Multiscale modeling of materials: (2) Dislocation structures → polycrystals

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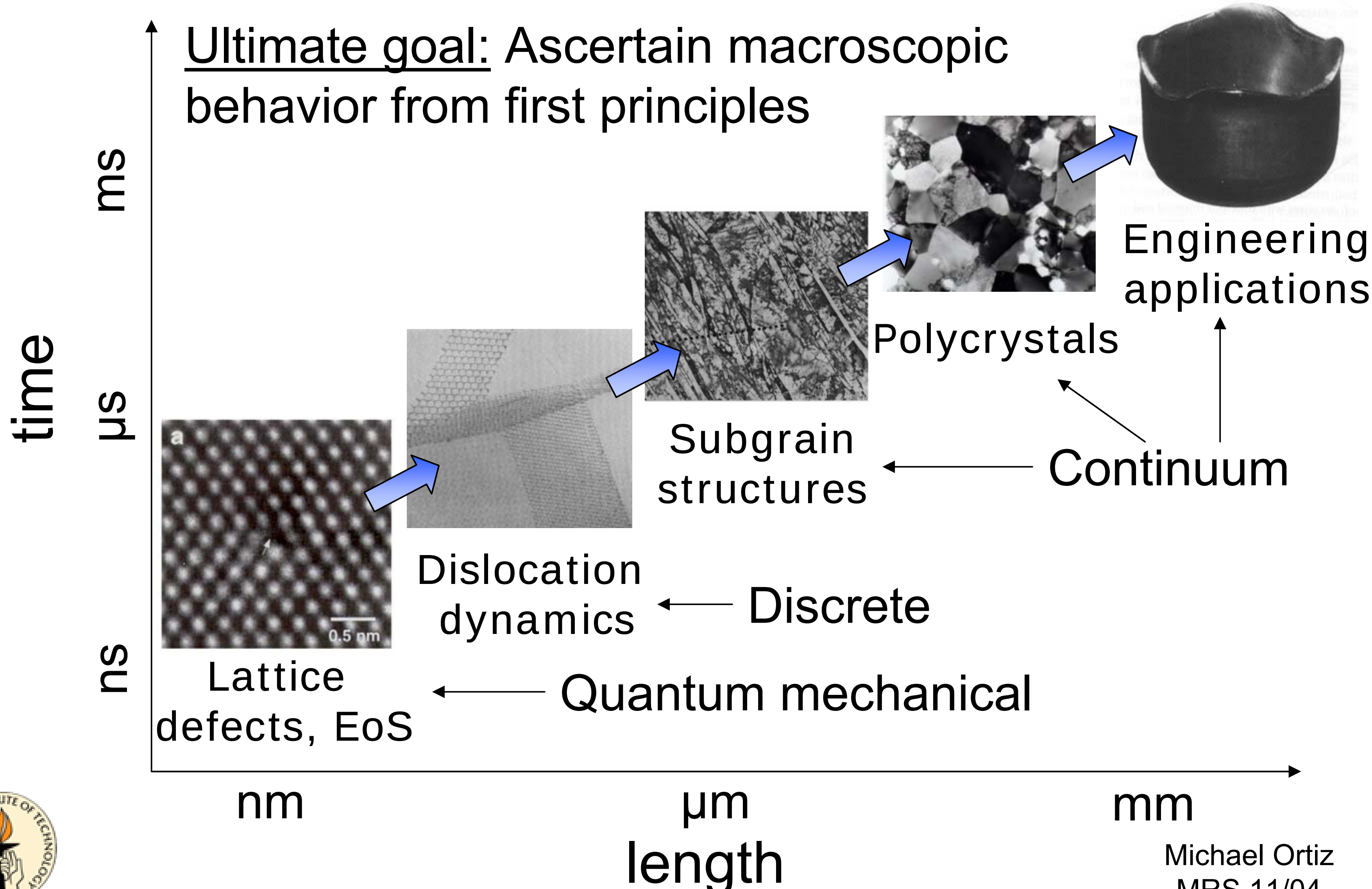
Metal plasticity − Multiscale hierarchy



