Nonconvex Plasticity and Microstructure

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Rodney Hill Prize Lecture

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Dedicated to Rodney Hill

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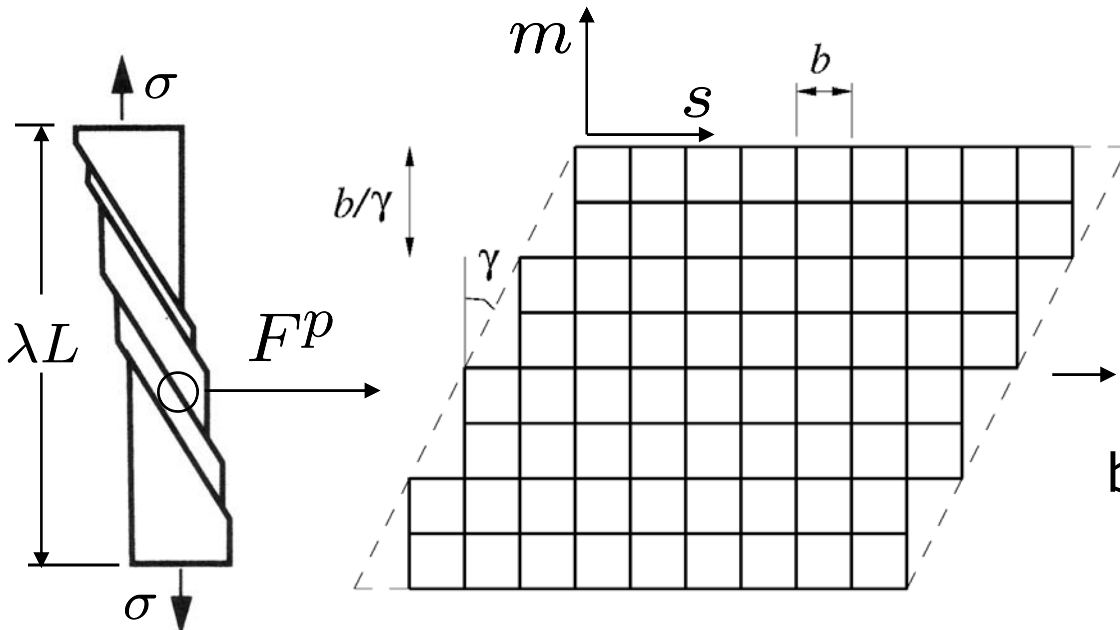
Dedicated to Rodney Hill

- "*Dr. Rodney Hill is widely regarded as among the foremost contributors to the foundations of solid mechanics over the second half of the 20th century. His early work was central to founding the* ***mathematical theory of plasticity****. This deep interest led eventually to general studies of* ***uniqueness and stability*** *in nonlinear continuum mechanics, work which has had a profound influence on the field of solid mechanics - theoretical, computational and experimental alike - over the past decades.*" (Excerpted from the ICTAM 2008 program)

Classical (convex) plasticity

- Plasticity's early development focused on establishing the elastic limit of materials → yield surface, elastic domain (Tresca, Coulomb, Föppl, Voigt, Huber, Mohr, Hencky, Prandtl, von Mises, Timoshenko…)
- The flow theory was formalized by Bishop, Nadai, **Hill**, Drucker, Prager…
- Heavy emphasis was placed on ensuring existence and uniqueness of solutions of the rate problem
- Drucker's postulates: **Convexity** of free energy (hardening) + **convexity** of elastic domain

Crystal plasticity – Deformation theory



Irreversible accommodation of shear deformation by crystallographic slip

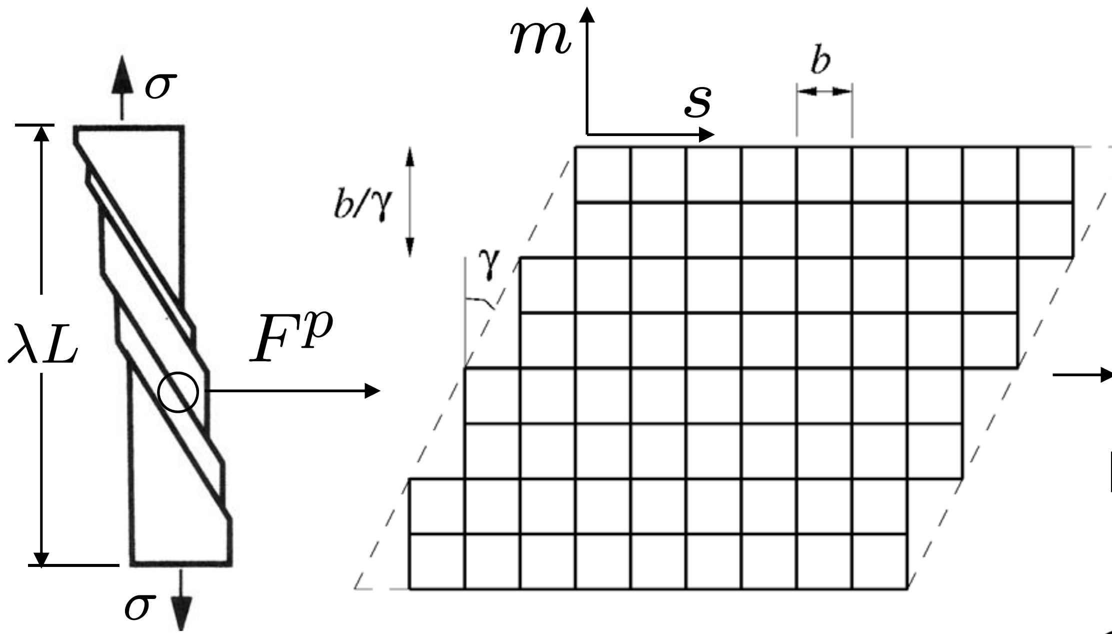
- Incremental flow rule: $F^p = \exp\left\{\sum \gamma s \otimes m\right\}$
- Pseudo-elastic strain energy density:

$$W(F) = \inf_{\gamma \geq 0} \left\{W^e(F\,F^{p-1}) + W^p(\gamma)\right\}$$

- Variational problem (static equilibrium):

$$F(y) = \int_\Omega W(\nabla y)\, dx + \text{forcing terms} \to \text{inf!}$$

Crystal plasticity – Deformation theory



Irreversible accommodation of shear deformation by crystallographic slip

- Incremental flow rule: $\epsilon^p = \text{sym}\left\{\sum \gamma s \otimes m\right\}$
- Pseudo-elastic strain energy density:

$$W(\epsilon) = \inf_{\gamma \geq 0} \{W^e(\epsilon - \epsilon^p) + W^p(\gamma)\}$$

- Variational problem (static equilibrium):

$$F(u) = \int_\Omega W(\epsilon(u))\, dx + \text{forcing terms} \to \text{inf!}$$

Convex crystal plasticity

- Pseudo-elastic energy density:

$$W(\epsilon) = \inf_{\gamma \geq 0} \{ W^e(\epsilon(u) - \epsilon^p(\gamma)) + \underbrace{W^p(\gamma)} \}$$

- Drucker's postulates: Convex!
- Convexity + growth $\Rightarrow$ **Existence + uniqueness**

Theorem Let W be strictly convex and coercive: $W(\epsilon) \geq \alpha_1 |\epsilon|^p - \alpha_2$. Then, the variational Dirichlet problem

$$\inf_{u \in u_0 + W_0^{1,p}(\Omega)} \int_\Omega W(\epsilon(u)) dx$$

has one solution.

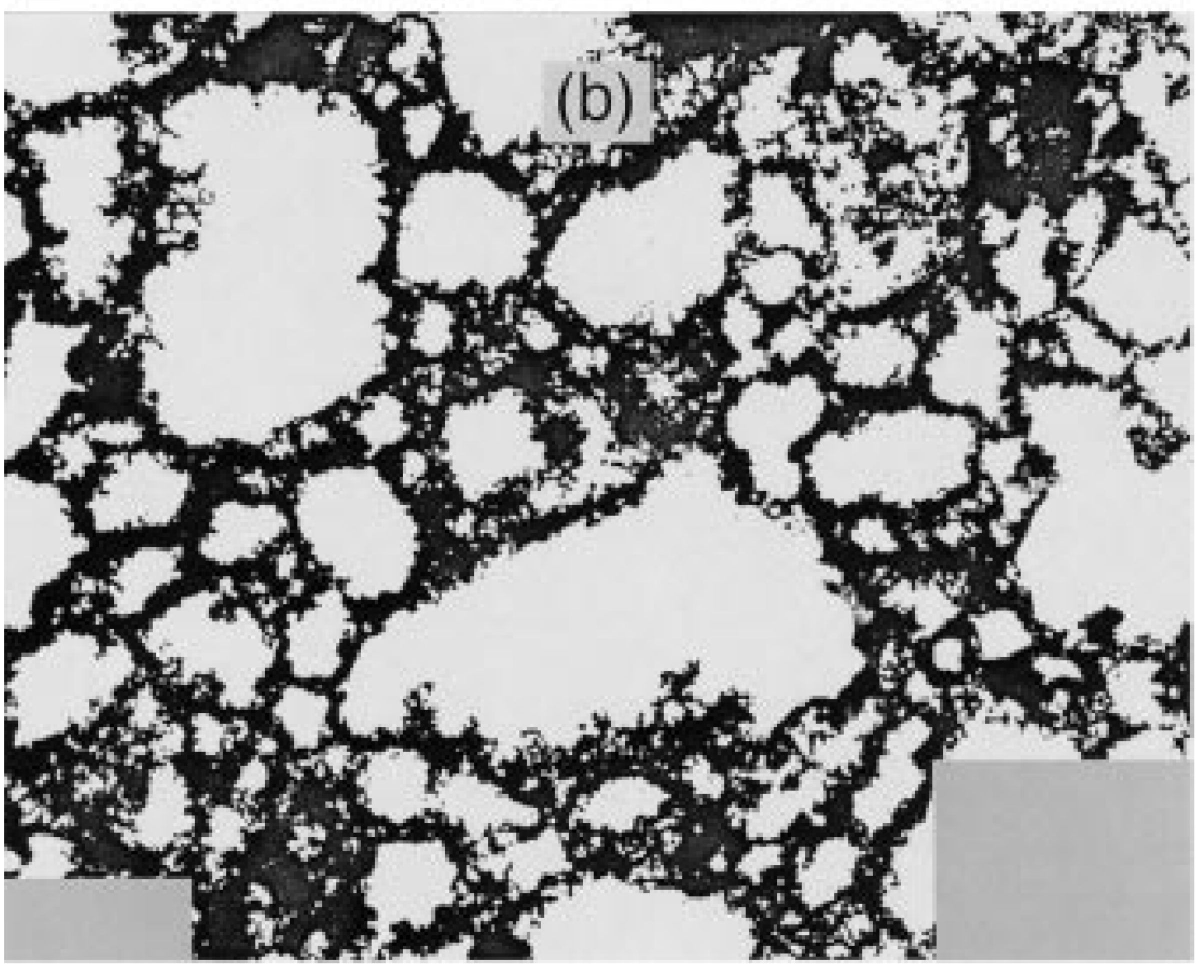
Convex crystal plasticity

But reality looks nothing like!

"How empty is theory in the presence of fact!"

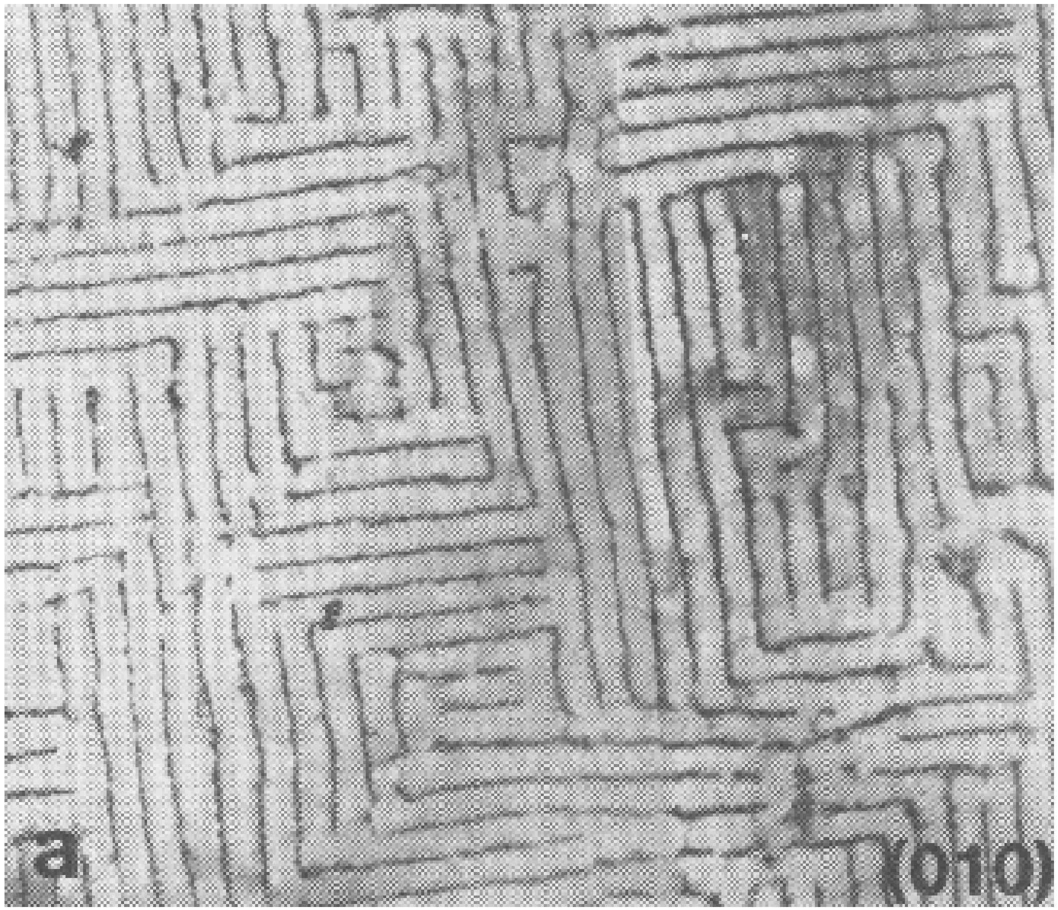
-- Mark Twain

Dislocation structures – Cells



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

Dislocation structures – Fatigue



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

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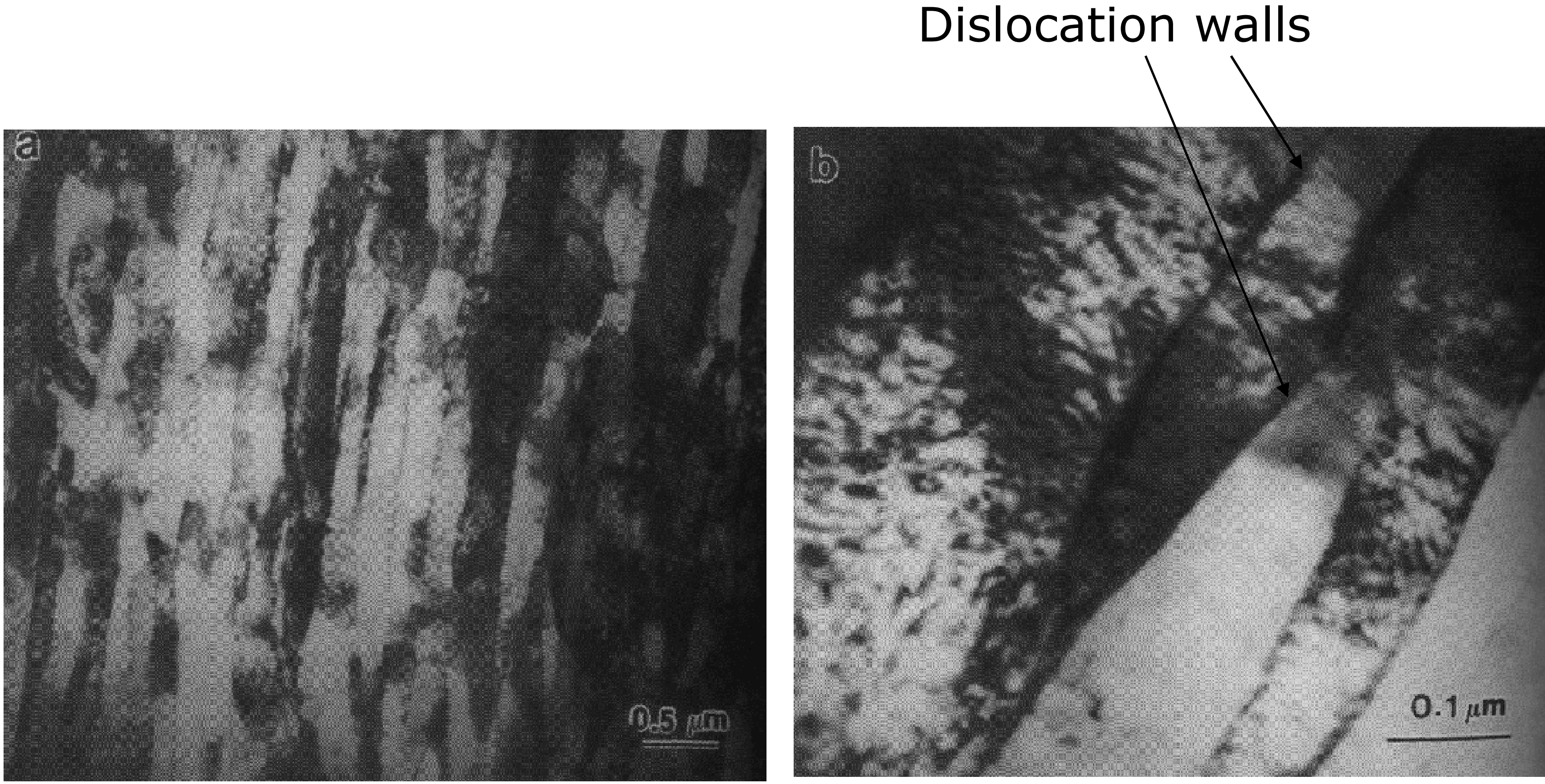
Dislocation structures – Lamellar



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

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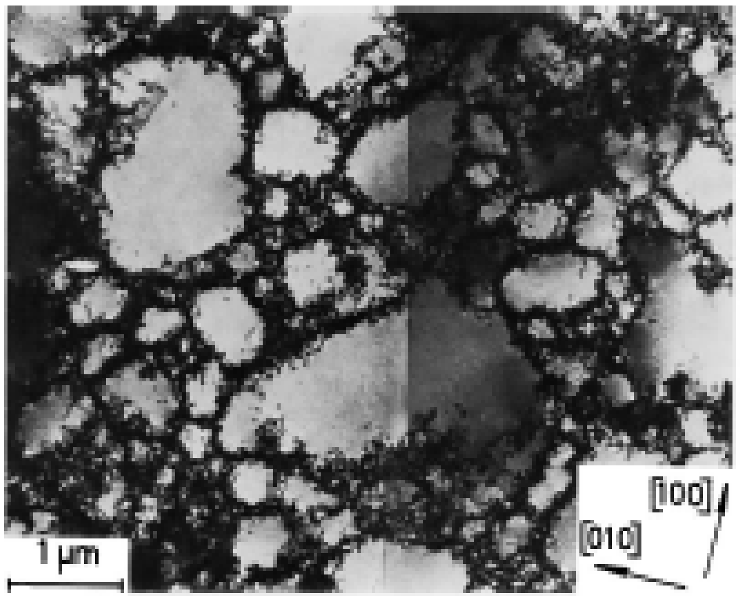
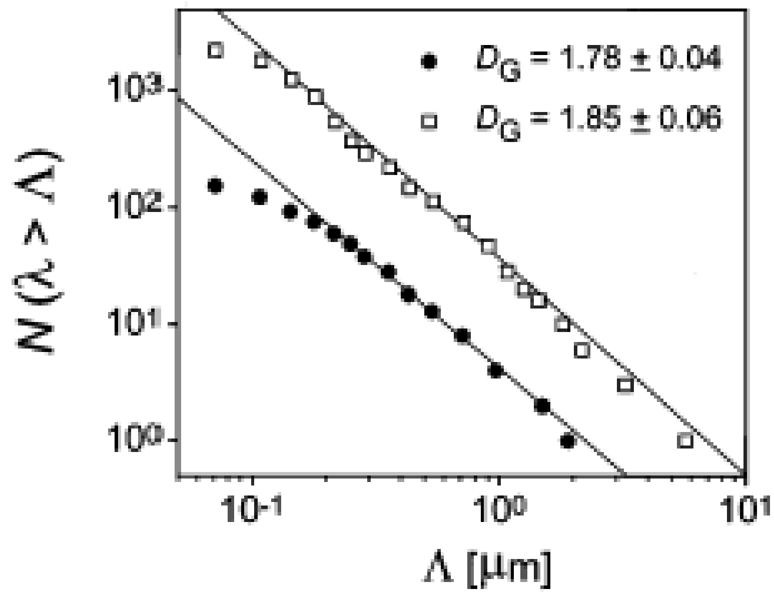
Dislocation structures – Fractality



