crystal plasticity – Local





- Incremental flow rule: $\epsilon^p(\gamma) = \sum \gamma s \odot m$
- Pseudo-elastic strain energy density:

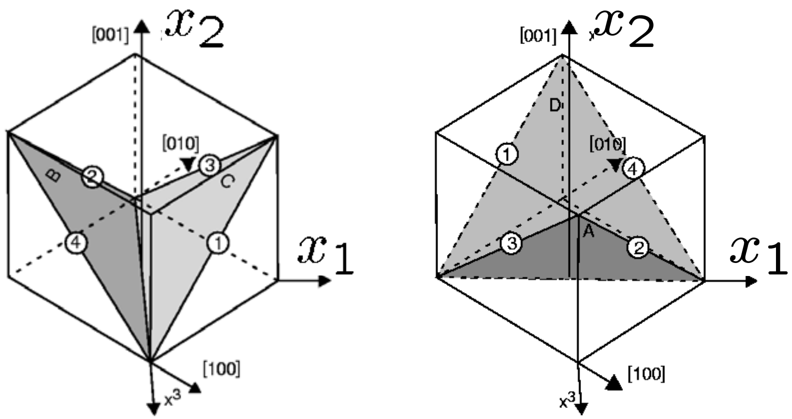
$$W(\epsilon) = \inf_{\gamma \in \mathbb{K}} \{W^e(\epsilon - \epsilon^p(\gamma)) + W^p(\gamma)\}$$

- Variational problem (static equilibrium):

$$F(u) = \int_\Omega W(\epsilon(u))\, dx \to \inf!$$

Non-convexity - Strong latent hardening

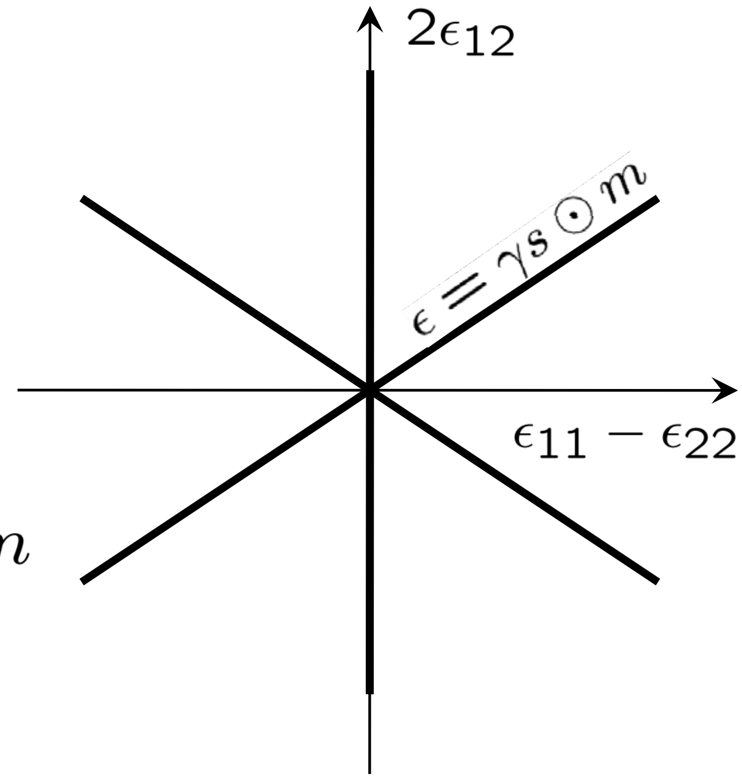
- Example: FCC crystal deforming on $(1\bar{1}0)$-plane



- Rigid-plastic case:

$$W = \begin{cases} 0, & \text{if } \epsilon = \gamma s \odot m \\ +\infty, & \text{otherwise.} \end{cases}$$

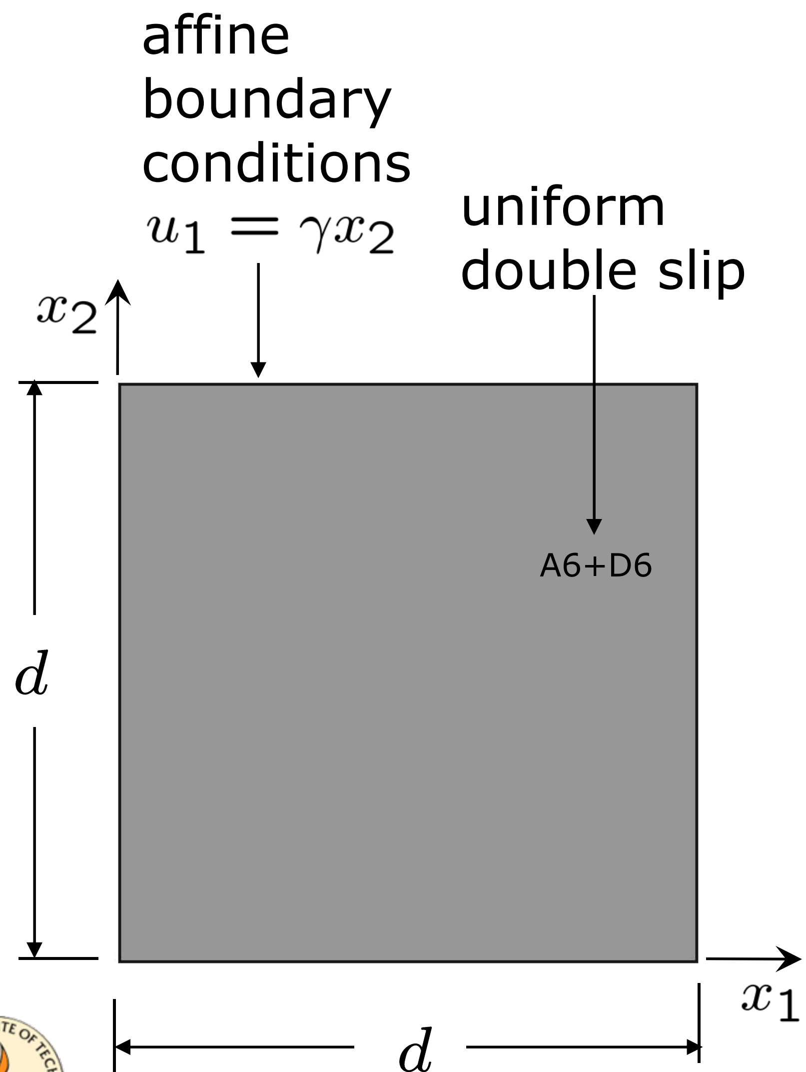
- $W(\epsilon)$ non-convex!

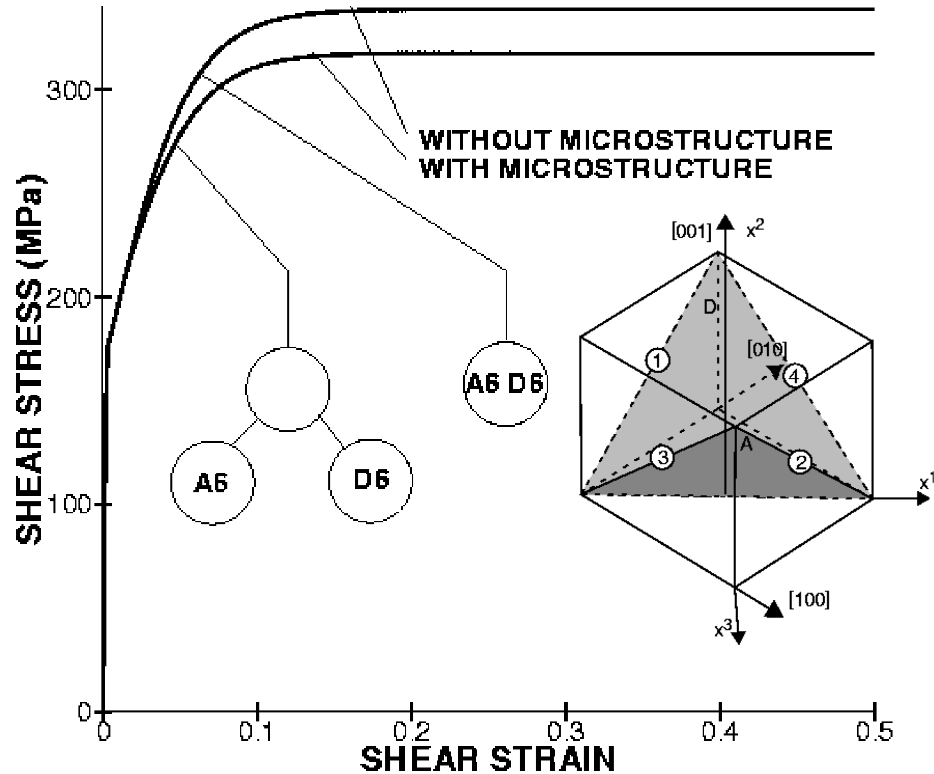


$W(\epsilon)$

(Ortiz and Repetto, *JMPS*, **47**(2) 1999, p. 397)