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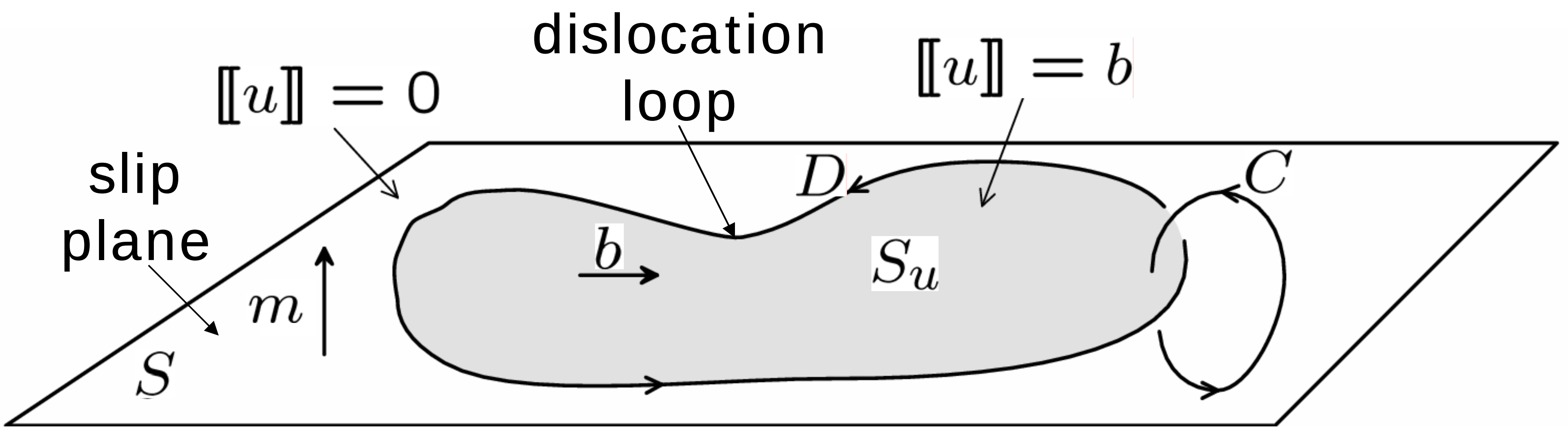
Continuum models of crystal plasticity

- Aim: 'Cook up' empirical models of crystal plasticity 'inspired' in dislocation mechanics that explain observed behavior (miscrostructure, macroscopic stress-strain behavior, scaling laws).
- To date: 'Deformation theory of plasticity' (one incremental step from initial to final state), energy minimization, relaxation, Γ-convergence.
- Open question: Which continuum models (energy + kinetics) are limits of discrete (hence more fundamental) models?
- Open question: General deformation paths?

General linear elastic dislocations



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

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

elastic deformation (β^e)
plastic deformation (β^p)

- Dislocation density: $\alpha = -\text{curl}\beta^e = \text{curl}\beta^p$

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General dislocations − Energy

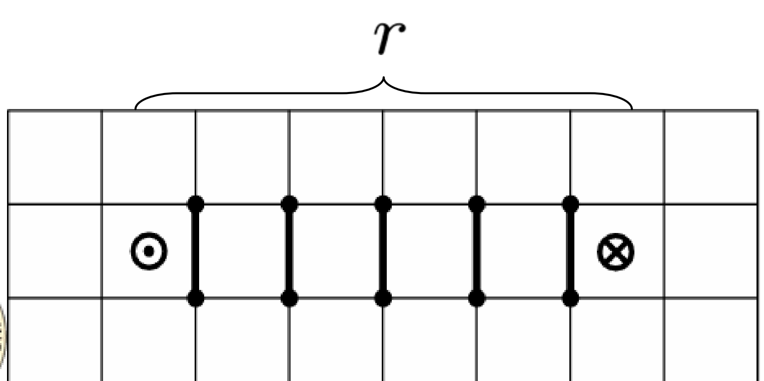
- Stored energy:

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

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

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

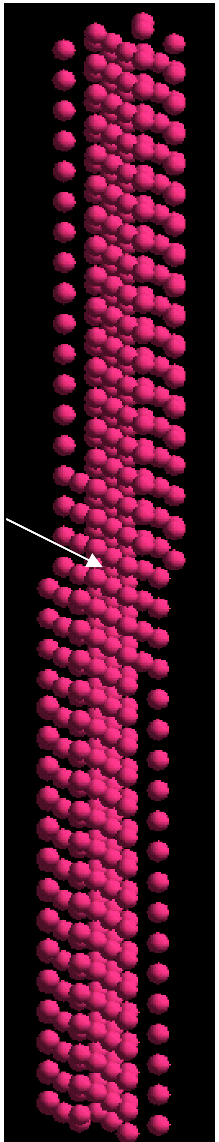
and: $G = \Delta^{-1} \equiv$ Green's function of the Laplacian.