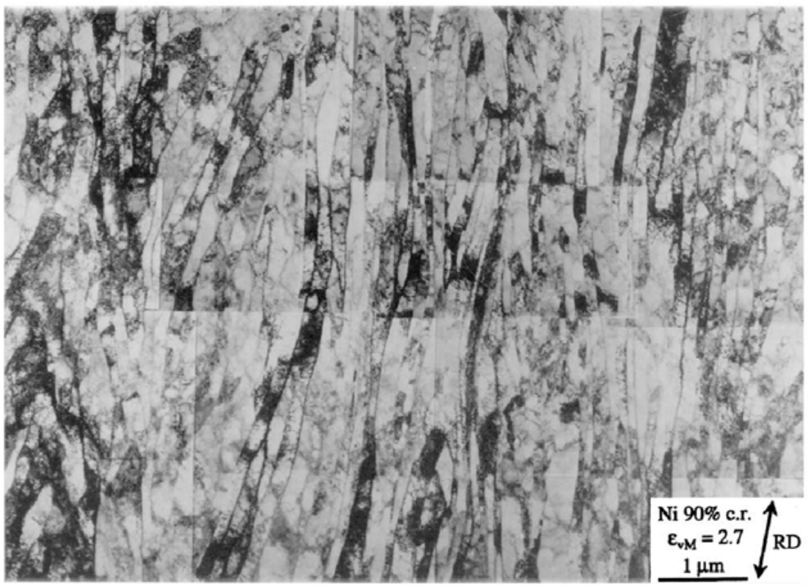
TEM micrograph of dislocation cells of single copper deformed at 75.6MPa
(Mughrabi *et al.*, 1986)



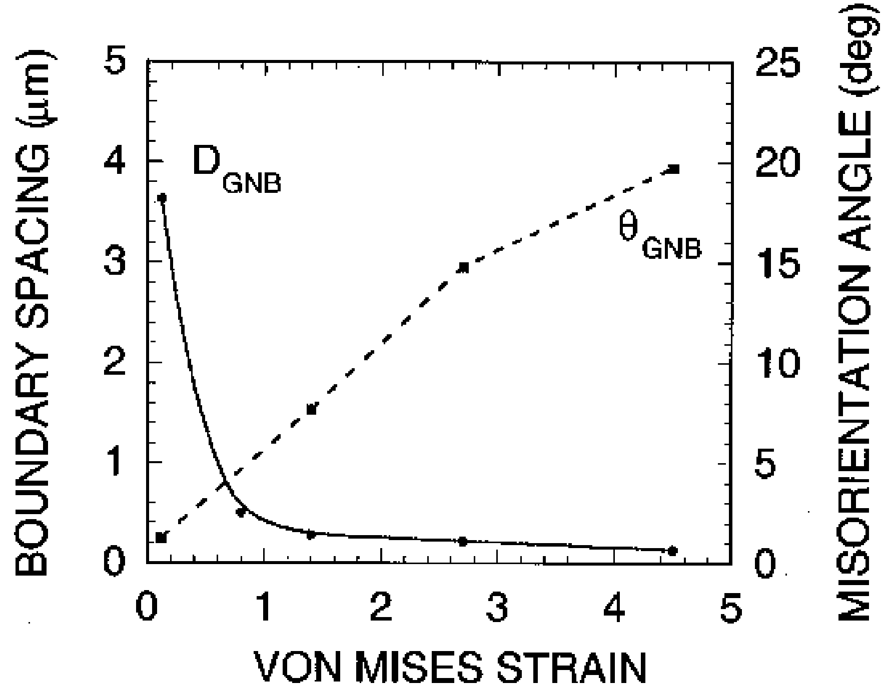
Cell distribution for deformed single crystal of copper and determination of the fractal dimension
(Haehner *et al.*, 1998).

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



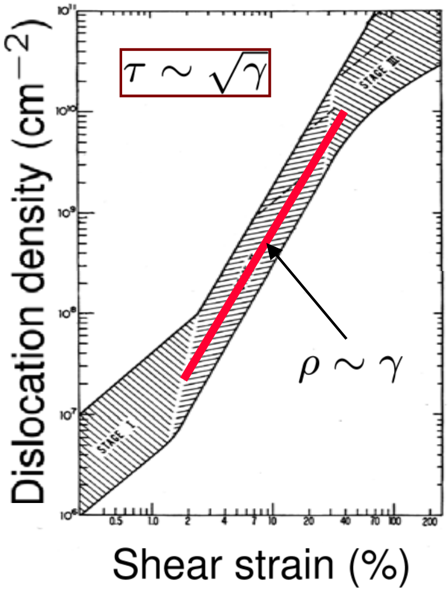
Pure nickel cold rolled to 90%
Hansen *et al., Mat. Sci. Engin*. A**317** (2001).



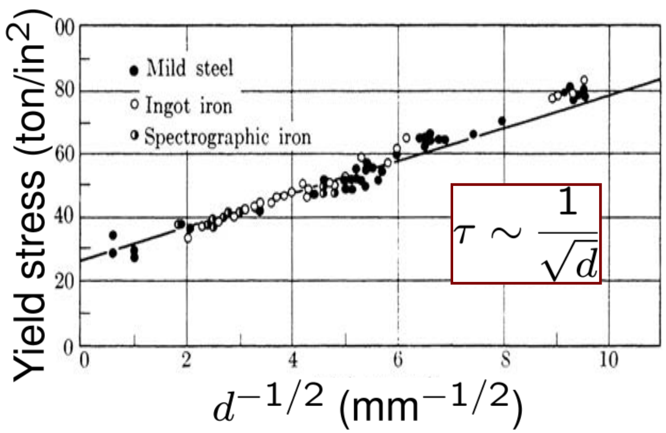
Lamellar width and misorientation angle as a function of deformatation
Hansen *et al., Mat. Sci. Engin*. A**317** (2001).

Scaling of lamellar width and misorientation angle with deformation

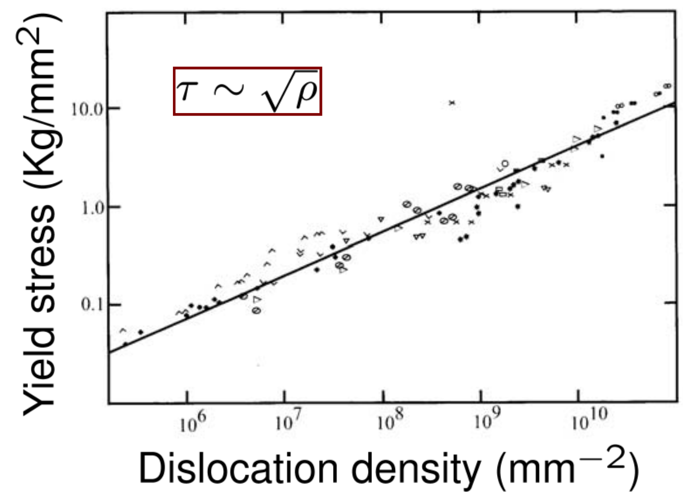
Dislocation structures – Scaling



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.)



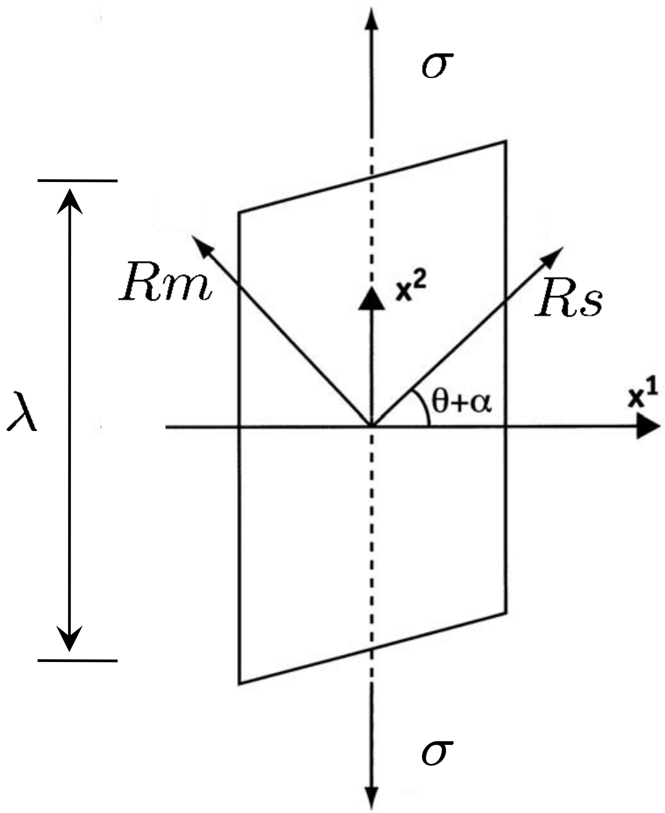
Taylor scaling
(SJ Basinski and ZS Basinski,
Dislocations in Solids,
FRN Nabarro (ed.)
North-Holland, 1979.)

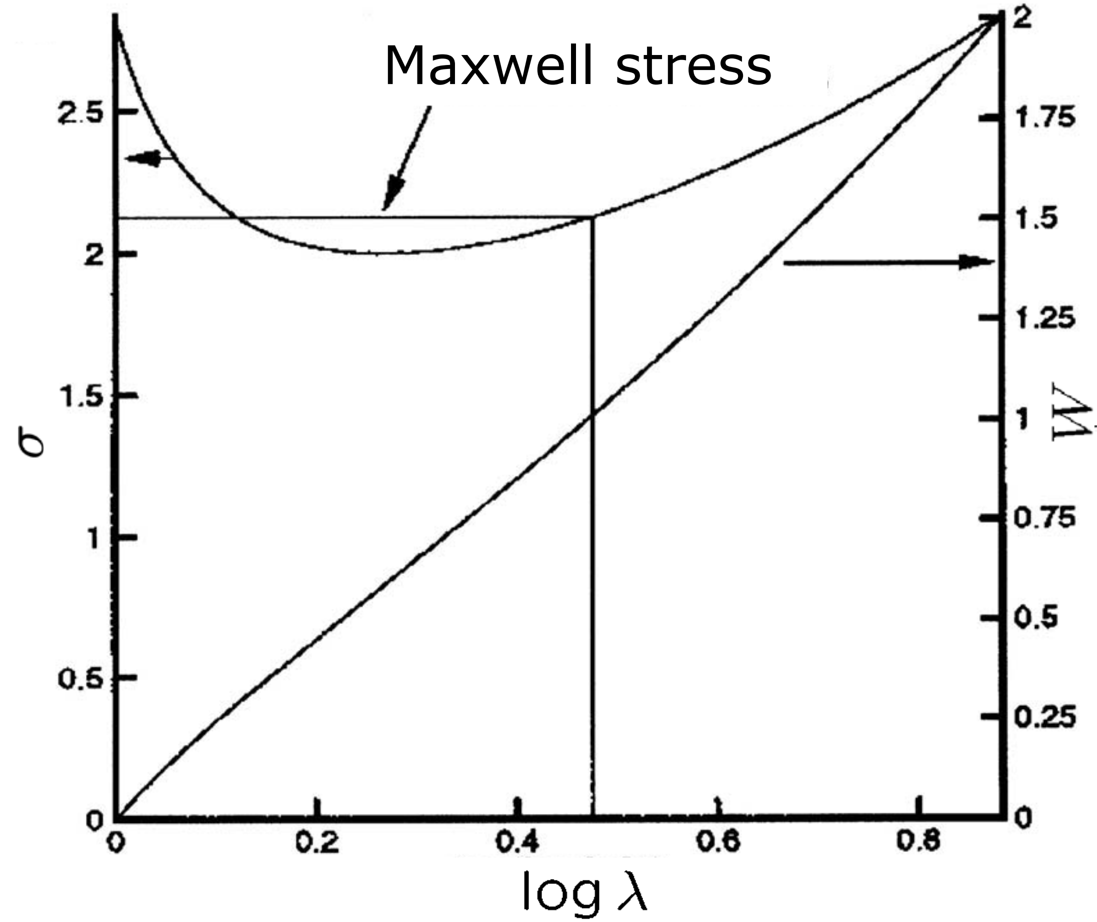
The classical scaling laws of single crystal plasticity

Non-convex non-local plasticity

- Druckerian (convex) plasticity is inconsistent with observation at the subgrain level
- Ubiquitous observation of subgrain dislocation structures strongly suggests that single crystal plasticity is **non-convex**
- Robust scaling relations strongly suggest that single crystal plasticity in **non-local**
- **Questions:**
  - *What are the physical sources of non-convexity, non-locality, in single crystals?*
  - *Connection between material stability, well-posedness of the equilibrium problem, microstructure, scaling behavior?*

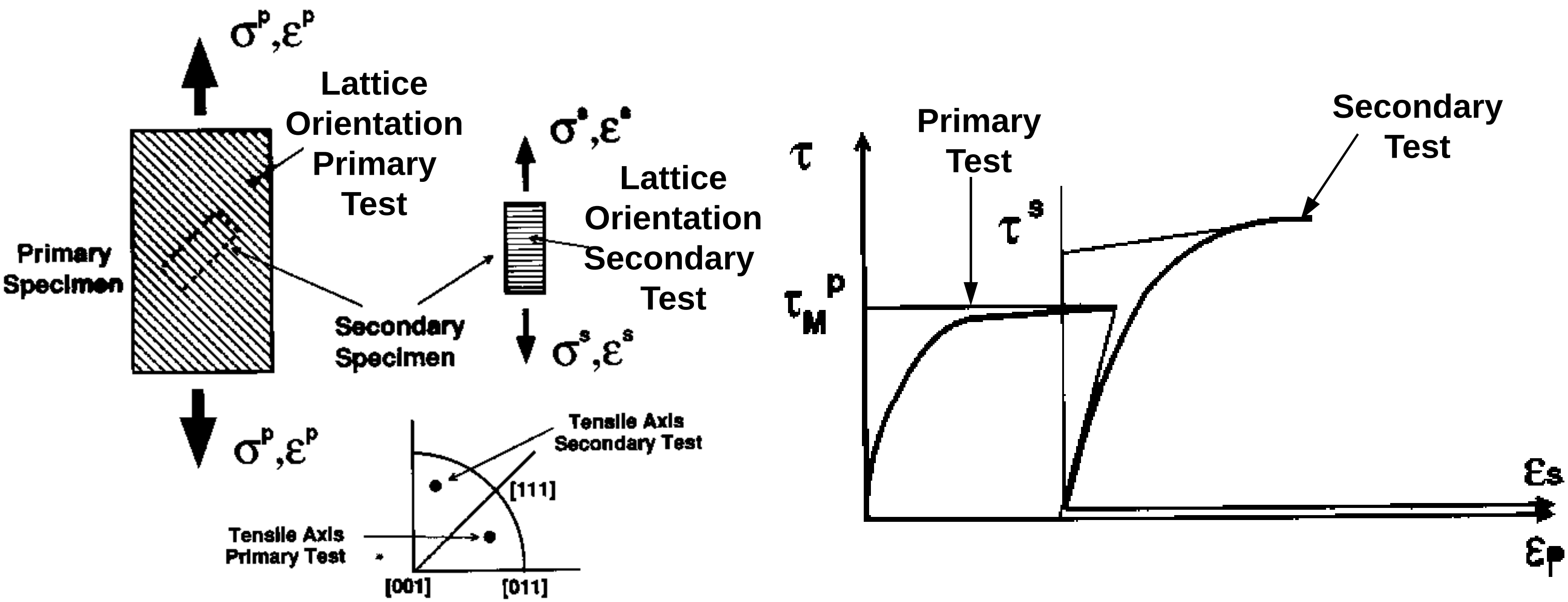
Non-convexity – Geometrical softening





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

Non-convexity - Strong latent hardening



Latent hardening experiments

UF Kocks, *Acta Metallurgica*, **8** (1960) 345

UF Kocks, *Trans. Metall. Soc. AIME*, **230** (1964) 1160

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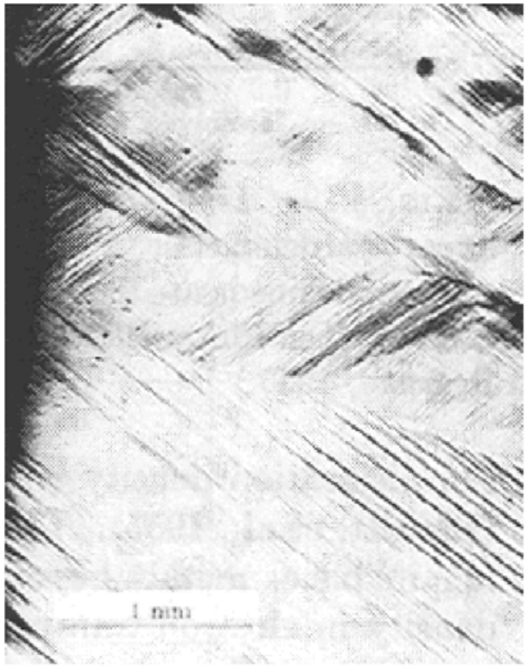
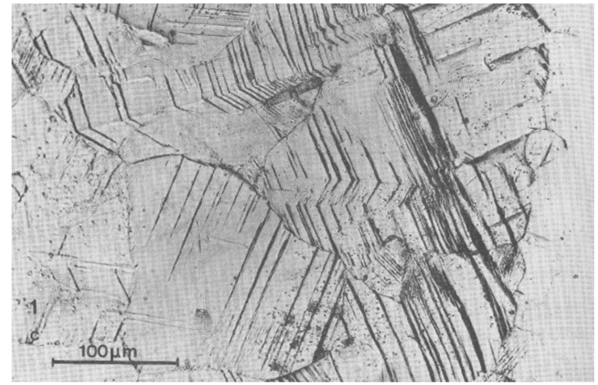
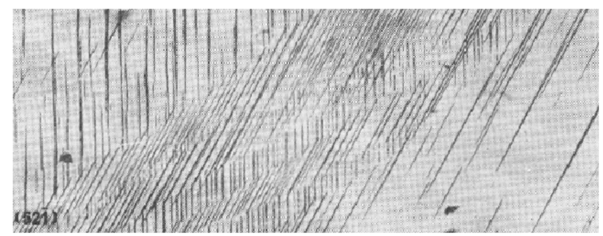
Non-convexity - Strong latent hardening



(Saimoto, 1963)



(Ramussen and Pedersen, 1980)

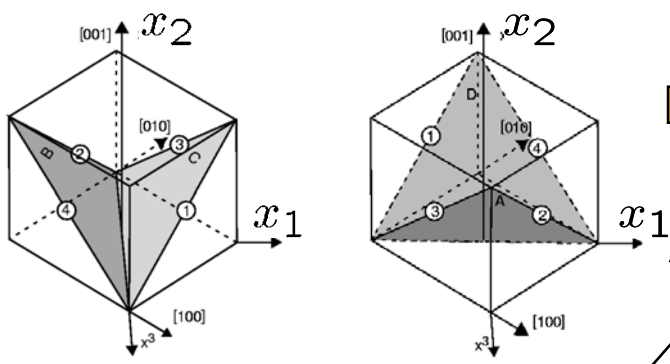


(Jin and Winter, 1984)

- **Latent hardening**: *"These results prove the reality of latent-hardening, in the sense that the slip lines of one system experience difficulty in breaking through the active slip lines of the other one"* (Piercy, G. R., Cahn, R. W., and Cottrell, A. H., *Acta Metallurgica*, **3** (1955) 331-338).

Non-convexity - Strong latent hardening

- Linear hardening: $W^p = \tau_0 \sum_\alpha \gamma^\alpha + \sum_\alpha \sum_\beta h_{\alpha\beta}\gamma^\alpha\gamma^\beta$
- Example: FCC crystal deforming on $(1\bar{1}0)$-plane

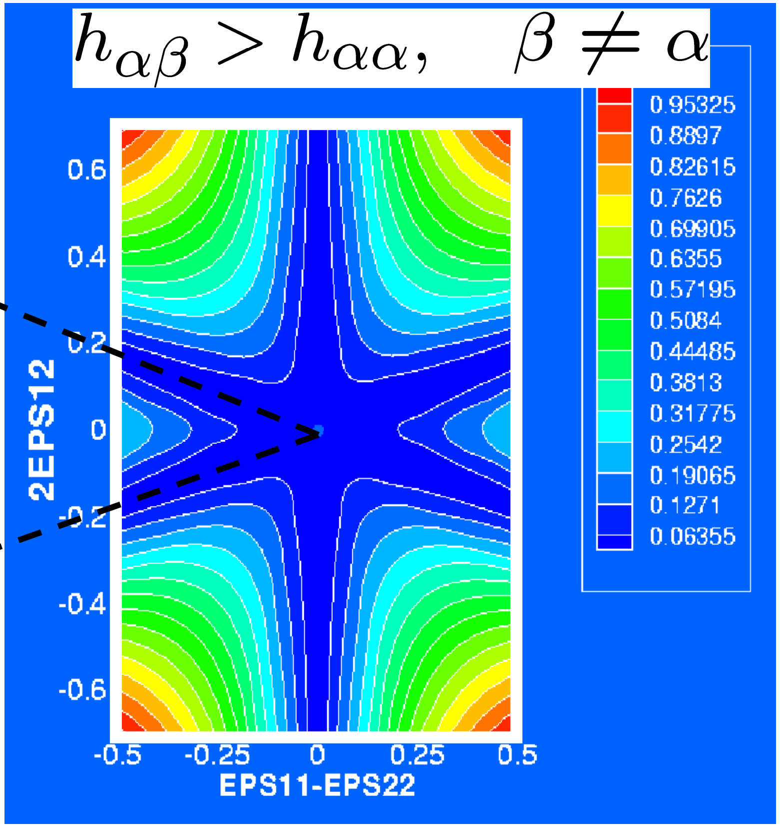


$\beta^p \in \gamma s \otimes m + so(3)$

(Single slip)

- $W(\nabla u)$ non-convex!