Strong latent hardening & microstructure

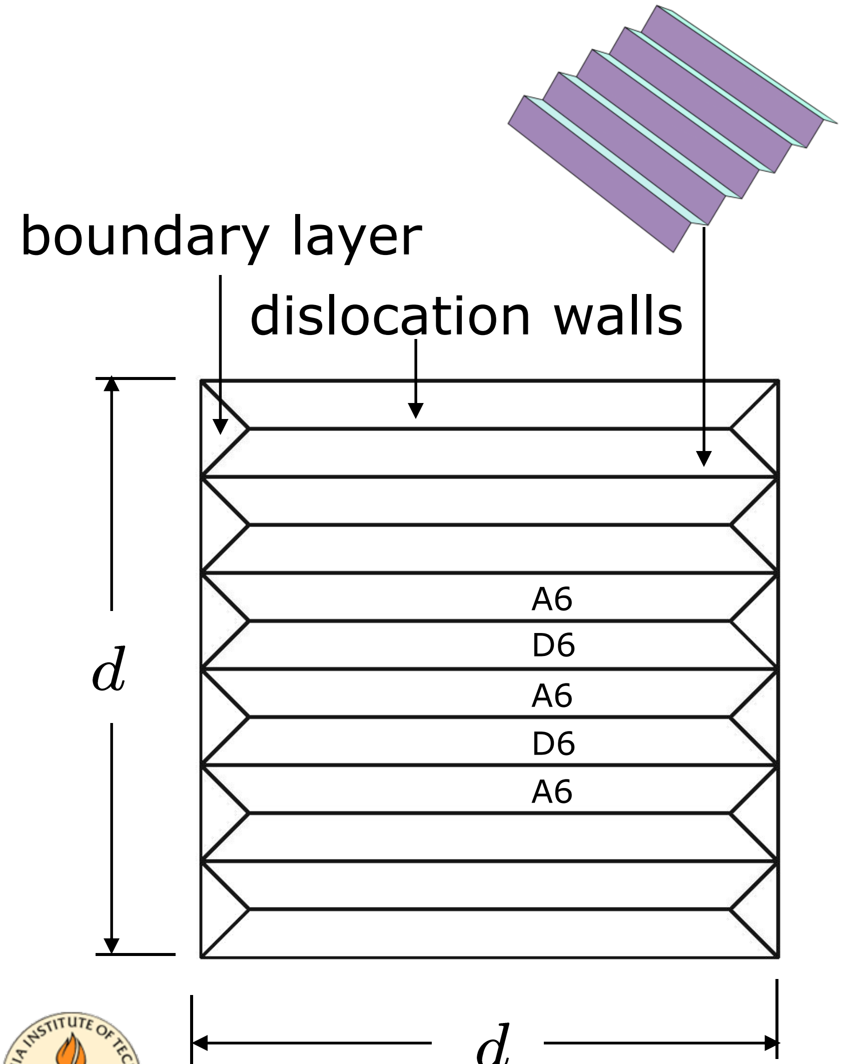


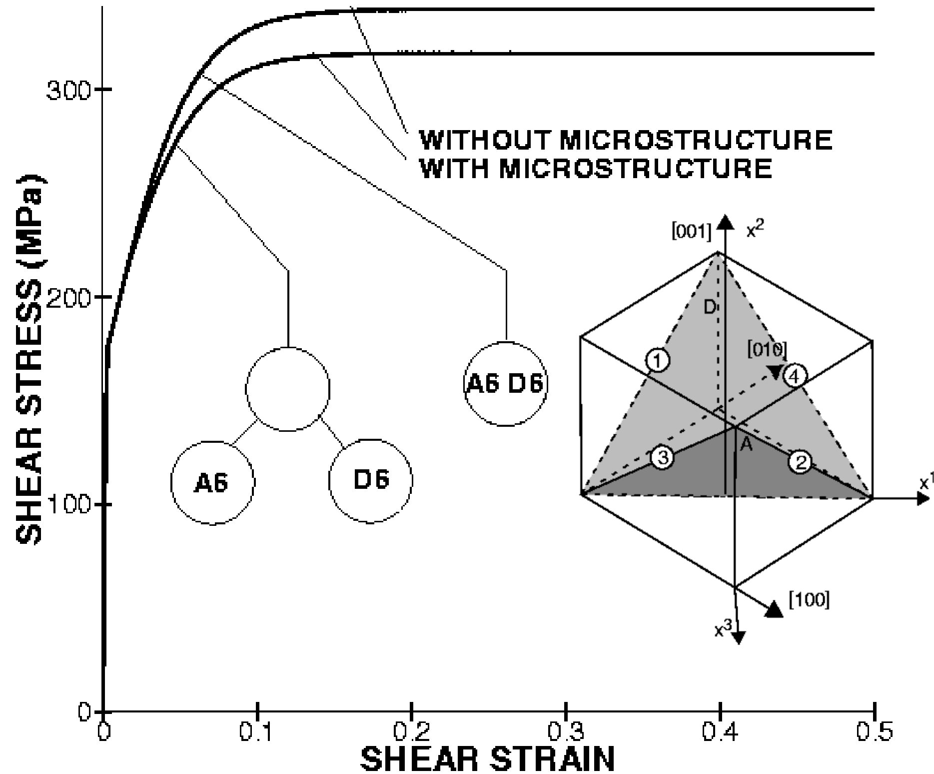


FCC crystal deformed in simple shear on (001) plane in [110] direction

(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure





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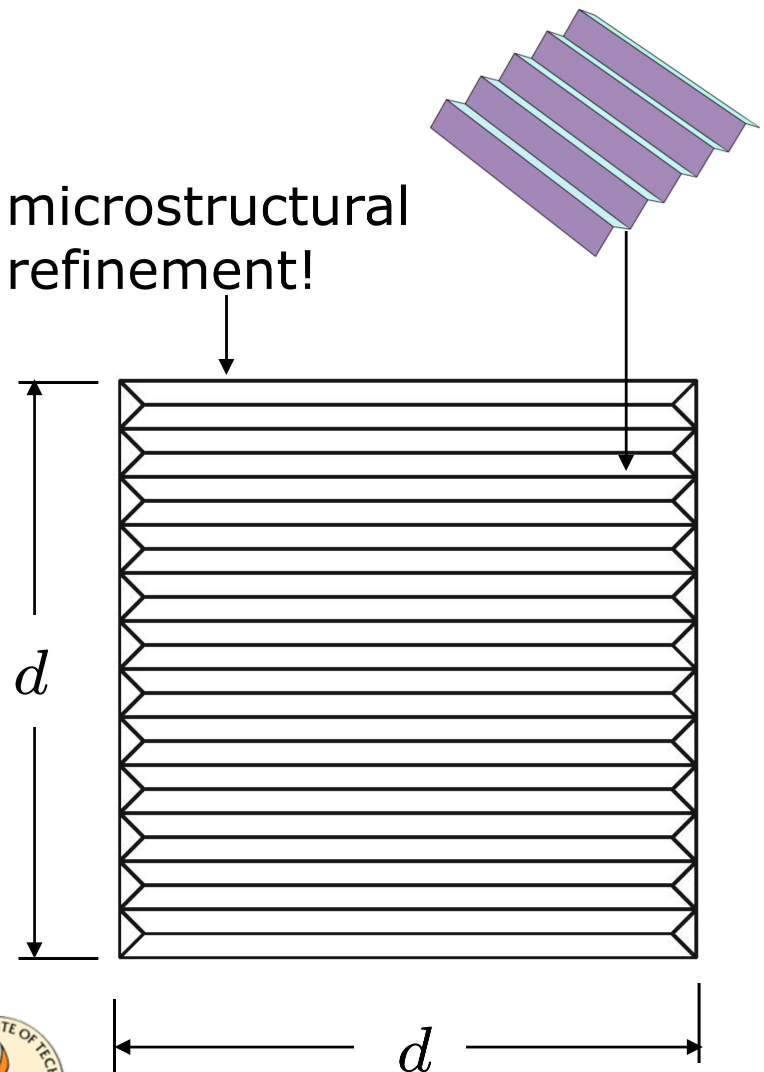
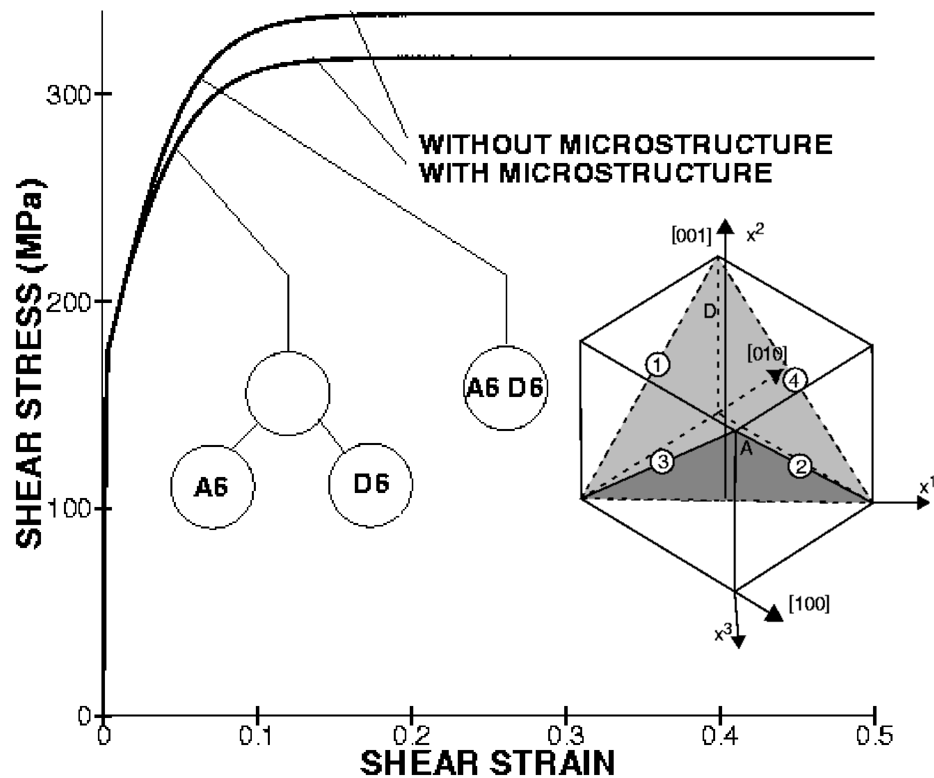
(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure

microstructural refinement!





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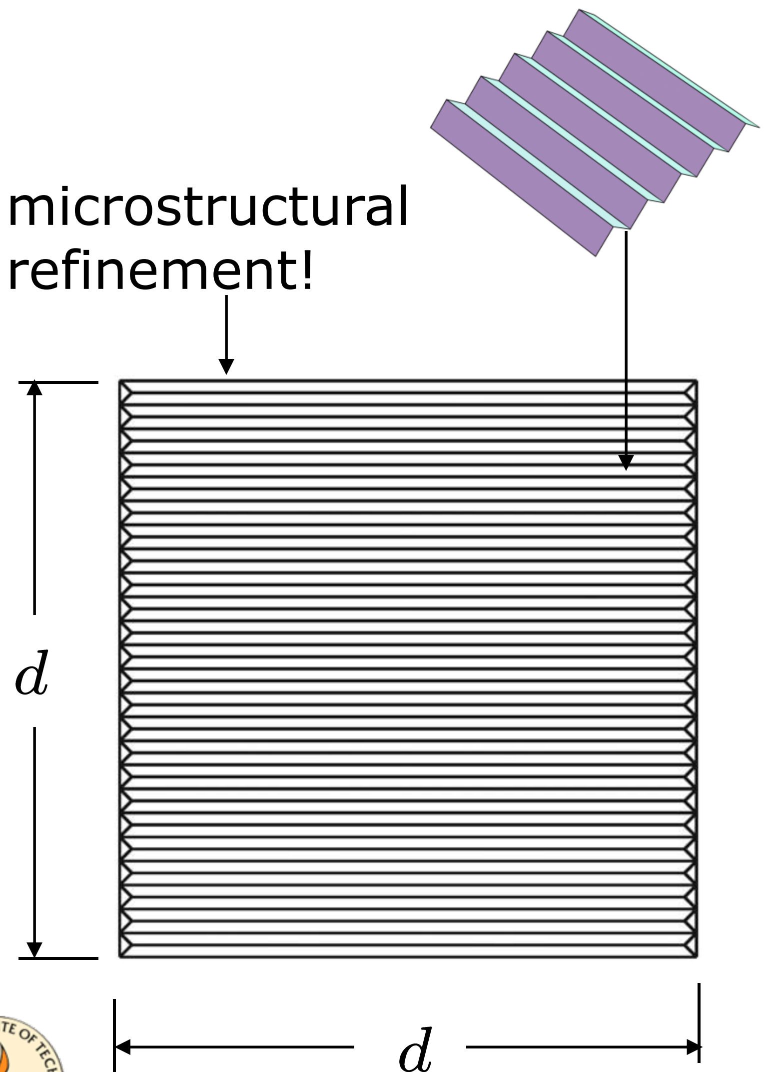
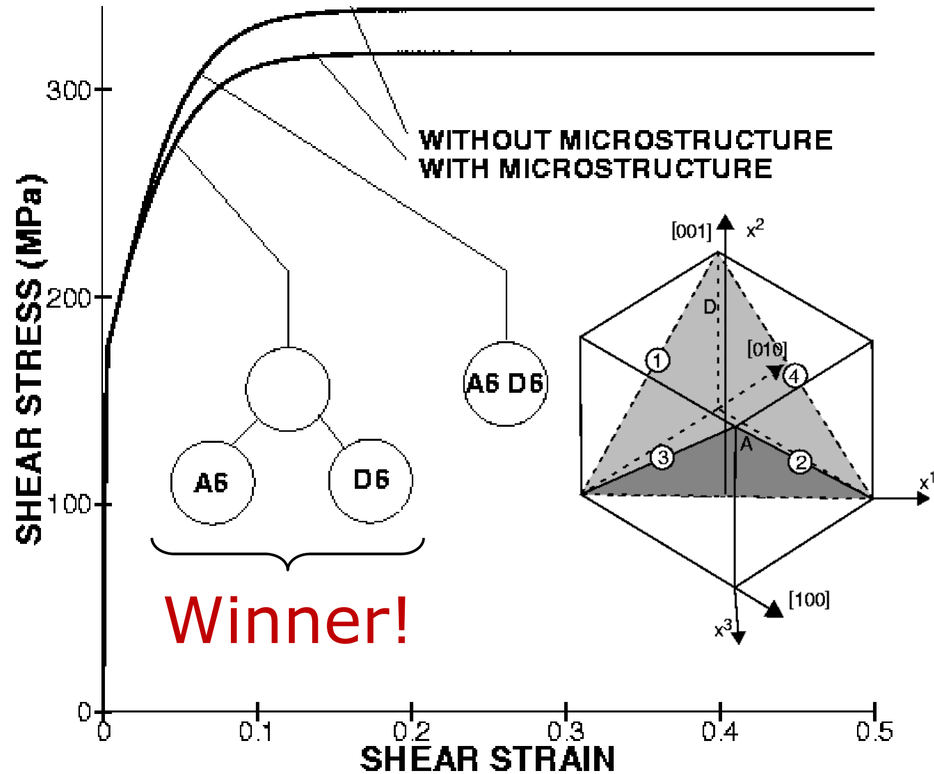
Strong latent hardening & microstructure





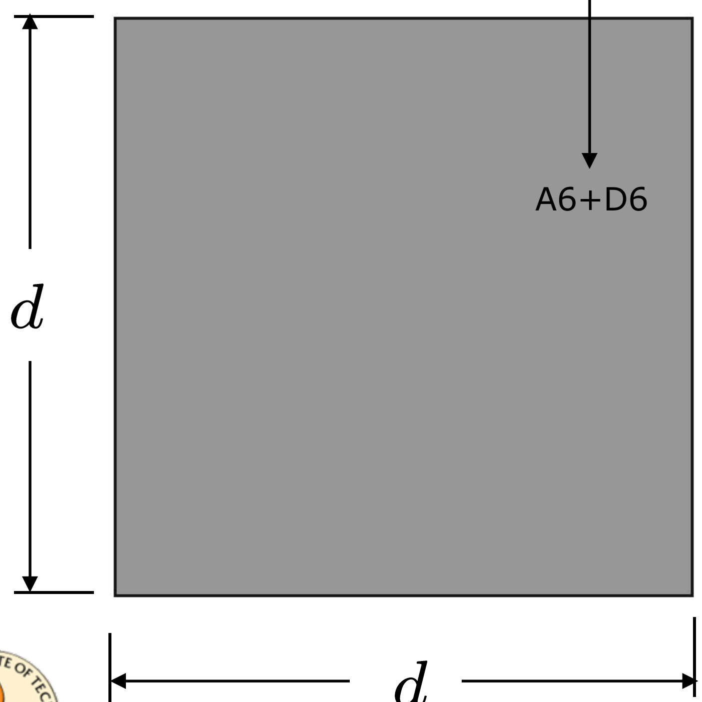
FCC crystal deformed in simple shear on (001) plane in [110] direction

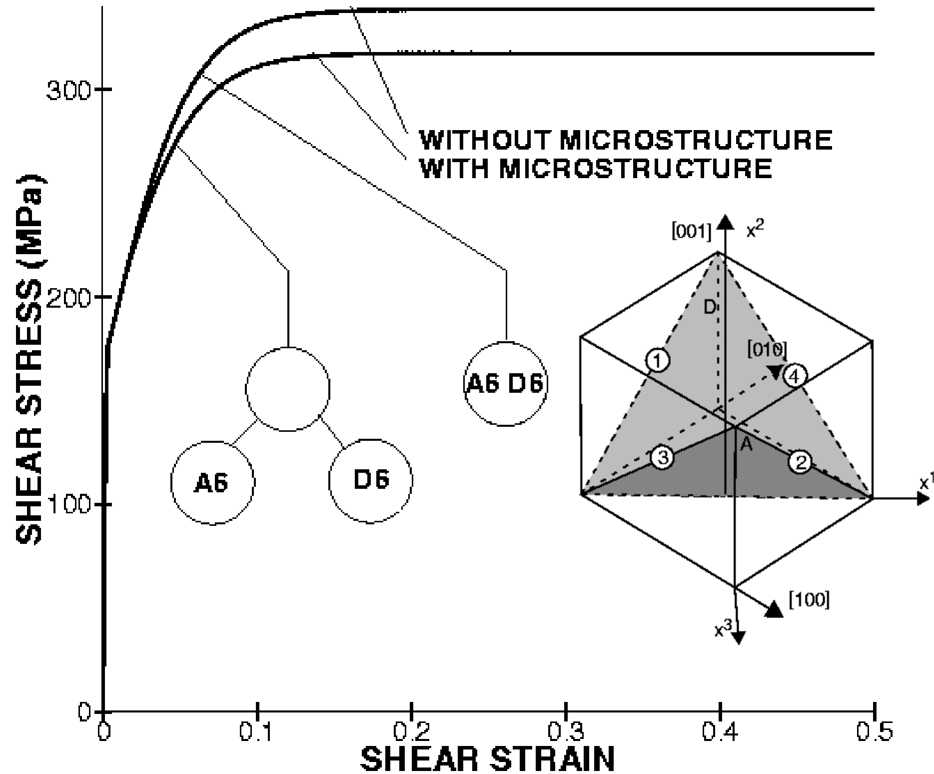
(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure

Pass to the limit…

uniform double slip!