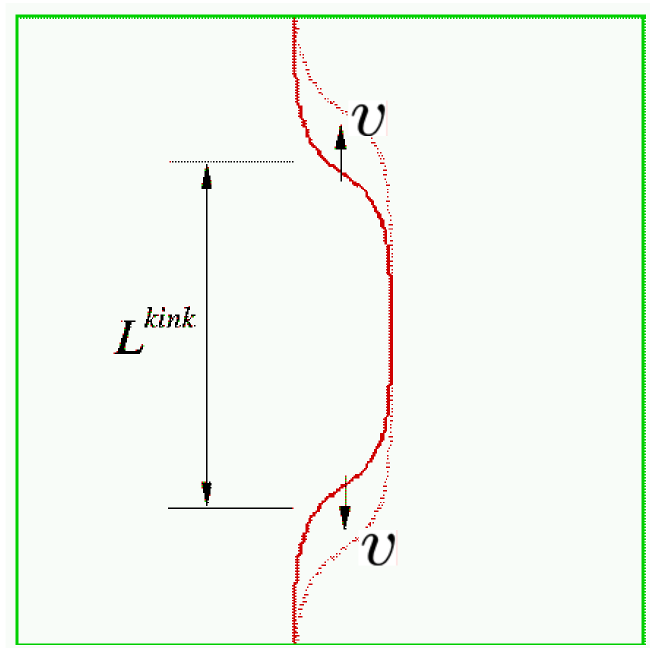


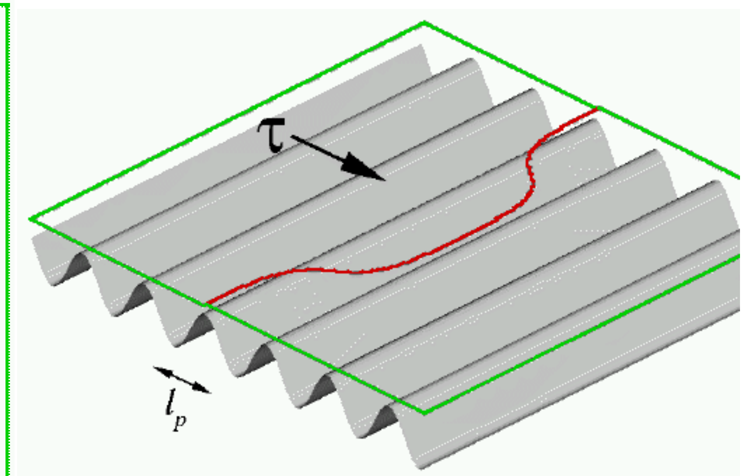
$$\longleftarrow \quad \frac{E}{L} \sim \frac{Gb^2}{2\pi} \log \frac{r}{r_0}$$

Straight dislocations – Dissipation

Kink







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

lattice friction

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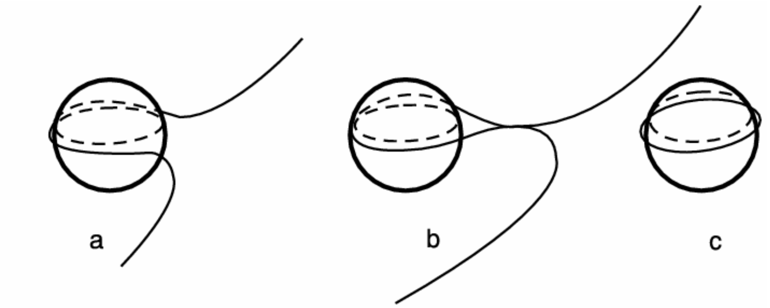
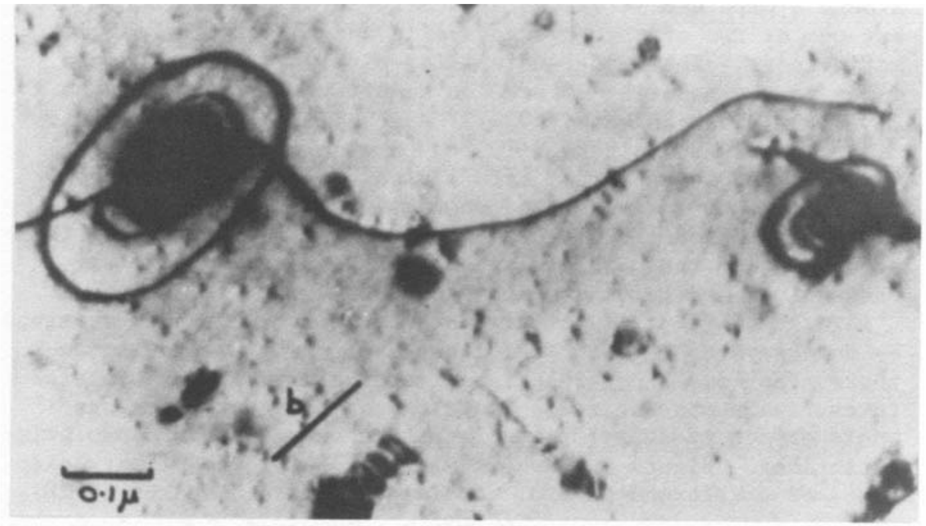
Obstacles – Topological obstructions