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



$W(\nabla u)$

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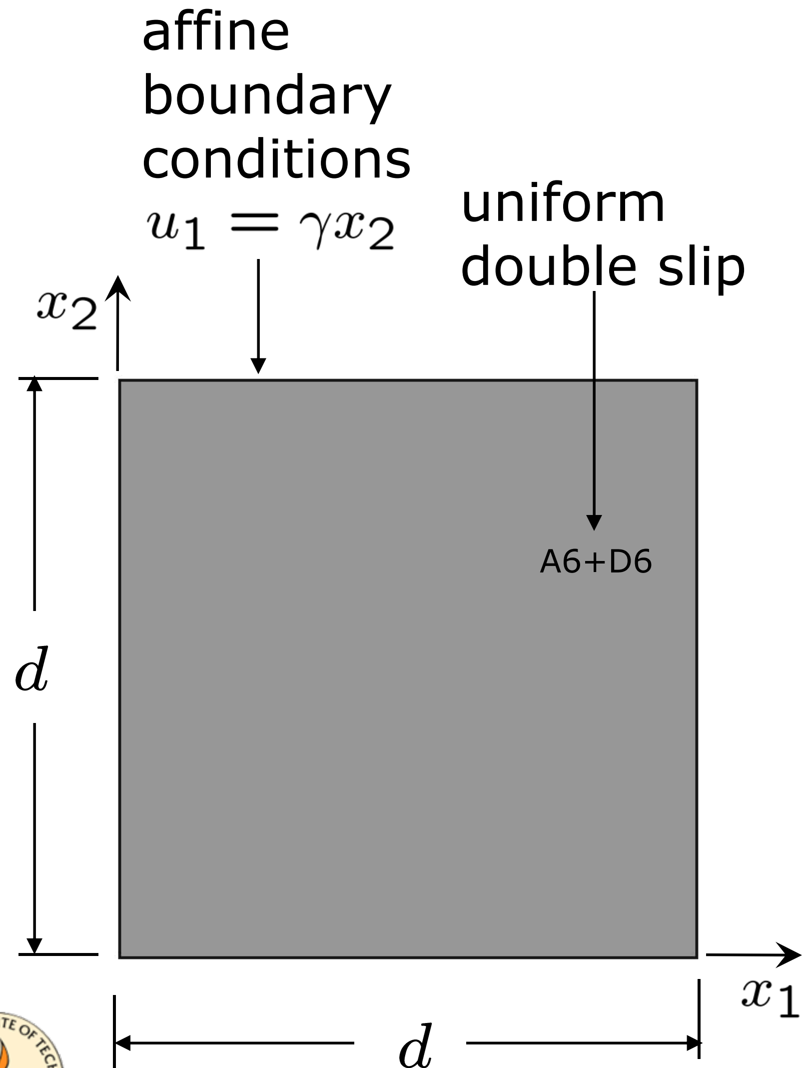
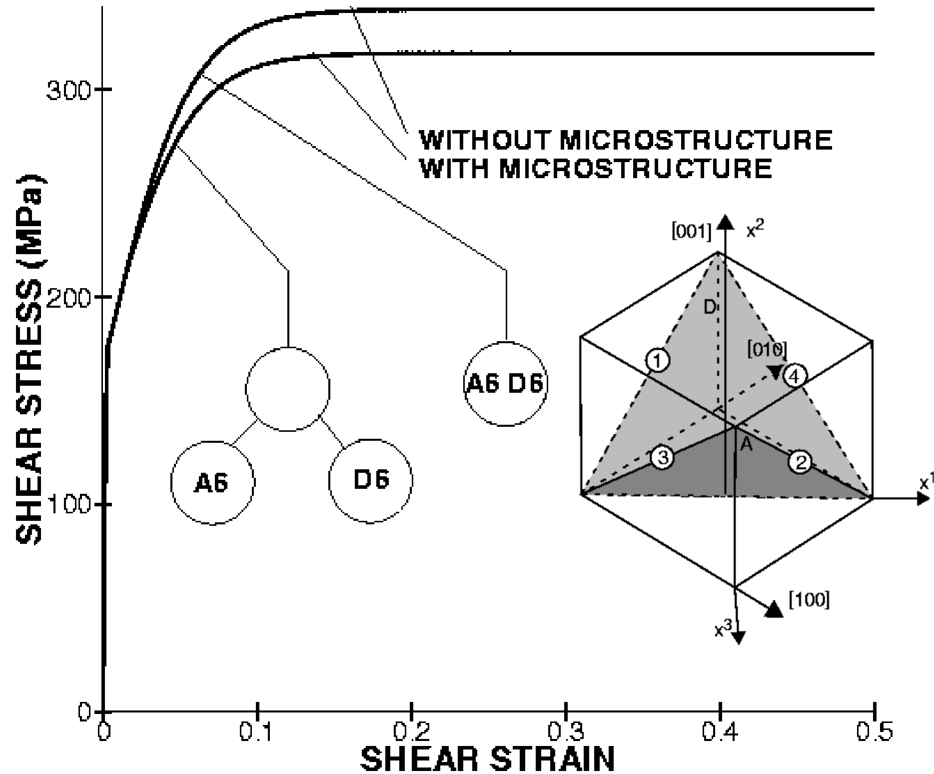
Non-convexity - Strong latent hardening

Single crystal energy density is non-convex due to geometrical softening and strong latent hardening → Consequences of non-convexity?

Strong latent hardening & microstructure

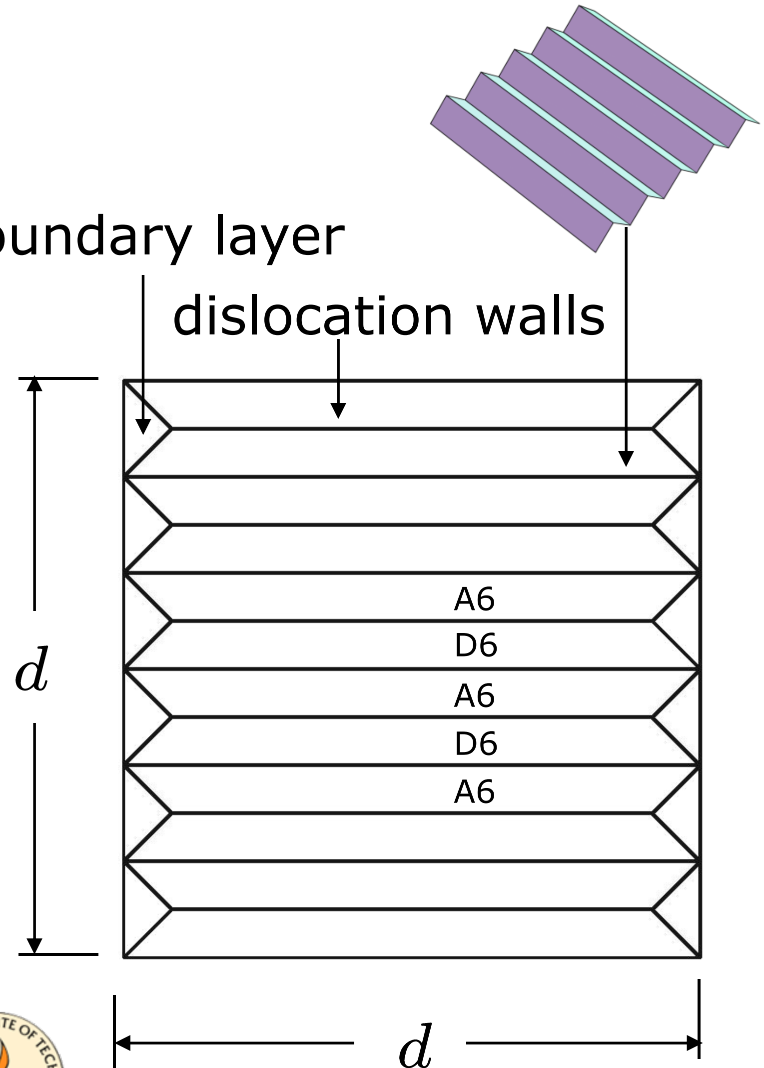


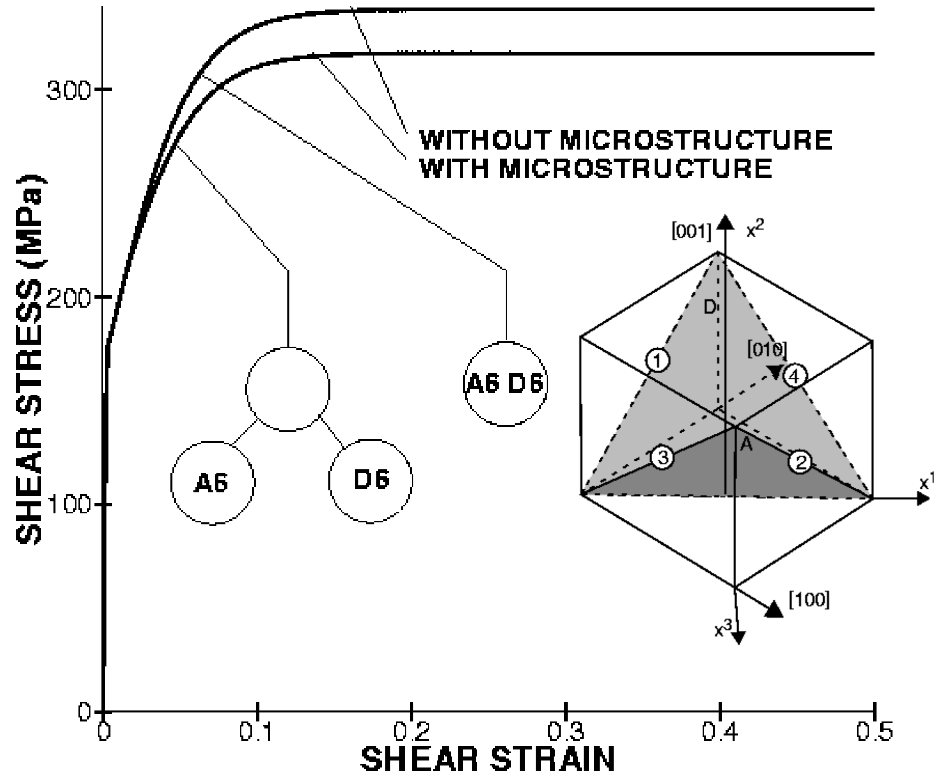


FCC crystal deformed in simple shear on (001) plane in [110] direction

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

Strong latent hardening & microstructure





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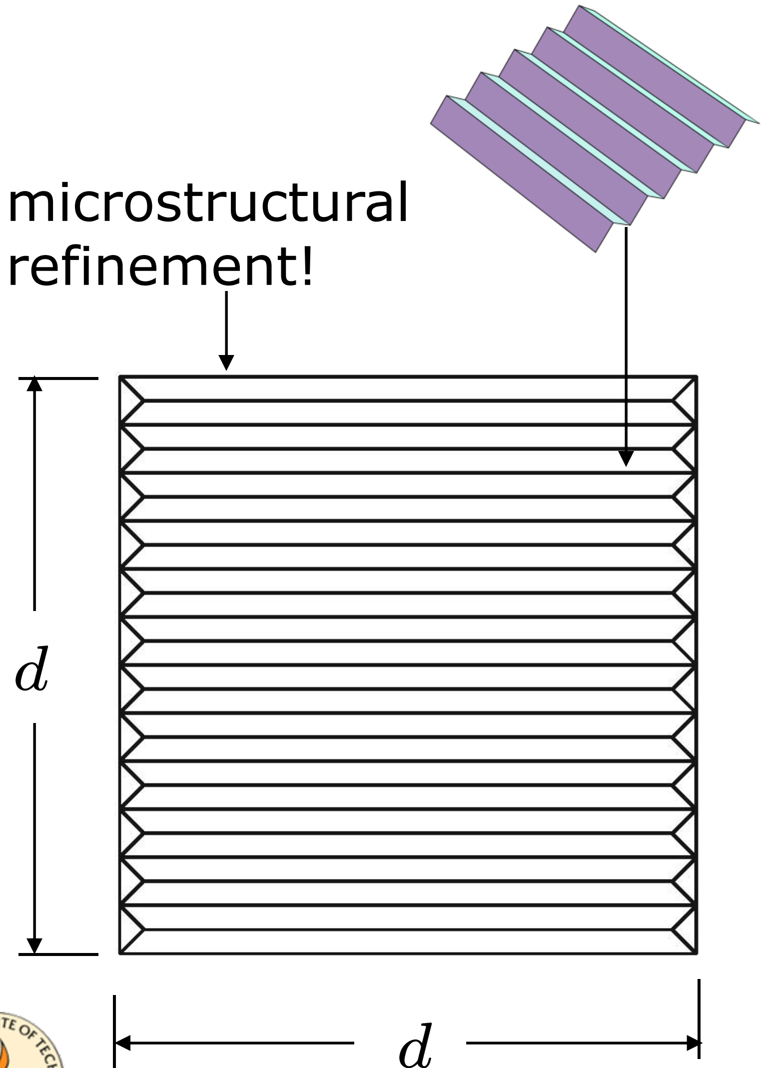

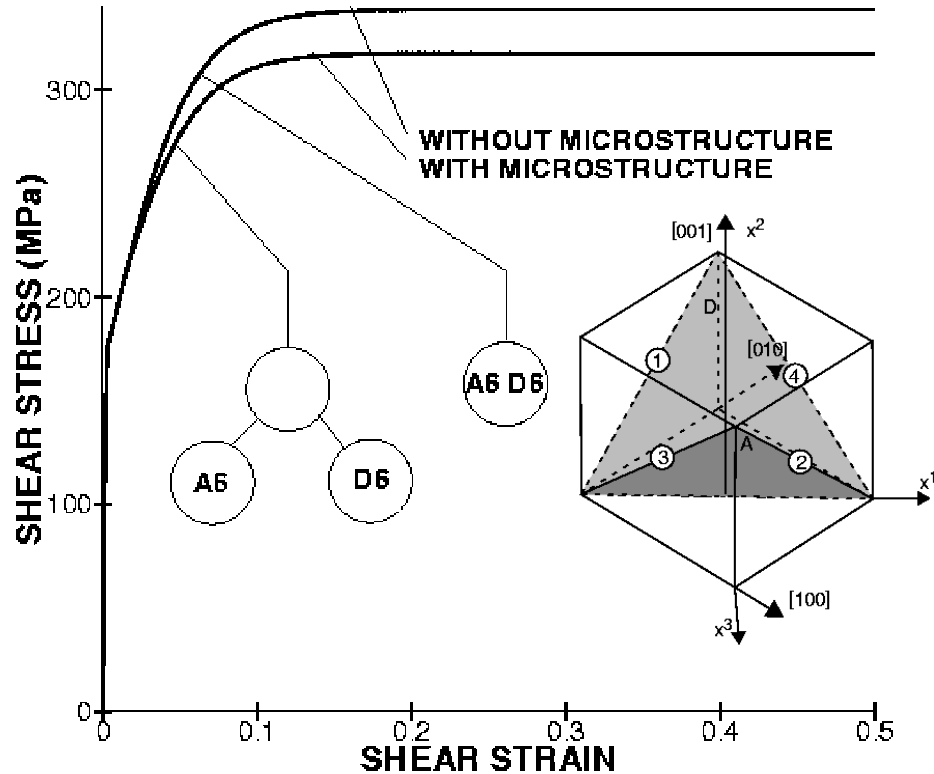

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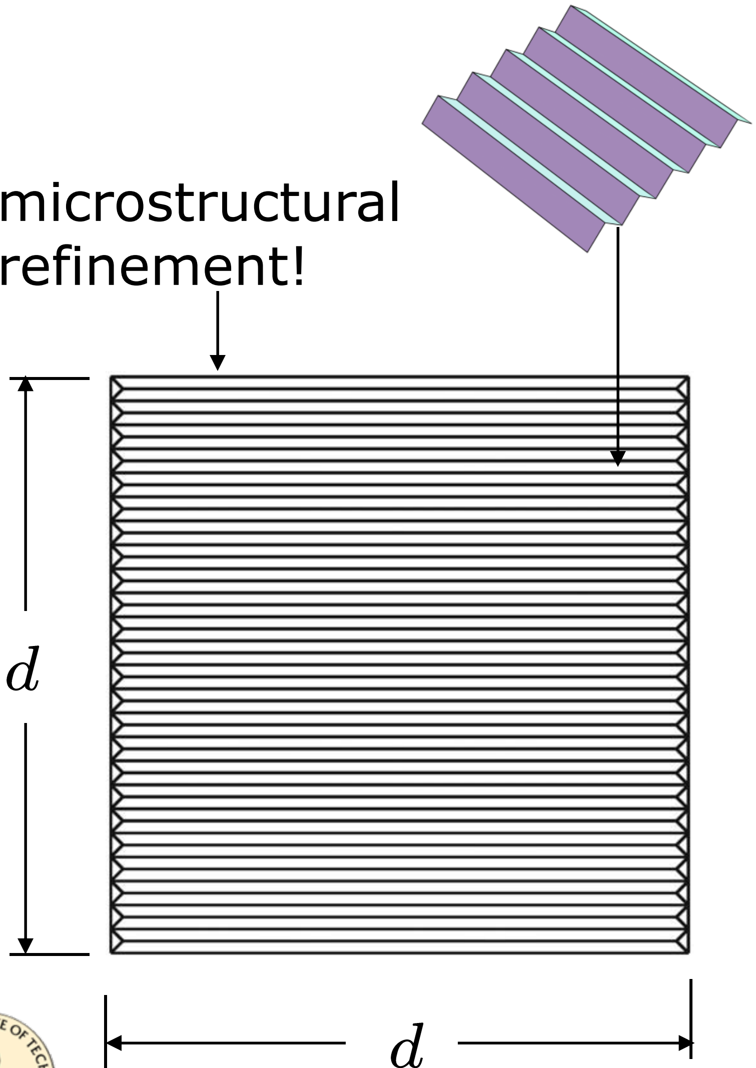
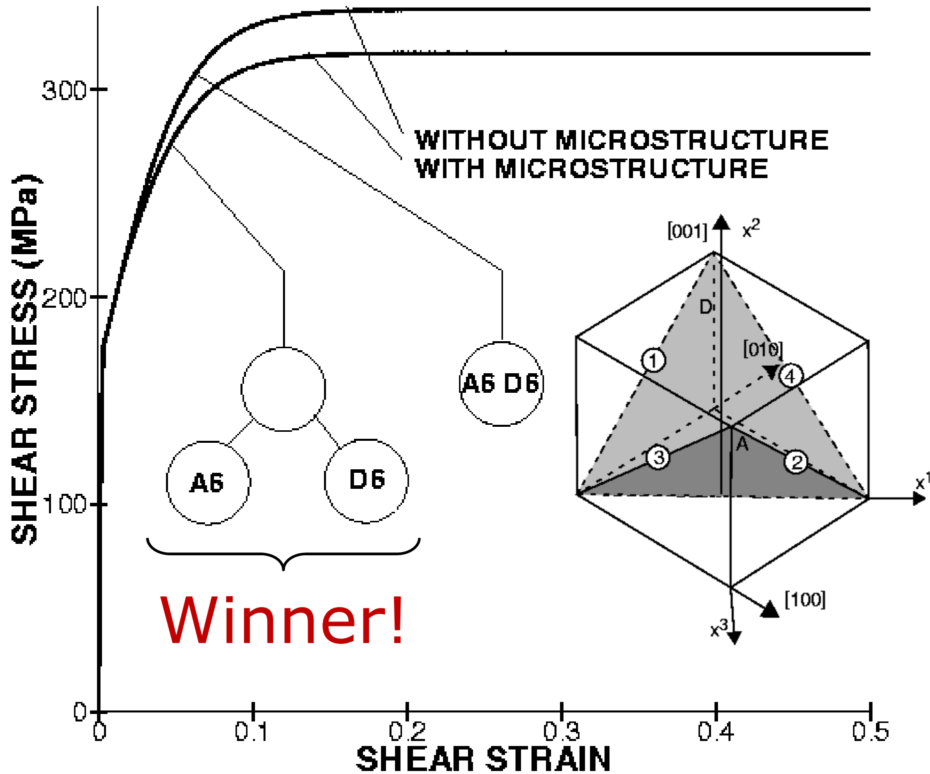
(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure

microstructural refinement!