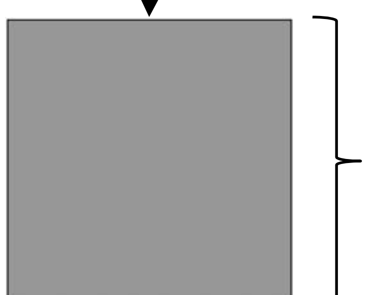
FCC crystal deformed in simple shear on (001) plane in [110] direction

(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Calculus of variations and microstructure

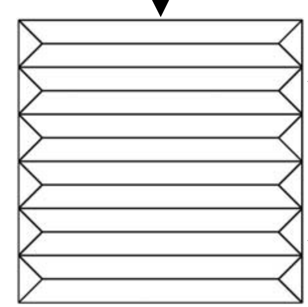
- $F : u_0 + H^1_0(\Omega, \mathbb{R}^3) \to \bar{\mathbb{R}}$ not weakly lower semi-continous (lsc) $\Rightarrow$ non-attainment, non-existence!
- Relaxed problem: $sc^- F(u) \to \inf!$
- $sc^- F \equiv$ largest lsc functional majorized by F
- Quasiconvex envelop:

$$QW(\beta) = \inf_{v \in W^{1,\infty}_0(E)} \frac{1}{|E|} \int_E W(\beta + \nabla v)\, dx$$



representative volume *E*

uniform deformation



$u = \beta x$

microstructure

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Relaxation as ‘exact’ multiscale method

- The relaxed problem is well-posed, exhibits no microstructure (attainment)
- The relaxed and unrelaxed problems deliver the same macroscopic response (e.g., force-displacement curve)
- All microstructures are pre-accounted for by the relaxed problem (no physics lost)
- Microstructures can be reconstructed from the solution of the relaxed problem (no loss of information)
- Relaxation is the ‘perfect’ multiscale method!

Crystal plasticity − Relaxation

- Convex envelop: $W^{**}(\beta) =$

$$\inf \left\{ \sum_i \lambda_i W(\beta_i) : \lambda_i \geq 0,\, \sum_i \lambda_i = 1,\, \beta_i \in \mathbb{R}^{3\times 3} \right\}.$$

  - Linear growth on traceless symmetric matrices
  - Quadratic growth on the trace

- Regression function: $W^{\infty}(\beta) = \lim_{t\to\infty} \frac{1}{t} W^{**}(t\beta)$.

Definition. *A set of slip systems* $\mathcal{S} = \{s_i \otimes m_i\}$ *is* complete *if the symmetric lamination convex hull of* $\{\pm(s_i \otimes m_i)^{\text{sym}}\}$ *contains a neighbourhood of the origin in the space of symmetric traceless matrices.*

Crystal plasticity − Relaxation

Theorem (Conti & MO, *ARMA* '05) *Suppose that the set of slip systems is complete. Then,* $QW = W^{**}$*.*

- Let: $U(\Omega) = \left\{ u \in BD(\Omega, \mathbb{R}^3) : \mathrm{div} u \in L^2(\Omega) \right\}$

Theorem (Conti & MO, *ARMA* '05) *Suppose that the set of slip systems is complete. Then, the relaxation of* F *with respect to the strong* L^1 *topology is*

$$sc^- F(u) =$$

$$\begin{cases} \int_\Omega W^{**}(\epsilon(u))dx + \int_\Omega W^\infty \left(\frac{E_s u}{|E_s u|} \right) d|E_s u|, & \text{if } u \in U(\Omega) \\ +\infty, & \text{otherwise.} \end{cases}$$

Crystal plasticity – Relaxation

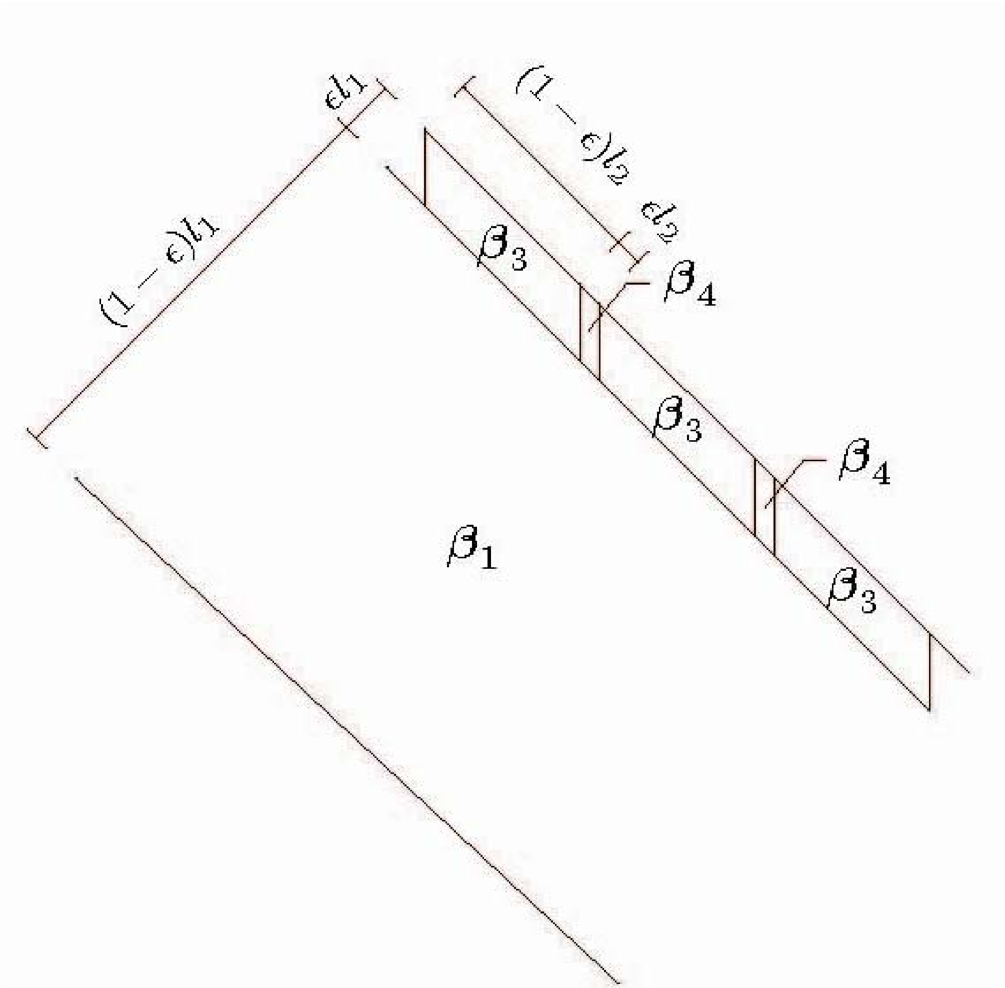
- Proof: Match upper & lower bounds, $QW = W^{**}$.
- Lower bound: $sc^{-}F(u)$ convex functional of measure Eu, $sc^{-}F(u) \leq F(u)$.

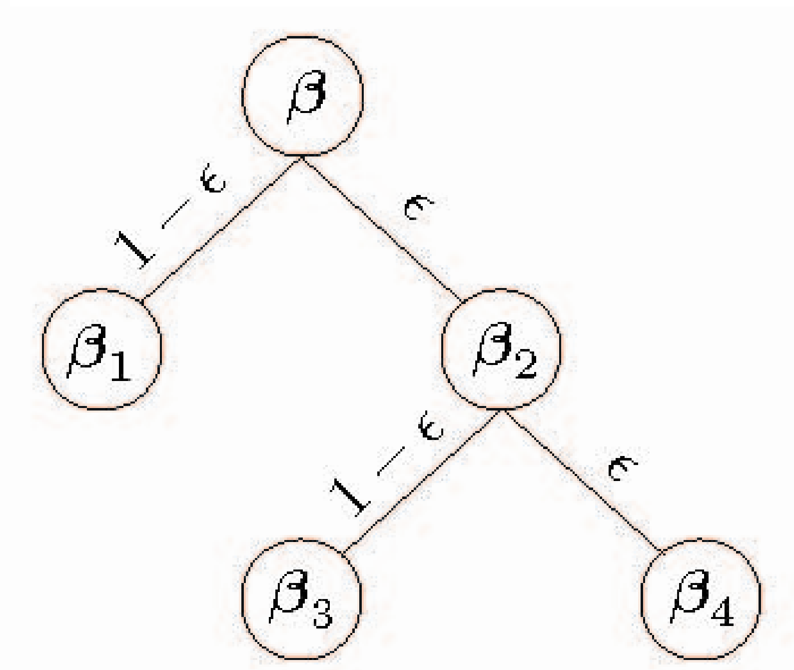
Lemma *Let $\mathcal{S}$ be a complete set of slip systems. For any $\beta \in \mathbb{R}^{3\times 3}$ and any $\epsilon > 0$ there is a laminate ν (of finite order) such that*

$$\langle \nu, \mathrm{Id} \rangle = \beta \qquad \textit{and} \qquad \langle \nu, W \rangle \leq W^{**}(\beta) + \epsilon \, .$$

- Some of the deformations in the laminate may become unbounded as $\epsilon \to 0$ and become slip lines in the limit.

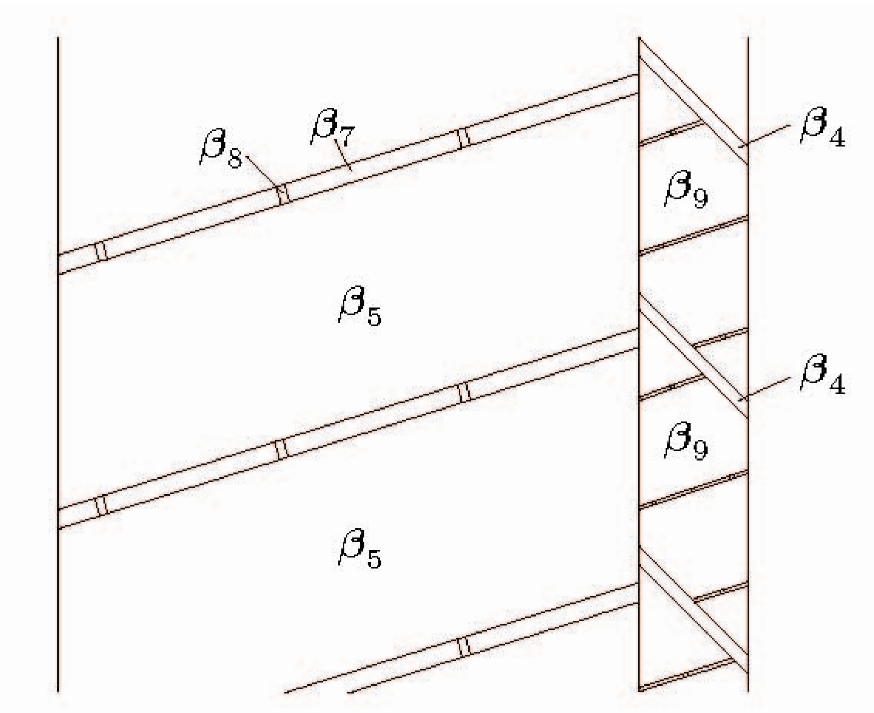
Crystal plasticity – Relaxation

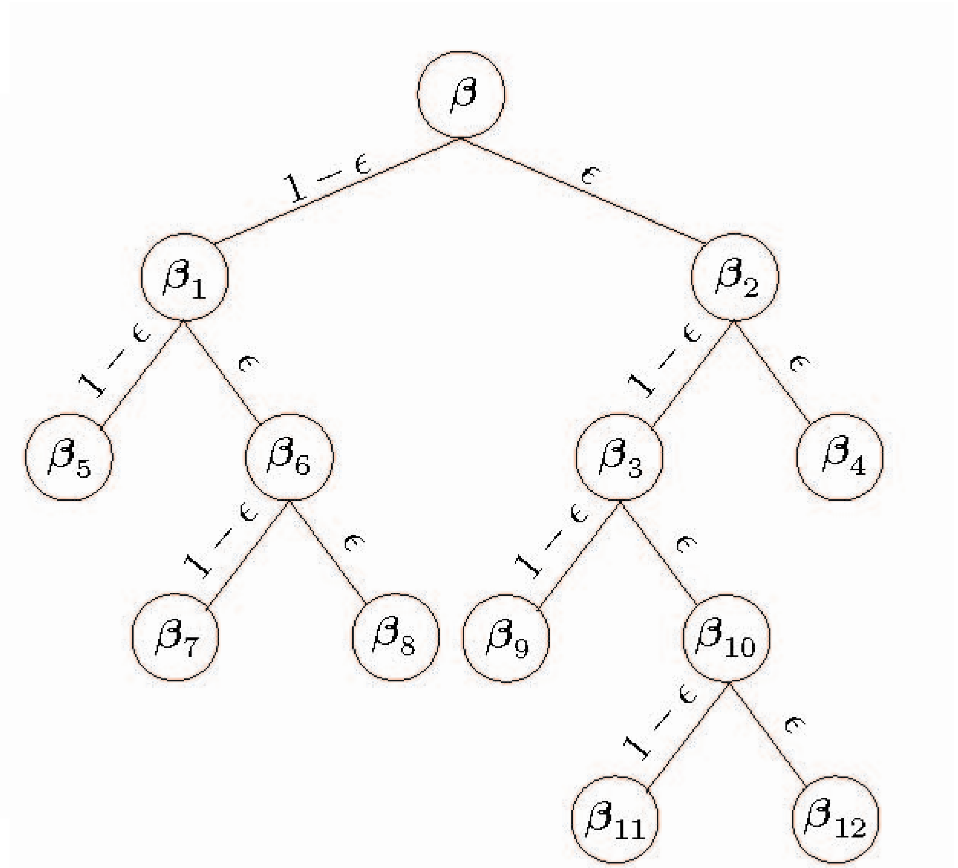




Optimal microstructure construction in double slip
(Conti and Ortiz, ARMA, 2004)