- Example: Precipitates.

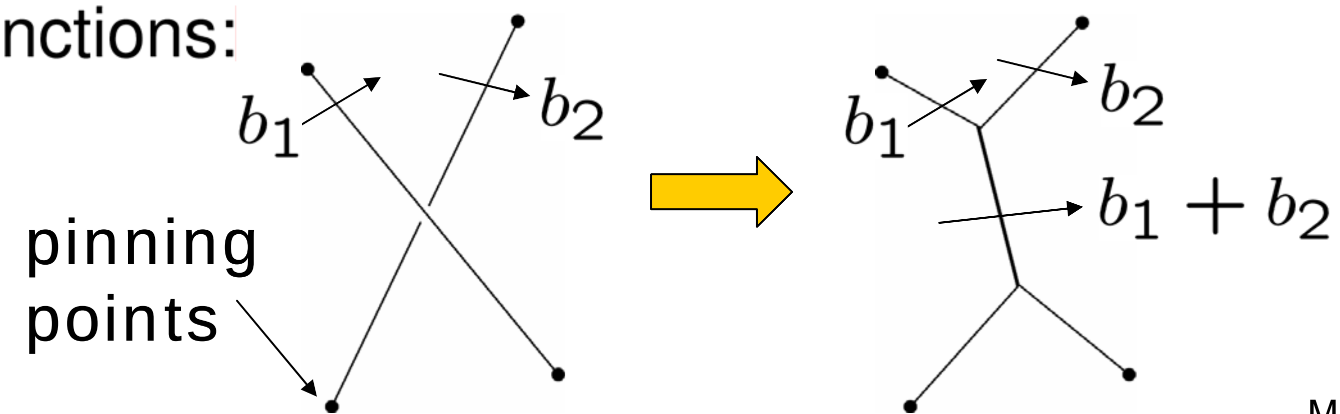


Impenetrable obstacles



(Humphreys and Hirsch '70)

- Junctions:



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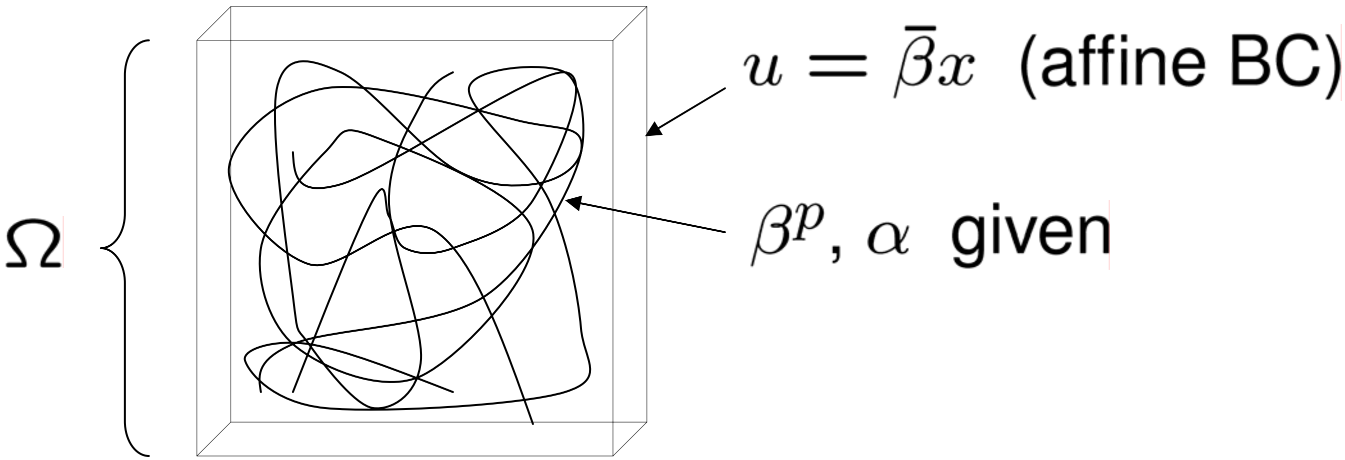
The standard continuum model



