Variational Methods in Convex and Non-Convex Plasticity

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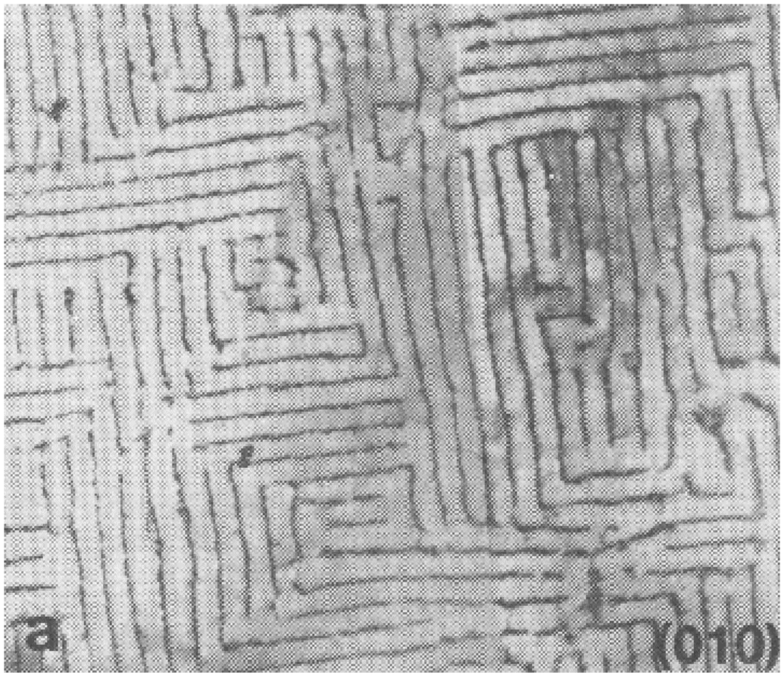
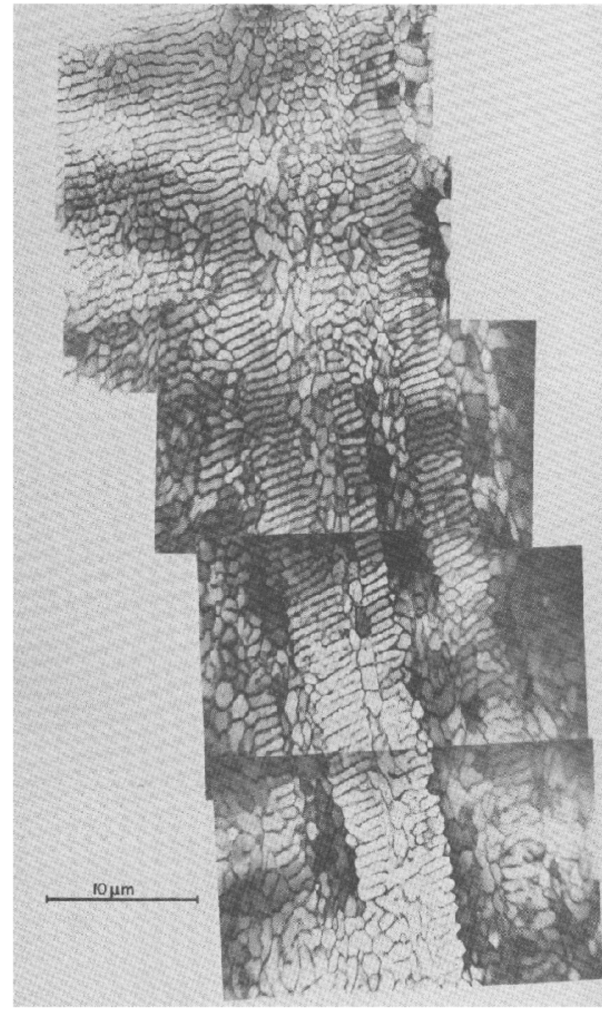
Subgrain dislocation structures - Fatigue

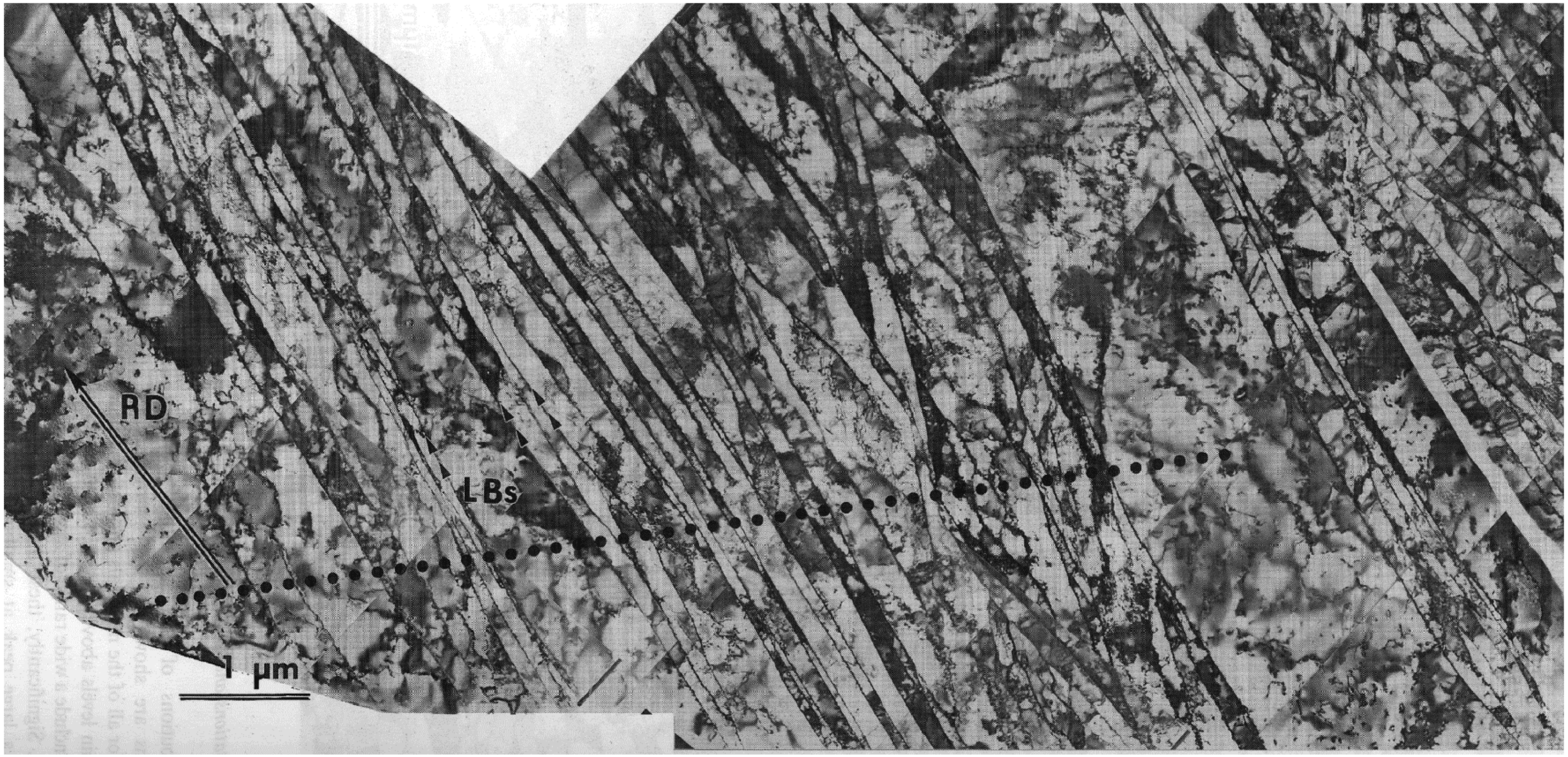


Labyrinth structure in fatigued copper single crystal (Jin and Winter, 1984)

Nested bands in copper single crystal fatigued to saturation (Ramussen and Pedersen, 1980) →

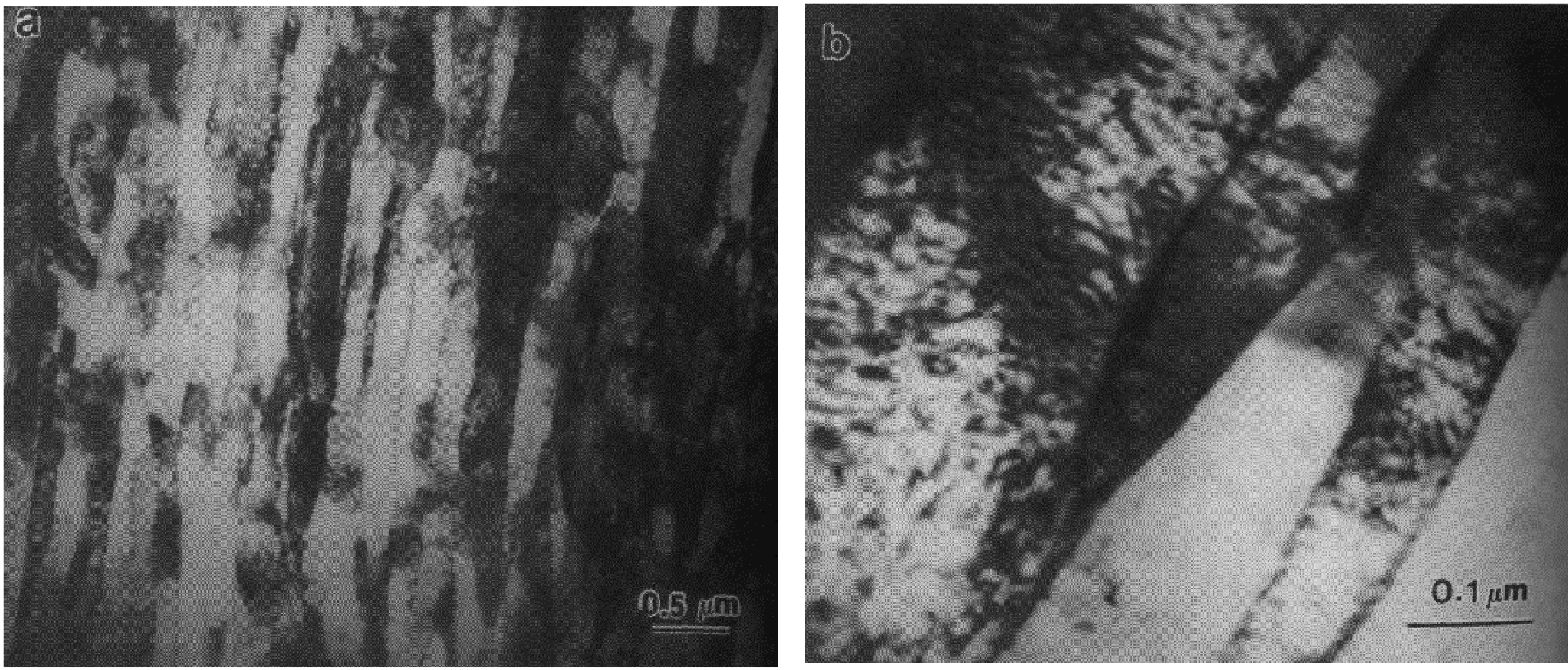


Subgrain dislocation structures - Static



90% cold rolled Ta (Hughes and Hansen, 1997)

Subgrain dislocation structures - Shock



Shocked Ta (Meyers et al., 1995)

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Overview

- Objective: To develop a theory of single-crystal plasticity with microstructure (subgrain dislocation structures):
  - *To understand the physical mechanisms underlying the formation and evolution of microstructures in ductile single crystals*
  - *The predict the effective macroscopic behavior of crystals with microstructure*
  - *To ascertain the scaling laws which govern the behavior of crystals with microstructure, including size effects*
- Assumption: Separation of scales. Multiscale approach:
  - *Macroscopic fields (e.g., finite elements) governed by effective behavior, computed `on the fly'*
  - *Microstructure handled explicitly at the subgrid level*
- Building blocks of the theory:
  - *Variational formulation of finite-deformation plasticity based on time discretization*
  - *Minimization of non-convex work-of-deformation functionals*
  - *Nonlocal regularization*

Initial Boundary-Value Problem

- **Initial boundary value problem**: Suppose that the crystal is subject to affine boundary conditions, i. e., $y_i(\boldsymbol{x}, t) = \bar{F}_{ij}(t) x_j$ on $\partial\Omega$, and that the state $(\boldsymbol{y}, \boldsymbol{F}^p, \boldsymbol{\gamma})$ of the crystal is known at $t = 0$. We wish to determine the state of the crystal for $t > 0$.