Winner!

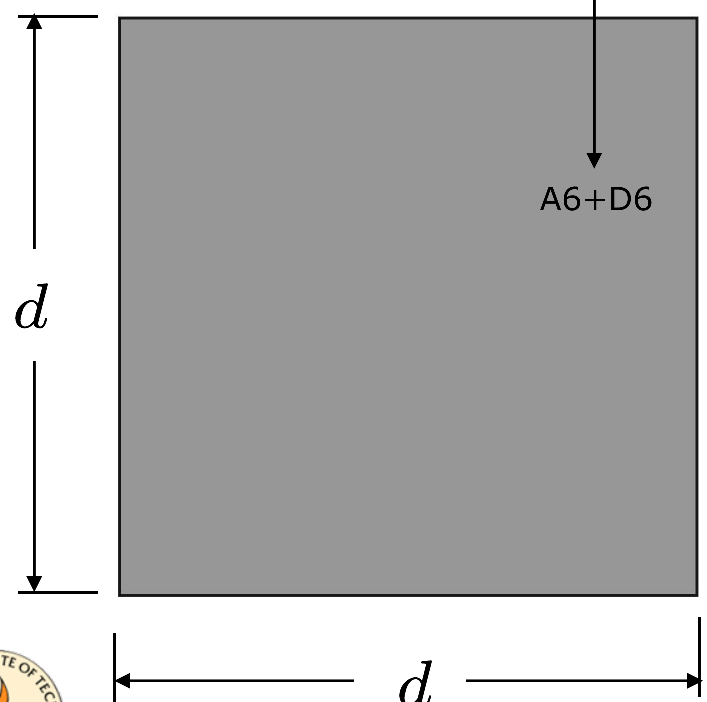
FCC crystal deformed in simple shear on (001) plane in [110] direction

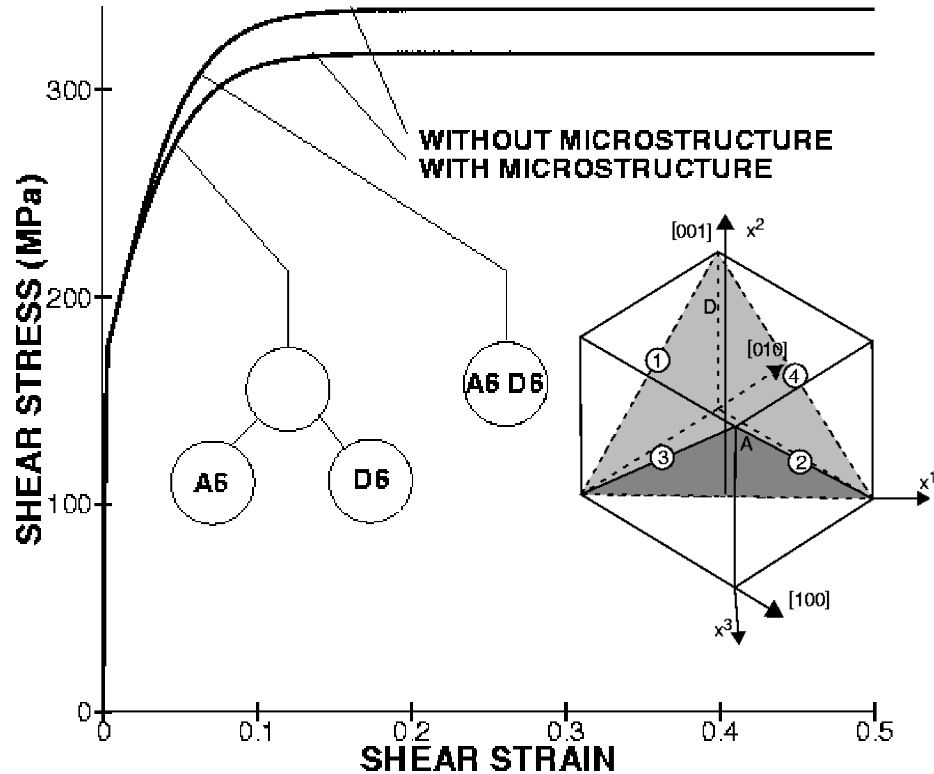
(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure

Pass to the limit…

uniform double slip!





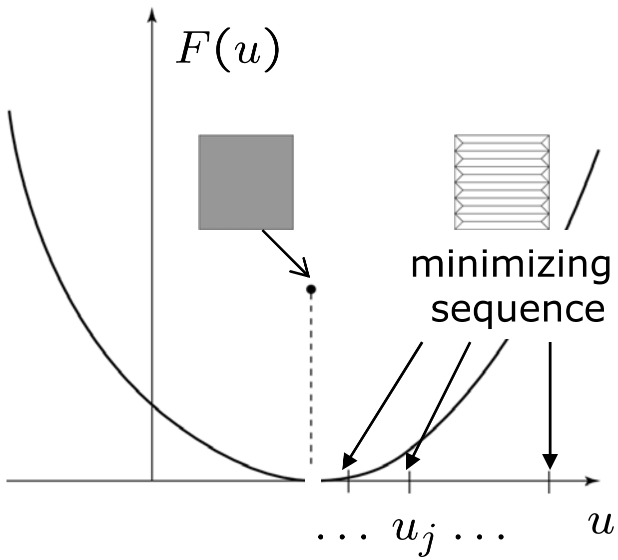
FCC crystal deformed in simple shear on (001) plane in [110] direction

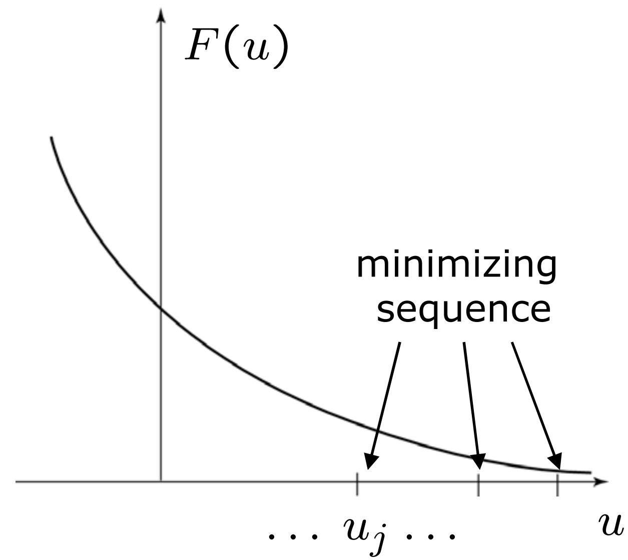
(M Ortiz, EA Repetto and L Stainier *JMPS*, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure

The energy of the limiting (uniform) deformation is greater than the limit of the energies of the microstructures!

Calculus of variations – Direct method





Lack of lower semi-continuity: u_j is a minimizing sequence but *lim* u_j is not a minimizer of $F(u)$

Lack of lower coerciveness: u_j is a minimizing sequence that contains no convergent sub-sequence

Theorem (Tonelli) $F(u)$ lower-semicontinuous and coercive in $X \Rightarrow$ problem $\inf_X F(u)$ has solutions.

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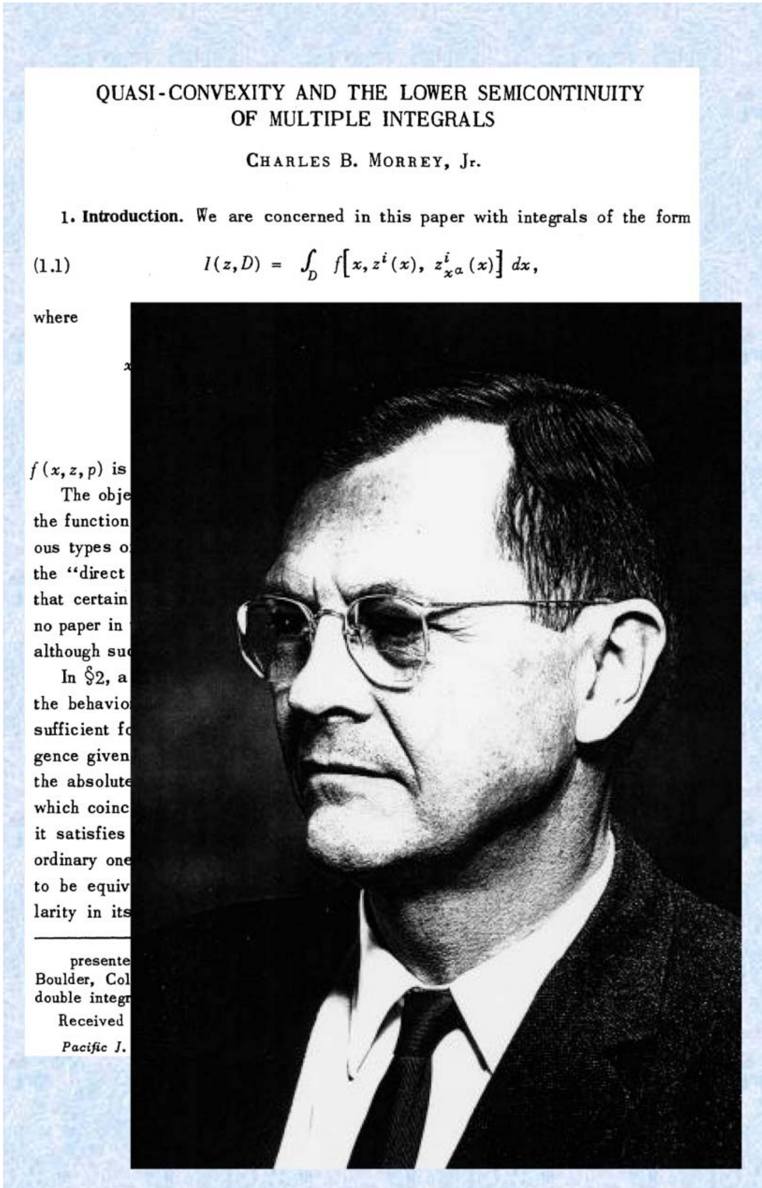
Calculus of variations – Direct method

Single crystals are ‘unstable’ with respect to microstructure: Variational Dirichlet problem has no solution in general! (“non-attaiment”)

Microstructure and material stability

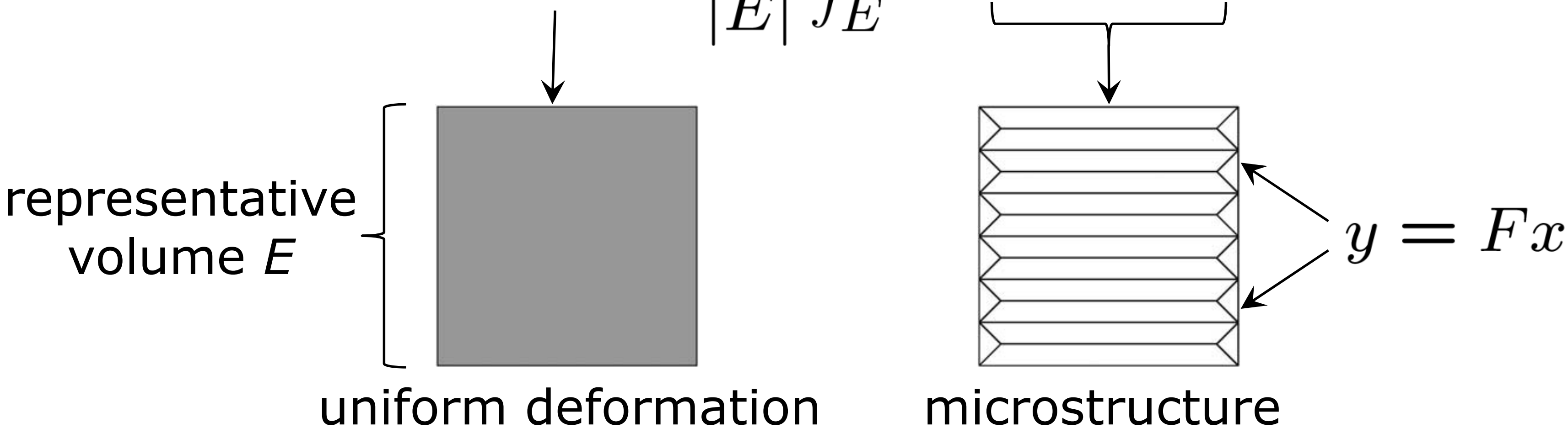


Morrey, C.B. Jr., "Quasi-convexity and the semicontinuity of multiple integrals," *Pacific J. Math*., Vol. 2 (1952) pp. 25-53.

Microstructure and material stability

- A material is *quasiconvex* (stable with respect to microstructure) if, for all $v \in W_0^{1,p}(E)$,

$$W(F) \leq \frac{1}{|E|} \int_E W(F + \nabla v)\, dx$$



Theorem (Morrey) $W(F)$ quasi-convex $\Leftrightarrow$ $F(u) = \int_\Omega W(\nabla u) dx$ lower semicontinuous in $W_0^{1,p}(\Omega)$.

Microstructure and material stability

Material stability (in the sense of Morrey) + coercivity => Existence of solutions of the variational Dirichlet problem ("attainment")

Microstructure and material stability

- Single-crystal plasticity is ill-posed due to geometrical softening, strong latent hardening
- Single crystals are unstable with respect to microstructure (in the sense of Morrey)
- NB: In 3d, the Hill-Hadamard condition is not sufficient for material stability (Sverak, V., *Proc. Roy. Soc. Edinburgh*, **A120** (1992) 185.)
- How can we make sense of such ill-posed problems?
  - *Minimizing sequences as "solutions"?*
  - *Corresponding macroscopic behavior?*

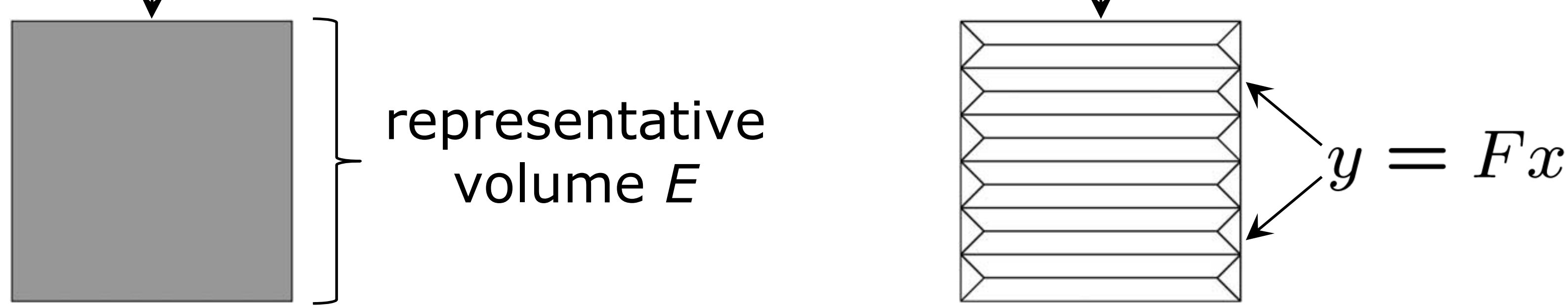
Calculus of variations and microstructure

De Giorgi, E., "Sulla convergenza di alcune successioni di integrali del tipo dell'area," *Rend. Mat.*, Vol. 8 (1975) pp. 277-294.

Calculus of variations and microstructure

- *Quasiconvex envelope* of an energy density $W(F)$:

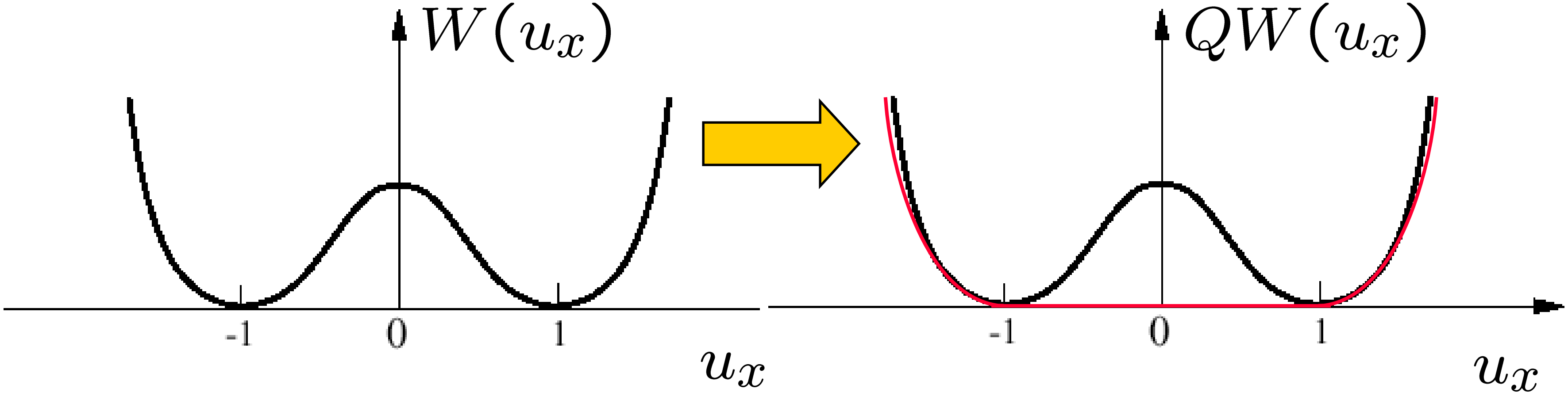
$$QW(F) = \inf_{v \in W_0^{1,p}(E)} \frac{1}{|E|} \int_E W(F + \nabla v)\, dx$$

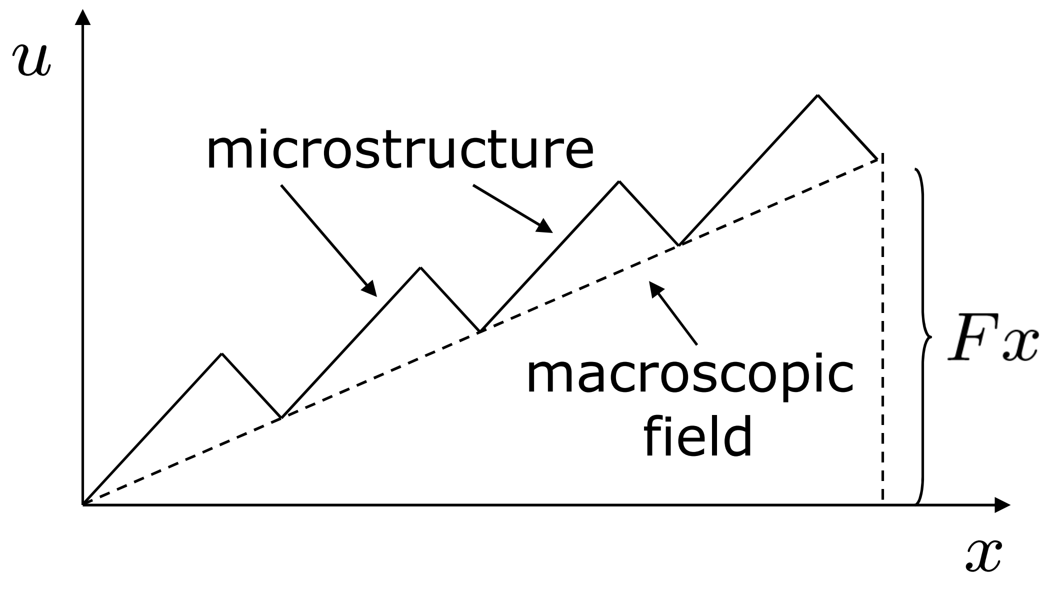


uniform deformation | microstructure

- $QW(F)$ is the largest quasi-convex (stable) energy density majorized by $W(F)$.
- Relaxed problem: $$\inf_{u \in u_0 + W_0^{1,p}(\Omega)} \int_\Omega QW(\nabla u) dx$$

Calculus of variations and microstructure





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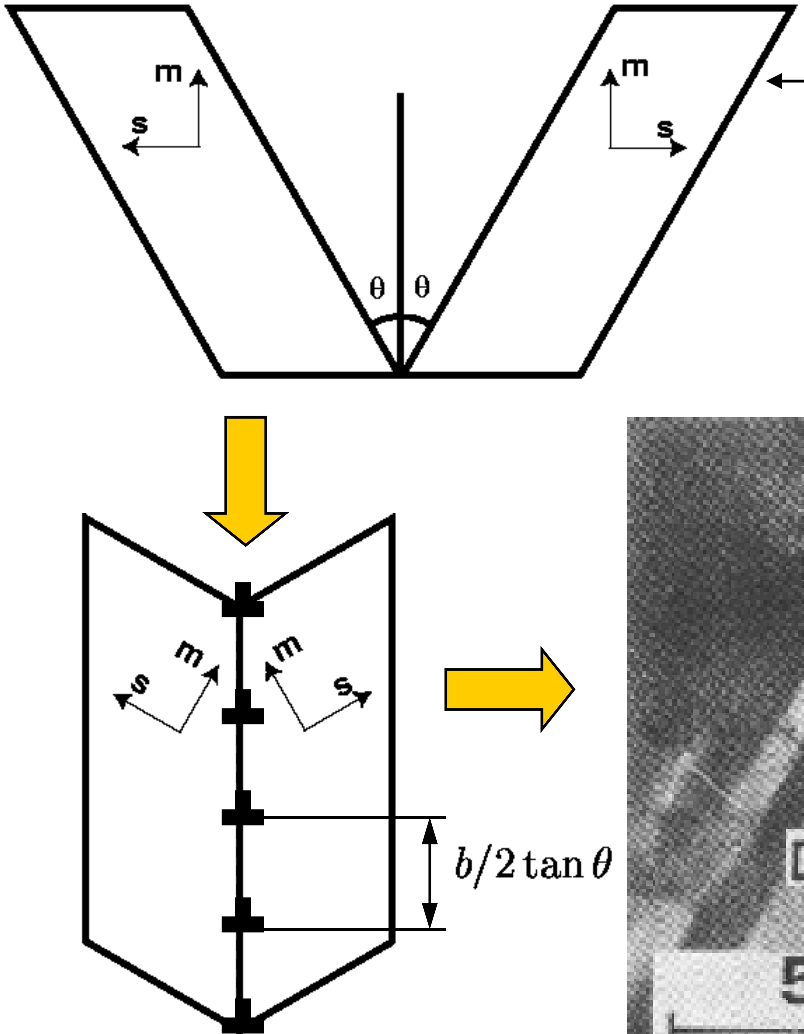
Relaxation as 'exact' multiscale method

- 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!