Crystal plasticity – Relaxation

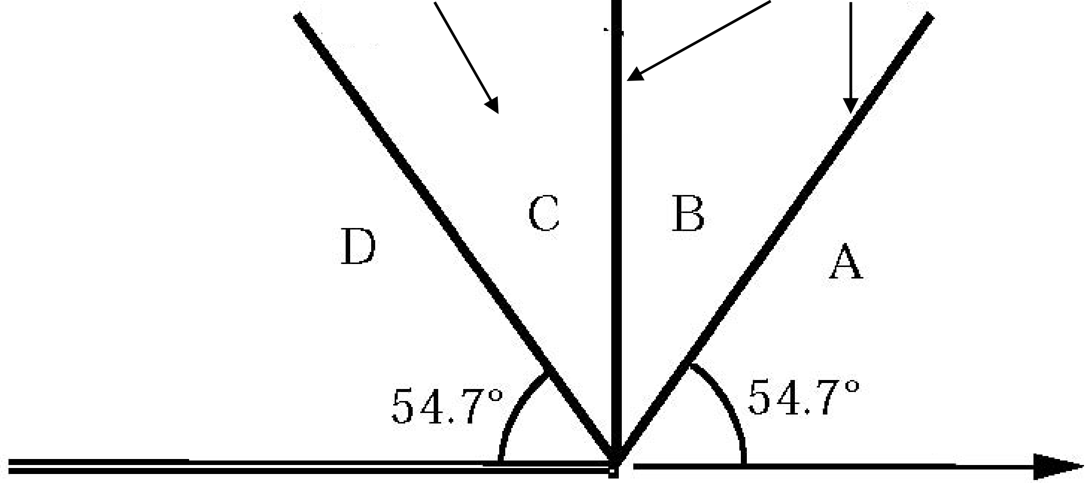




Optimal microstructure construction in triple slip
(Conti and Ortiz, ARMA, 2004)

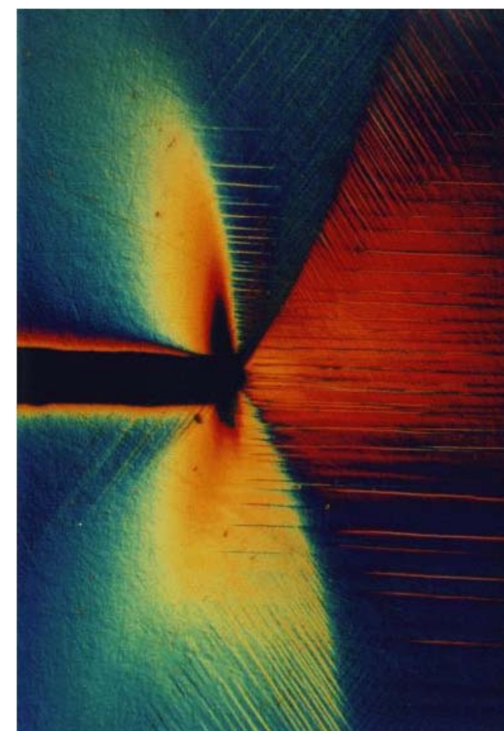
Standard model – Relaxation

$$sc^{-}F(u) = \underbrace{\int_\Omega W^{**}(\epsilon(u))dx}_{\text{Ideal plasticity}} + \underbrace{\int_\Omega W^{\infty}\left(\frac{E_s u}{|E_s u|}\right) d|E_s u|}_{\text{Slip-line energy}}$$

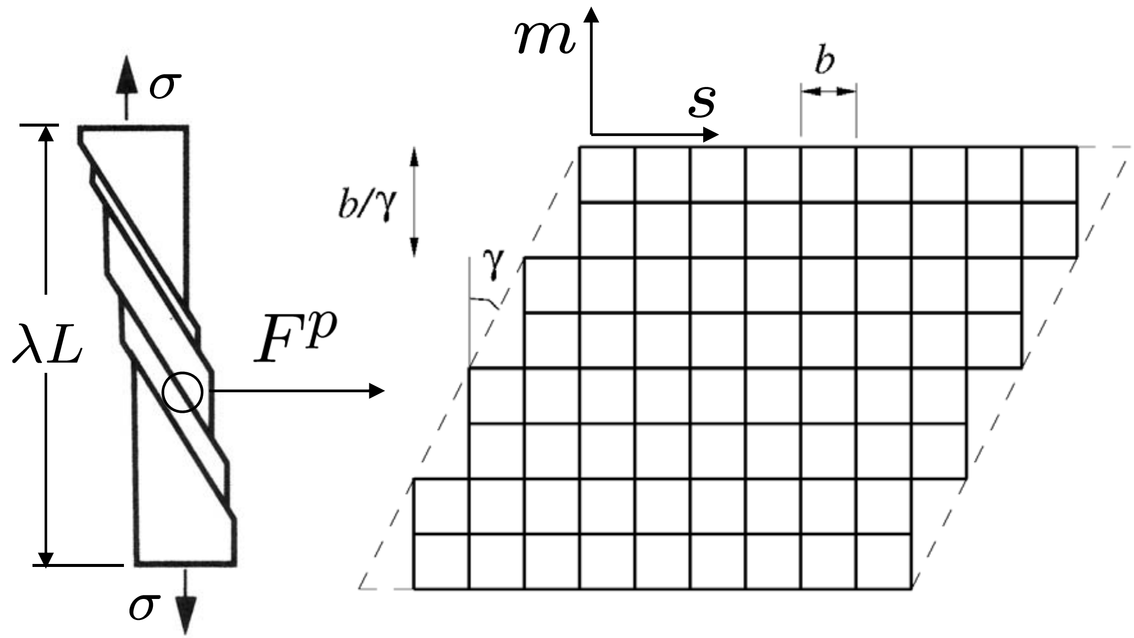


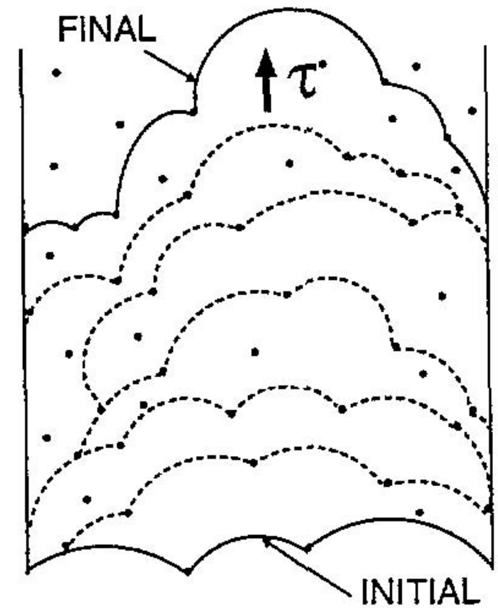
(Rice, *Mech. Mat.*, 1987)

(Crone and Shield, *JMPS*, 2002) →



Crystal plasticity – Finite kinematics





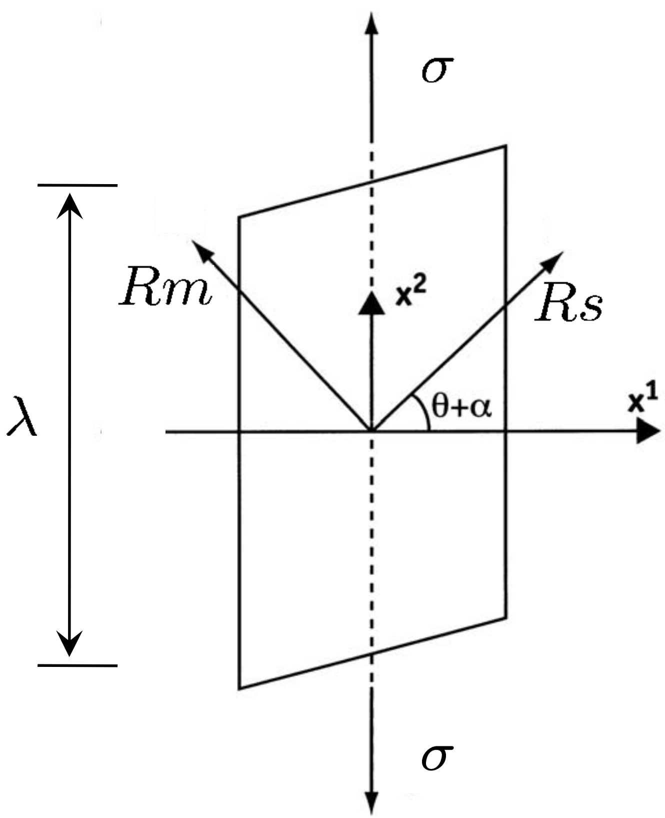
- Energy:

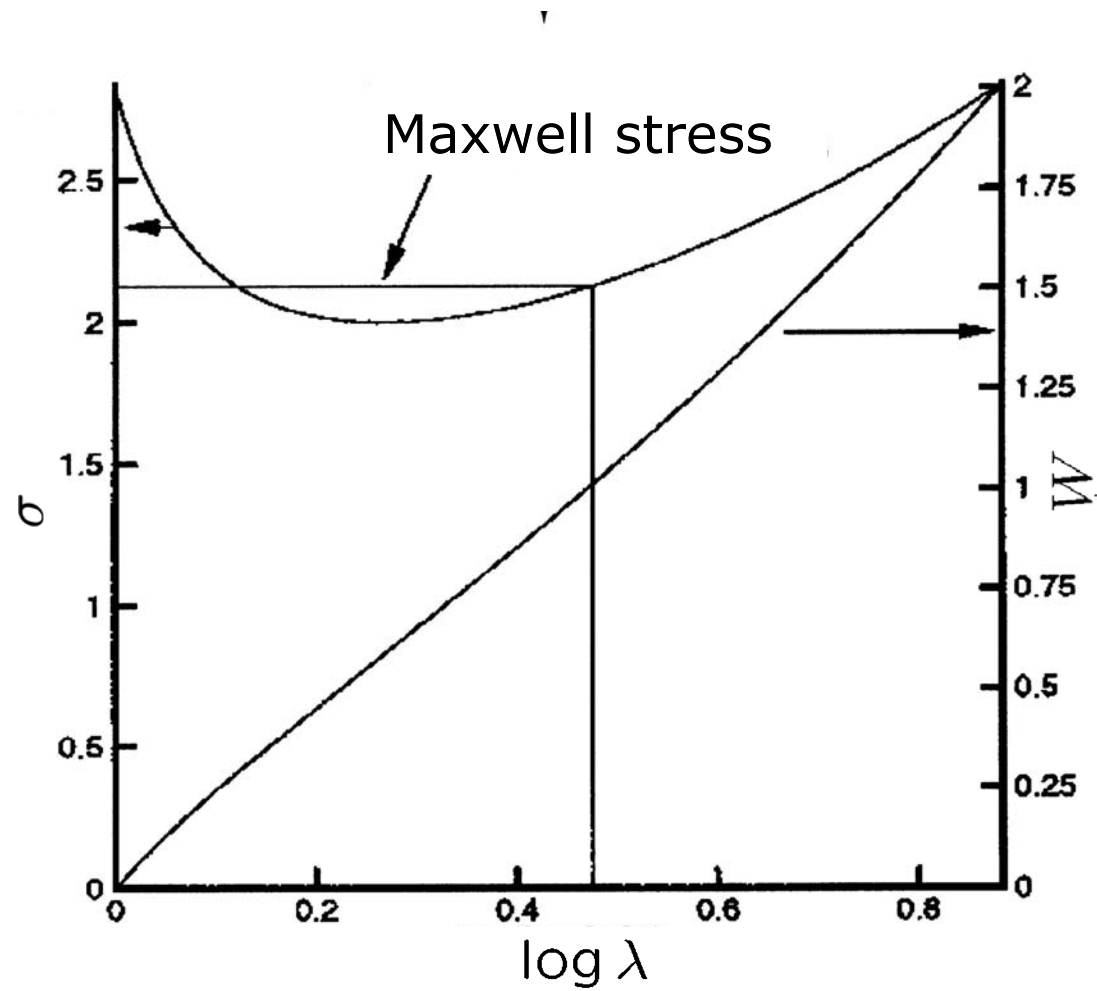
$$E(y, F^p, \gamma) = \int_\Omega [\, W^e(\nabla y F^{p-1}) + T\,|\nabla\gamma \times m|\,]\, dx$$

- Dissipation:

$$\psi(\dot\gamma, \dot F^p, F^p) = \begin{cases} \tau_c|\dot\gamma|, & \text{if single slip,} \\ & \dot F^p F^{p-1} = \sum \dot\gamma s \otimes m \\ +\infty, & \text{otherwise.} \end{cases}$$

Crystal plasticity – Geometrical softening





(Ortiz and Repetto, *JMPS*, **47**(2) 1999, p. 397)