- For all $t > 0$,

Nonconvex dependence, requires regularization

$$\inf_{\boldsymbol{y}} \int_\Omega A(D\boldsymbol{y}, \boldsymbol{F}^p, \boldsymbol{\gamma}) dx$$

← **(BVP)**

- For all $x \in \Omega$,

$$\dot{\boldsymbol{F}}^p \boldsymbol{F}^{p-1} = \sum_{\alpha=1}^{N} \dot{\gamma}^\alpha \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha$$

← **(System of nonholonomic constraints)**

$$\dot{\boldsymbol{\gamma}} = \partial\psi(\boldsymbol{Y}) \equiv \mathbf{f}(\boldsymbol{F}, \boldsymbol{F}^p, \boldsymbol{\gamma})$$

← **(System of ODE's)**

(Convex, proper, lower semi-continuous)

Variational constitutive updates

(Ortiz and Stainier, CMAME, 1999; Ortiz, Repetto and Stainier, JMPS, 2001)

- **Discretize time**: Wish to approximate the deformation mapping at discrete times $t_0 = 0,\ t_1 = \Delta t,\ \ldots,\ t_n = n\Delta t$ $\ldots \Rightarrow \boldsymbol{y}_0,\ \boldsymbol{y}_1,\ \ldots\ \boldsymbol{y}_n,\ \ldots.$
- Integrate flow rule in time: $\boldsymbol{F}^p_{n+1} = \exp\left\{\sum_{\alpha=1}^{N} \Delta\gamma^\alpha \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha\right\} \boldsymbol{F}^p_n$

  (Ortiz et al., IJNME, 2001) → exp
- Incremental work density function:

$$f_n(\boldsymbol{F}_{n+1}, \boldsymbol{\gamma}_{n+1}) = A(\boldsymbol{F}_{n+1}, \boldsymbol{F}^p_{n+1}, \boldsymbol{\gamma}_{n+1}) - A_n + \Delta t\, \psi^* \left(\frac{\Delta\gamma}{\Delta t}\right)$$

- Incremental work density: $W_n(\boldsymbol{F}_{n+1}) = \min_{\boldsymbol{\gamma}_{n+1} \geq \boldsymbol{\gamma}_n} f_n(\boldsymbol{F}_{n+1}, \boldsymbol{\gamma}_{n+1})$
- Incremental stress-strain relations: $\boldsymbol{P}_{n+1} = \dfrac{\partial W_n}{\partial \boldsymbol{F}_{n+1}}(\boldsymbol{F}_{n+1})$

Incremental BVP -Variational formulation

(Ortiz and Repetto, JMPS, 1999)

- **Incremental *minimum* principle**:

$$I_n[\boldsymbol{y}_{n+1}] \equiv \int_\Omega W_n(D\boldsymbol{y}_{n+1})dx \Rightarrow \boxed{\inf_{\boldsymbol{y}_{n+1}} I_n[\boldsymbol{y}_{n+1}]}$$

- Euler-Lagrange equations:

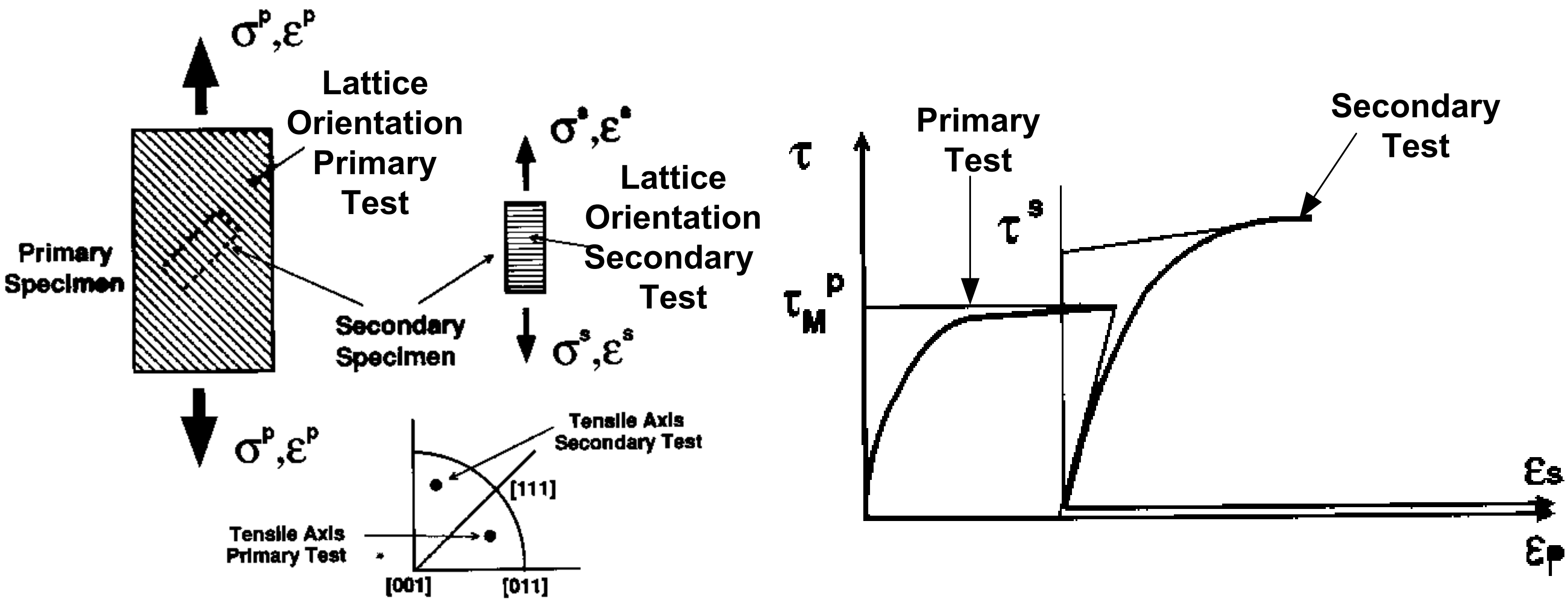
$$\delta I_n[\boldsymbol{y}_{n+1}] = \int_\Omega \boldsymbol{P}_{n+1} \cdot \nabla \delta \boldsymbol{y}_{n+1} dx = 0$$

$\equiv$ equilibrium equations (weak form).

- Classical platicity, small strains: $W_n(\boldsymbol{\epsilon}_{n+1})$ ***convex*** $\Rightarrow$ ***uniqueness!*** (no microstructures).

- Single-crystal plasticity: $W_n(\boldsymbol{F}_{n+1})$ not quasi-convex $\Rightarrow$ (evolving) ***microstructures***.

Strong latent hardening



Kocks, U. F., “Polyslip in single crystals”, *Acta Metallurgica*, **8** (1960) 345.

Kocks, U. F., “Latent hardening and secondary slip in aluminum and silver” *Trans. Metall. Soc. AIME*, **230** (1964) 1160.

Franciosi, P. Berveiller, M., Zaoui, A., “Latent hardening in copper and aluminum single crystals”, *Acta Metallurgica*, **28** (1980) 273.

Strong latent hardening

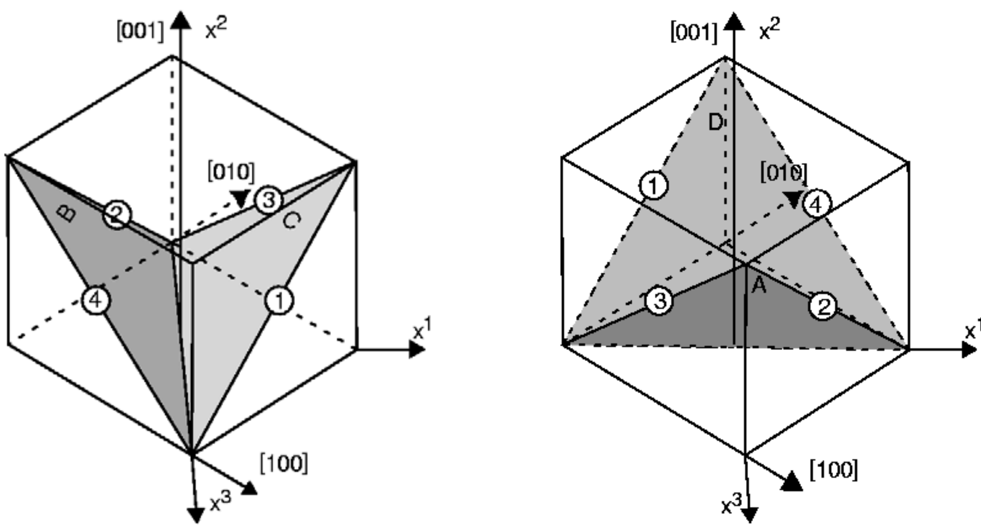
- Linear-hardening model:

$$A(\boldsymbol{F}, \boldsymbol{F}^p, \boldsymbol{\gamma}) = W^e(\boldsymbol{F}\boldsymbol{F}^{p-1}) + W^p(\boldsymbol{\gamma})$$

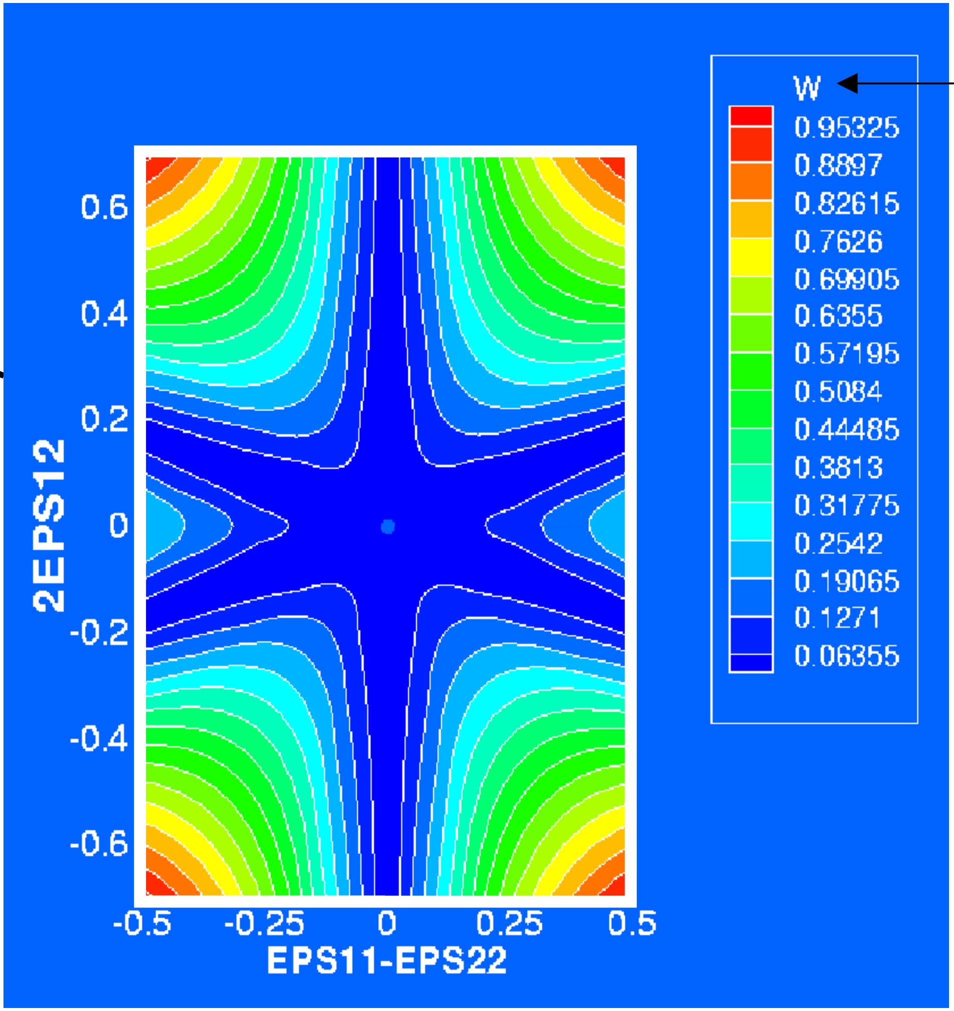
$$W^p = \tau_0 \sum_{\alpha=1}^{N} \gamma^\alpha + \frac{1}{2} \sum_{\alpha=1}^{N} \sum_{\beta=1}^{N} h_{\alpha\beta} \gamma^\alpha \gamma^\beta$$

with $h_{\alpha\alpha} = h_0, \; h_{\alpha\beta} = h_1 > h_0, \; \beta \neq \alpha$

- Two-dimensional example:



Strong latent hardening



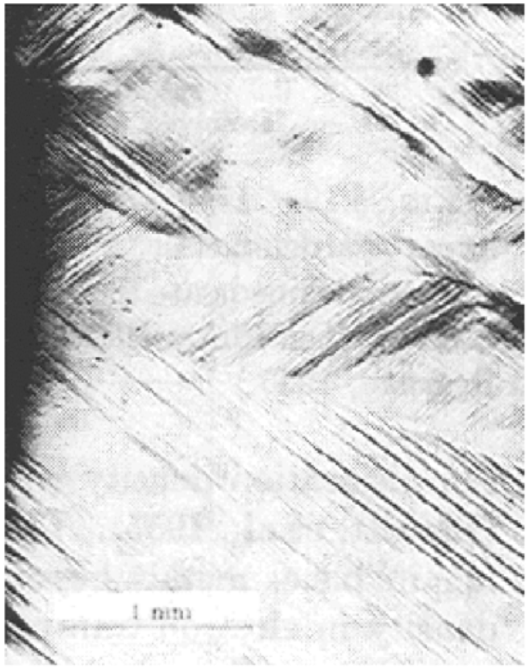
Single-slip directions

Nonconvex!

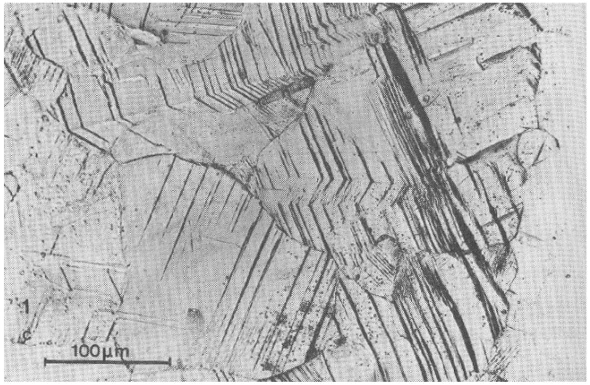
Patchy slip!

Incremental work density function, quadratic model, two-dimensional geometry

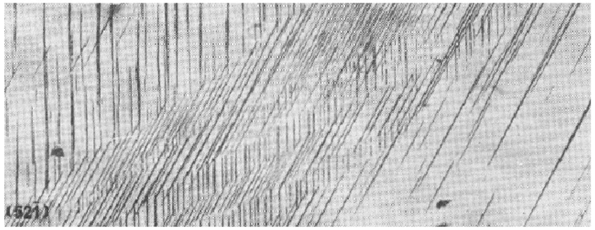
Strong latent hardening



(Saimoto, 1963)



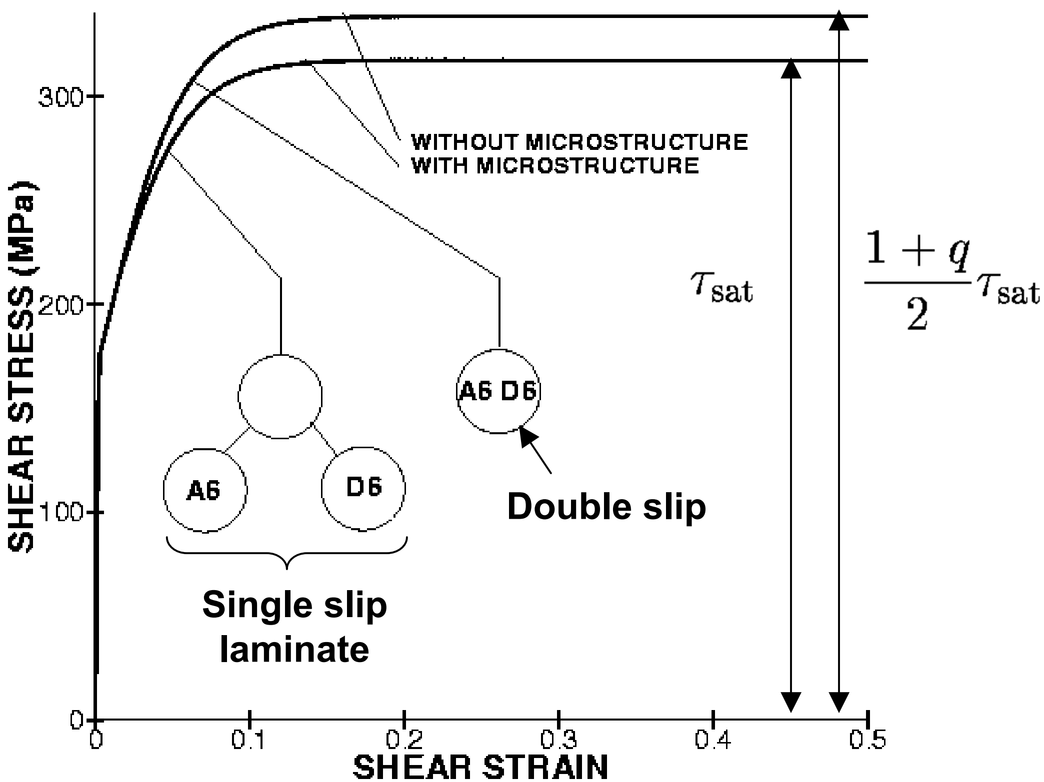
(Ramussen and Pedersen, 1980)

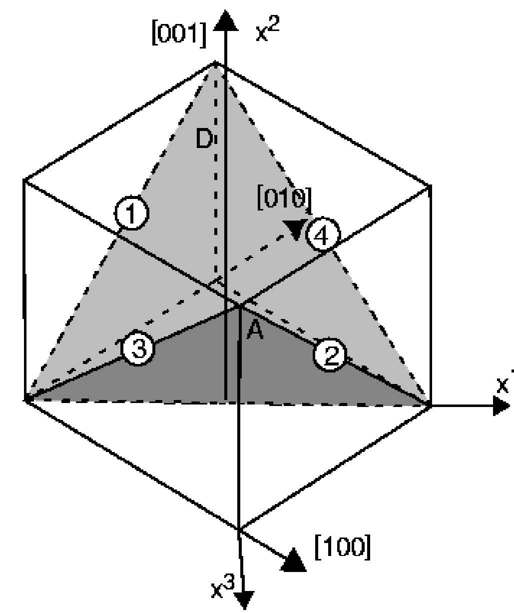


(Jin and Winter, 1984)

- **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).