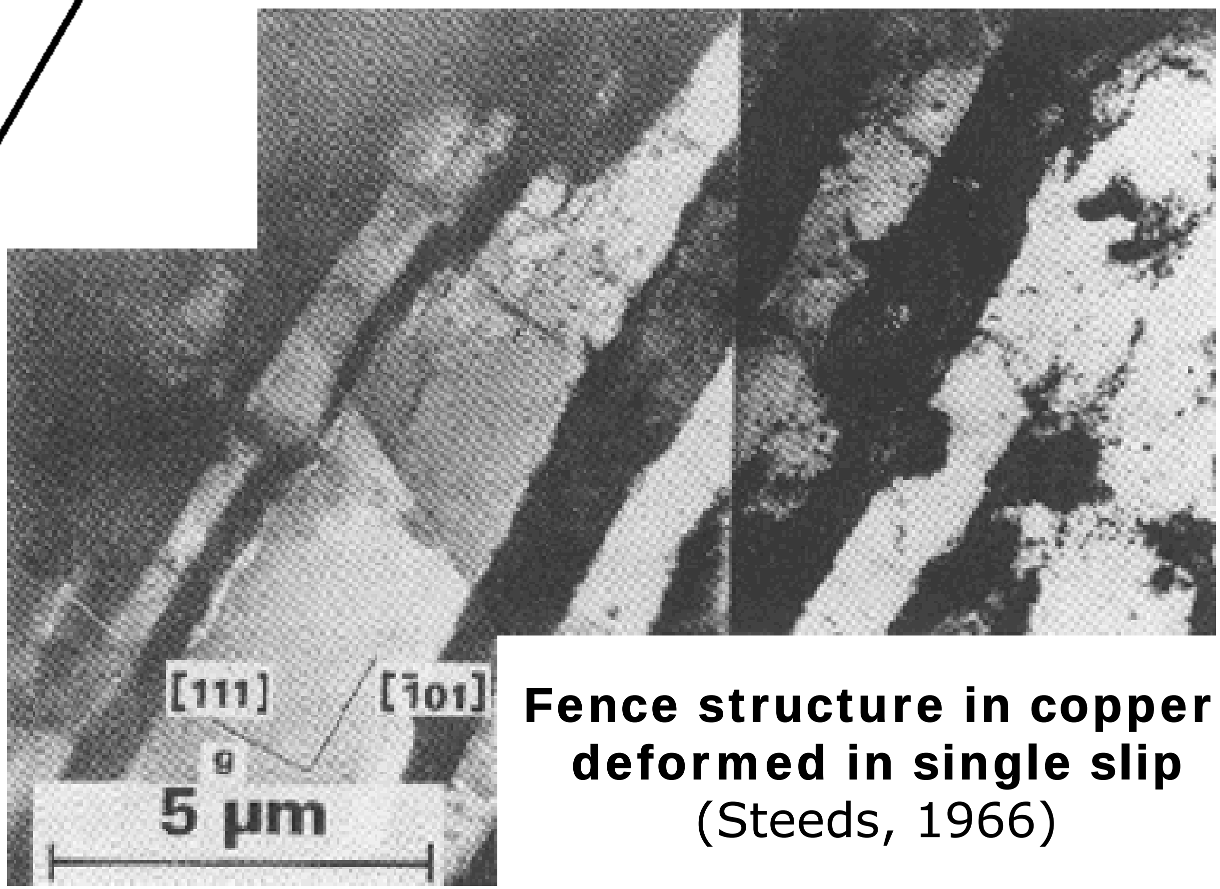
Relaxation as ‘exact’ multiscale method

- General strategy for computing the relaxation:
  - *Exhibit a microstructure construction that ‘beats’ uniform deformations over representative volumes*
  - *Prove that the material cannot do better (optimality)*
- Optimality is difficult to prove in general => Exact relaxation is known for few material models
- However: Inspired constructions (even in the absence of a proof of optimality) can explain experimental observations of microstructure
- Application to single-crystal plasticity?
  - *Laminates*
  - *Cell structures*

Constructions – Fence structures

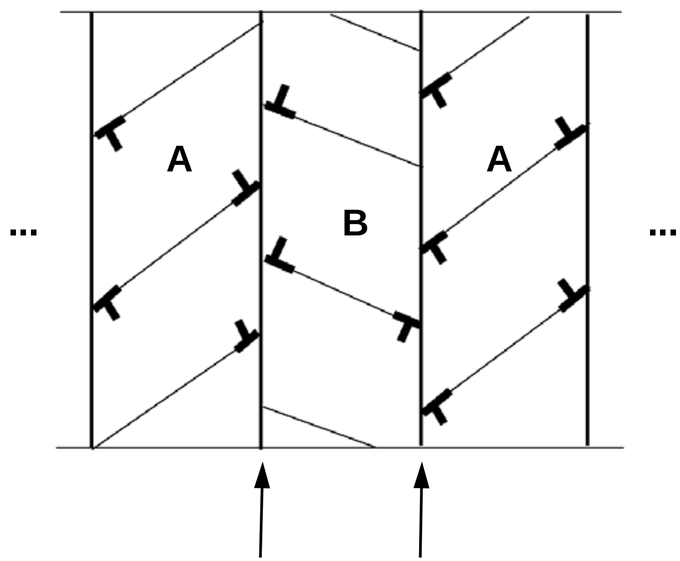


Symmetric tilt boundary construction

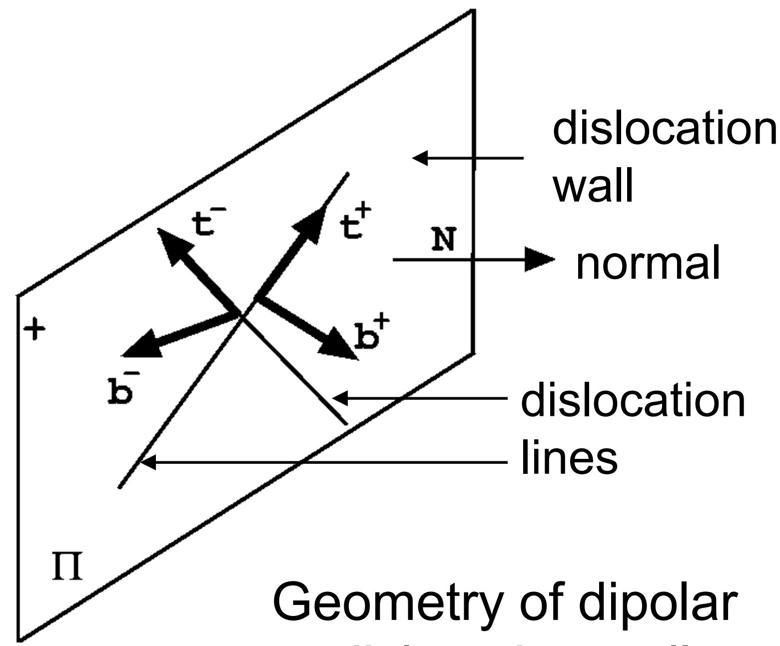


Fence structure in copper deformed in single slip
(Steeds, 1966)

Constructions – Dipolar dislocation walls



Dipolar dislocation walls



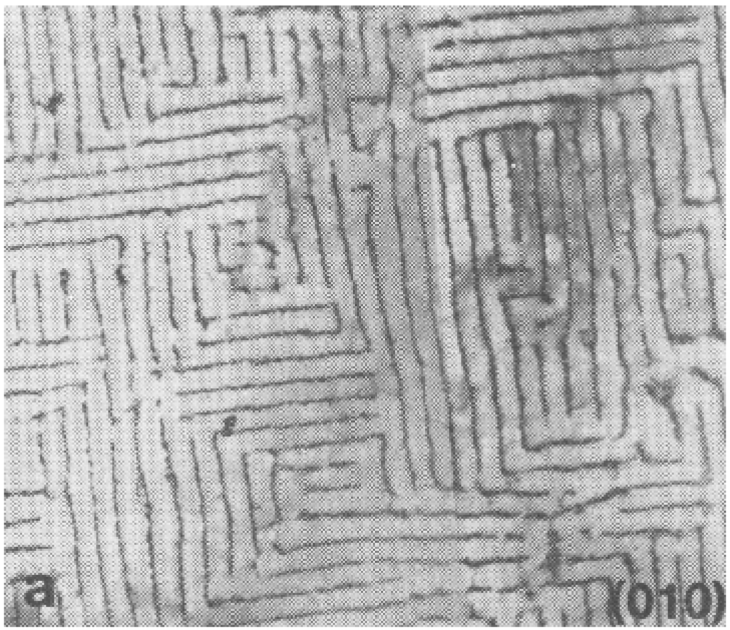
Geometry of dipolar dislocation wall

- Infinite latent hardening: $F^p = I + \gamma s \otimes m$
- Rigid-plastic behavior: $F = R(I + \gamma s \otimes m)$
- Rank-1 compatibility: $[\![F]\!] = a \otimes N$
- **Problem:** Find all possible dipolar walls

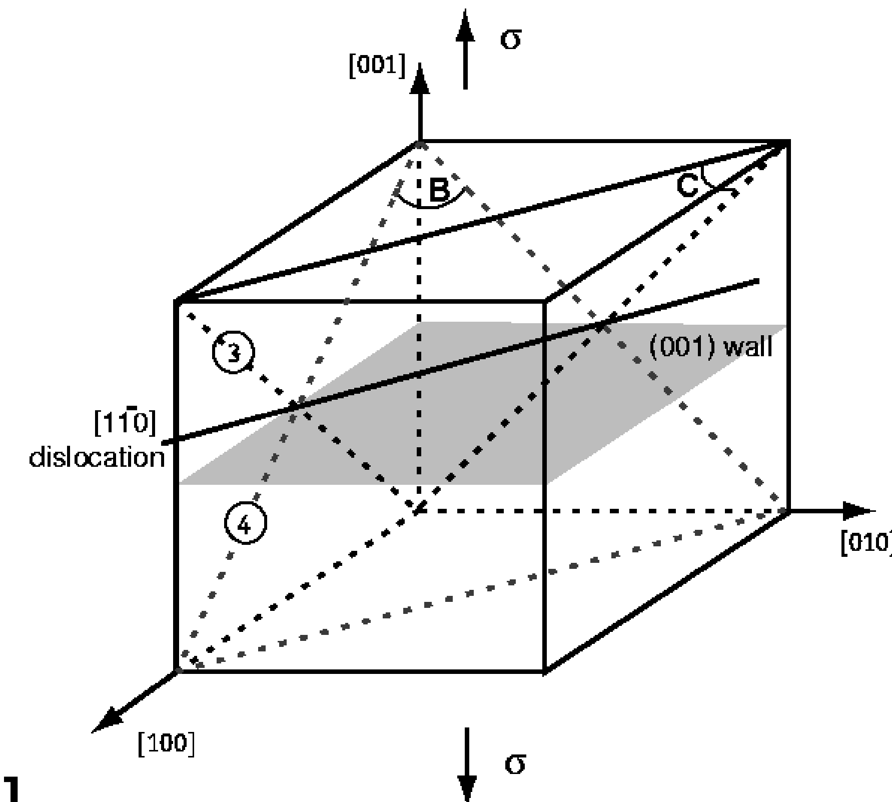
Constructions – Dipolar dislocation walls

Only possible dipolar dislocation walls are: (001), (110), (111), (112), (113)!

Constructions – Dipolar dislocation walls

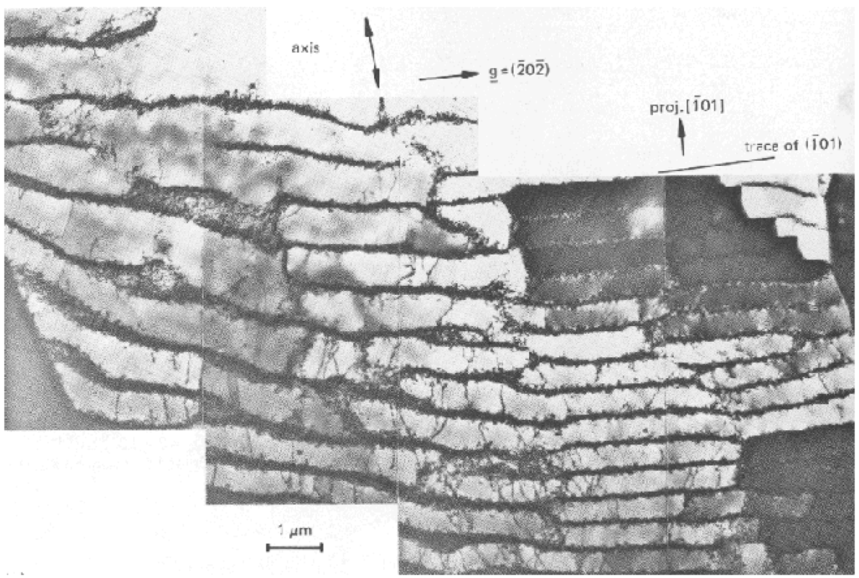


Copper single crystal fatigued with tensile axis [001] showing labyrinth structure
(Jin and Winter, 1984)

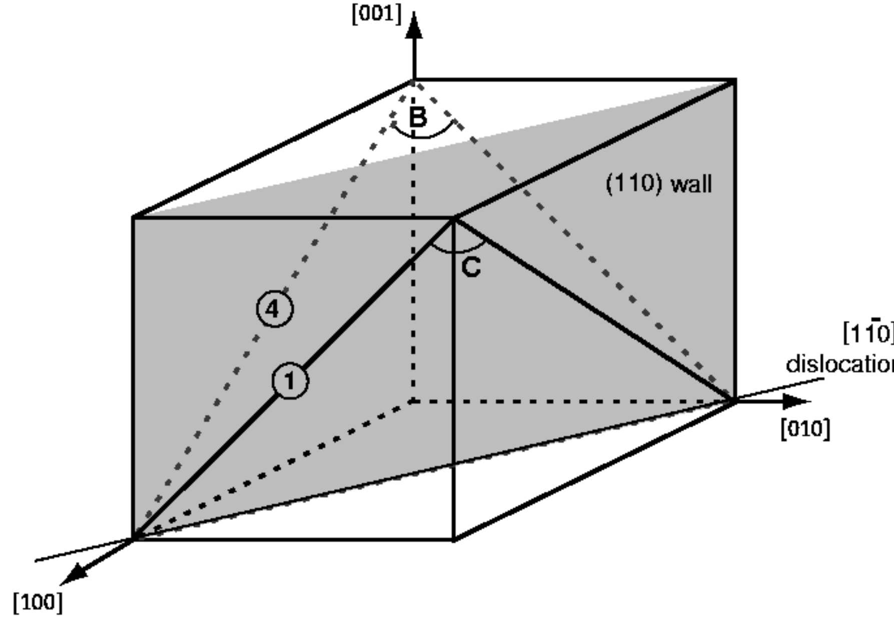


Geometry of B4-C3 interface
(M Ortiz and EA Repetto, *JMPS,* **47**(2) 1999, p. 397)

Constructions – Dipolar dislocation walls



(101) wall structure in fatigued polycrystalline copper
(Wang and Mughrabi, 1984)



Geometry of B4-C1 interface
(M Ortiz and EA Repetto, *JMPS,* **47**(2) 1999, p. 397)

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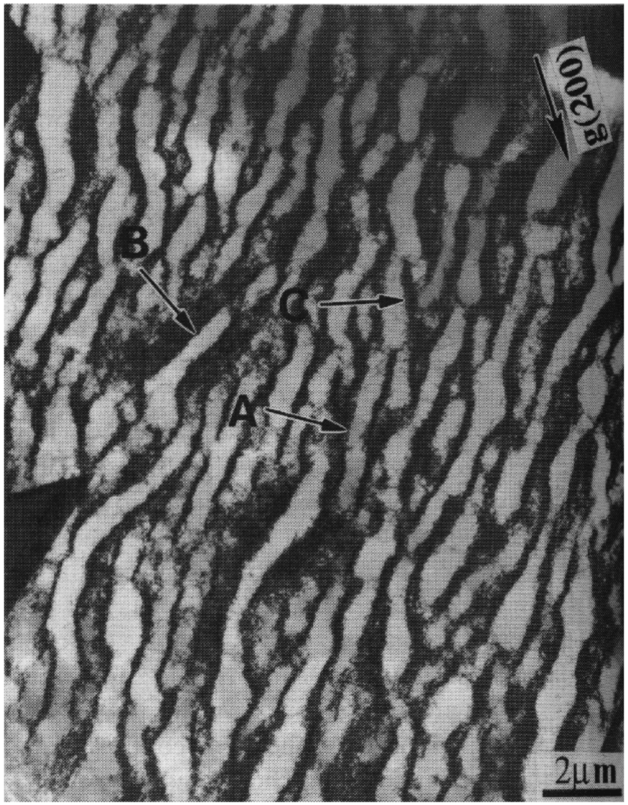
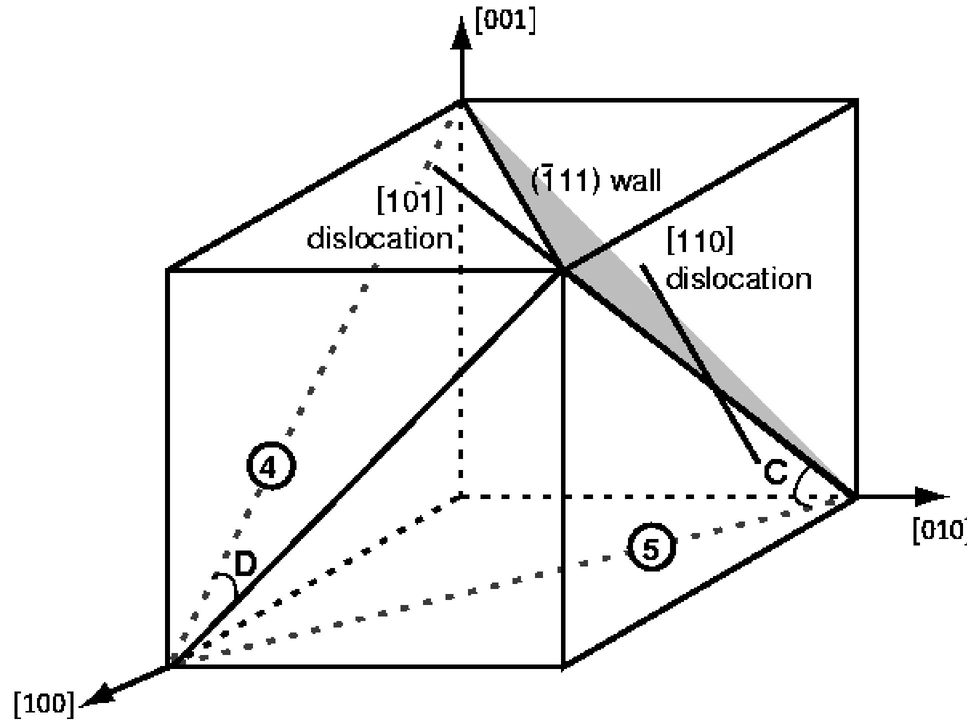
Constructions – Dipolar dislocation walls



(111) wall structure in fatigued polycrystalline copper
(Yumen, 1989)



Geometry of C5-D4 interface
(M Ortiz and EA Repetto, *JMPS,* **47**(2) 1999, p. 397)