- Elastic energy: $\inf_u \int_{\Omega \setminus S_u} \left(\frac{1}{2} |\epsilon(u)|^2 - \epsilon(u) \cdot \epsilon^p \right) dx$

$$= |\Omega| \underbrace{\left(\frac{1}{2} |\bar{\epsilon}|^2 - \bar{\epsilon} \cdot \bar{\epsilon}^p \right)}_{\text{strain energy}} + \underbrace{E(\alpha)}_{\text{stored energy}}$$

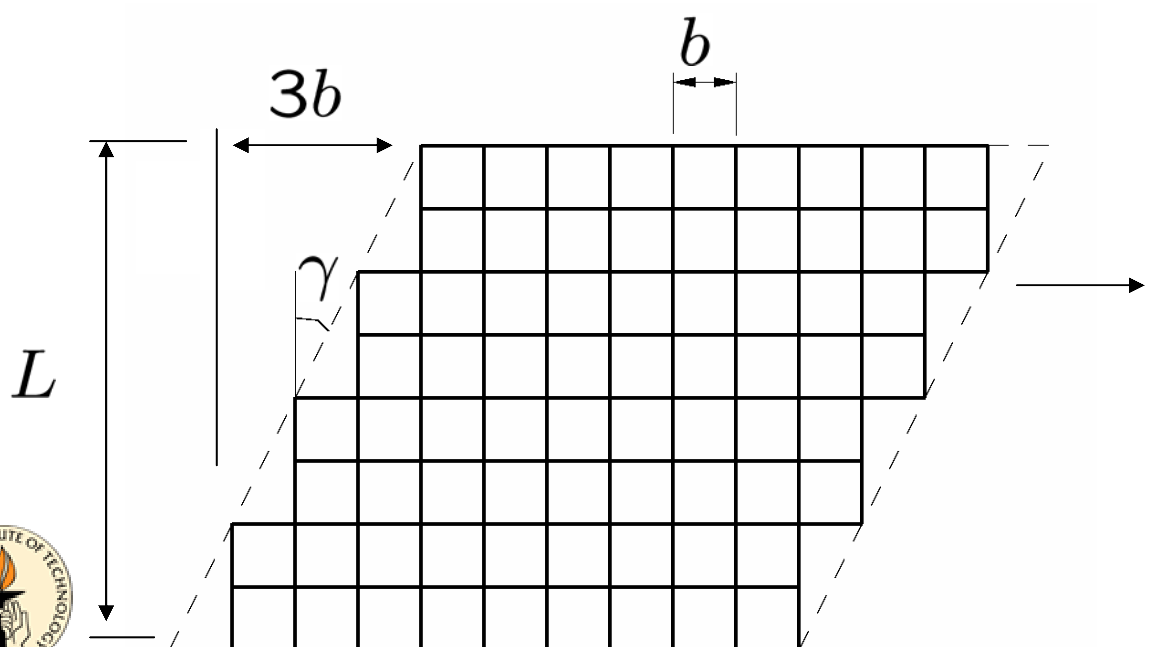
$$\bar{\beta}^p = \frac{1}{|\Omega|} \int_{\Omega} \beta^p \, dx \equiv \text{average plastic deformation}$$

The standard continuum model

- Average plastic deformation: $\bar{\beta}^p = \frac{1}{|\Omega|} \int_\Omega \beta^p \, dx$

$$\bar{\beta}^p = \frac{1}{|\Omega|} \int_{S_u} [\![u]\!] \otimes m \, d\mathcal{H}^2 \equiv \sum_{i=1}^{N} \gamma_i s_i \otimes m_i$$

where $\gamma_i \equiv$ slip strain on system i.