Example – fcc crystal in simple shear





Two-dimensional geometry
Potentially active slip systems

Stress-strain curves for an fcc crystal subjected to simple shear on the (001) plane in the [110] direction, showing the softening of microstructre development. The curves are obtained using Hutchinson [36] and Pierce *et al.* [70] model of hardening, with material constants representative Al-Cu alloys [3, 12].

Nonlocal core-energy regularization

- Dislocation density tensor: $\boldsymbol{A} = -\nabla \times \boldsymbol{F}^p = \boldsymbol{b} \otimes \boldsymbol{t}\delta_L$.
- Identity: $\int_\Omega |\boldsymbol{A}| dx = bL$, where $L \equiv$ dislocation length.
- Isotropic line-energy approximation:

$$E^{\text{core}} = TL = \int_\Omega \frac{T}{b} |\boldsymbol{A}| dx = \int_\Omega \frac{T}{b} |\nabla \times \boldsymbol{F}^p| dx$$

where $T = U^{\text{core}}$ is the dislocation core-energy per unit length, or *line tension*.

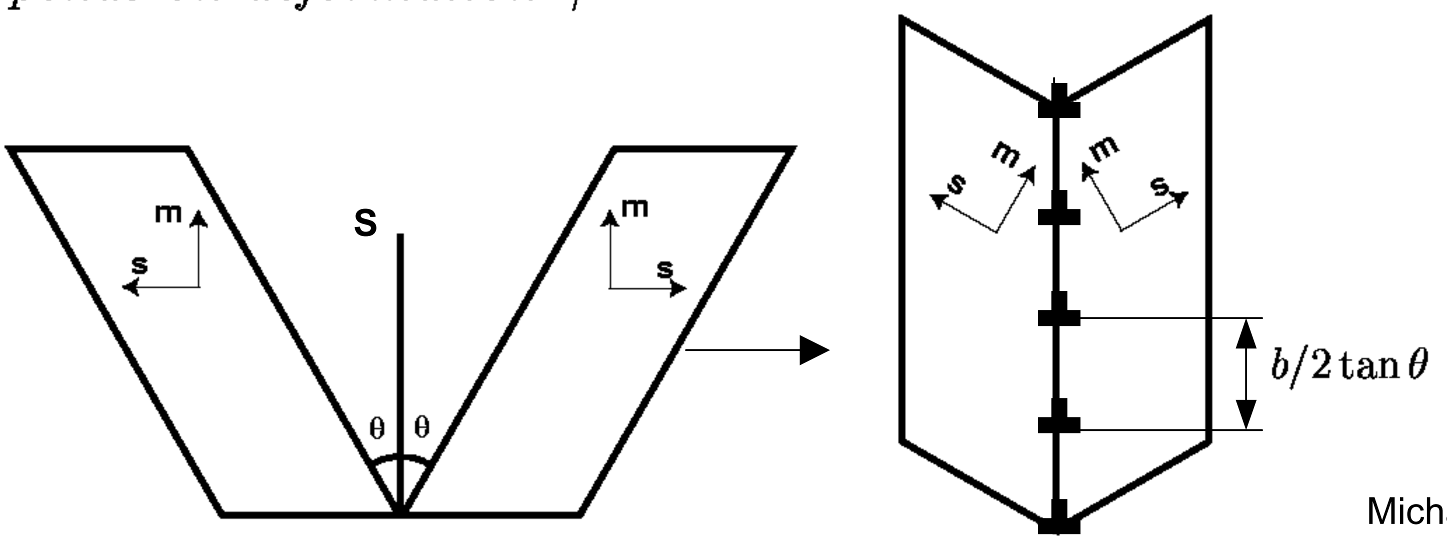
- Regularized problem: $\inf_{\boldsymbol{y}_{n+1}} I_n[\boldsymbol{y}_{n+1}]$, where:

$$I_n[\boldsymbol{y}_{n+1}] \equiv \int_\Omega W_n(D\boldsymbol{y}_{n+1}) dx + \int_\Omega \frac{T}{b} |\nabla \times \boldsymbol{F}^p_{n+1}| dx$$

(Ortiz and Repetto, JMPS, 1999)

Analysis: Symmetric tilt boundary

- Variant deformation: $\boldsymbol{F}^{\pm} = \boldsymbol{R}(\boldsymbol{s}\times\boldsymbol{m};\pm\theta)\,[\boldsymbol{I}\pm\tan\theta\,\boldsymbol{s}\otimes\boldsymbol{m}]$, Here, $\gamma = \tan\theta$, $\boldsymbol{F}^p = \boldsymbol{I}\pm\tan\theta\,\boldsymbol{s}\otimes\boldsymbol{m}$; $\boldsymbol{F}^e = \boldsymbol{R}(\boldsymbol{s}\times\boldsymbol{m};\pm\theta) \in SO(3) \Rightarrow$ *no elastic long-range stresses!*.
- Dislocation density tensor: $\boldsymbol{A}(\boldsymbol{x}) = 2\tan\theta\,\boldsymbol{s}\otimes(\boldsymbol{s}\times\boldsymbol{m})\,\delta_S(\boldsymbol{x})$ $\equiv$ planar array of parallel edge dislocations, *tilt boundary*.
- Wall energy density: $\Gamma = 2\gamma(T/b) = T/(b/2\tan\theta)$, *depends on deformation* γ.



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Incremental BVP - Relaxation

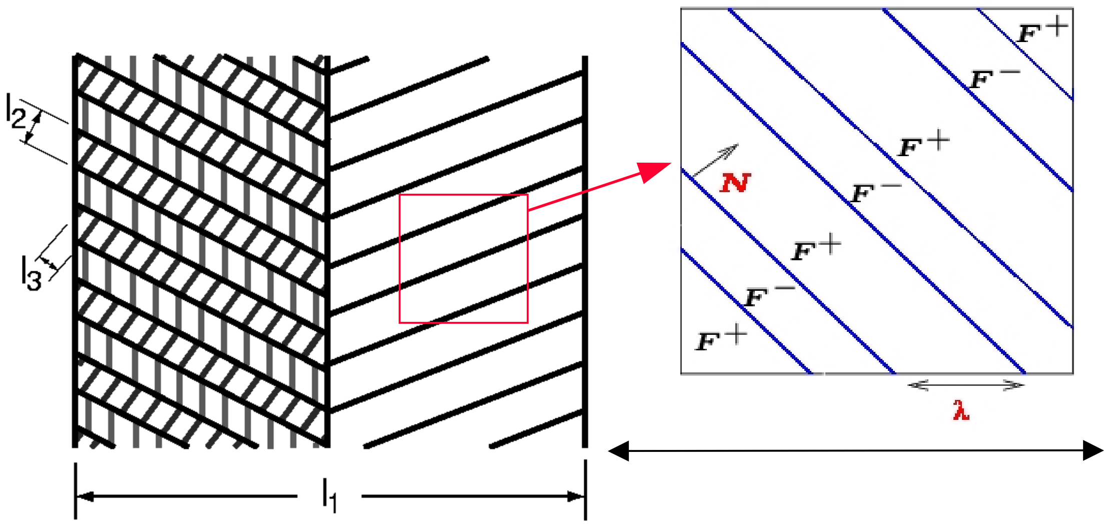
- Relaxed problem: $\inf_{\boldsymbol{y}_{n+1}} \int_\Omega QW_n(D\boldsymbol{y}_{n+1})dx$

  where: $QW_n(\boldsymbol{F}) = \frac{1}{|E|} \inf_{\boldsymbol{u} \in W_0^{1,\infty}(E)} \int_E W_n(\boldsymbol{F} + D\boldsymbol{u})dx$

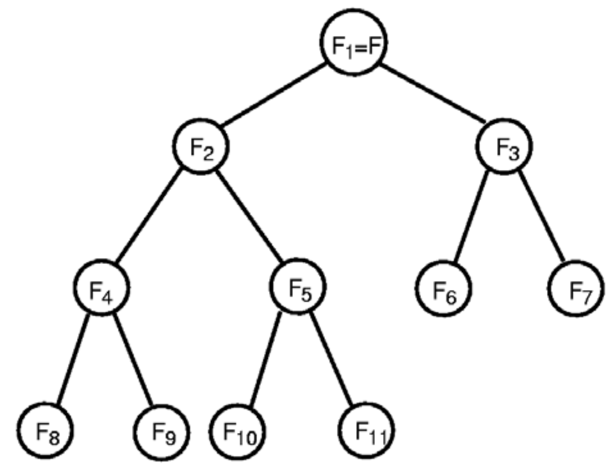
- Relaxed energy density: Minimum energy density attainable by consideration of all possible microstructures consistent with a macroscopic or average deformation.
- No constructive method is known for relaxing general energy densities $\Rightarrow$ consider special microstructures
- Sequential laminates $\Rightarrow$ Rank-1 convexification
- No practical algorithm is known for computing the rank-1 convexification of a general energy density exactly

Incremental BVP - Relaxation

- Special microstructures: Sequential laminates



Sequential laminate



Graph of laminate

- Compatibility equations: $F_i^+ - F_i^- = a_i \otimes N_i$

- Averaging: $F_i = \lambda_i^- F_i^- + \lambda_i^+ F_i^+,$

$$1 = \lambda_i^- + \lambda_i^+$$

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Incremental BVP – Relaxation

(Ortiz, Repetto and Stainier JMPS, 2001; Aubry, Fago and Ortiz, 2001)

- Objective: To formulate a practical rank-1 convexification algorithm.
- Laminate energy: $$LW(F) = \sum_{i \in \text{leaves}} \nu_i W(F_i)$$
- For fixed graph, enforce mechanical and configurational equilibrium:

$$\langle DLW(F), \delta a_i \rangle = 0 \Rightarrow [\![P_i]\!] \cdot N_i = 0$$

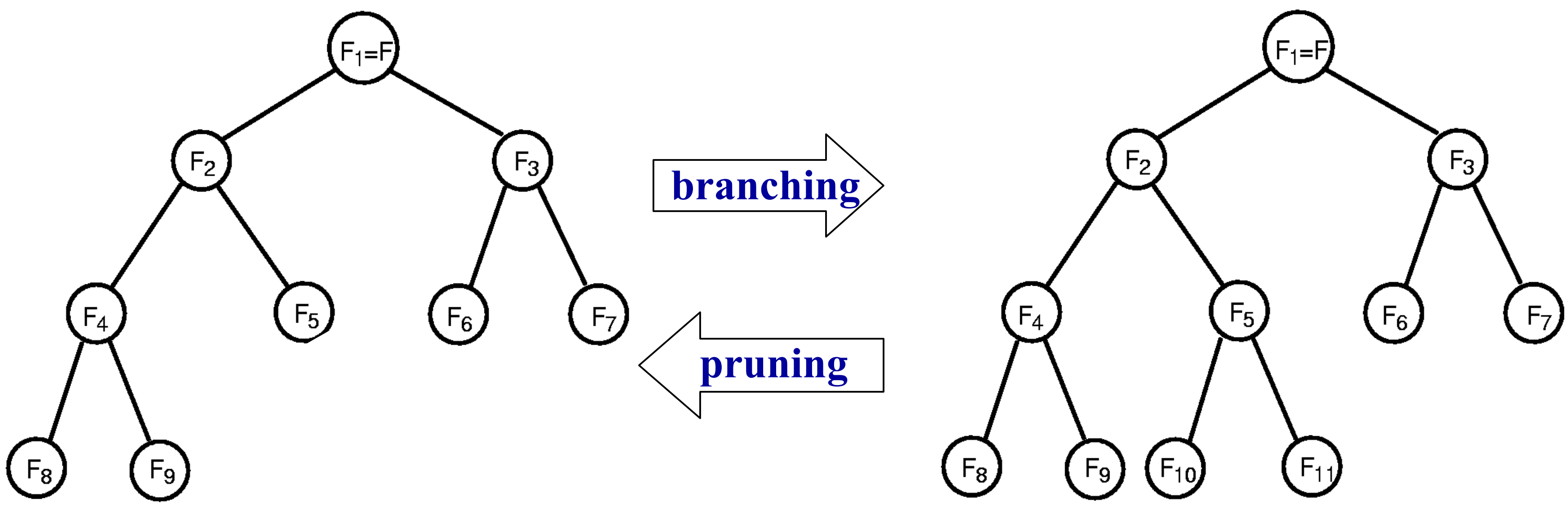
$$\langle DLW(F), \delta N_i \rangle = 0 \Rightarrow a_i \cdot [\![F_i]\!] = \mu_i N_i$$

$$\langle DLW(F), \delta \lambda_i \rangle = 0 \Rightarrow f_i \equiv [\![W_i]\!] - \langle P_i \rangle \cdot [\![F_i]\!] = 0$$