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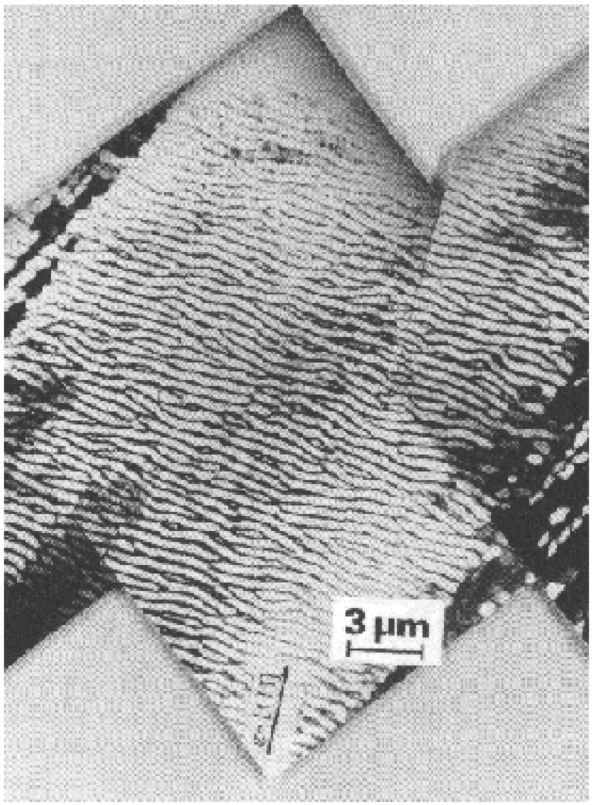
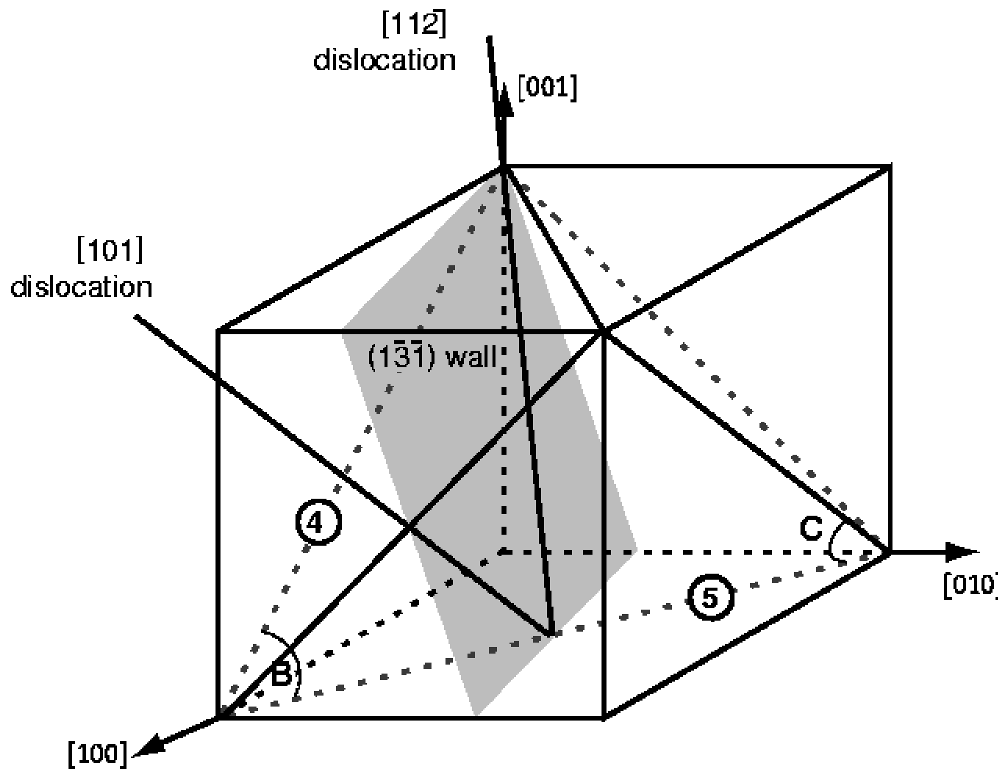
Constructions – Dipolar dislocation walls



(131) wall structure in fatigued [111] copper single crystal
(Lepisto et al., 1986)



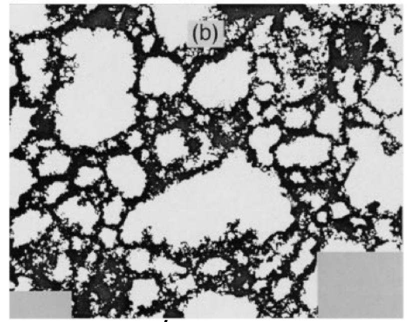
Geometry of B4-C5 interface
(M Ortiz and EA Repetto, *JMPS,* **47**(2) 1999, p. 397)

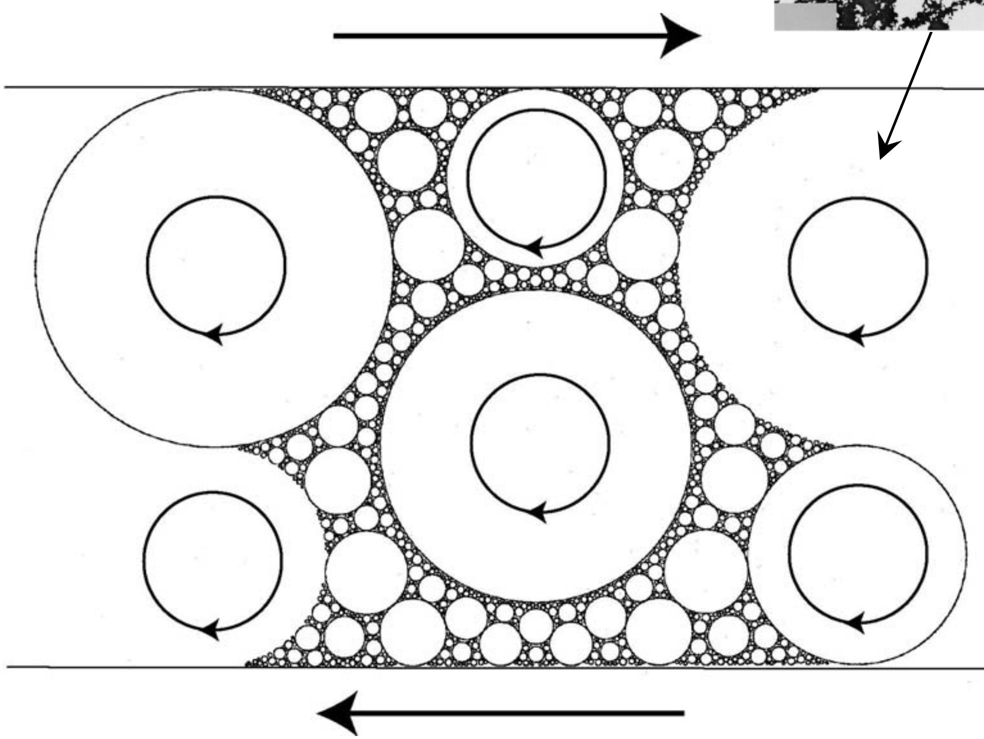
Constructions – Dipolar dislocation walls

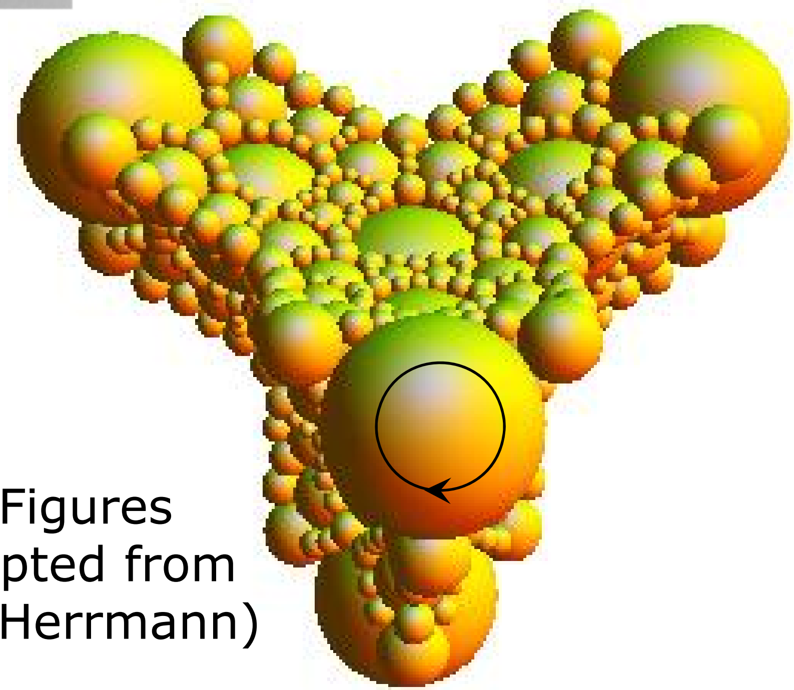
Simple algebraic construction explains the geometry of dipolar dislocation walls in fatigued fcc crystals!

Constructions – Cell structures

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







(Figures adapted from H.J. Herrmann)

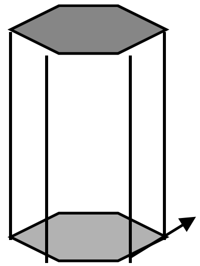
Ball-bearing kinematical model of dislocation cell structures

Constructions – Cell structures

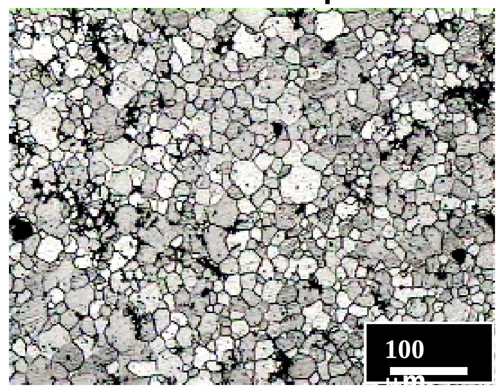
Can dislocation cell structures be described as space-filling ball-bearing mechanisms?

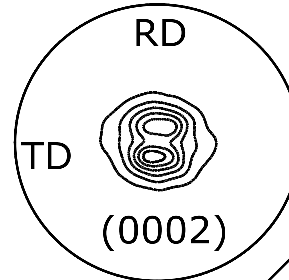
Constructions – Cell structures

Magnesium slip systems: (0001) [1120]