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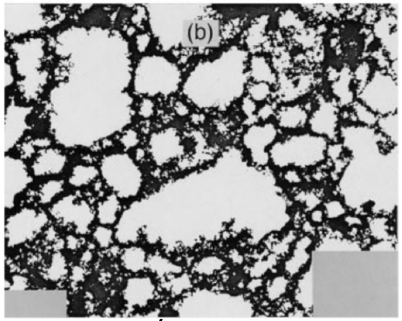
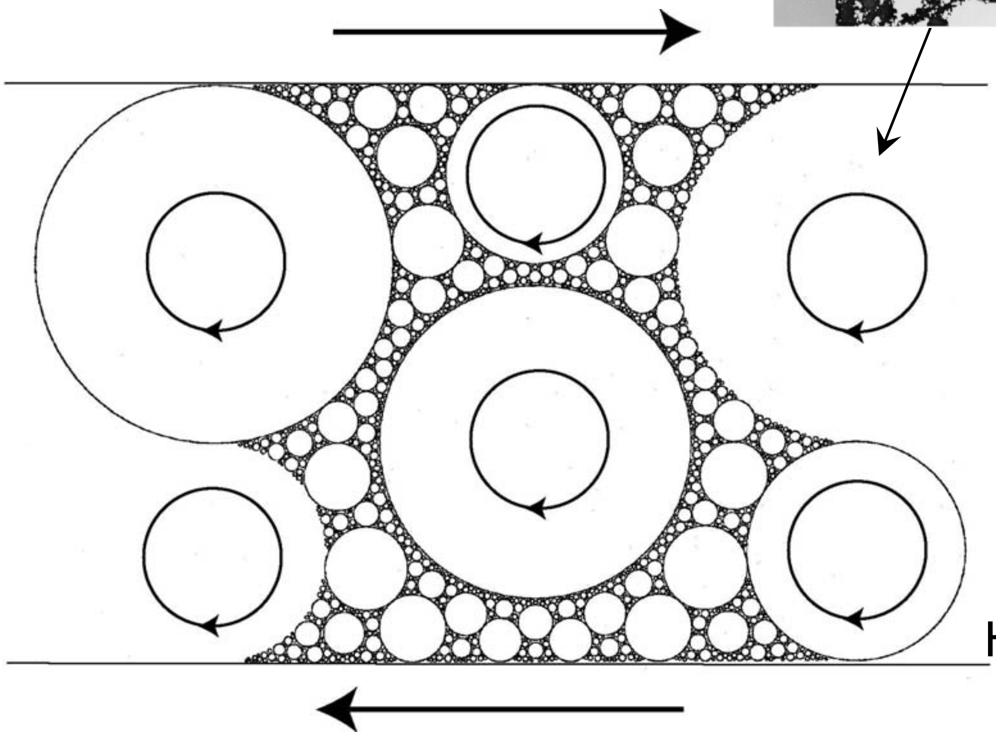
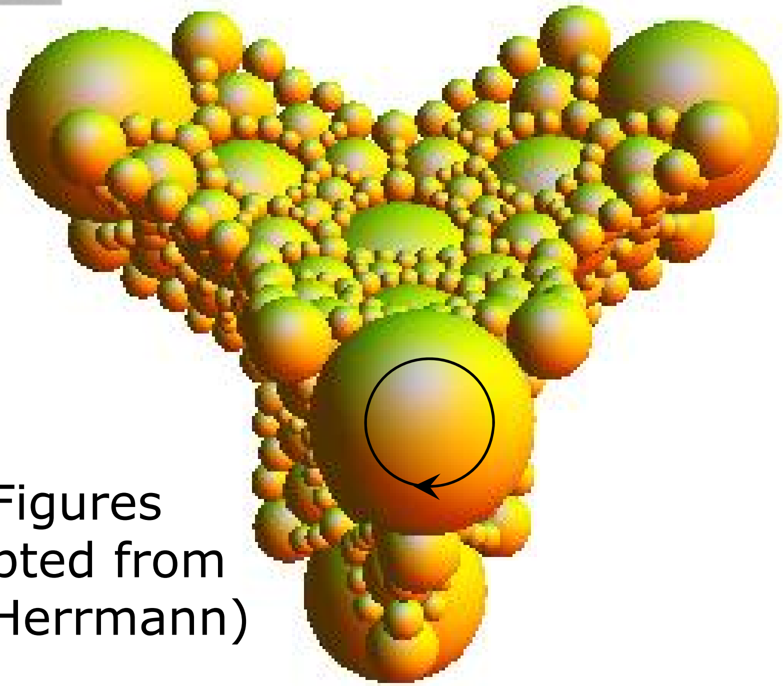
Constructions – Cell structures

Cell structures in copper
Mughrabi, Phil. Mag. **23**, 869 (1971)





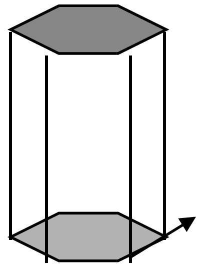


(Figures adapted from H.J. Herrmann)

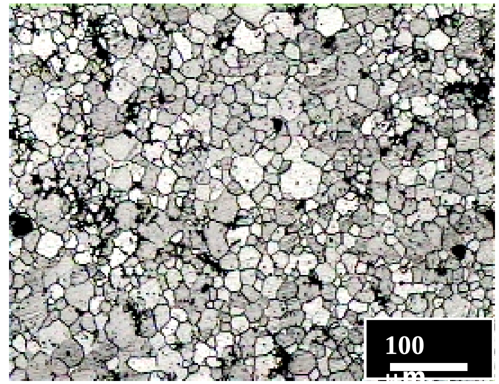
Ball-bearing kinematical model of dislocation cell structures

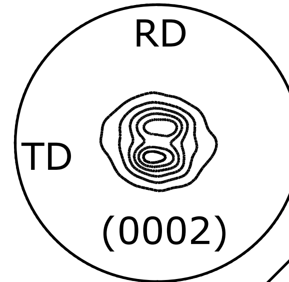
Constructions – Cell structures

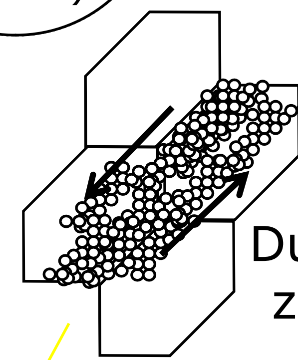
Magnesium slip systems: (0001) [1120]