- Microstructural evolution: Branching and pruning of leaves

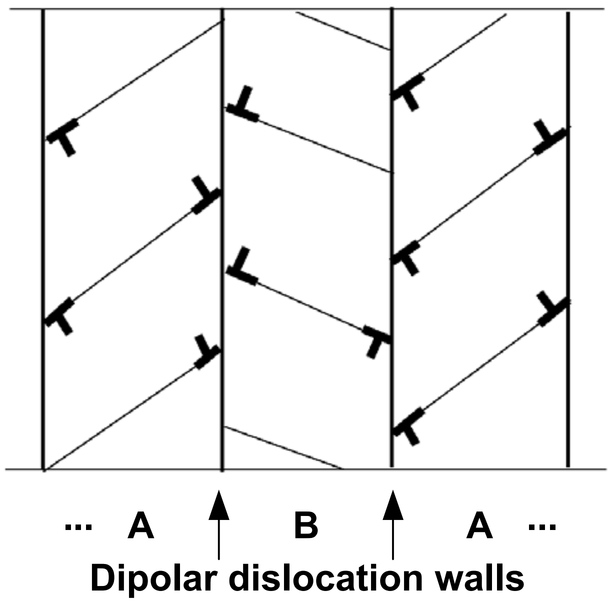
Incremental BVP – Relaxation

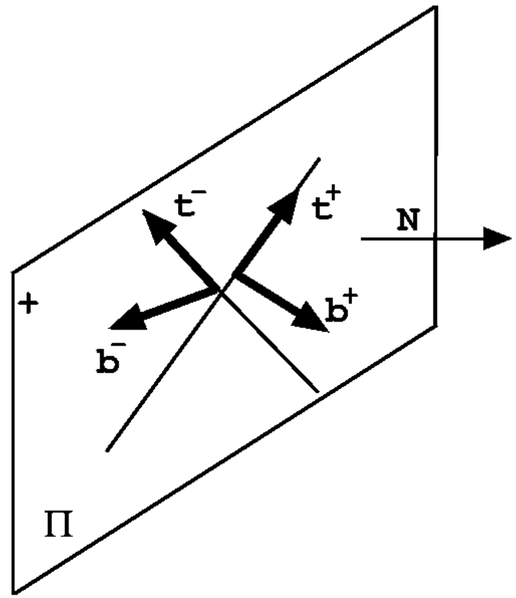
(Aubry, Fago and Ortiz, 2001)



- Accept branching if and only if it lowers the energy of the laminate
- Prune a leaf of its volume fraction goes to 0 or 1
- Re-equilibrate laminate after each transition
- Apply algorithm at Gauss points as part of constitutive update
- No FE interpolation enhancement

Analysis – Dipolar dislocation walls





- Dislocation-density tensor: $\boldsymbol{A} = -[\![\boldsymbol{F}^p]\!] \times \boldsymbol{N}\,\delta_\Pi(\boldsymbol{x})$. This consists of the two sets of parallel dislocations:

$$\rho^\pm = (\gamma^\pm/b)\delta_\Pi, \quad \boldsymbol{b}^\pm = b\boldsymbol{s}^\pm, \quad \boldsymbol{t}^\pm = \boldsymbol{N} \times \boldsymbol{m}^\pm$$

$\Rightarrow$ ***dipolar dislocation walls.***

Analysis – Dipolar dislocation walls

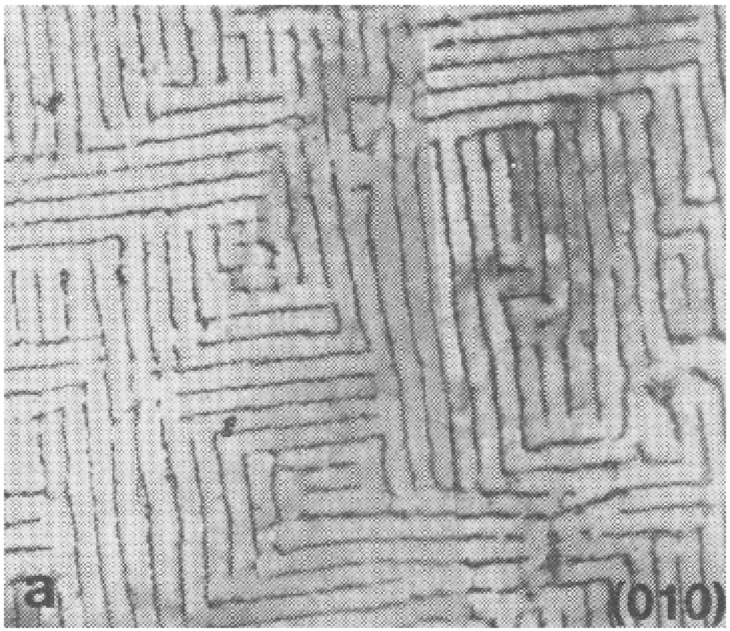
Theorem (*Ortiz and Repetto*). Let $(\boldsymbol{s}_1, \boldsymbol{m}_1)$, $(\boldsymbol{s}_2, \boldsymbol{m}_2)$, be a pair of slip systems. Then, there are two simple laminates involving single slip on system $(\boldsymbol{s}_1, \boldsymbol{m}_1)$ in one variant and single slip on system $(\boldsymbol{s}_2, \boldsymbol{m}_2)$ in the other.

Remarks:

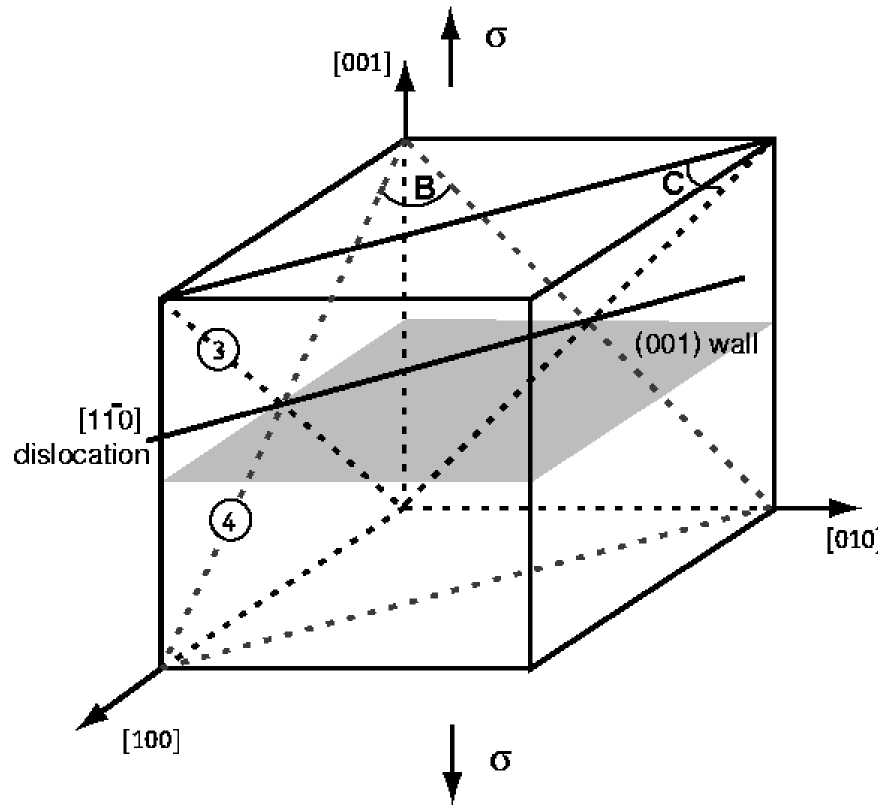
1. $\boldsymbol{N}$ and γ_2/γ_1 are determined by $\{(\boldsymbol{s}_1, \boldsymbol{m}_1), (\boldsymbol{s}_2, \boldsymbol{m}_2)\}$.
2. λ_1 and λ_2 may be chosen arbitrarily.
3. In small strains: $\boldsymbol{n} \in \{(100), (110), (111), (112), (113)\}$

same as observed experimentally in fatigued fcc crystals.

Analysis – Simple laminate structures

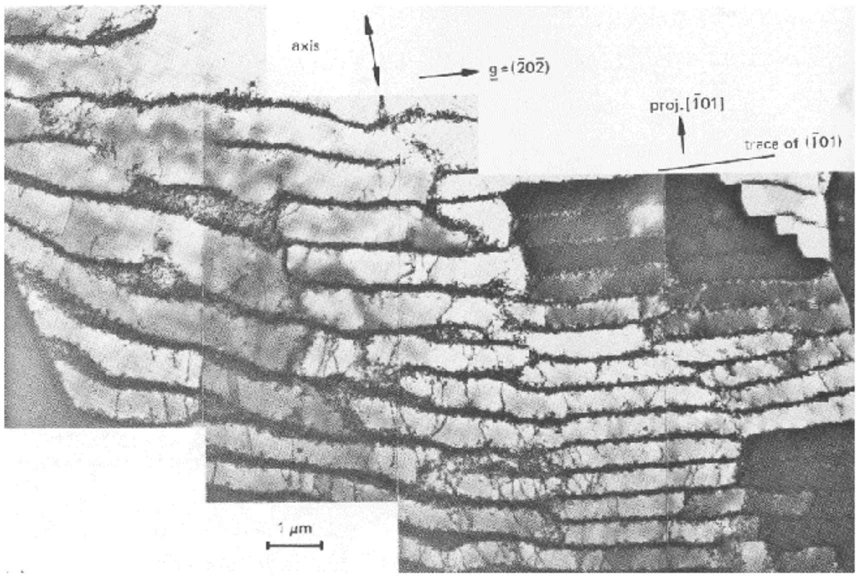


Copper single crystal fatigued with tensile axis [001], showing labyrinth wall structure(Jin and Winter, 1984)

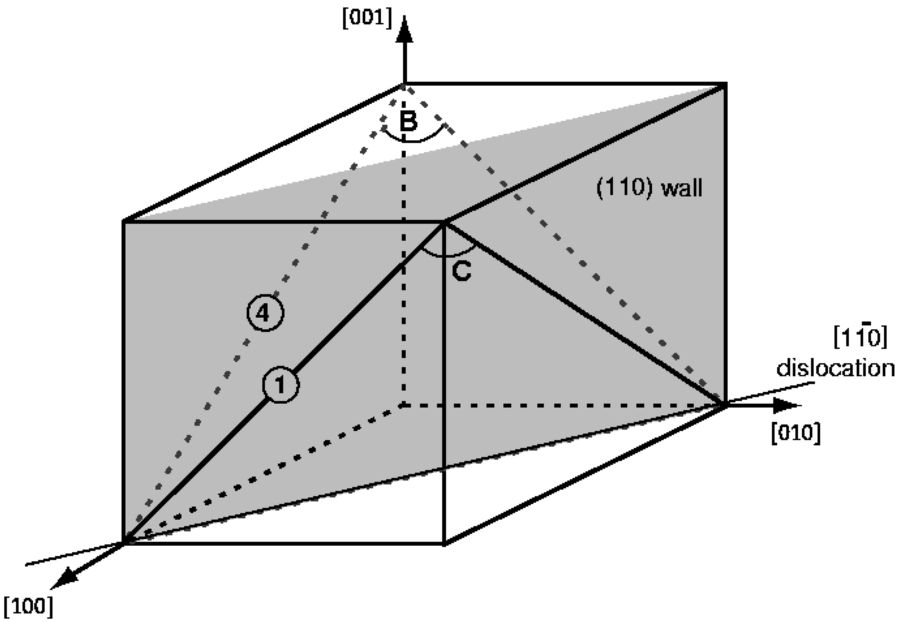


Geometry of the B4-C3 interface (Ortiz and Repetto, 1999)

Analysis – Simple laminate structures

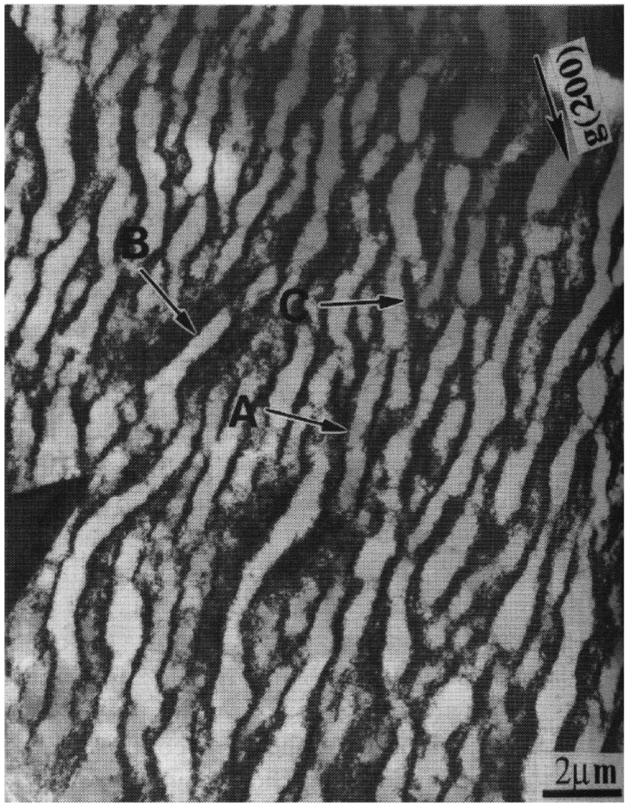


(101) wall structure in fatigued polycrystalline copper (Wang and Mughrabi, 1984)

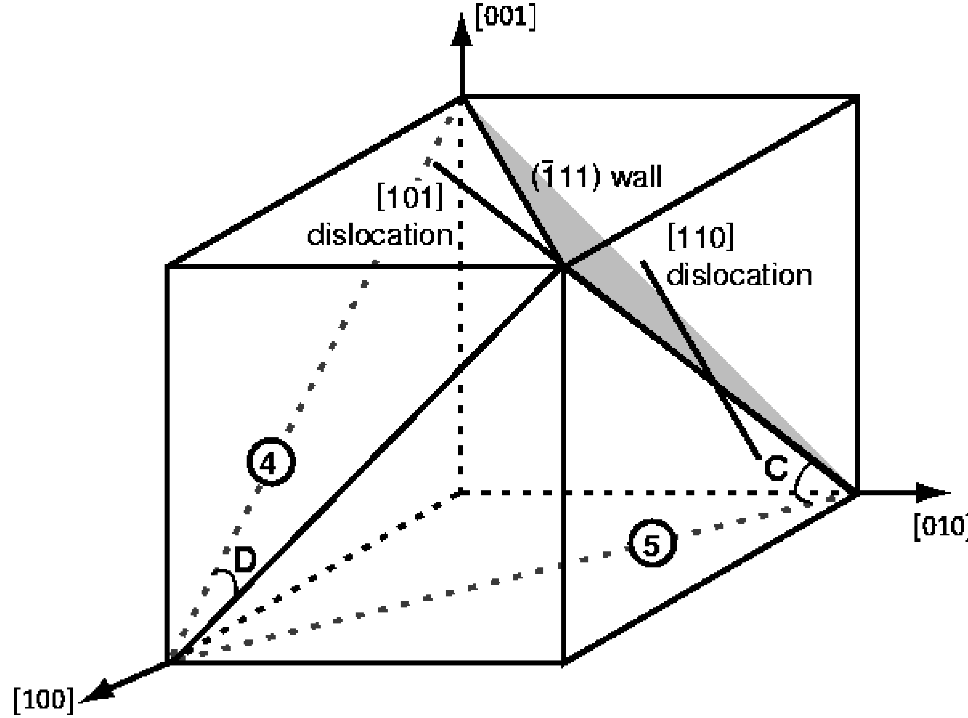


Geometry of the B4-C1 interface (Ortiz and Repetto, 1999)