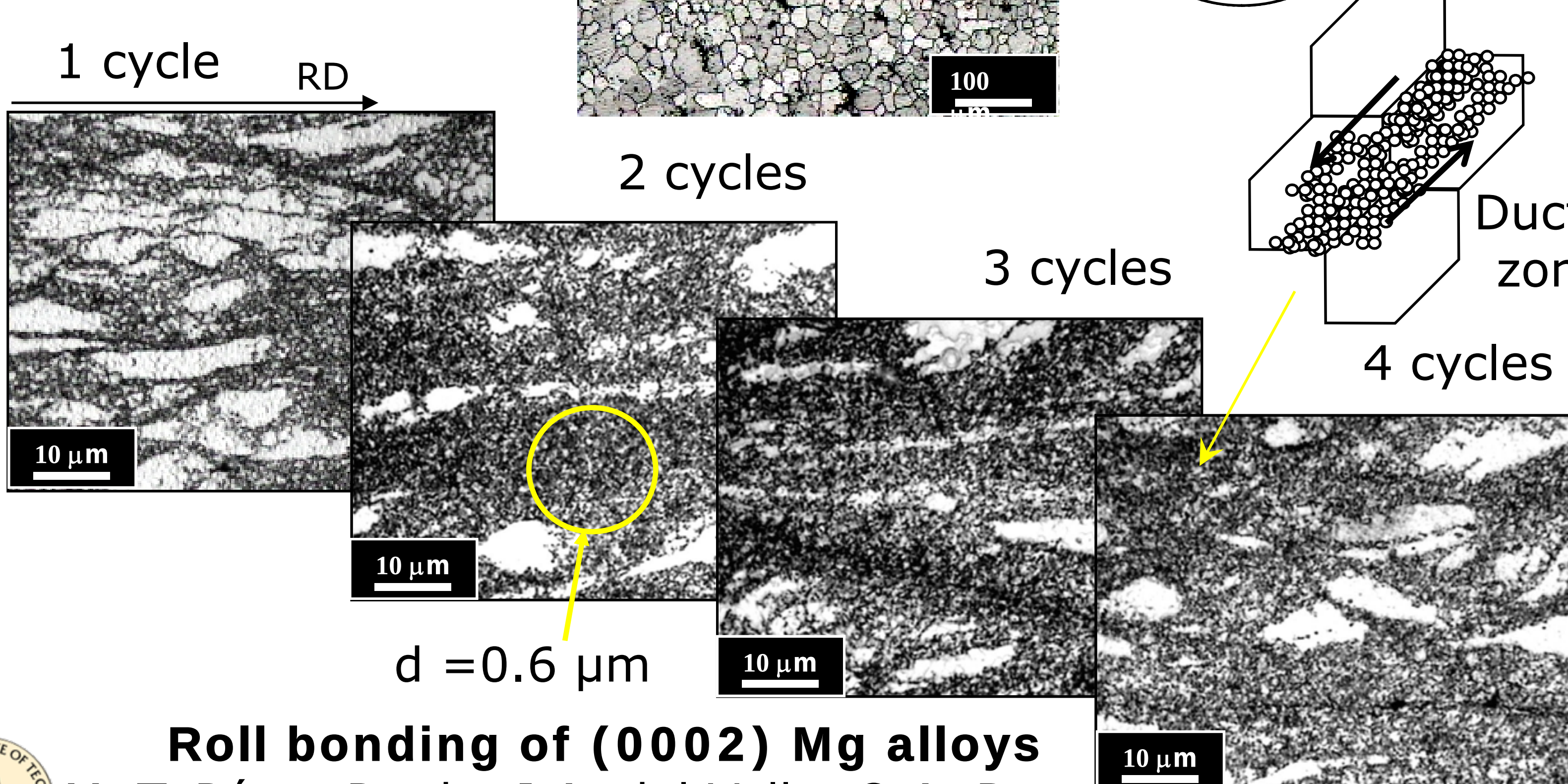


d = 40 μm





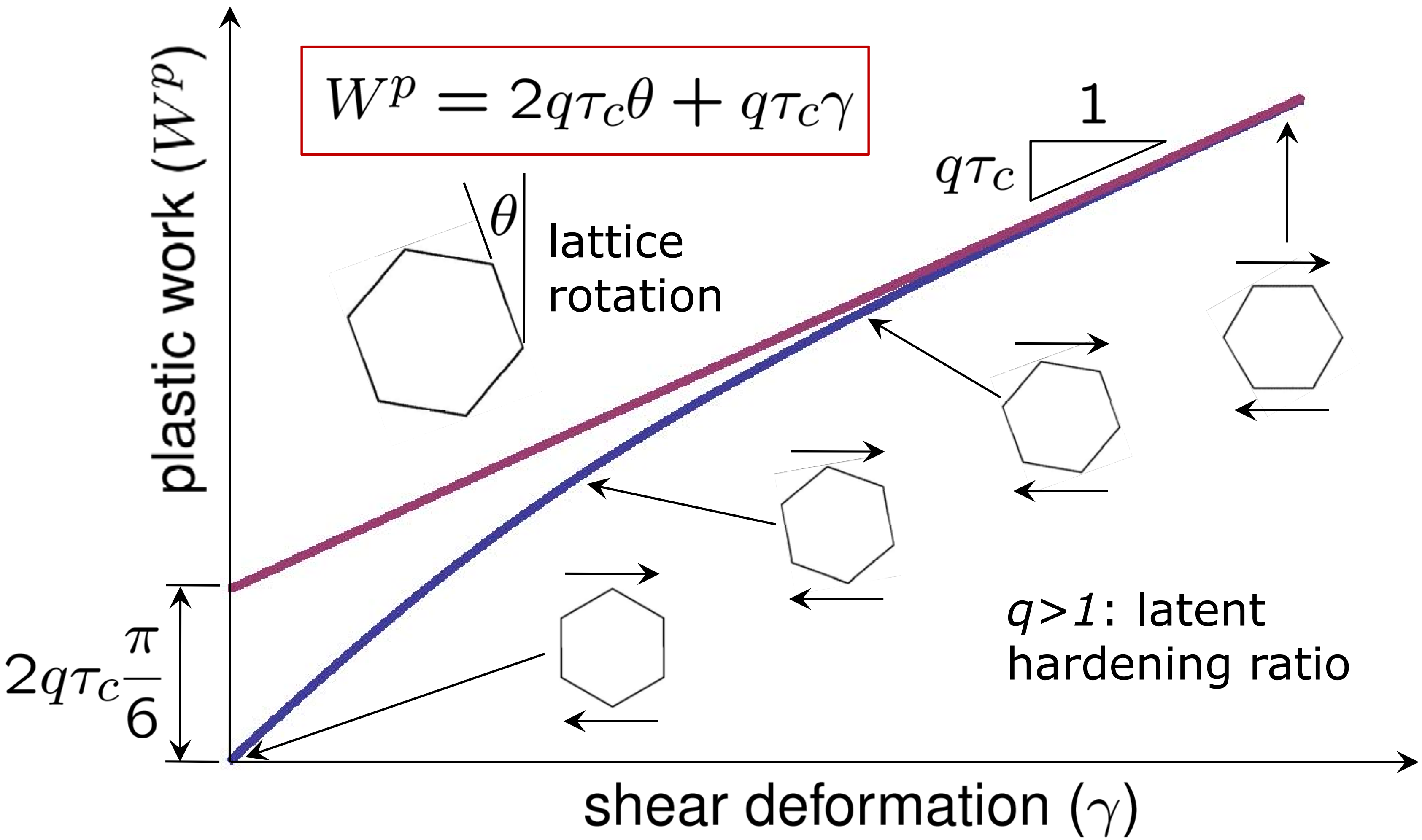
1 cycle RD



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

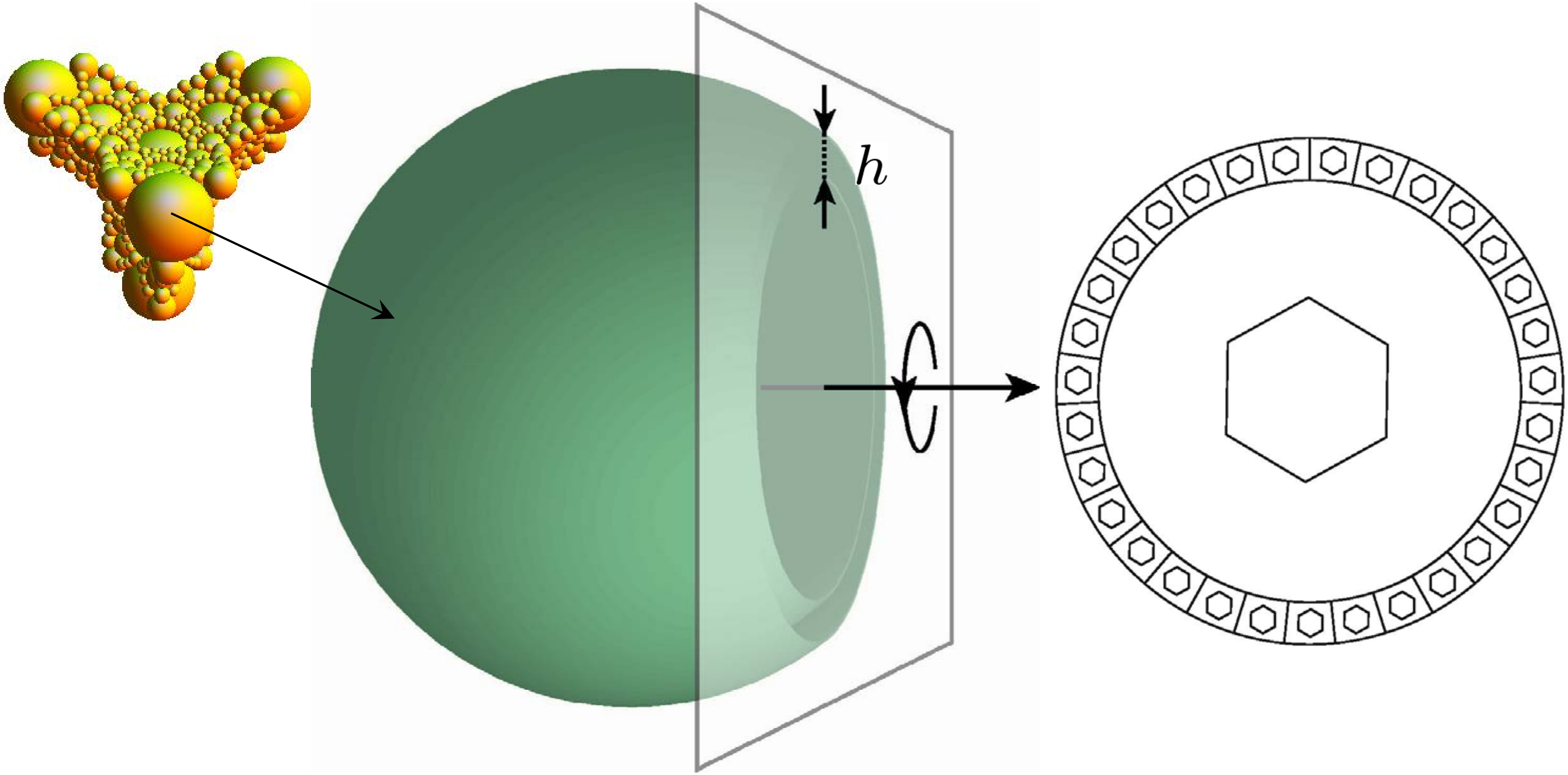


Simple shear on basal plane:
Uniform double slip

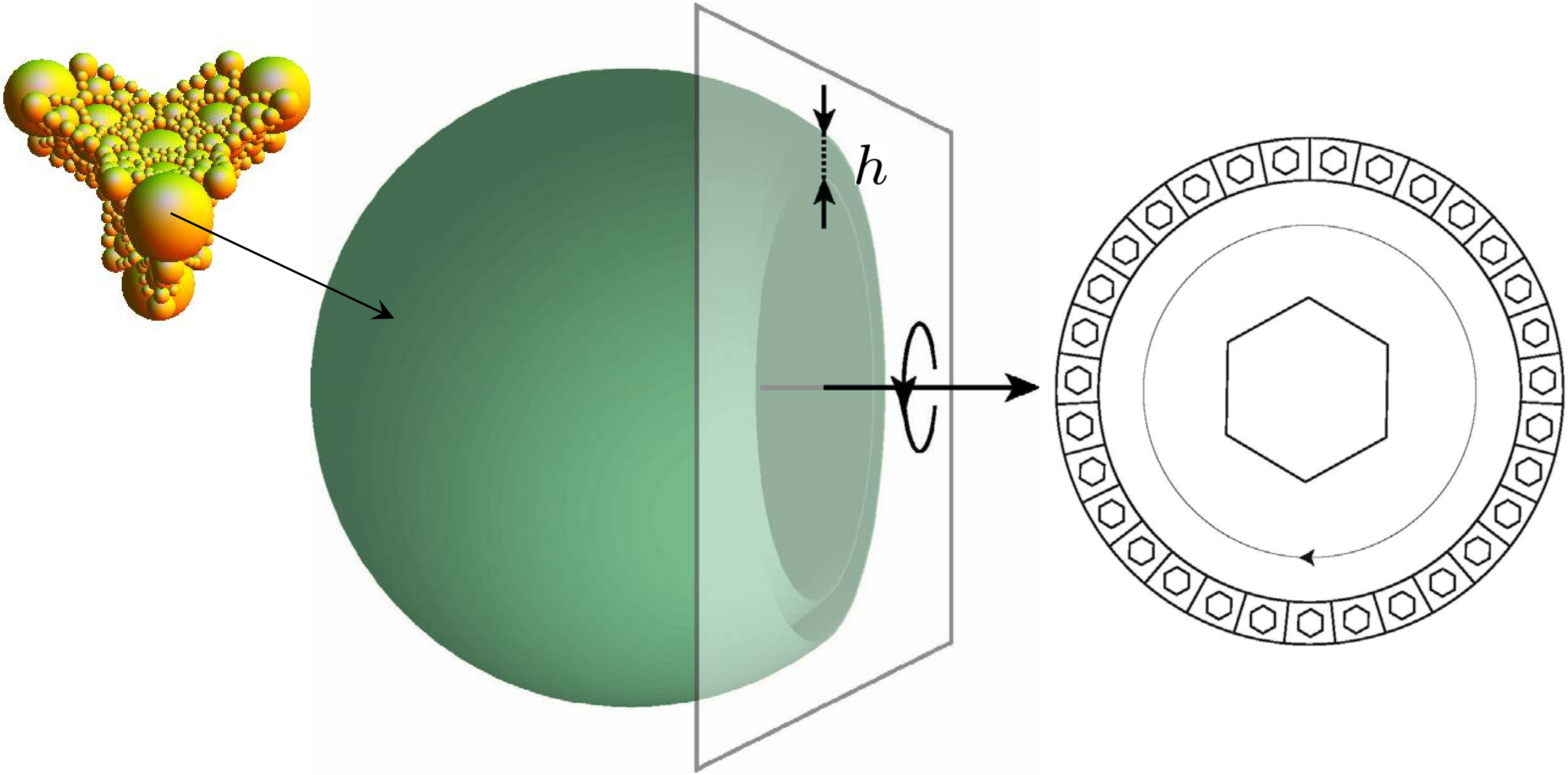
Constructions – Cell structures

Can uniform double slip be beaten by dislocation cell microstructures?

Dislocation cell structures



Dislocation cell structures



Step 1: Reorient cells for single slip

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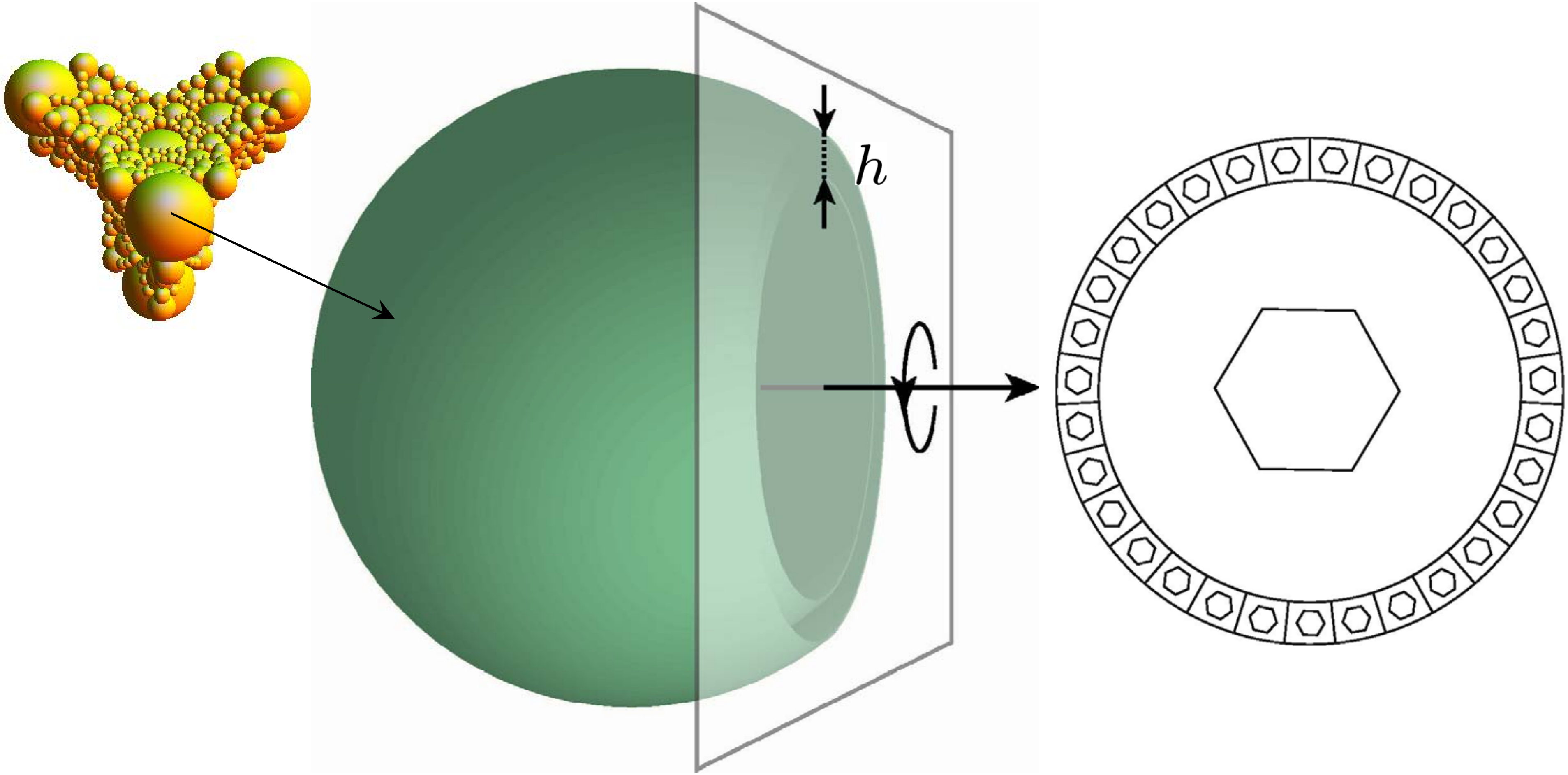
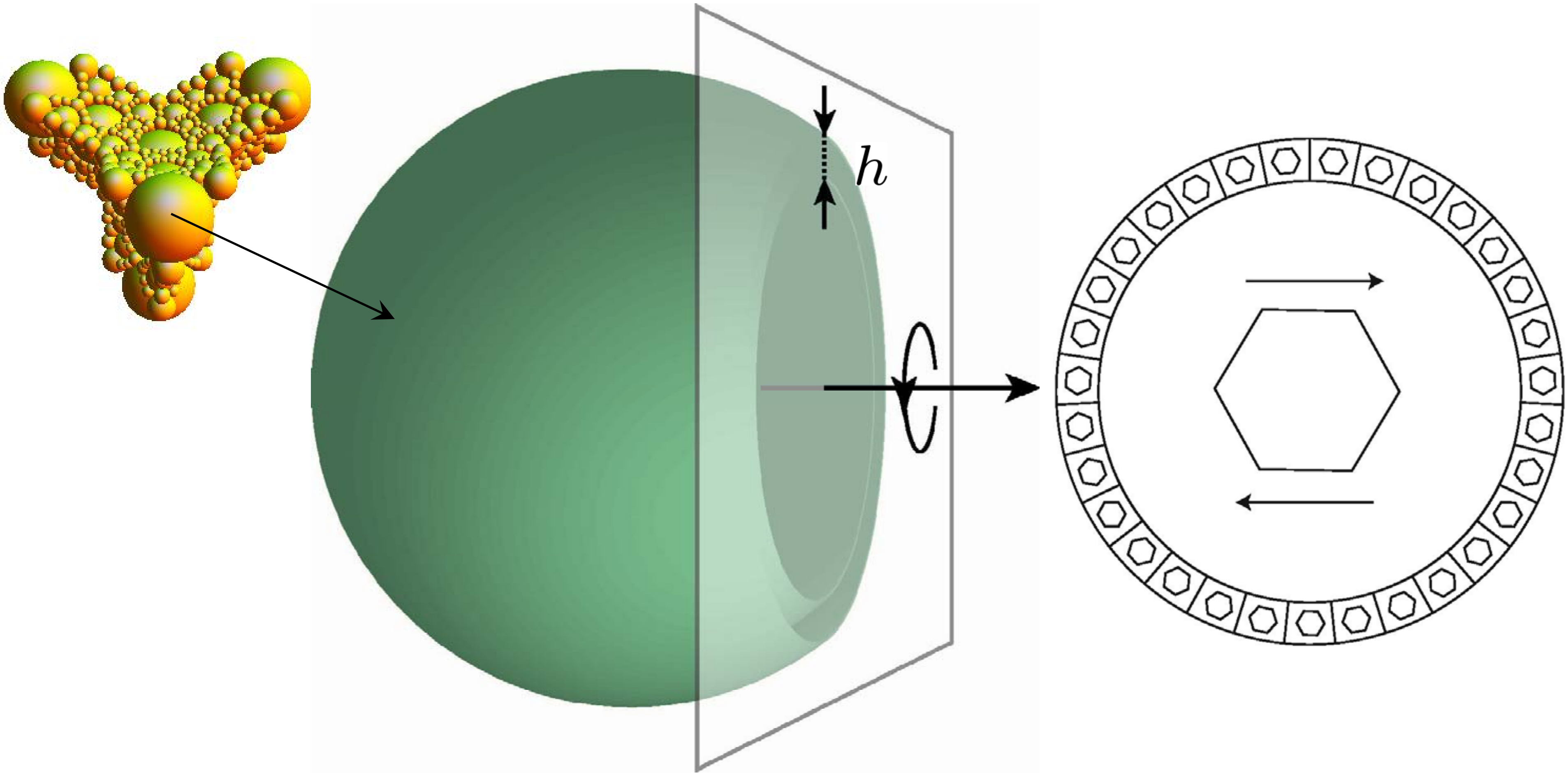
Dislocation cell structures



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

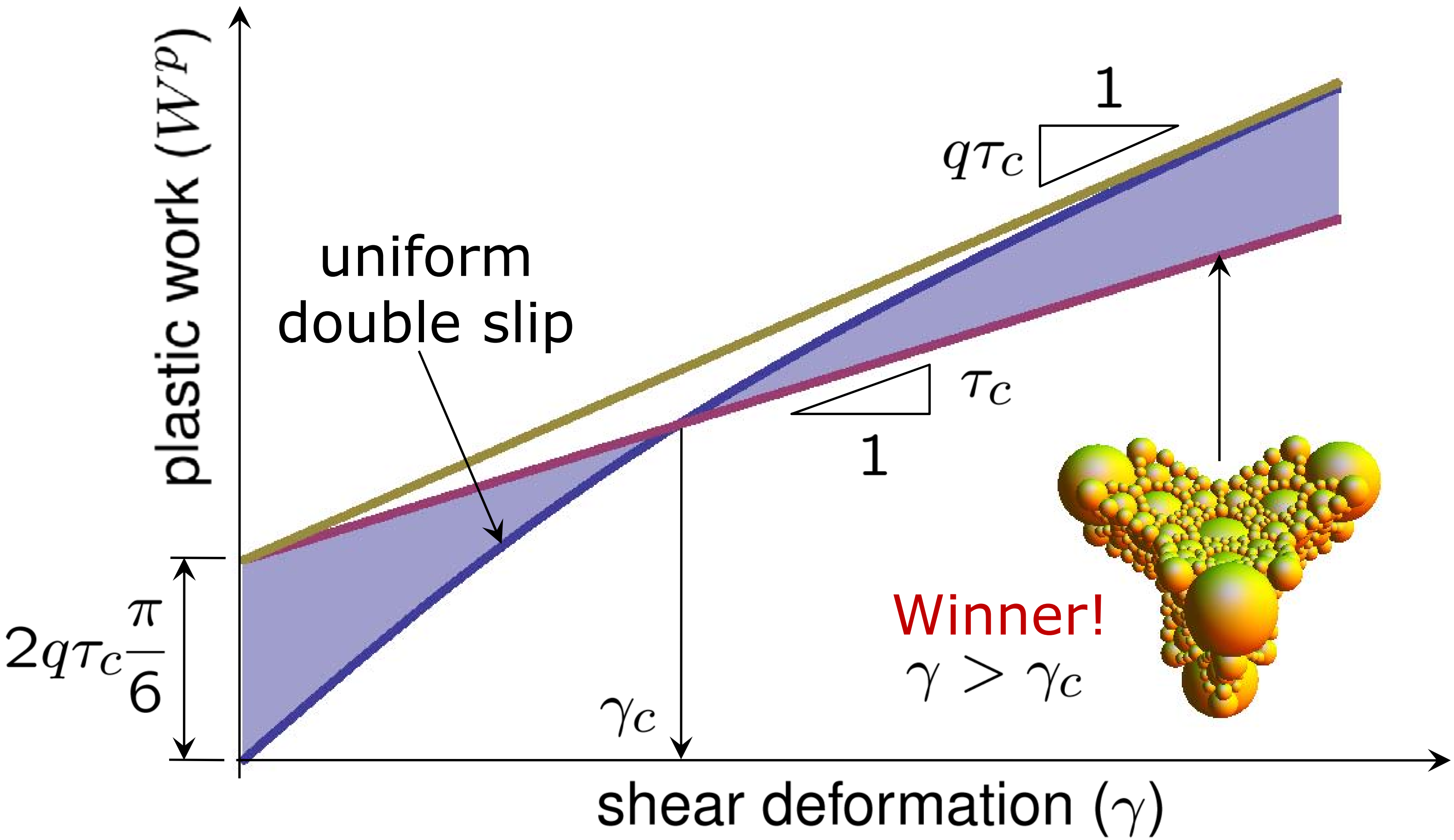
Dislocation cell structures



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

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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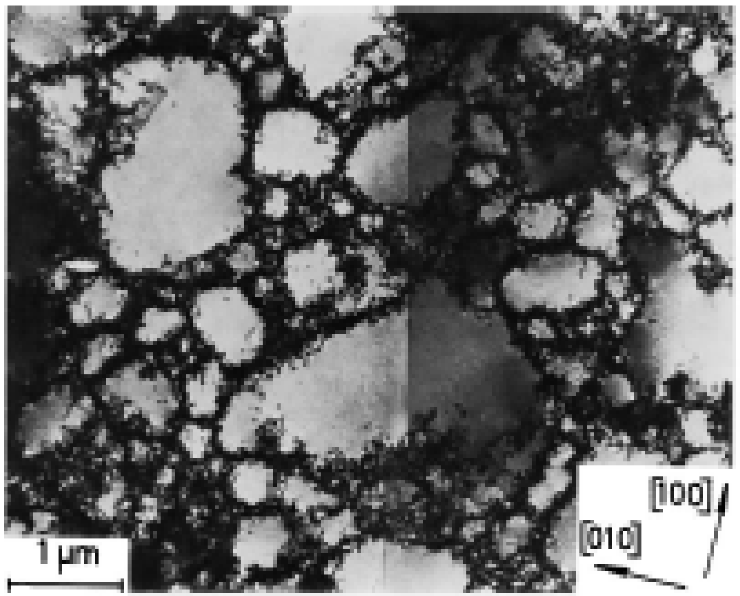
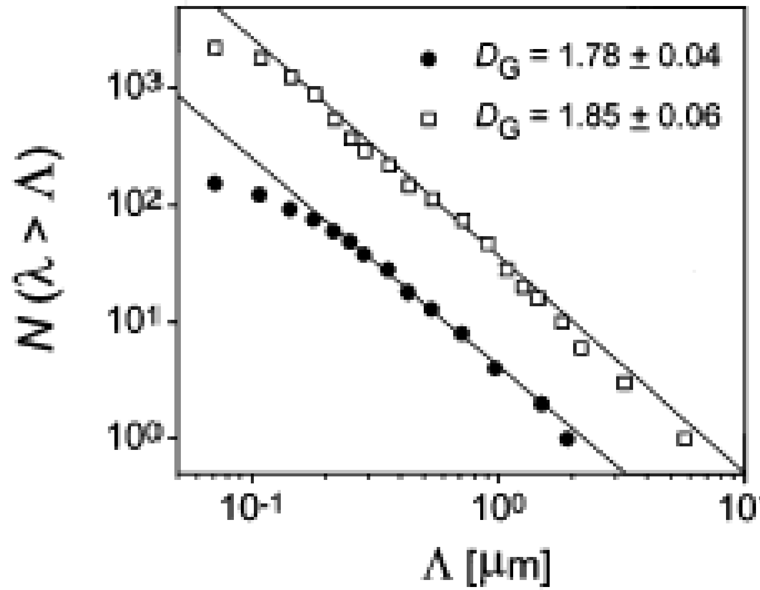
Constructions – Cell structures

Dislocation cell structures beat uniform double slip for sufficiently large deformations and sufficiently strong latent hardening

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)

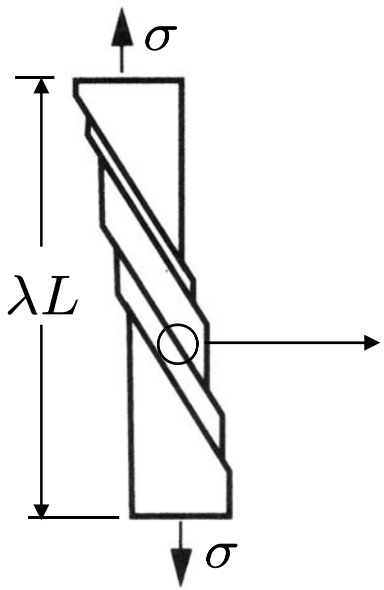
Dislocation structures – Fractality

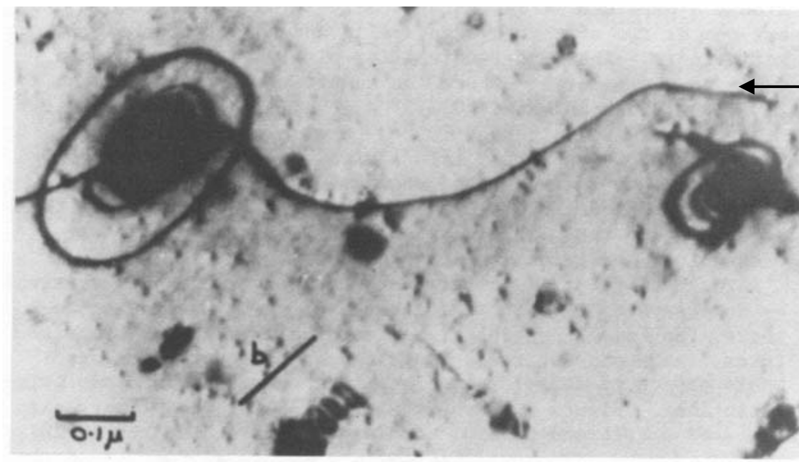
Dislocation cell construction is consistent with the observed self-similar structure of dislocation cells

Crystal plasticity – Exact relaxation

- Microstructures may be regarded as ‘failure mechanisms’ resulting from material instabilities
- Simple constructions (even in the absence of optimality) suffice to explain observed microstructures
- Exact relaxation is known for small-strain single crystal plasticity (Conti, S. and Ortiz, M., *Arch. Rat. Mech. Anal.*, **176** (2005) 103-147)
- Exact relaxation of finite-deformation plasticity is known for single slip (S. Conti and F. Theil, *Arch. Rat. Mech. Anal.*, **178** (2005) 125-148)
- The general finite-deformation case is open!