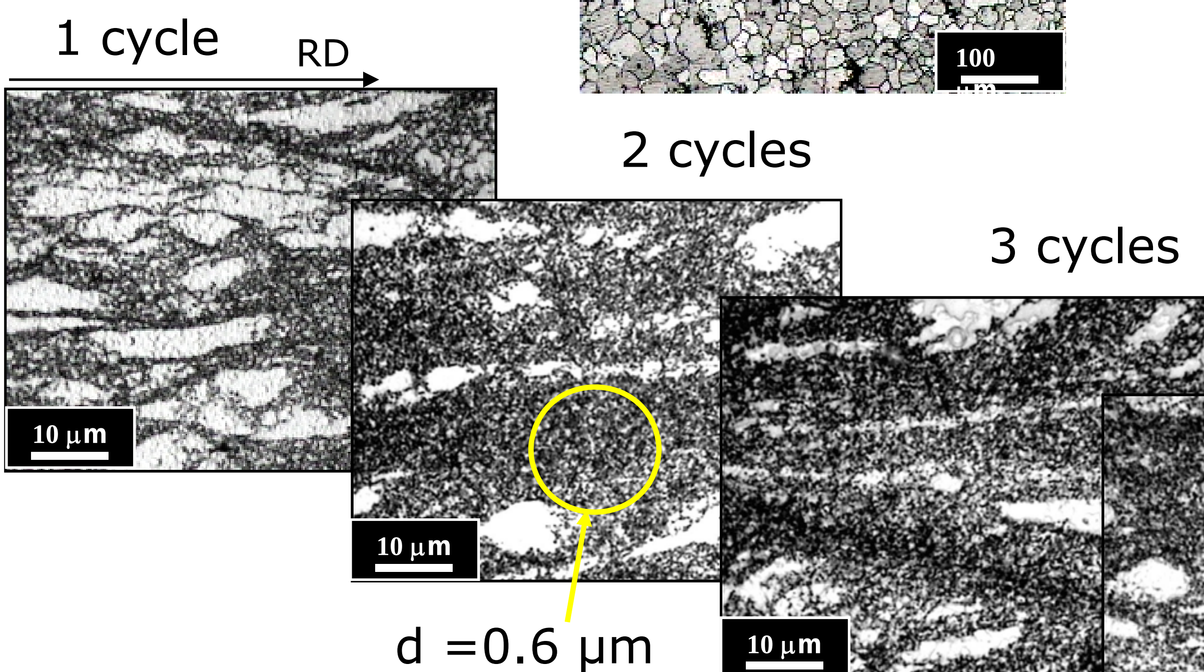
d = 40 μm

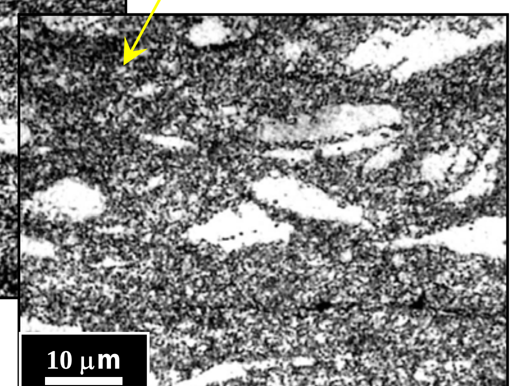






Ductile zones



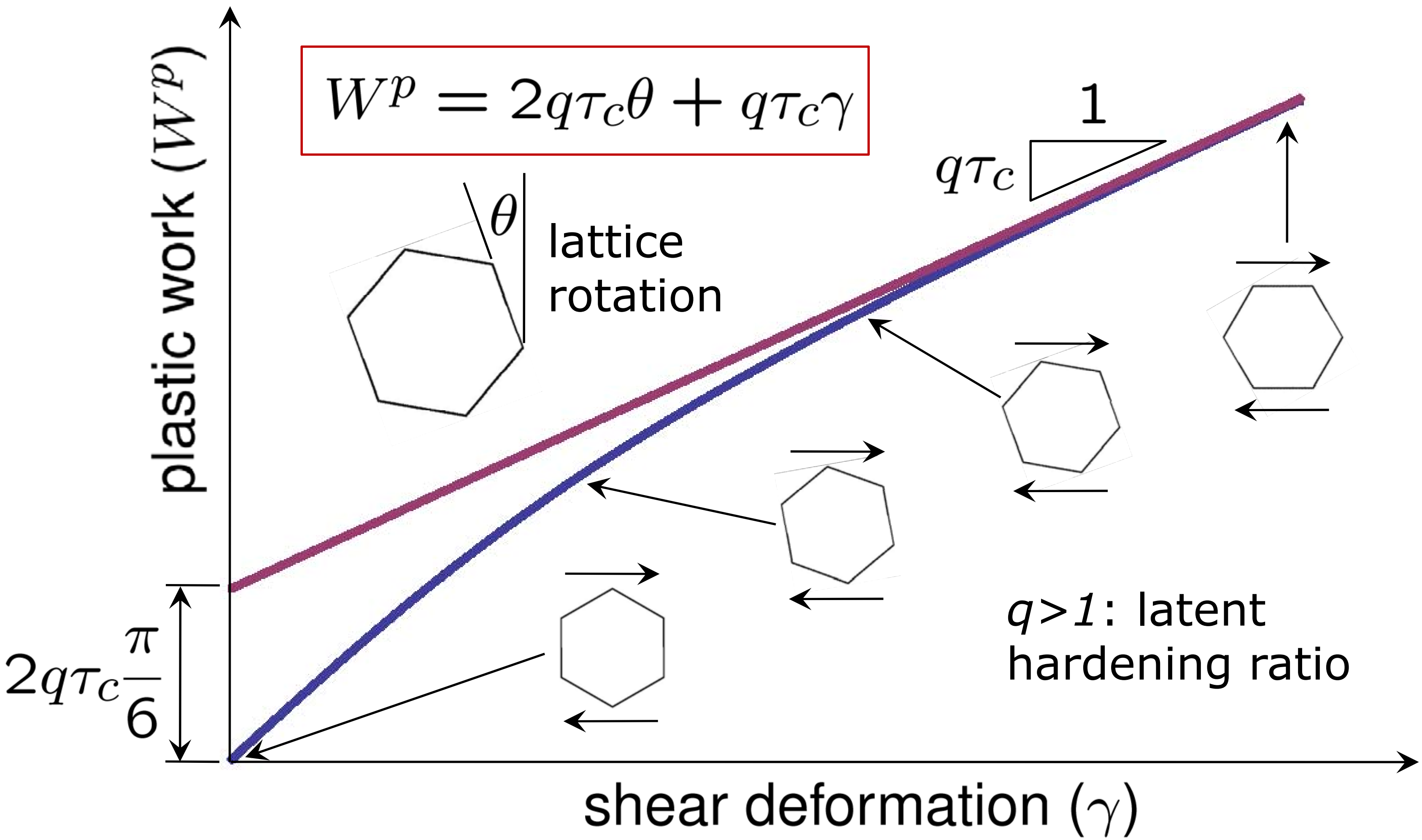


d =0.6 μm

Roll bonding of (0002) Mg alloys

M. T. Pérez-Prado, J.A. del Valle, O.A. Ruano, *Scripta Mater*., **51** (2004) 1093-1097.

Constructions – Cell structures



Simple shear on basal plane:
Uniform double slip

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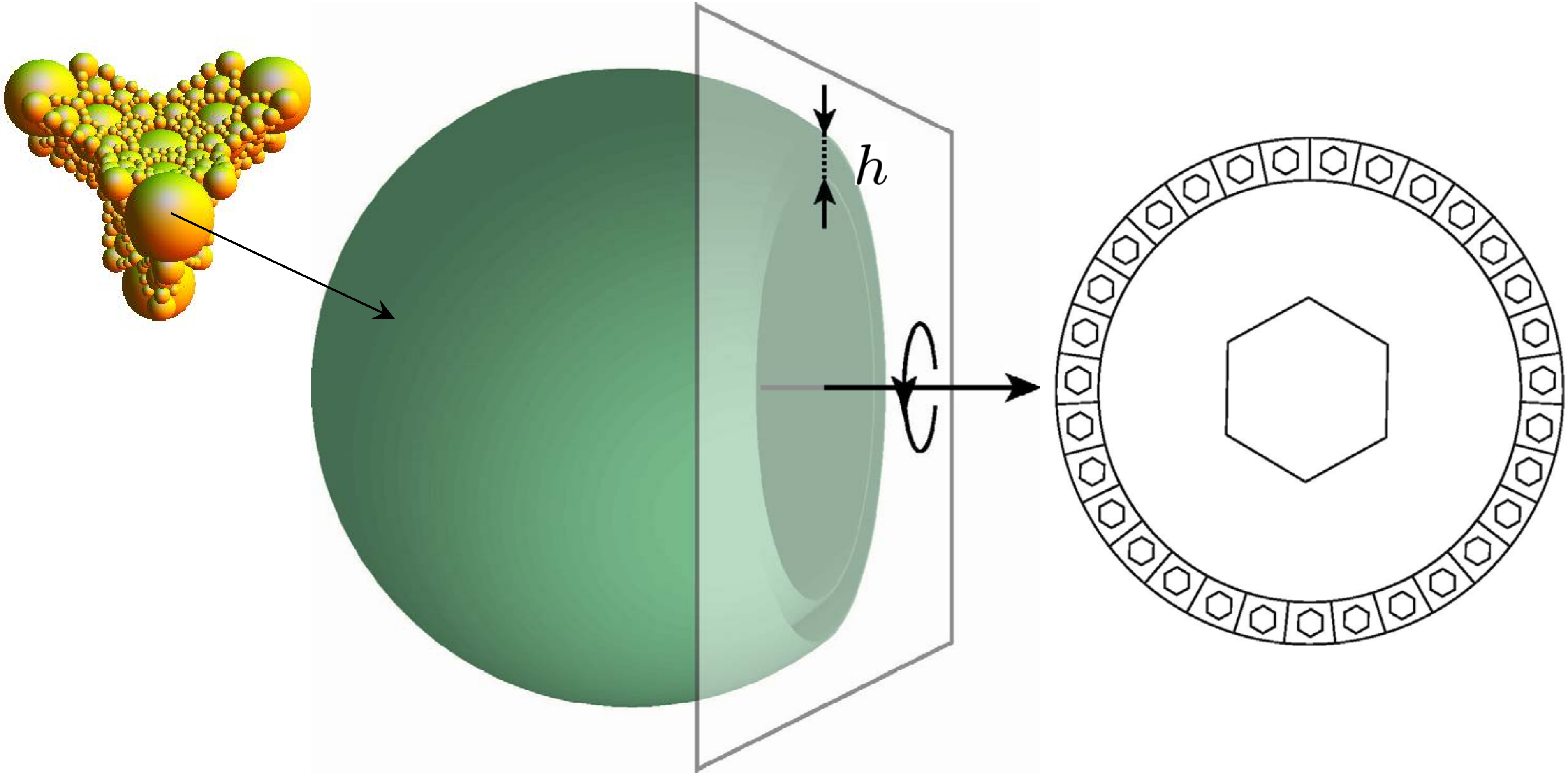
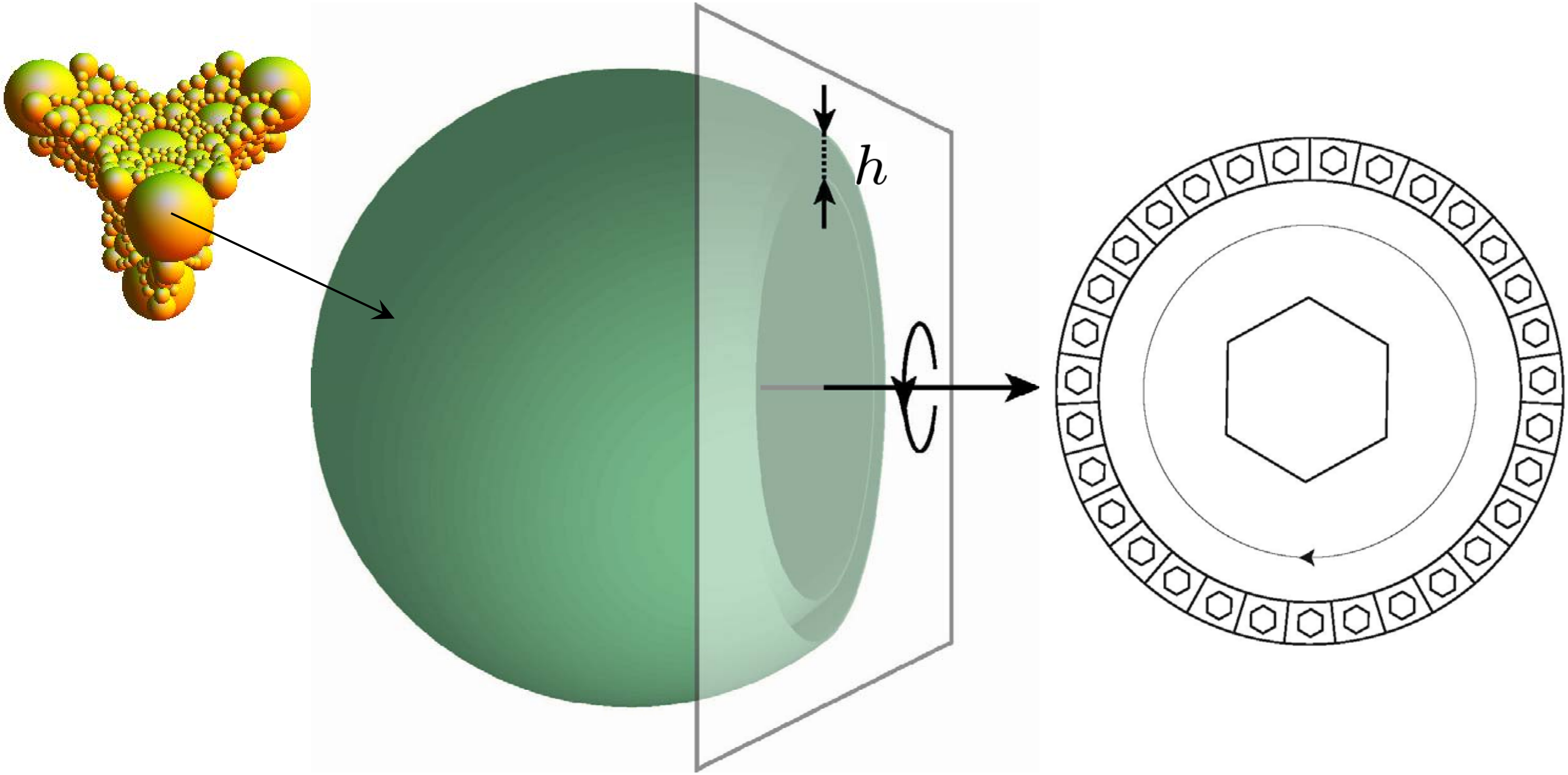
Dislocation cell structures