Analysis – Simple laminate structures

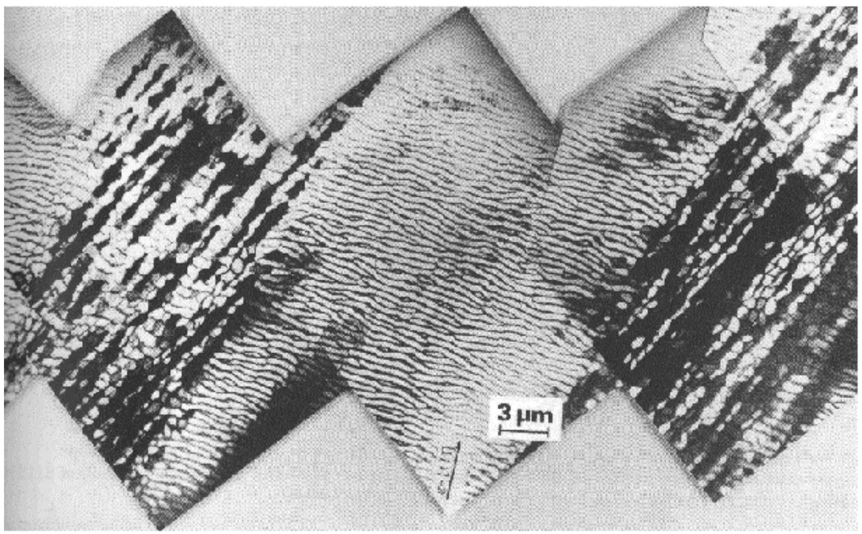


(111) wall structure in fatigued polycrystalline copper (Yumen, 1989)

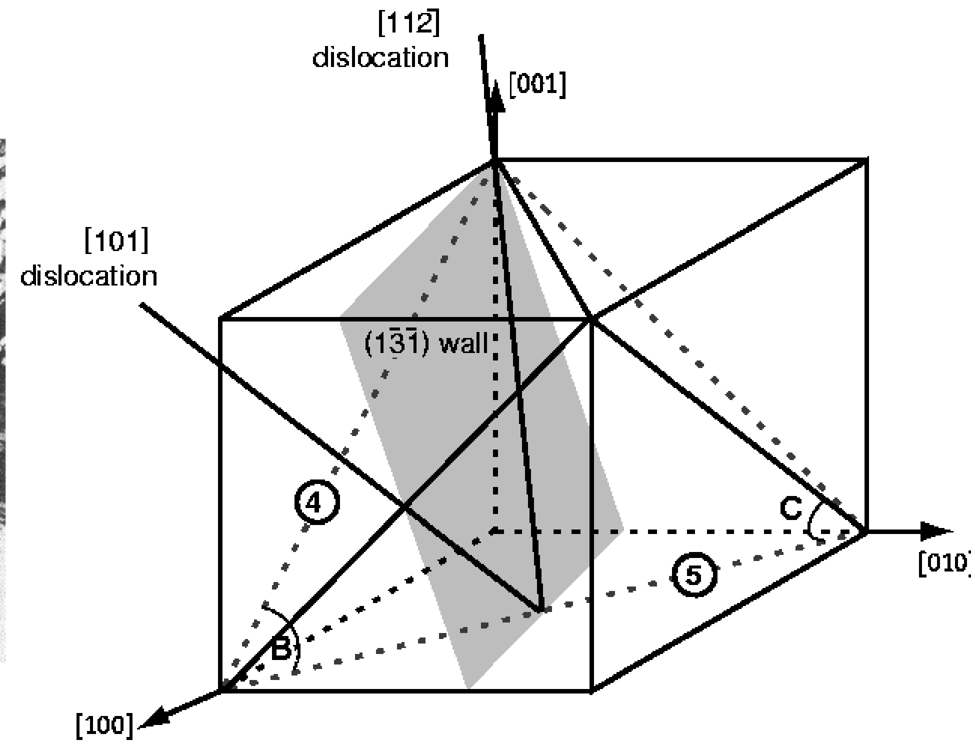


Geometry of the C5-D4 interface (Ortiz and Repetto, 1999)

Analysis – Simple laminate structures



(121) section of fatigued [111] single crystal showing possible (131) or (111) wall structure (Lepisto et al., 1986)



Geometry of the B4-C5 interface (Ortiz and Repetto, 1999)

Analysis – Sufficiency of laminates

Consider a crystal with slip-system set $\mathcal{S} = \{(\boldsymbol{s}_\alpha, \boldsymbol{m}_\alpha),\ \alpha = 1, \dots, N\}$.

Theorem (*Aubry, Bhattacharya and Ortiz*). Consider a strain of the form:

$$\bar{\boldsymbol{\epsilon}} = \sum_{\alpha=1}^{n} A_\alpha \, \mathrm{sym}(\boldsymbol{s}_\alpha \otimes \boldsymbol{m}_\alpha)$$

with $A_\alpha > 0$ and $(\boldsymbol{s}_\alpha, \boldsymbol{m}_\alpha) \in \mathcal{S}$, $\alpha = 1, \dots, n \leq N$. Then there is a sequential laminate of rank $n-1$ and average strain is $\bar{\boldsymbol{\epsilon}}$ consisting of single slip on one of the systems $(\boldsymbol{s}_\alpha, \boldsymbol{m}_\alpha) \in \mathcal{S}$, $\alpha = 1, \dots, n$ in each leave.

Remarks:

1. Rank $n-1$ of laminate is probably not optimal

Analysis – Sufficiency of laminates

Theorem (*Aubry, Bhattacharya and Ortiz*). The relaxed energy density of an elastic-perfectly plastic crystal with infinite latent hardening undergoing small strains is:

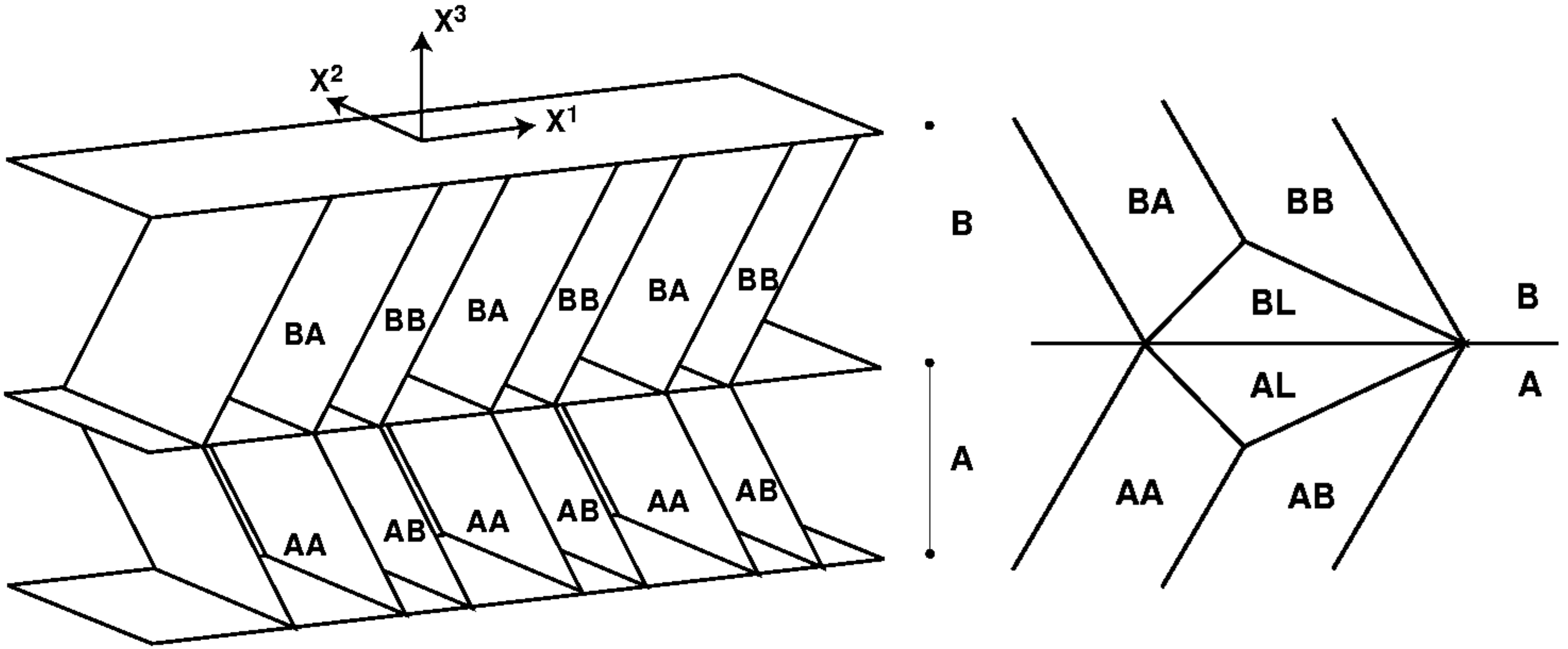
$$QW(\bar{\boldsymbol{\epsilon}}) = W^{e*}(P_C \boldsymbol{\sigma}^{\mathrm{pre}})$$

where: $\boldsymbol{\sigma}^{\mathrm{pre}} = W^e{}_{,\boldsymbol{\epsilon}}(\bar{\boldsymbol{\epsilon}})$, and P_C is the closest-point projection onto the elastic domain C.

Remarks:

1. Laminates are sufficient for relaxation.
2. Crystals can **beat** the single-slip constraint.
3. Effective behavior $\sim$ classical ideally plastic crystal.

Scaling relations



Boundary layers in sequential laminates.

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Scaling relations

- **Question**: What is the effect of the crystal size on the effective behavior?

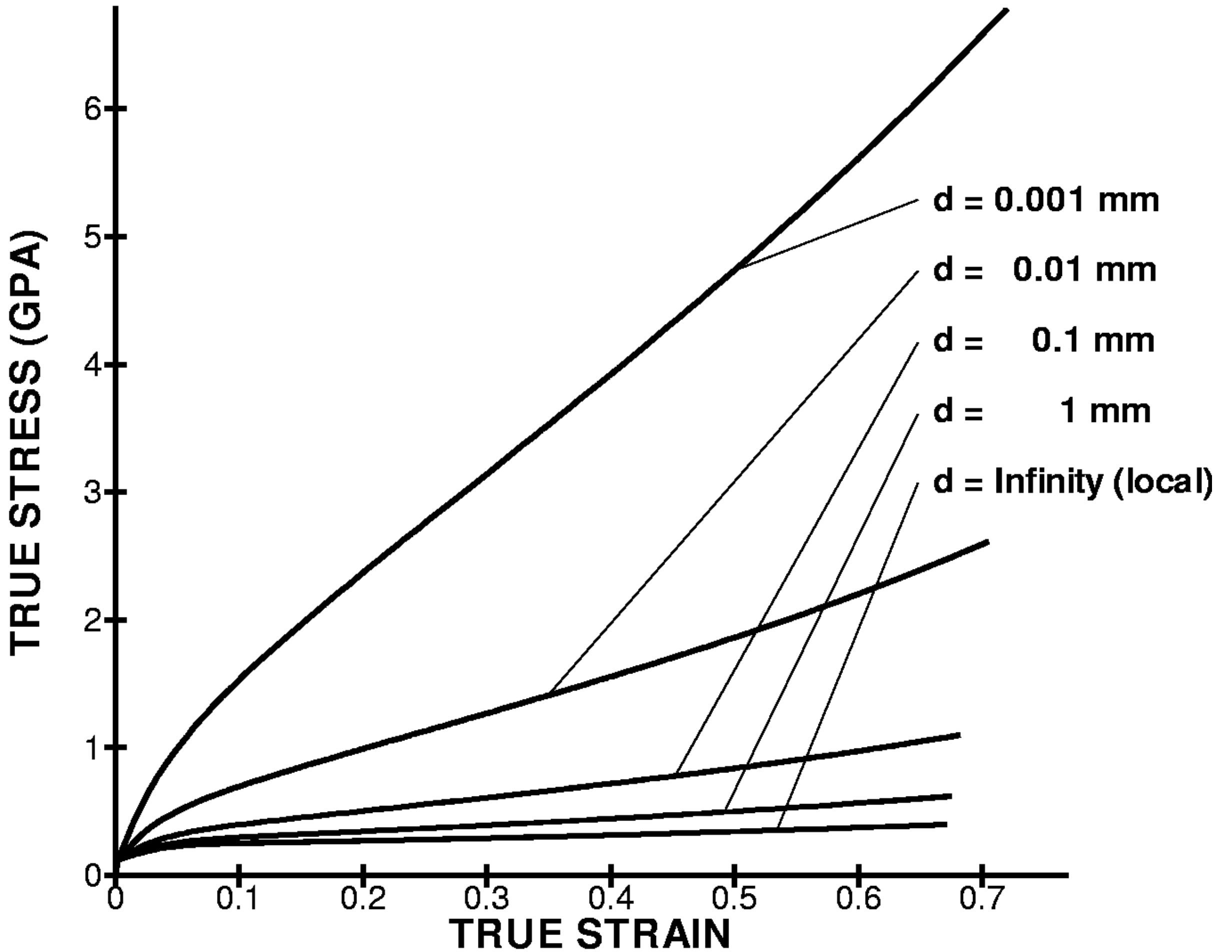
- Consider a crystal of size L containing a simple laminate of lamellar width l, slip strains $\sim \gamma$:

  - Boundary layer energy: $E^{\mathrm{BL}} \sim \mu \gamma^2 L^2 l$.
  - Wall energy: $E^{\mathrm{wall}} \sim \mu b \gamma L^3 / l$.
  - Optimize $E^{\mathrm{BL}} + E^{\mathrm{wall}}$ with respect to $l \Rightarrow l \sim \sqrt{bL}\gamma^{-1/2}$
  - Energy: $E \sim \mu \sqrt{b} \gamma^{3/2} L^{5/2}$.