Non-local extension - Scaling





(Humphreys and Hirsch '70)

dislocation lines carry additional energy

$$T \sim Gb^2$$

dislocation energy/ unit length

- Incremental flow rule: $F^p = \exp\left\{\sum \gamma s \otimes m\right\}$
- Local: $F_{\text{loc}}(y,\gamma) = \int_\Omega \left\{W^e(\nabla y\, F^{p-1}) + W^p(\gamma)\right\} dx$
- Nonlocal extension:

$$F(y,\gamma) = F_{\text{loc}}(y,\gamma) + \int_\Omega \sum \underbrace{T\left(\frac{\text{curl}(\gamma m)}{|\text{curl}(\gamma m)|}\right)}_{\text{anisotropic line tension}} \underbrace{|\text{curl}(\gamma m)|}_{\text{dislocation density}}\, dx$$

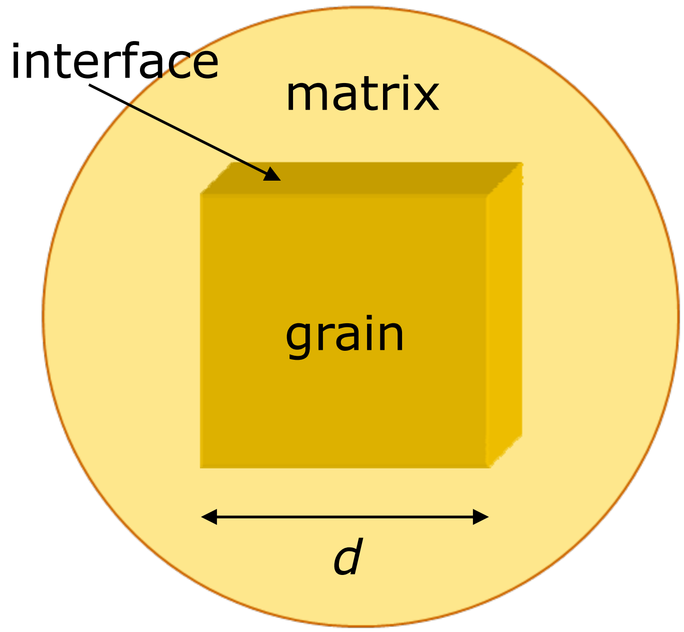
strain gradients! → anisotropic line tension   dislocation density

Nonlocal extension - Scaling

- Consideration of dislocation energies renders the energy **non-local**
- The anisotropic line-tension model follows as a rigorous limit of discrete dislocation dynamics (Garroni, A. and Müller, S., *SIAM J. Math. Anal.*, **36** (2005) 1943-1964; *ARMA* **3** (2006) 535-578)
- Non-attainment problem removed but solutions can still exhibit fine oscillations!
- **Questions**. What is the effect of non-locality on:
  - *Microstructure and patterning?*
  - *Macroscopic behavior and scaling?*

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

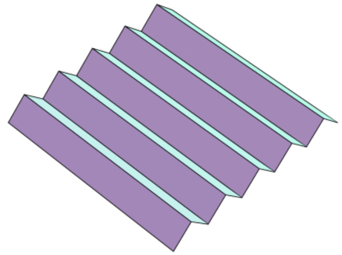


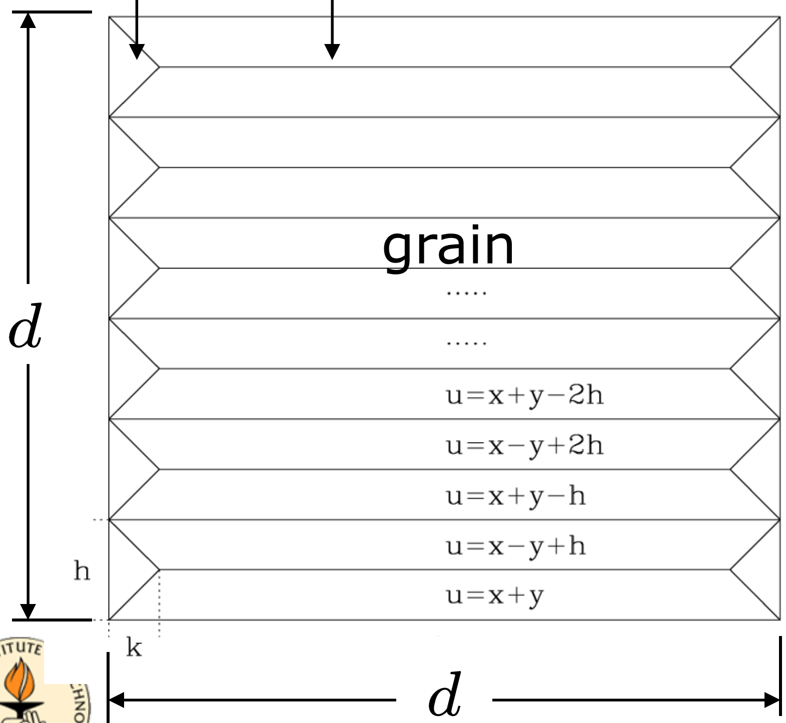
Grain in elastic matrix
(Conti, S. and Ortiz, M., *ARMA*, **176** (2005) 147)

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

macroscopic scaling laws!

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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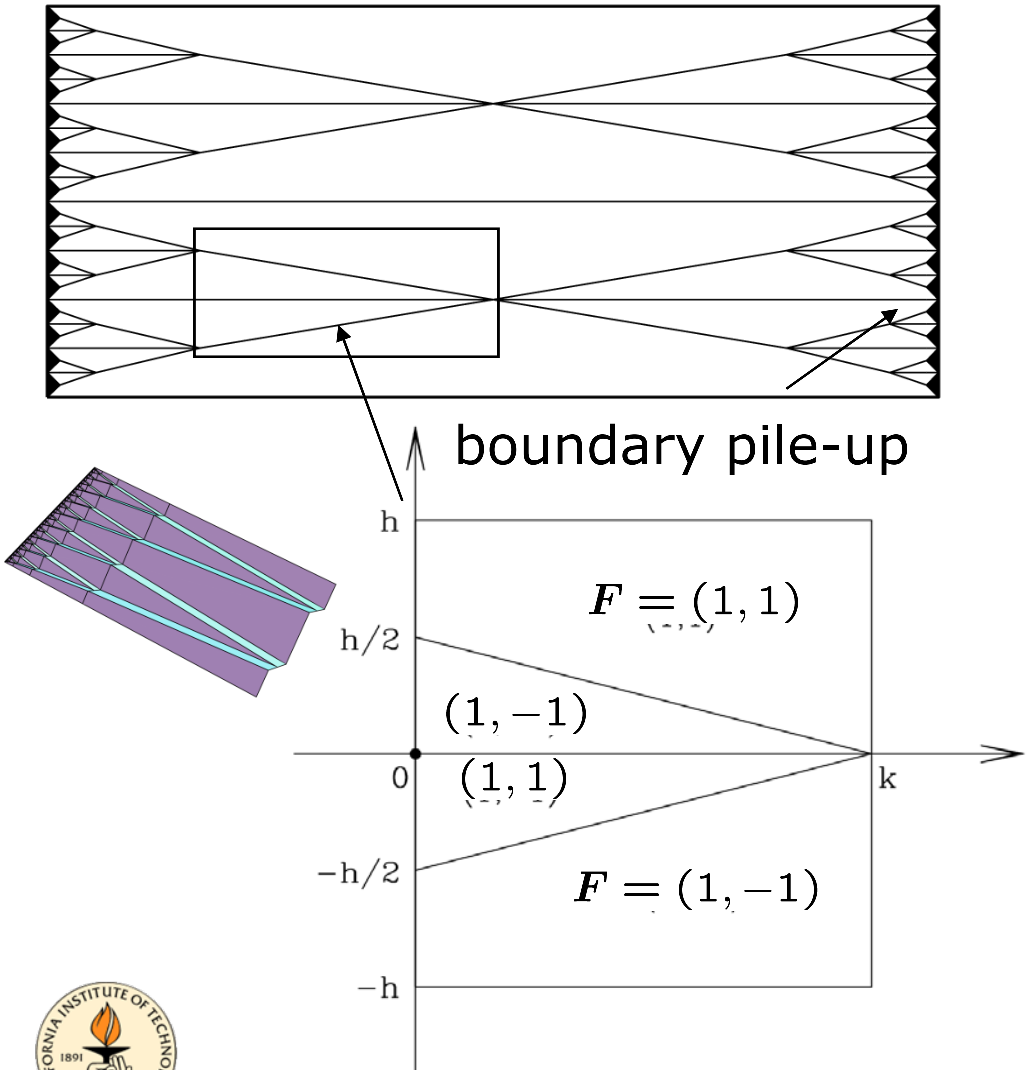
Optimal scaling – Branching construction



- Energy:

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

- Yield stress:

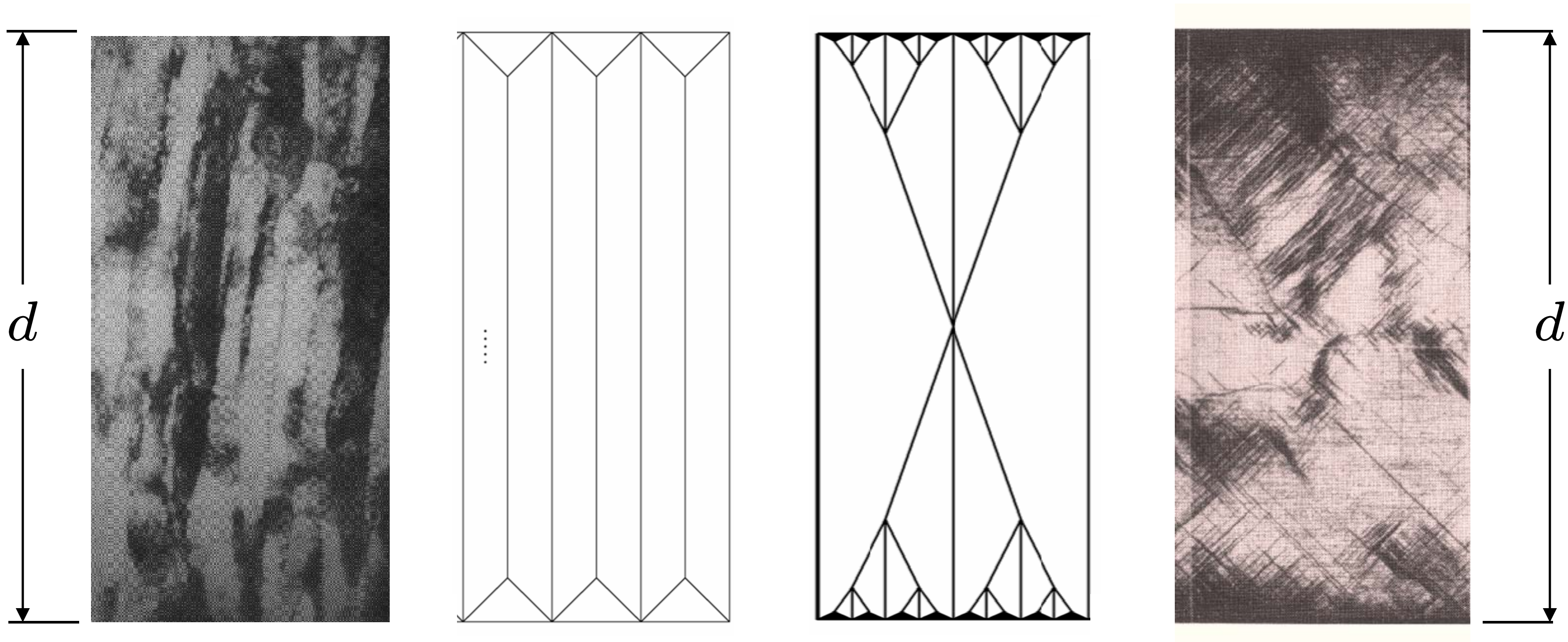
$$\tau \sim \tau_c + \left(\frac{T}{bd} \right)^{2/3} (G\gamma)^{1/3}$$

- Microstructure size:

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

refinement with strain!

Optimal scaling – 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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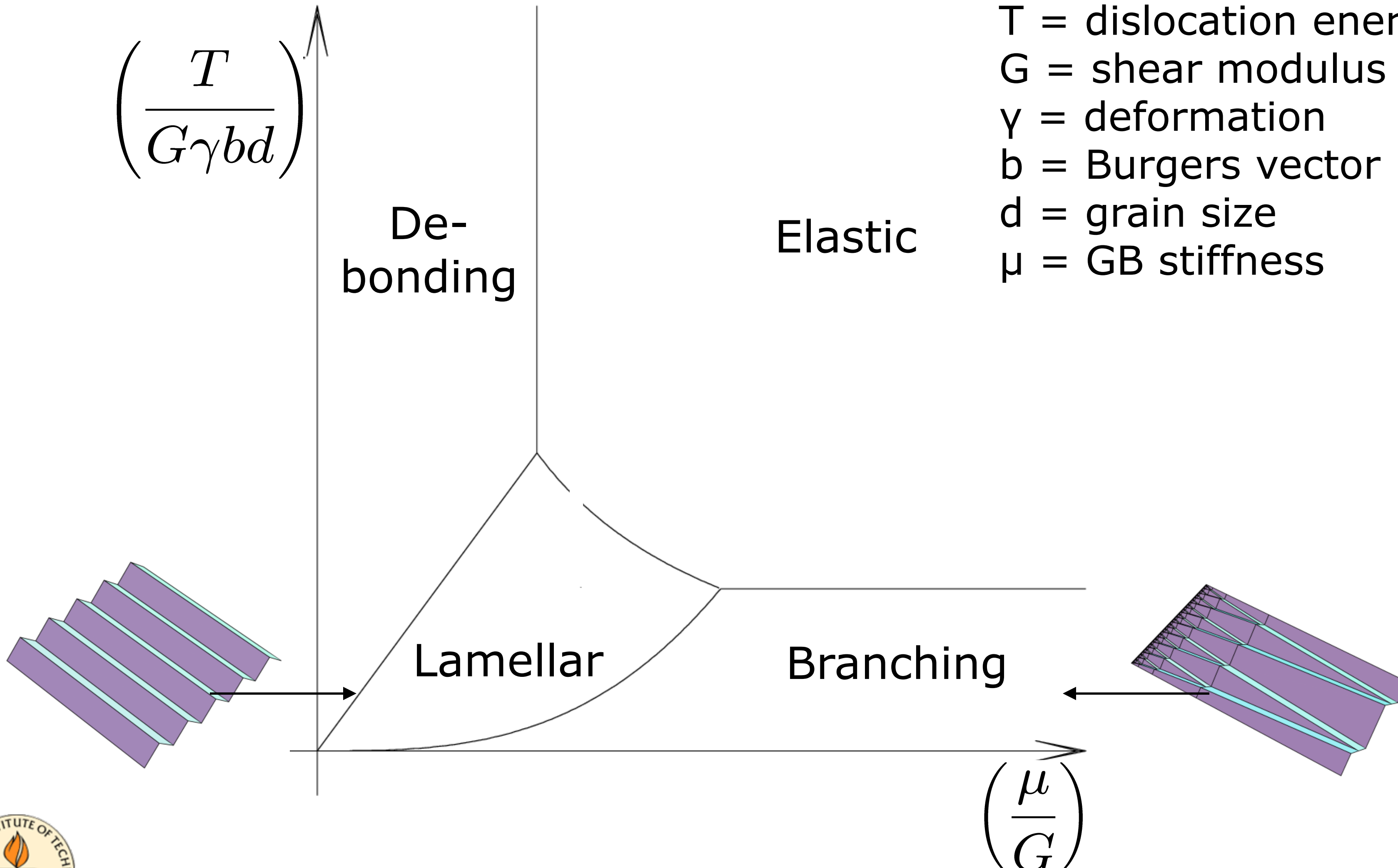
Optimal scaling – Mechanism map

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



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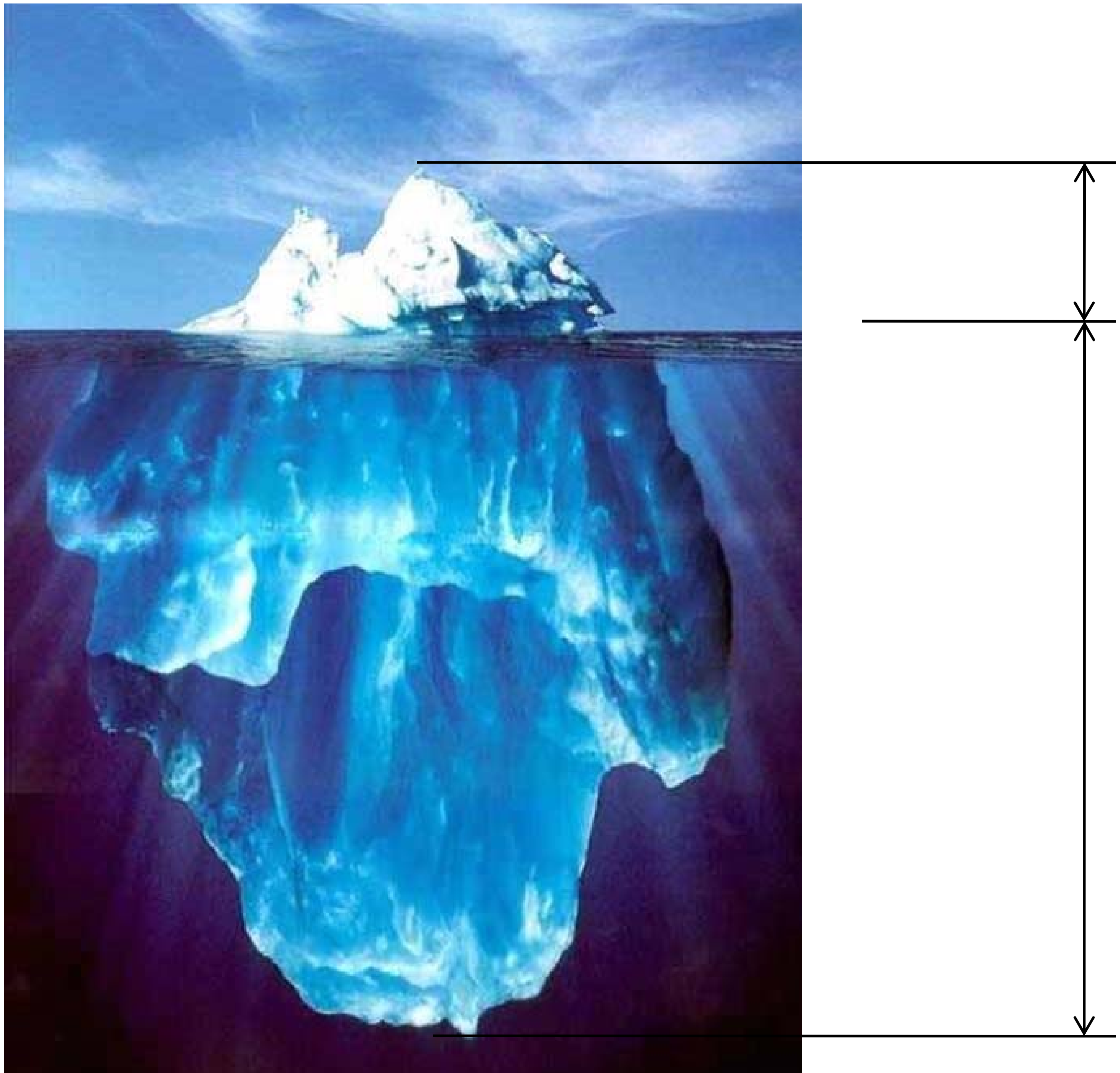
Optimal scaling – Mechanism map

Non-locality introduces a lengthscale (size cut-off) but can also radically change the microstructural pattern (e.g., branching)

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*
  - *…*

Convex *vs.* nonconvex-plasticity



Concluding remarks

THANK YOU!