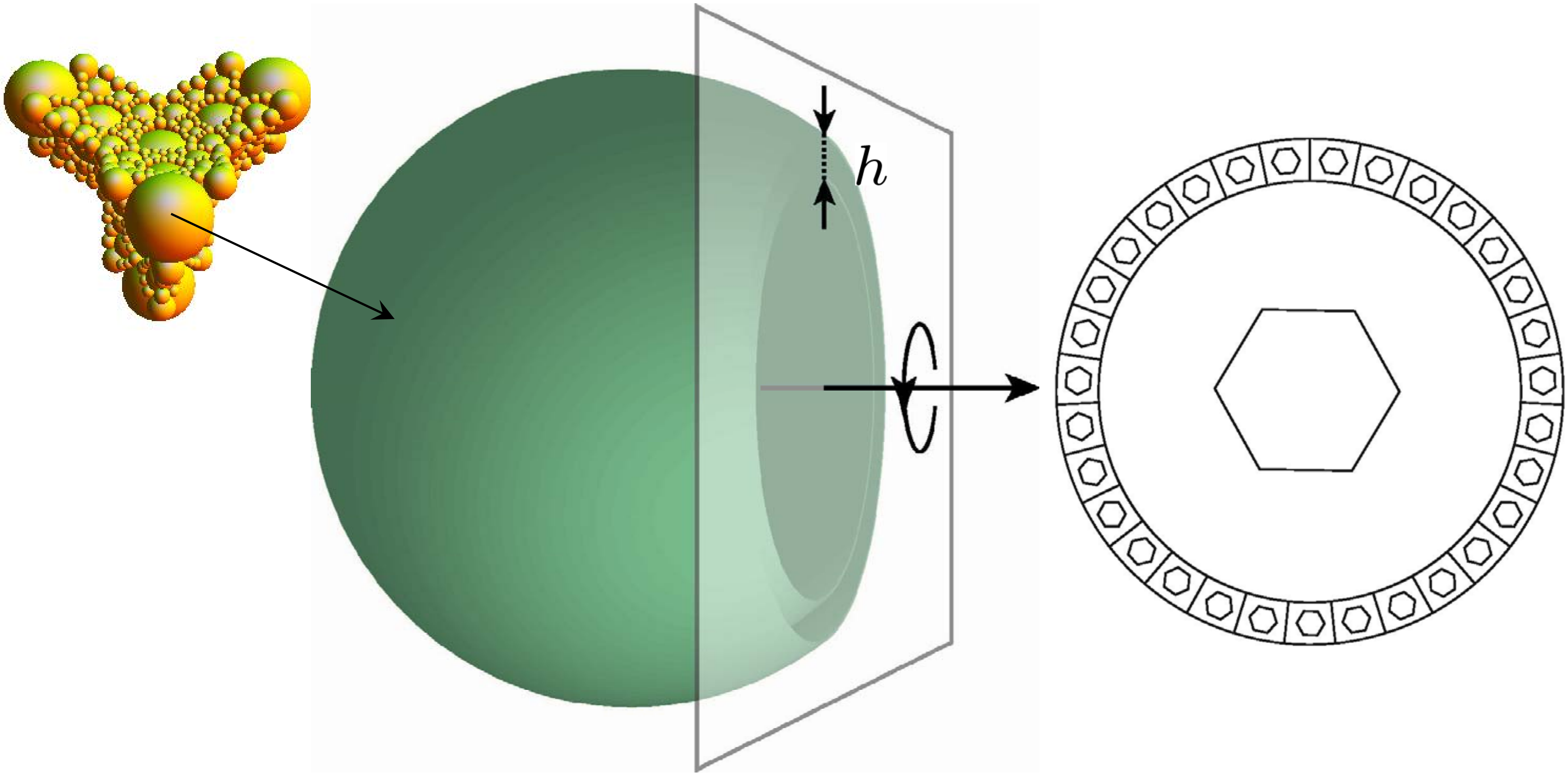


Dislocation cell structures



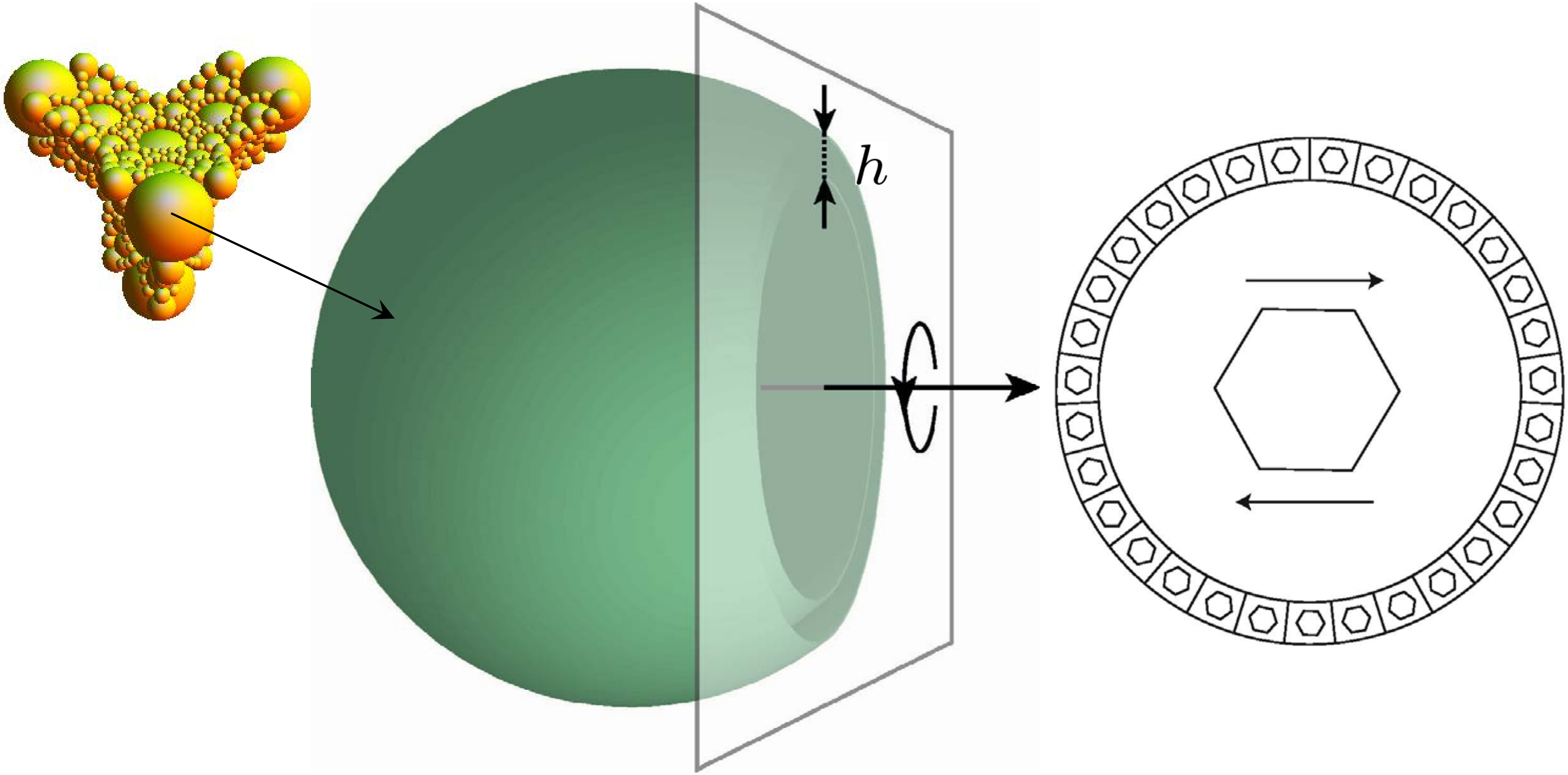
Step 1: Reorient cells for single slip

Dislocation cell structures



Step 1: Reorient cells for single slip $\Rightarrow W^p = 2q\tau_c\frac{\pi}{6}$

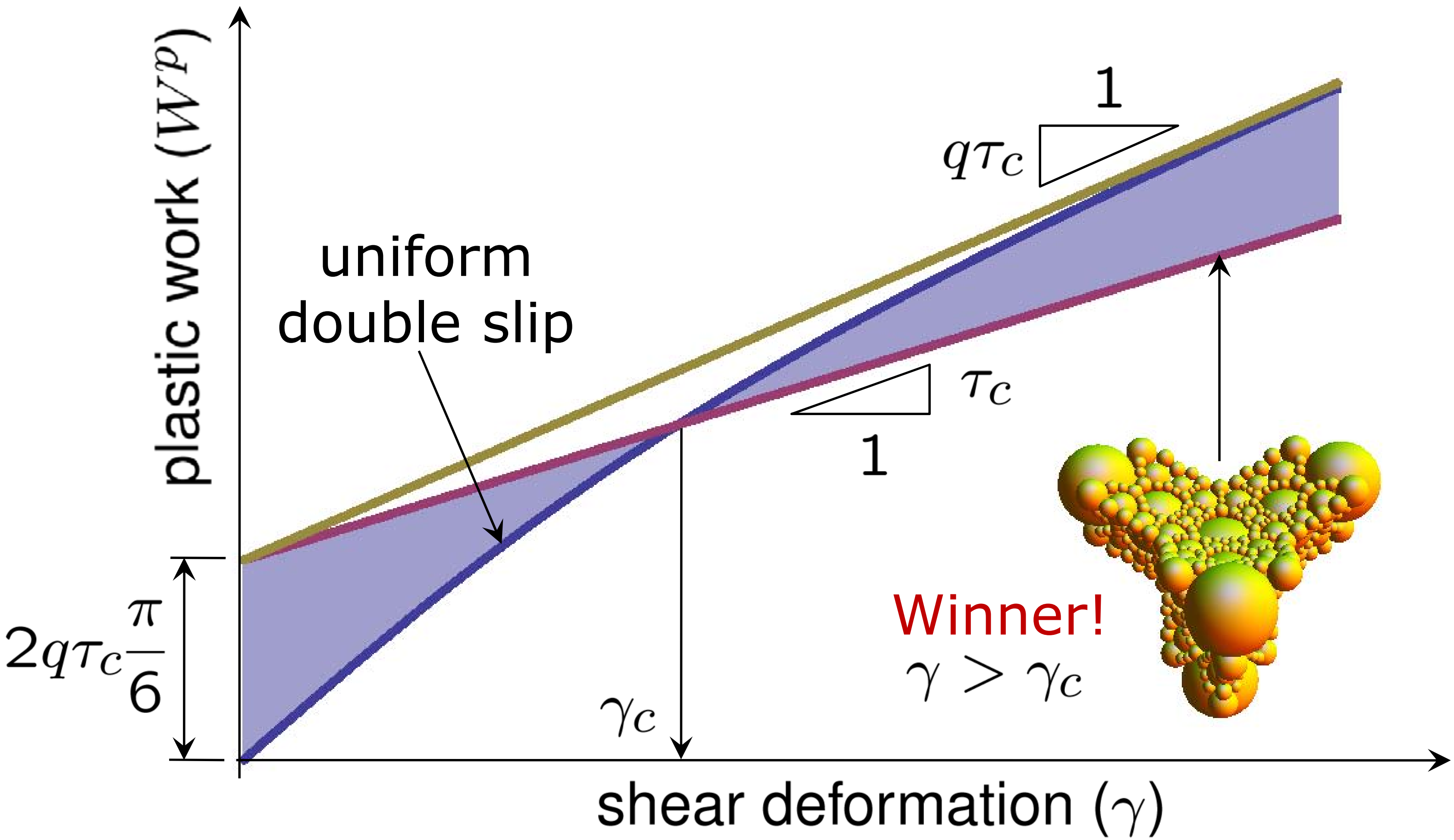
Dislocation cell structures



Step 1: Reorient cells for single slip $\Rightarrow W^p = 2q\tau_c\dfrac{\pi}{6}$

Step 2: Uniform single slip $\Rightarrow W^p = \tau_c\gamma$

Constructions – Cell structures



Simple shear on basal plane:
Uniform double slip *vs*. cell structure

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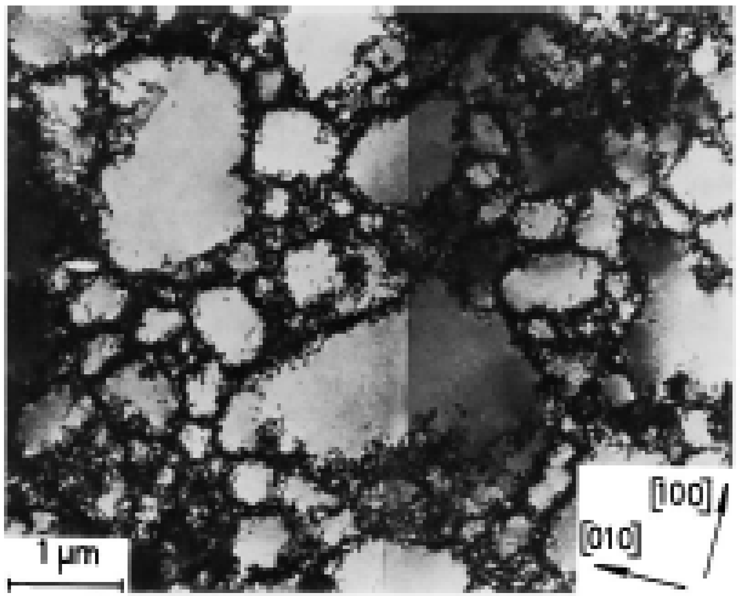
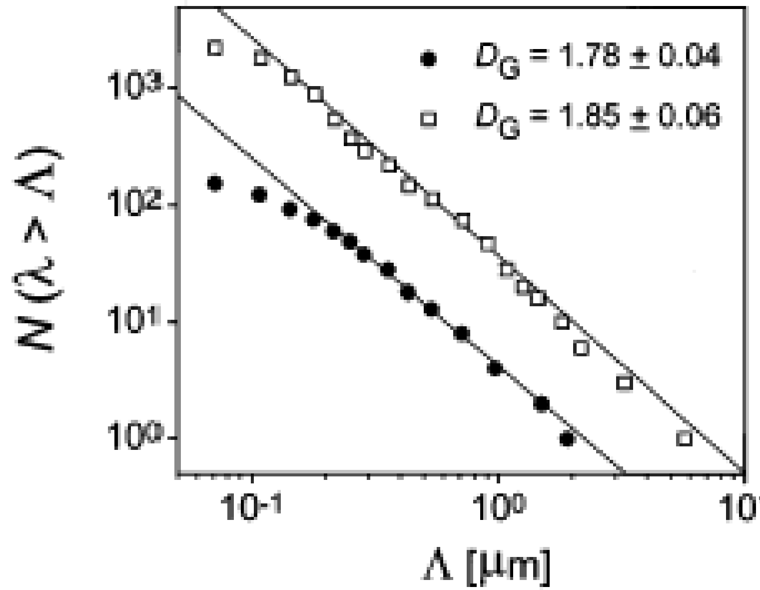
Dislocation structures – Fractality



TEM micrograph of dislocation cells of single copper deformed at 75.6MPa
(Mughrabi, et.al. 1986)

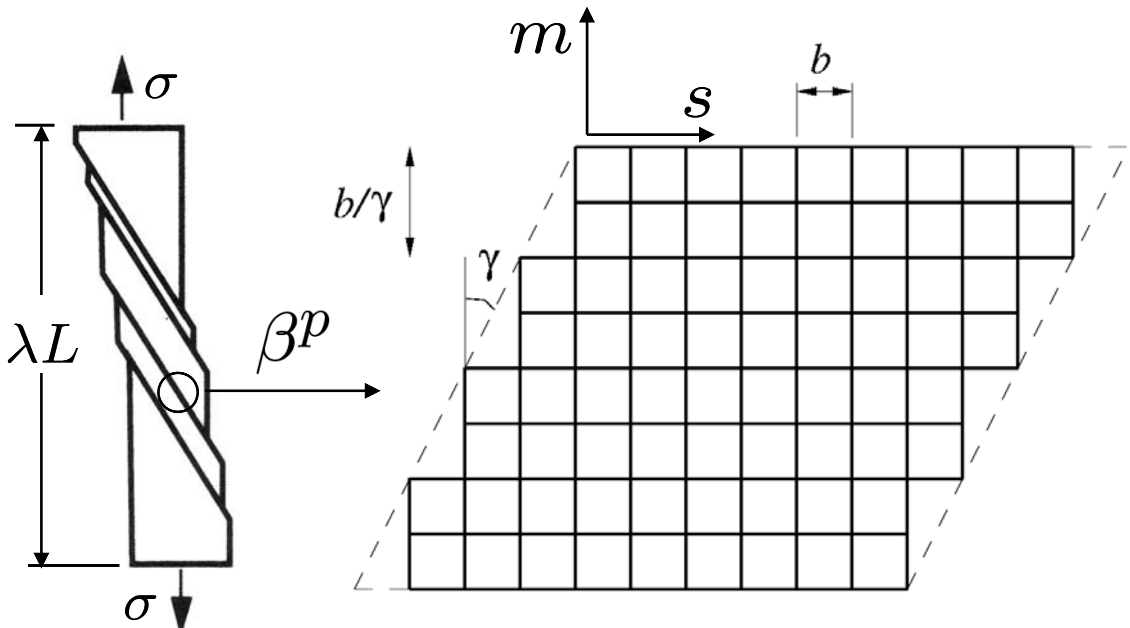


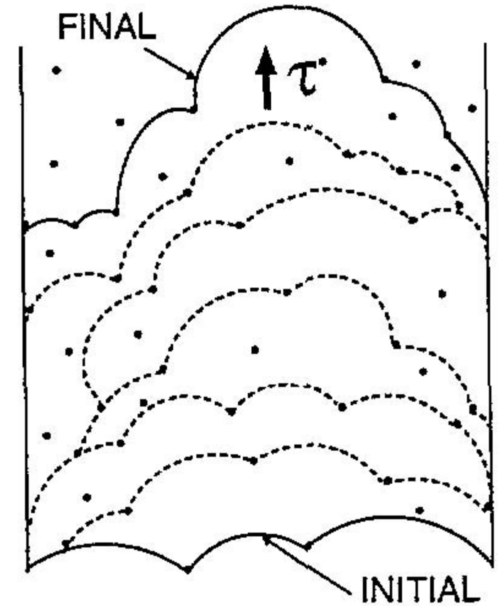
Cell distribution for deformed single crystal of copper and determination of the fractal dimension
(Hahner, et.al. 1998).

Fractal dimension of cuts of 3D sphere packings ~ 1.7—1.9!

(Lind, P.G., Baram, R.M. and Hermman, H.J., *Phys. Rev. E*, **77** (2008) 021304)

Crystal plasticity – Non local





- Kinematics: $\epsilon^p(\gamma) = \dfrac{1}{|\Omega|}\displaystyle\int_{J_u} [\![u]\!] \odot m \, d\mathcal{H}^2 \equiv \sum \gamma s \odot m$

- Energy: $E(u,\gamma) = \displaystyle\int_\Omega [\, W^e(\nabla u - \epsilon^p(\gamma)) + \underline{T\, |\nabla\gamma \times m|}\,]\, dx$

- Dissipation: $\psi(\dot\gamma) = \begin{cases} \tau_c |\dot\gamma|, & \text{if single slip,} \\ +\infty, & \text{otherwise.} \end{cases}$

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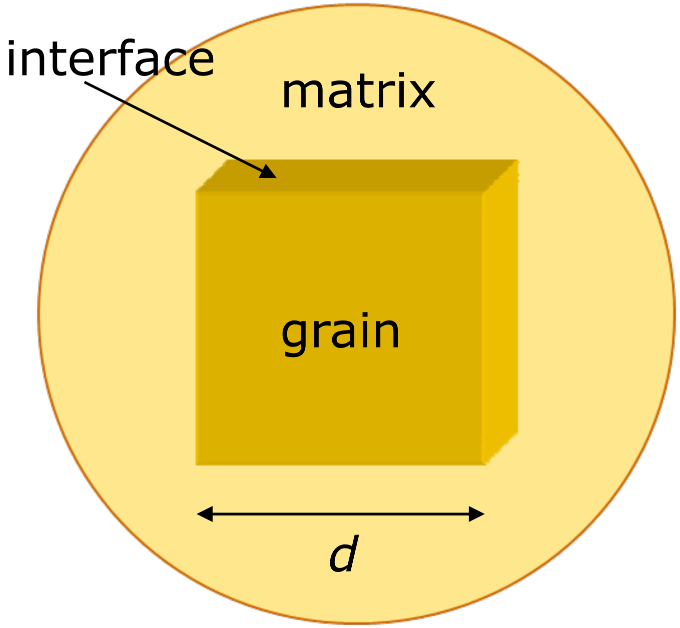
Nonlocal extension - Scaling

- Case study: Grain embedded in elastic matrix deforming in simple shear
- Assumptions:
  - *Cubic grain (d)*
  - *Collinear double slip (τ_c)*
  - *Antiplane shear deformation (γ)*
  - *Linear isotropic elasticity (G)*
  - *Compliant grain boundary (μ)*
  - *Infinite latent hardening*
- Objective: Find optimal upper and lower bounds



Grain in elastic matrix
(Conti, S. and Ortiz, M., *ARMA*, **176** (2005) 147)

$$cT^{\alpha_1}\gamma^{\alpha_2}\tau_c^{\alpha_3}\mu^{\alpha_4}d^{\alpha_5} \leq \inf F \leq c'T^{\alpha_1}\gamma^{\alpha_2}\tau_c^{\alpha_3}\mu^{\alpha_4}d^{\alpha_5}$$

macroscopic scaling laws!