- Let the crystal be loaded in uniaxial tension, and let the axial strain $\epsilon \sim \gamma$. Then $\sigma = W_{,\epsilon} \sim \sqrt{\gamma / L} \Rightarrow$ ***Taylor and Hall-Petch scaling***.

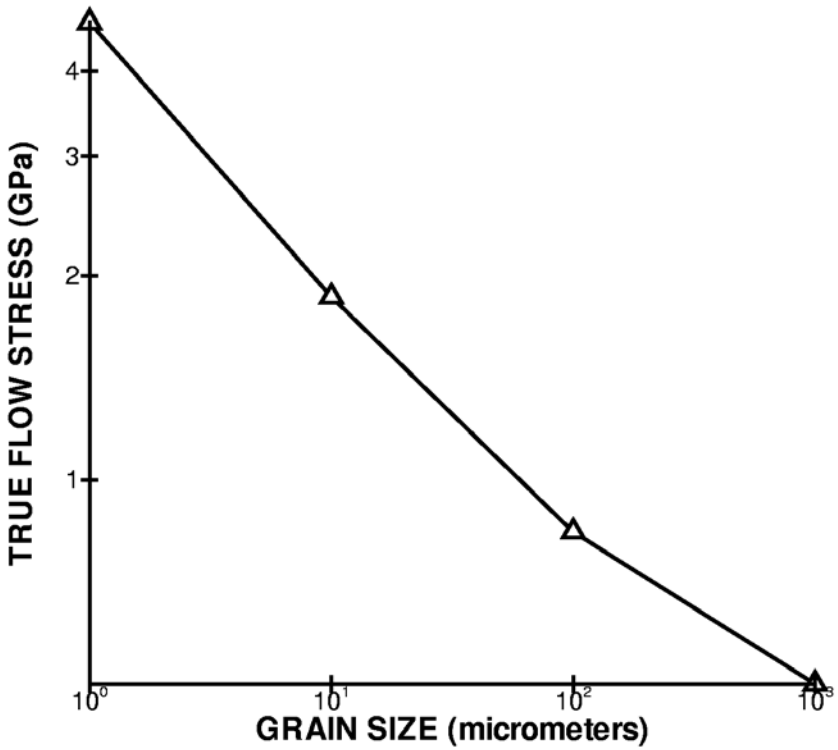
- For copper: $b = 2.56 \times 10^{-10}$ m, $\gamma \sim 2.5 \times 10^{-3}$, $L = 10^{-5}$ m $\Rightarrow l \sim 10^{-6}$ m, consistent with observation.

Subgrain dislocation structures

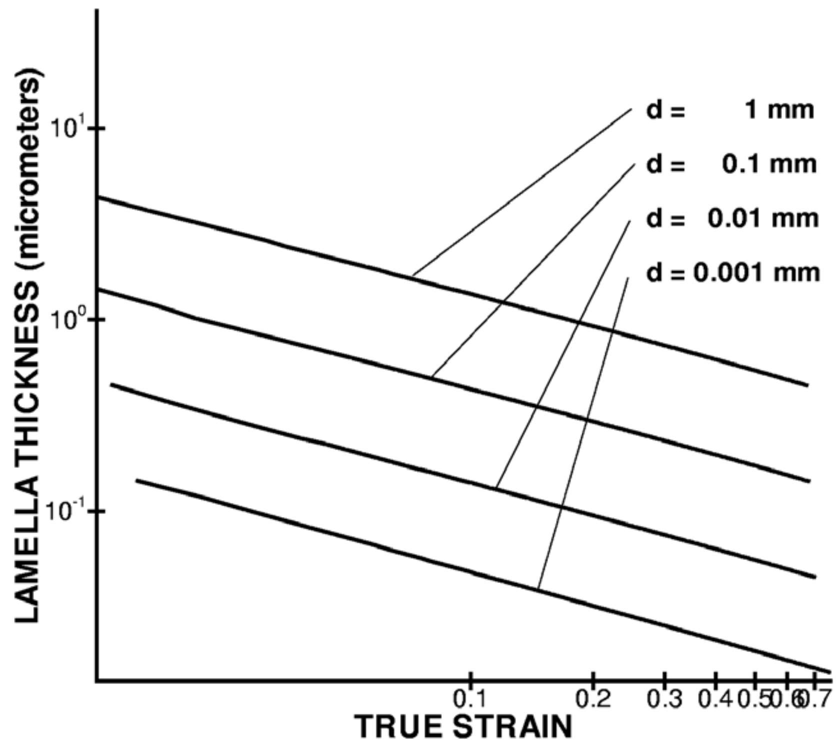


Uniaxial tension, (001) Cu.
(Ortiz, Repetto and Stainier, 2000)

Subgrain dislocation structures



Flow stress vs grain size.



Lamellar thickness vs strain and grain size.

(Ortiz, Repetto and Stainier, 2000)

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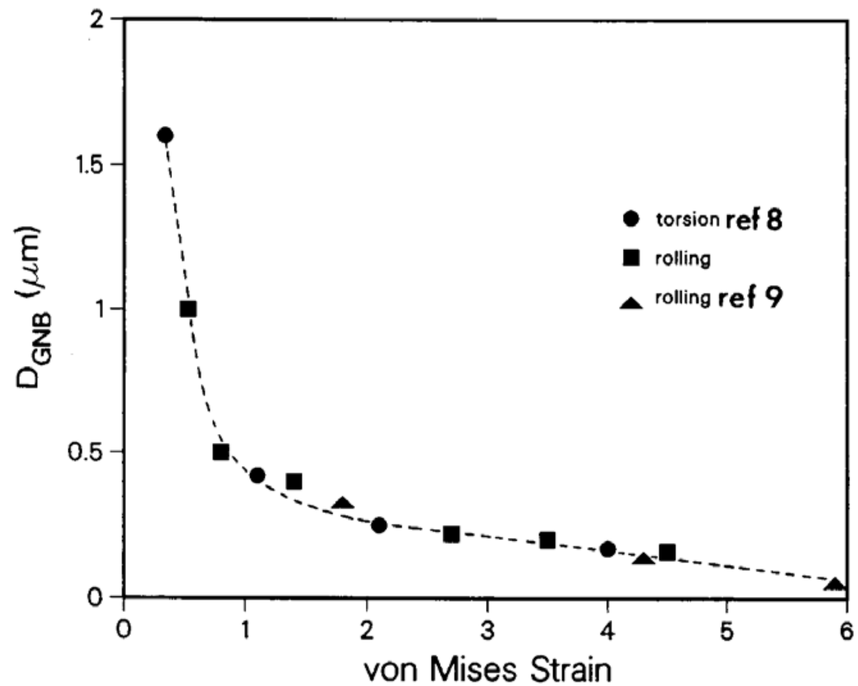
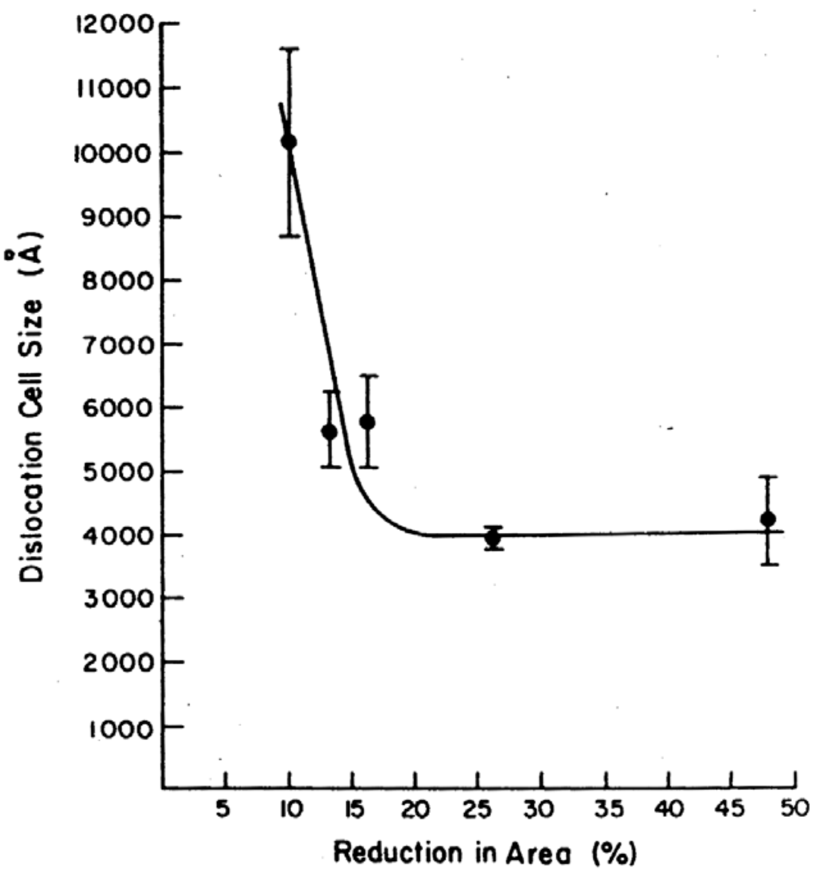
Subgrain dislocation structures



Hughes and Hansen, 1993)



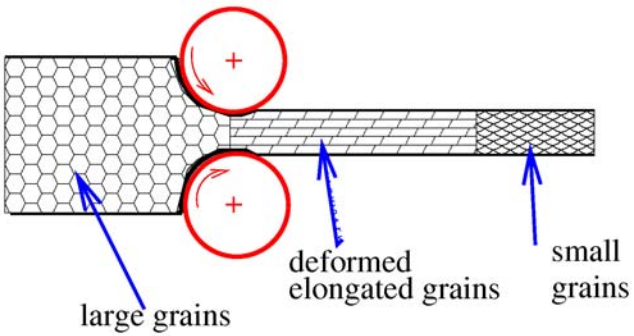
Bassin and Klassen, 1986)

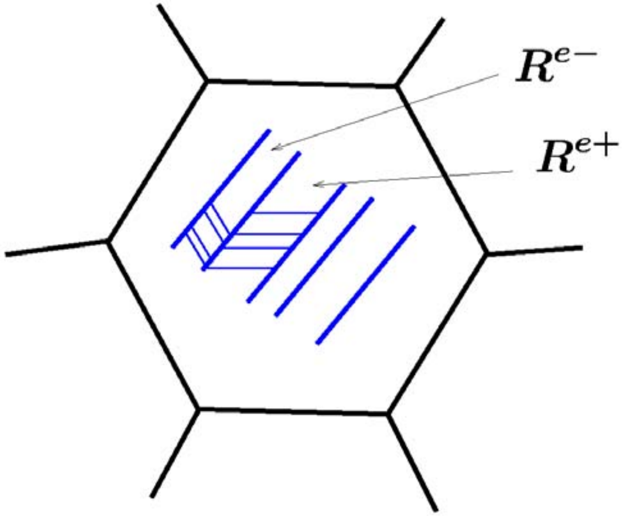
Subgrain structures - Validation

- **Experiments of D.A. Hughes *et al.*: Measure misorientation angle distribution following different amounts of deformation in cold-rolled metals.**

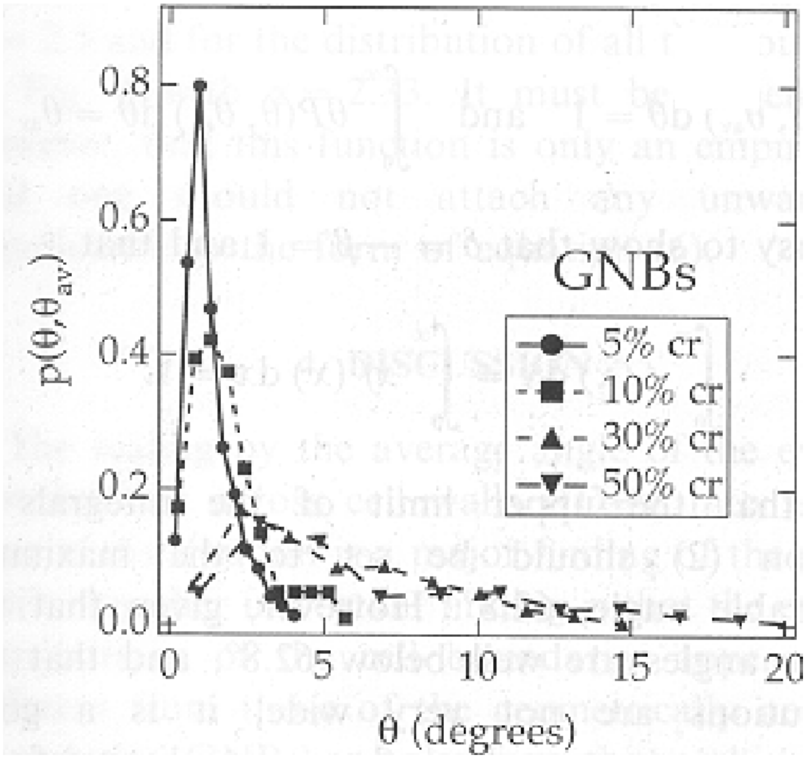
- **Numerical simulation of the misorientation angle: compute the angle of the relative rotation from one variant to the other: $R^{e+}(R^{e-})^{-1}$ for a random given orientation of the crystal.**

(Aubry and Ortiz, 2001)

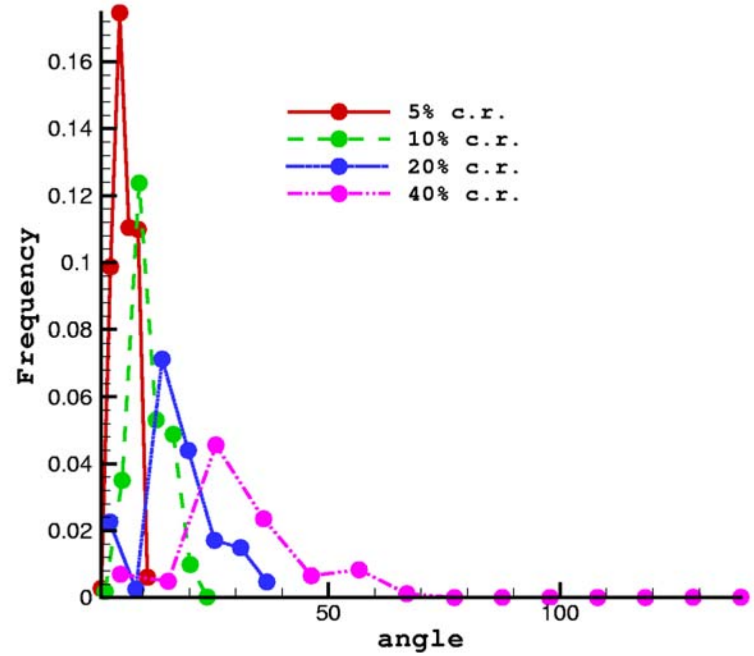




Subgrain structures - Validation



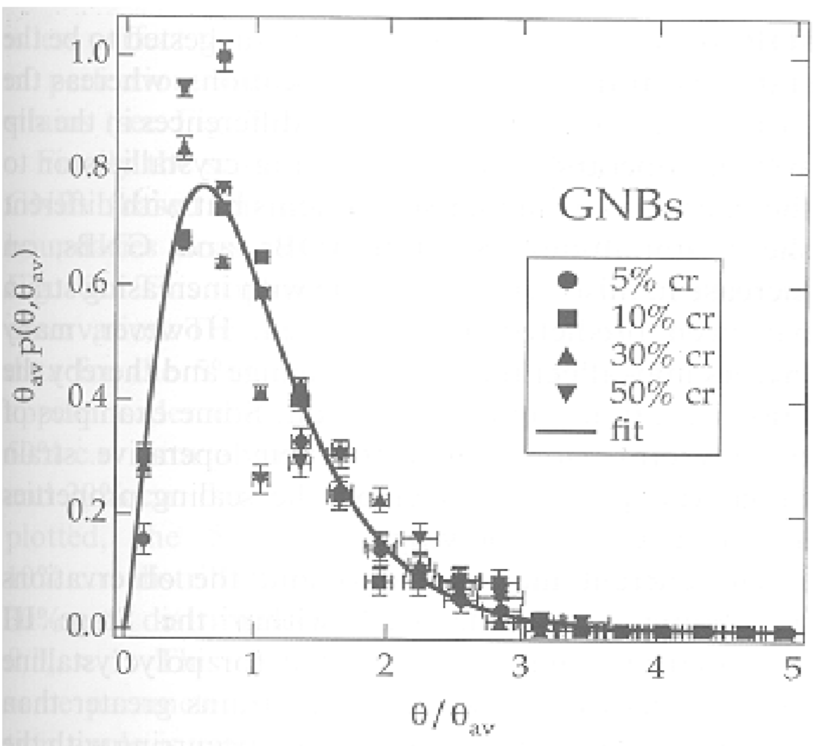
(Hughes *et al.*, 1997)



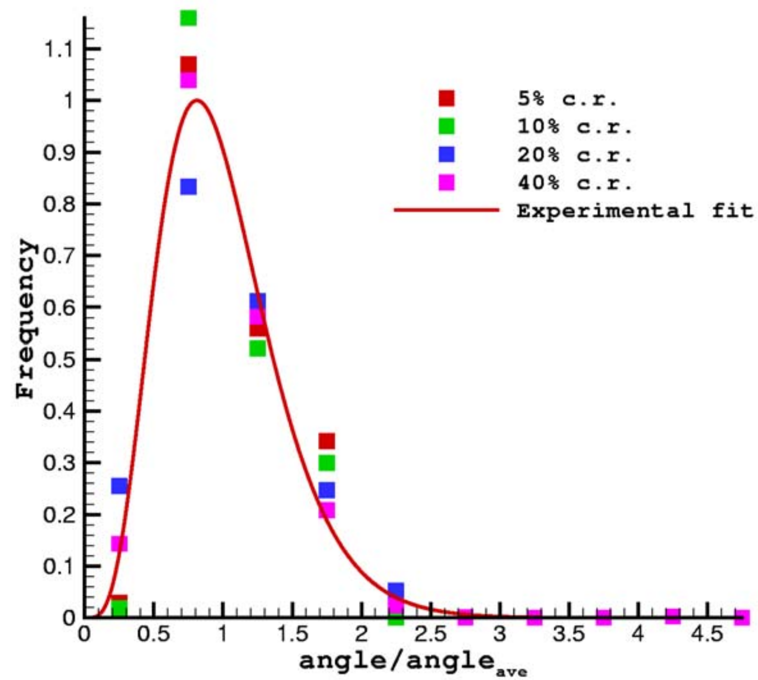
(Aubry and Ortiz, 2001)

Experimental *vs* computed histograms of misorientation angle

Subgrain structures - Validation



(Hughes and Hansen, 1997)



(Aubry and Ortiz, 2001)

Scaled probability density of misorientation angle

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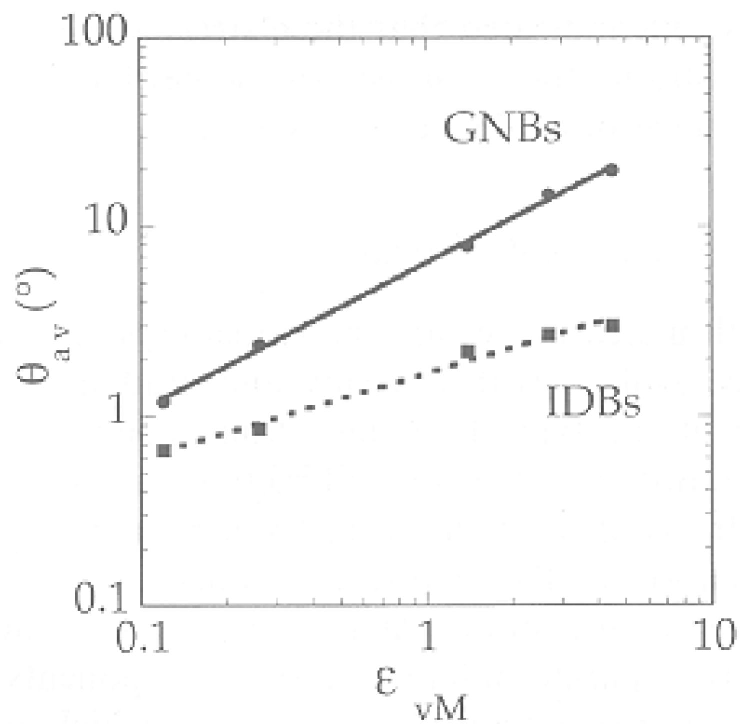
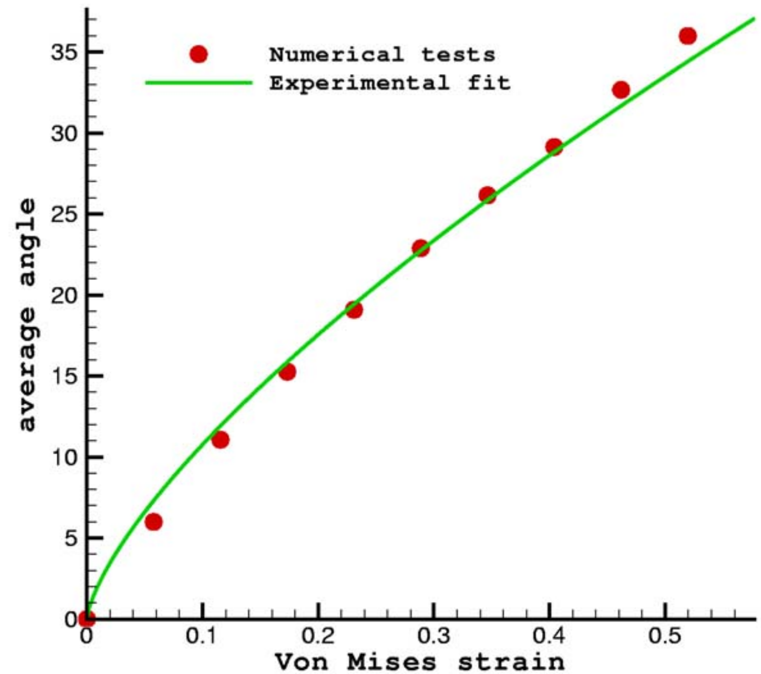
Subgrain structures - Validation



(Hughes *et al.*, 1997)



(Aubry and Ortiz, 2001)

Average misorienation angle *vs* strain

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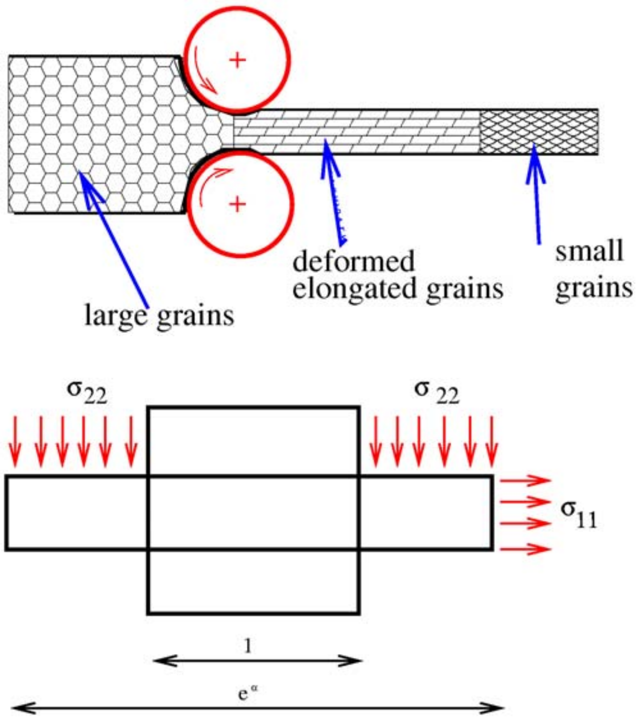
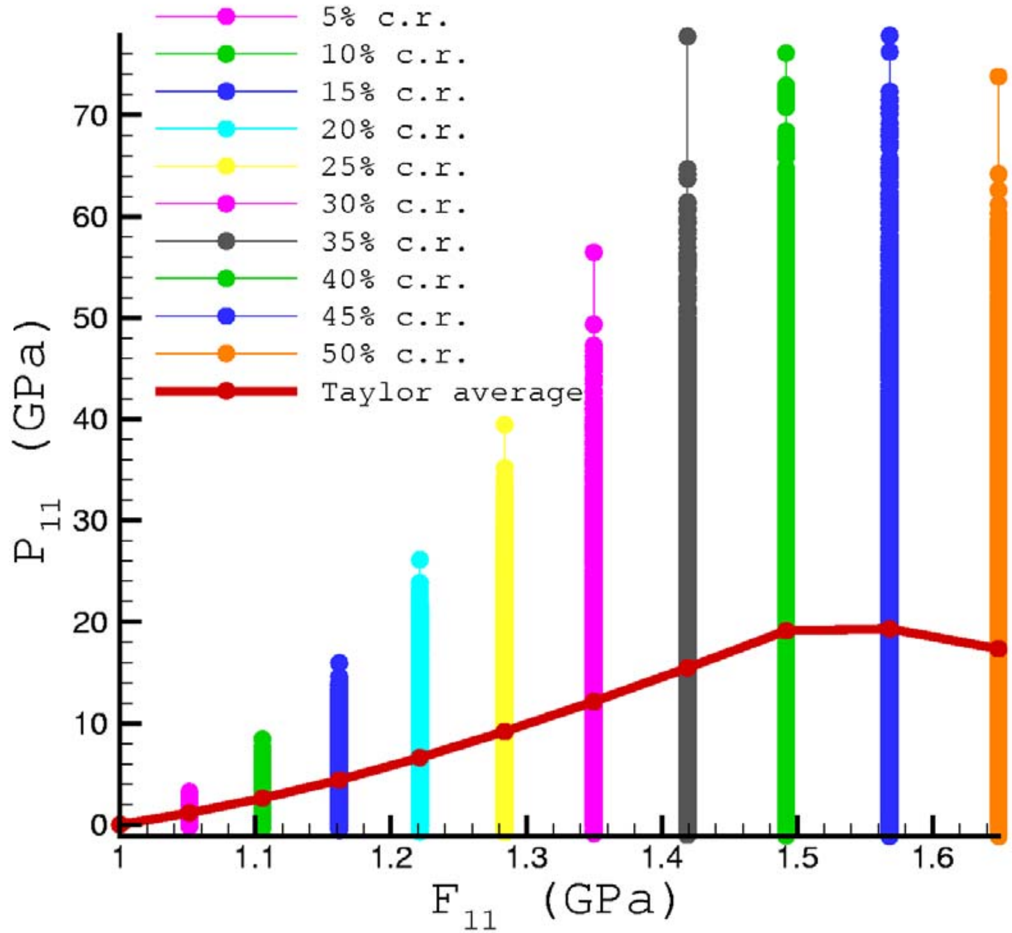
Subgrain structures - Validation