Nonlocal extension - Scaling

Theorem (Conti & MO, *ARMA* '05) *There are constants* c, c' *such that*

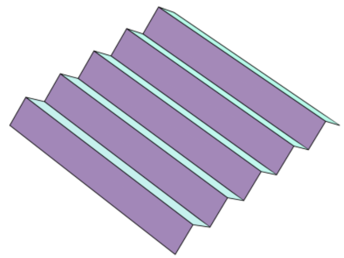
$$cF_0(T,\gamma,\tau_0,\mu,d) \leq \inf F \leq c' F_0(T,\gamma,\tau_0,\mu,d)$$

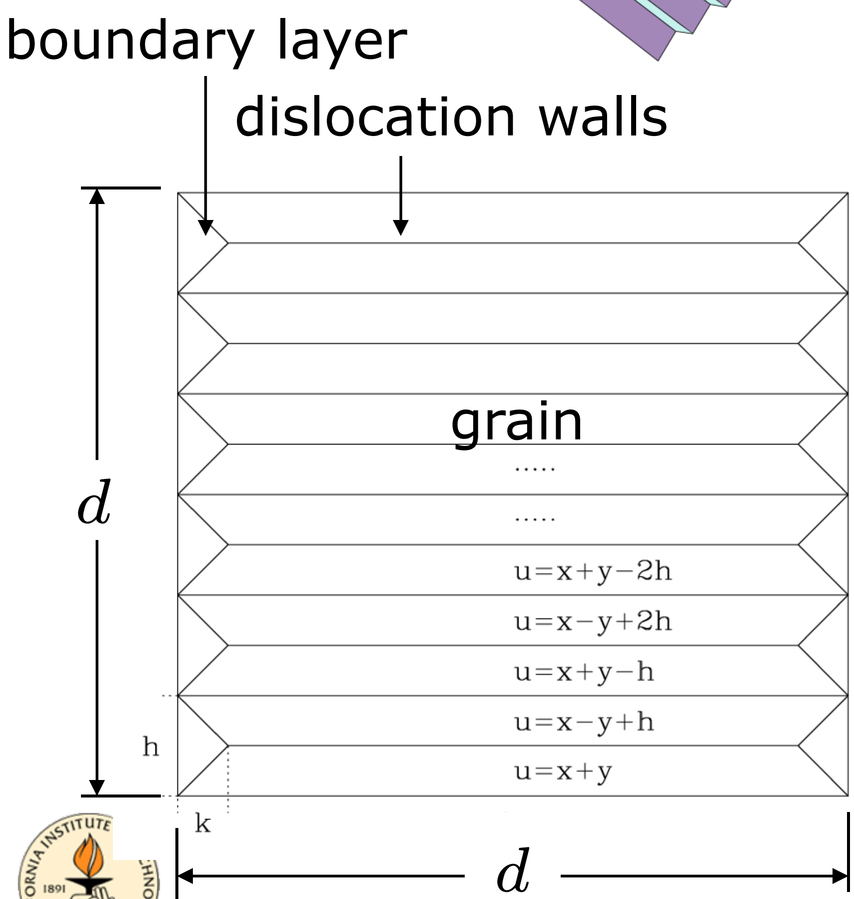
where $\quad F_0(T,\gamma,\tau_0,\mu,d)\Big/G\gamma^2 d^3 =$

$$\min\left\{1, \frac{\mu}{G}, \frac{\tau_0}{G\gamma} + \left(\frac{\mu}{G}\right)^{1/2}\left(\frac{T}{G\gamma bd}\right)^{1/2}, \frac{\tau_0}{G\gamma} + \left(\frac{T}{G\gamma bd}\right)^{2/3}\right\}$$

- Upper bounds determined by construction
- Lower bounds: Rigidity estimates, ansatz-free lower bound inequalities (Kohn and Müller '92, '94; Conti '00)

Optimal scaling – Laminate construction





- Energy:

$$W \equiv \frac{F_0}{d^3} \sim \tau_c \gamma + \left(\frac{\mu T \gamma^3}{bd} \right)^{1/2}$$

- Yield stress:

$$\tau \equiv \frac{\partial W}{\partial \gamma} \sim \tau_c + \frac{1}{2} \left(\frac{\mu T \gamma}{bd} \right)^{1/2}$$

parabolic hardening + Hall-Petch scaling

- Lamellar width:

$$l \sim \left(\frac{Td}{G\gamma b} \right)^{1/2}$$

refinement with strain!

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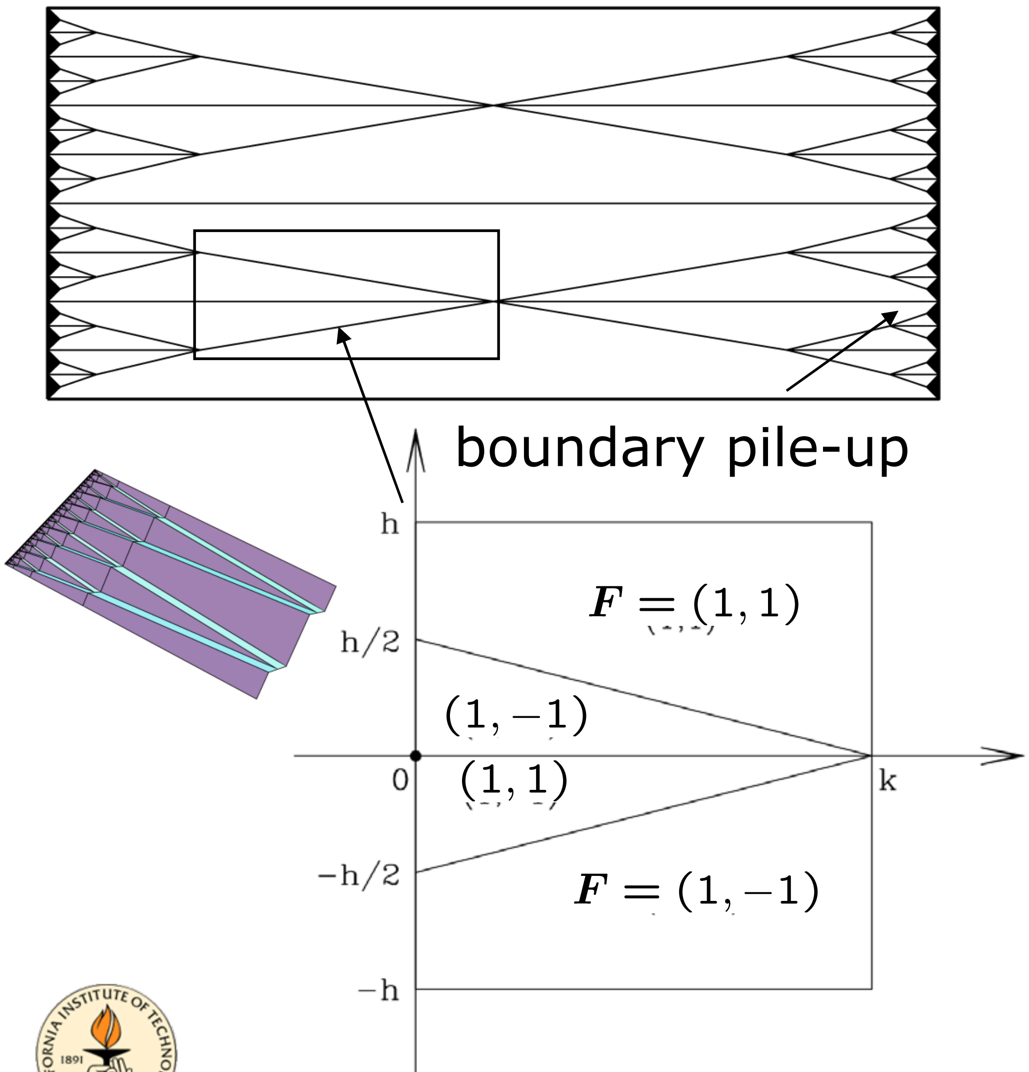
Optimal scaling – Branching construction



- Energy:

$$W \sim \tau_c \gamma + G \left(\frac{T\gamma^2}{Gbd} \right)^{2/3}$$

- Yield stress:

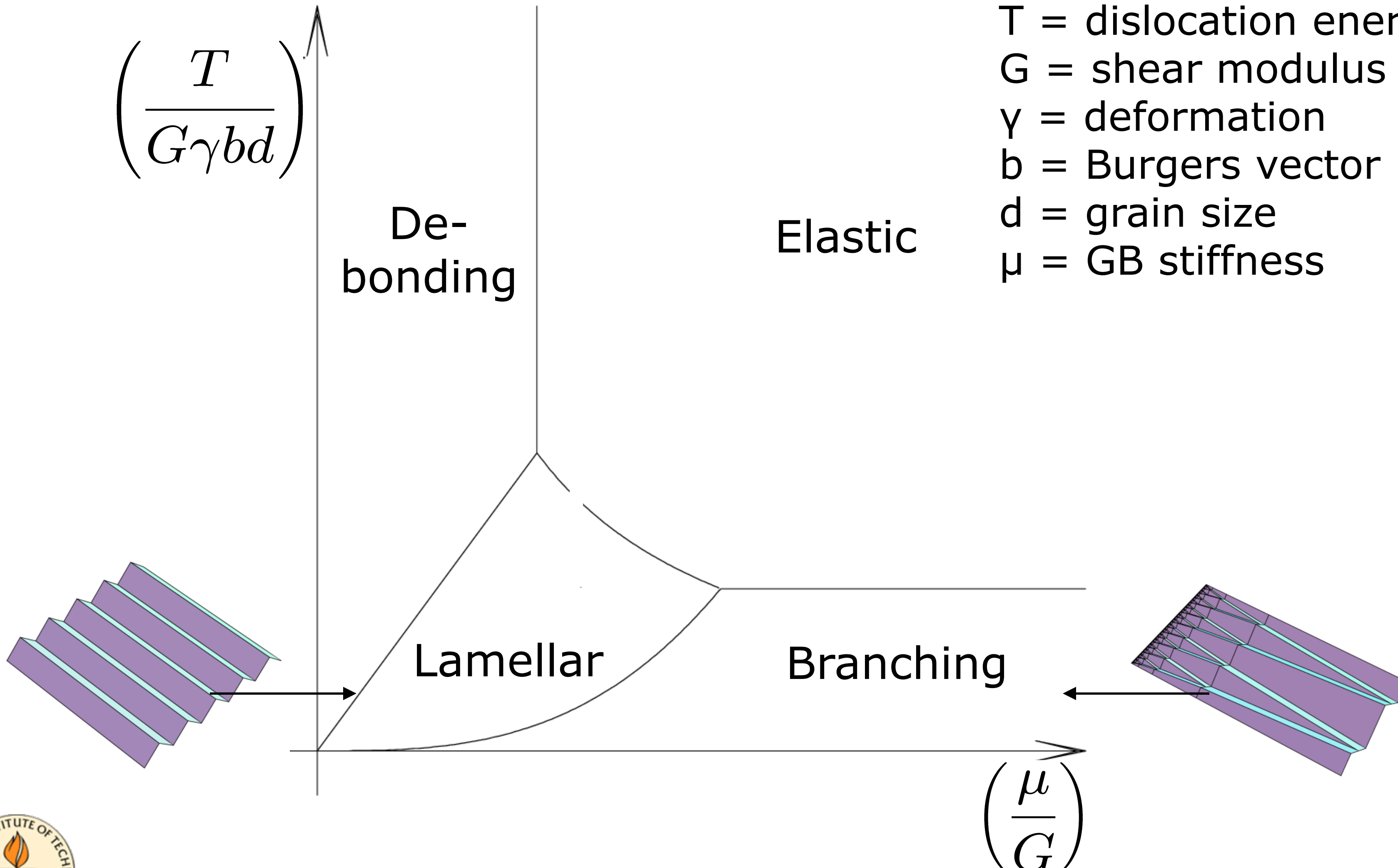
$$\tau \sim \tau_c + \left(\frac{T}{bd} \right)^{2/3} (G\gamma)^{1/3}$$

- Microstructure size:

$$l \sim \left(\frac{Td^2}{G\gamma b} \right)^{1/3}$$

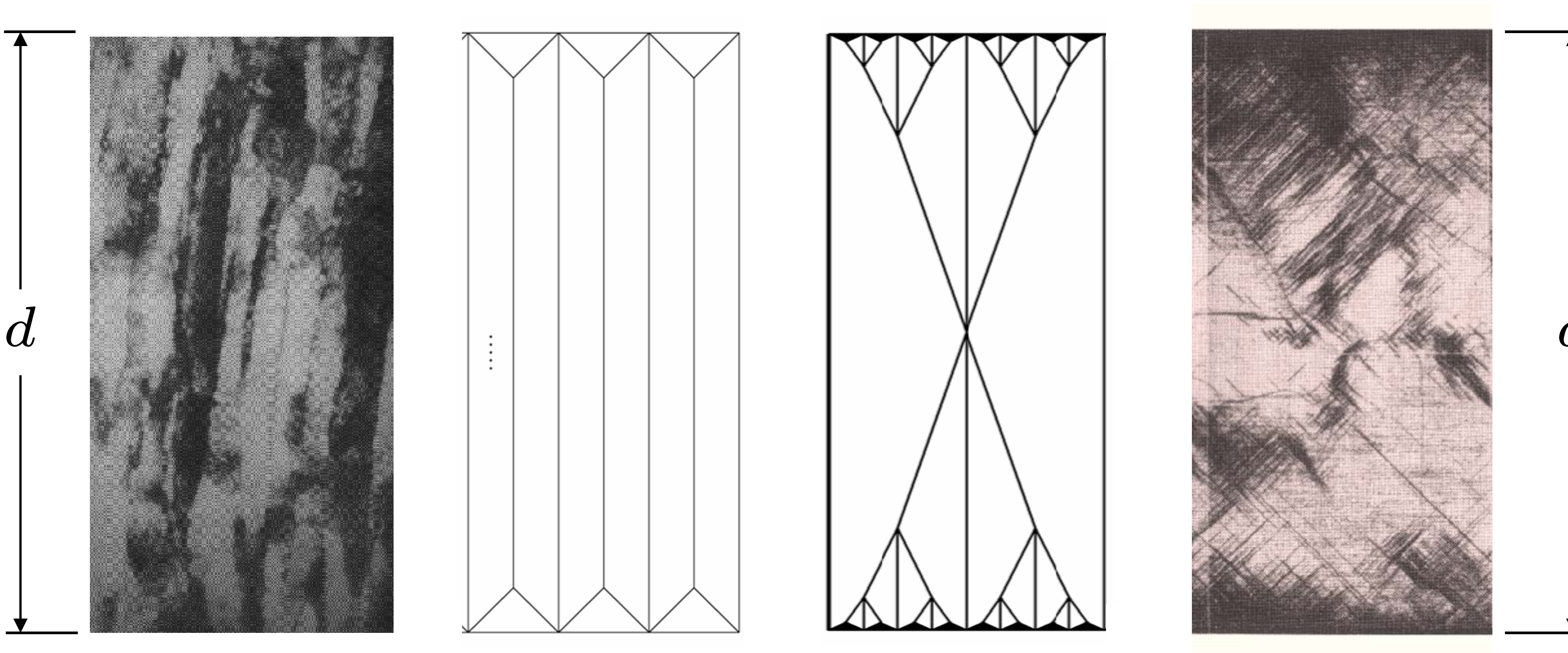
refinement with strain!

Optimal scaling – Mechanism map



T = dislocation energy
G = shear modulus
γ = deformation
b = Burgers vector
d = grain size
μ = GB stiffness

Optimal scaling – Microstructures



Shocked Ta (Meyers et al ´95) | Laminate $\tau \sim d^{-1/2}$ | Branching $\tau \sim d^{-2/3}$ | LiF impact (Meir and Clifton ´86)

Dislocation structures corresponding to the lamination and branching constructions

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Concluding remarks

- Within the framework of deformation theory of crystal plasticity there is a strong connection between non-convexity, non-locality, subgrain microstructures and macroscopic scaling relations
- Relaxation constructions match many observed sub-grain microstructures
- Scaling relations such as Taylor, Hall-Petch, are a manifestation of the non-locality introduced by the dislocation line energy
- Exact relaxations provide 'perfect' multiscale models for use, e.g., in numerical calculations
- Many problems of interest remain open:
  - *General relaxation accounting for finite kinematics*
  - *Microstructural evolution for arbitrary loading paths*
  - *…*