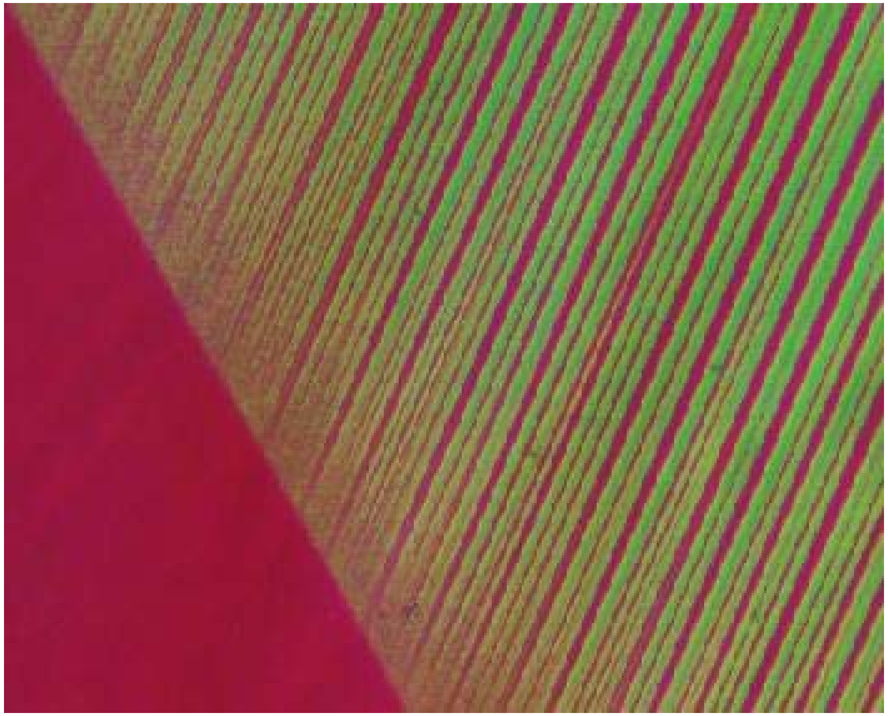


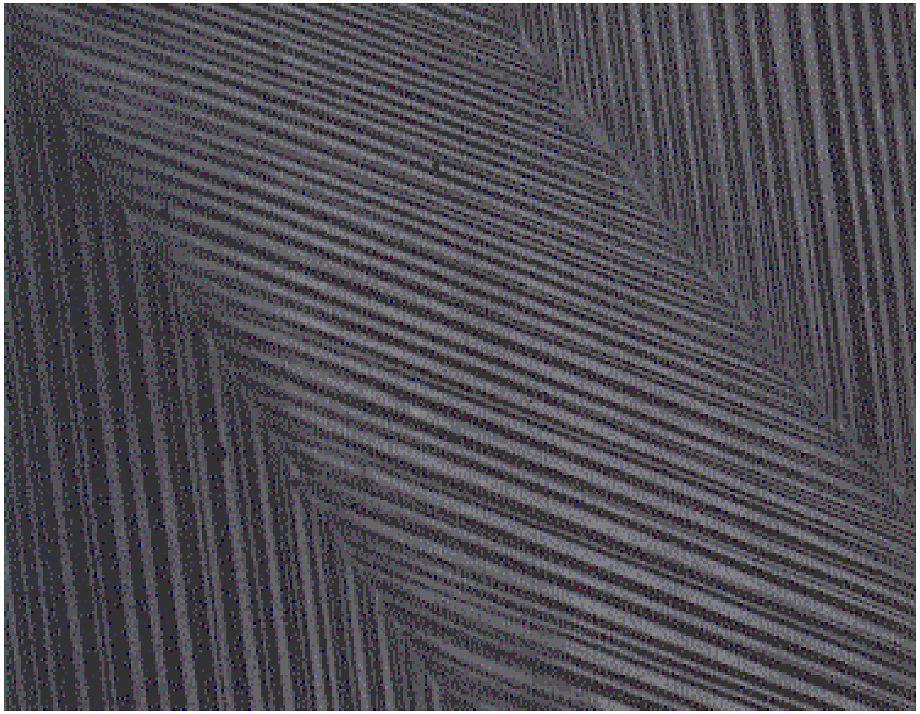
Cold rolling



Effective polycrystalline stress-strain curve
(Aubry and Ortiz, 2001)

Martensitic materials – Continuum theory

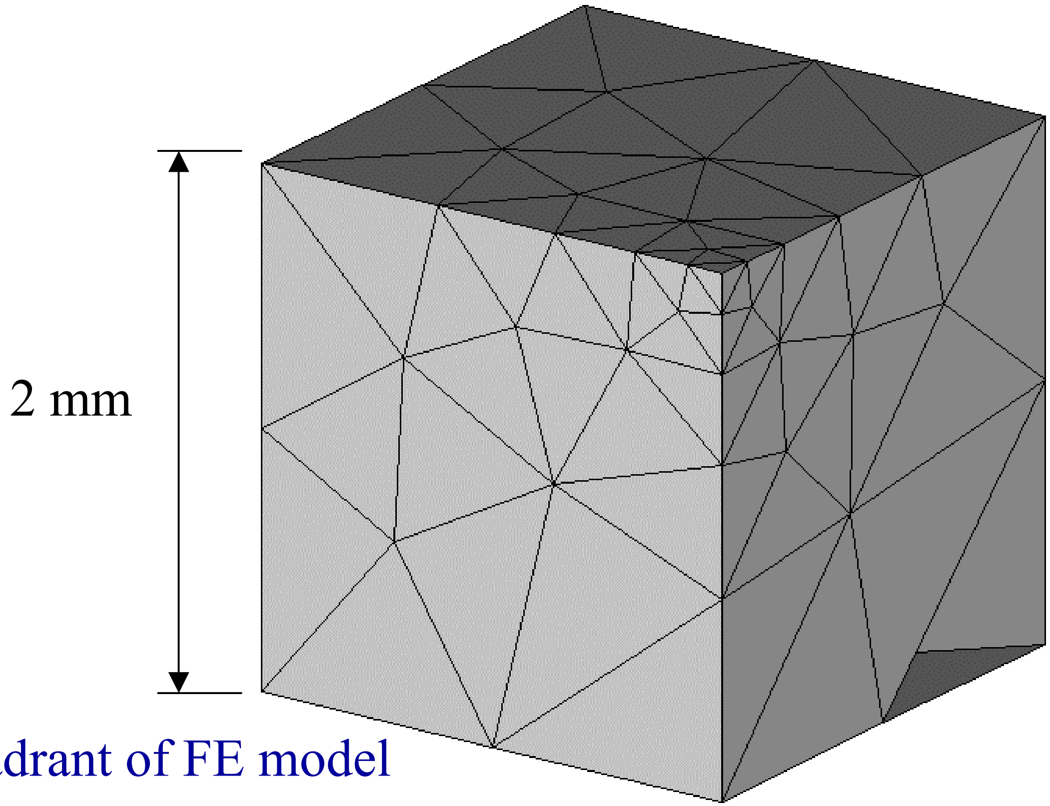




Observed microstructures in Cu-Al-Ni
(Chu and James, 1999)

FE Simulation of indentation in Al-Cu-Ni

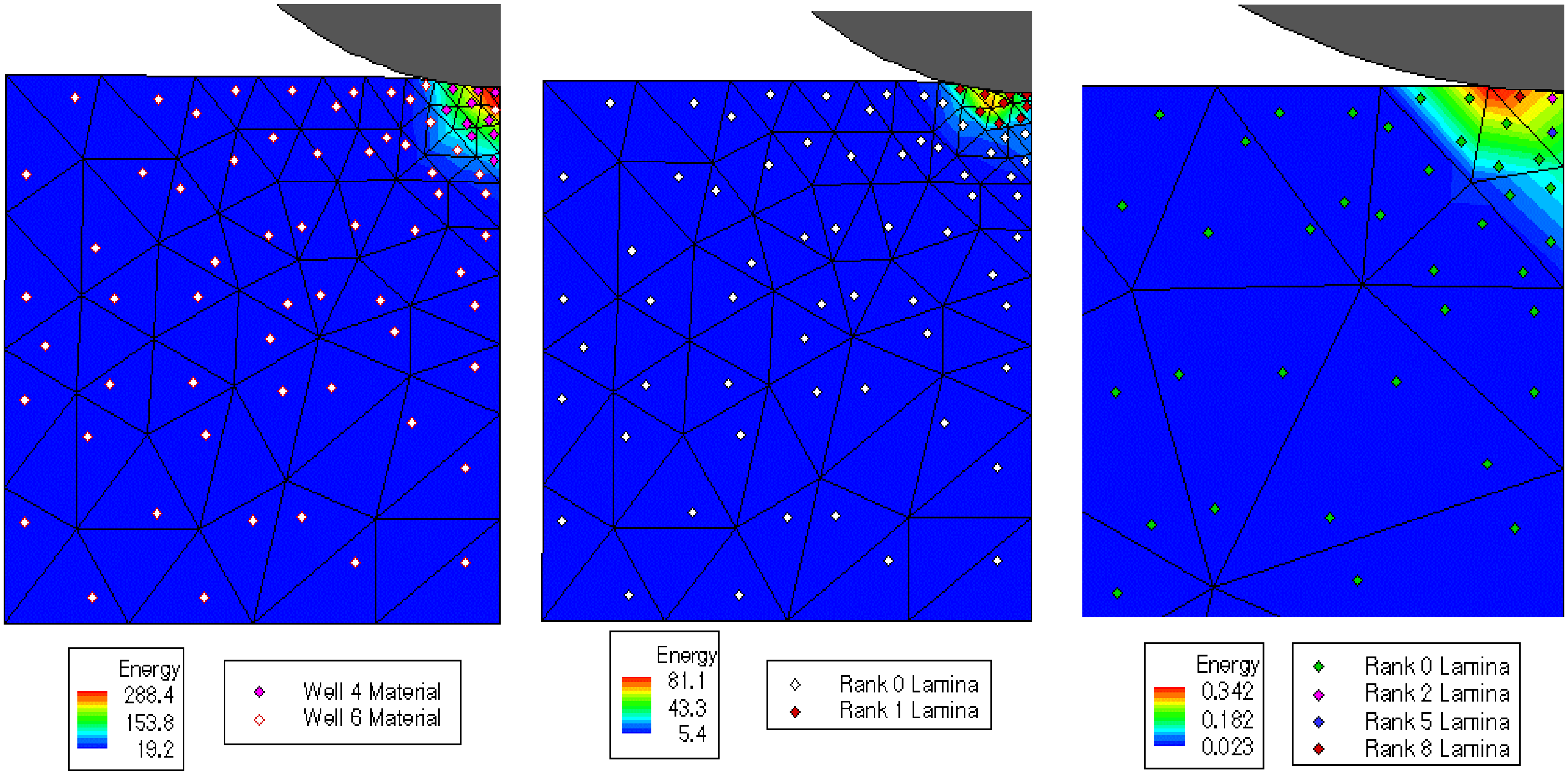
- Spherical indenter (1.5mm radius)
- Lamination algorithm applied at each (on the fly) quadrature point



Quadrant of FE model

FE Simulation of indentation in Al-Cu-Ni

(indenter radius = 1.5 mm)



Unrelaxed Relaxed, small grain Relaxed, large grain

(Aubry, Fago and Ortiz, 2001)

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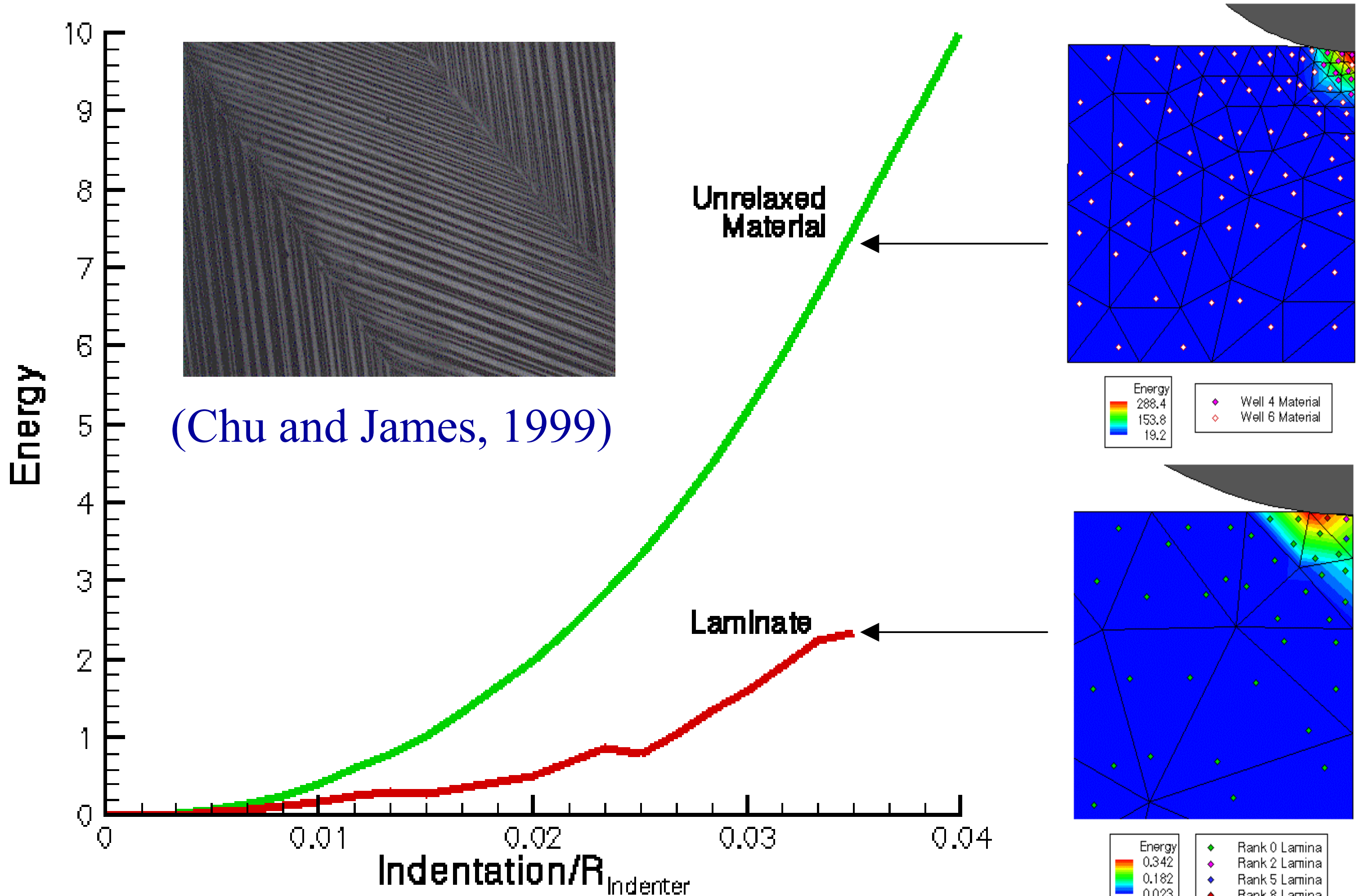
FE simulation of indentation in Al-Cu-Ni



(Chu and James, 1999)

(Aubry, Fago and Ortiz, 2001)

Concluding remarks

- The incremental IBVP of finite-deformation single-crystal plasticity may be reduced to a sequence of minimization problems by recourse to variational constitutive updates
- For crystals with strong latent hardening the work-of-deformation functional is non-convex, which promotes fine microstructure
- Relaxation (probably) requires consideration of sequential laminates of finite depth only
- Multiscale approach:
  - *Finite elements endowed with effective behavior, no enhancement*
  - *Effective behavior computed by lamination algorithm at Gauss points*
- Theory predicts:
  - *Dipolar walls in fatigued fcc crystals*
  - *Misorientation data of Hughes and Hansen.*
  - *Hall-:Petch scaling (cf Ortiz and Repetto, JMPS, 1999; Ortiz et al., JMPS, 2001).*

References

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R. Radovitzky and M. Ortiz, "Error Estimation and Adaptive Meshing in Strongly Nonlinear Dynamic Problems," *Computer Methods in Applied Mechanics and Engineering*, **172** (1999) 203-240.

M. Ortiz and E. A. Repetto, "Nonconvex Energy Minimization and Dislocation Structures in Ductile Single Crystals," *Journal of the Mechanics and Physics of Solids*, **47** (1999) 397-462.

M. Ortiz, E. A. Repetto and L. Stainier "A Theory of Subgrain Dislocation Structures," *Journal of the Mechanics and Physics of Solids* (2000) to appear.