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

$$= \frac{b \times \text{Area}}{\text{Volume}}$$

The standard continuum model

- Standard model: $E(u,\gamma) =$

$$\int_\Omega \Big(\underbrace{\frac{1}{2}|\epsilon(u) - \bar{\epsilon}^p(\gamma)|^2}_{\text{strain energy}} + \underbrace{W^p(\gamma)}_{\text{plastic work}} + \underbrace{(T/b)|\text{curl}\,\bar{\beta}^p(\gamma)|}_{\text{core energy}} \Big)\, dx$$

- Plastic work (infinite latent hardening):

$$W^p(\gamma) = \begin{cases} \tau_i|\gamma_i| & \text{if } \gamma_j = 0, \quad \forall j \neq i \\ \infty & \text{otherwise,} \end{cases}$$

- Core energy: $T \sim Gb^2 \equiv$ dislocation line tension, $T/b \sim Gb \sim O(\epsilon)$

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Standard model − Local

- Minimize slip strains pointwise:

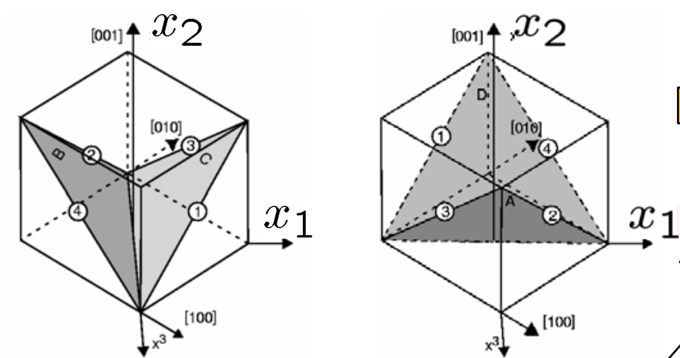
$$\inf_{\gamma} E(u,\gamma) = I(u) = \int_{\Omega} W(\epsilon(u))\, dx$$

where: $$W(\epsilon) = \min_{\gamma} \left(\frac{1}{2} |\epsilon - \bar{\epsilon}^p(\gamma)|^2 + W^p(\gamma) \right)$$

- Properties of $W(\epsilon)$:
  - Linear growth along orbits of $s_i \otimes m_i$, $i = 1, \dots, N$.
  - Quadratic growth in all other directions.
- Question: Relaxation of $I(u)$?

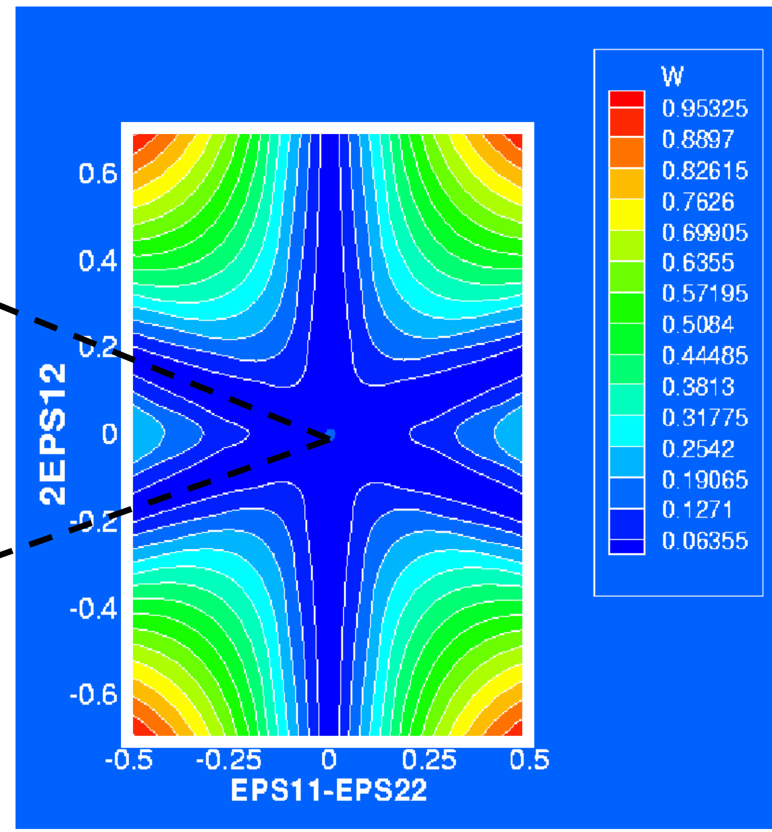
Standard model – Local

- 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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Standard model − 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.*

Standard model − Relaxation

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

Theorem (Conti and Ortiz, ARMA '05) *Suppose that the set of slip systems is complete. Then, the relaxation of $I(u)$ with respect to the strong L^1 topology is*

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

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Standard model − Relaxation

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

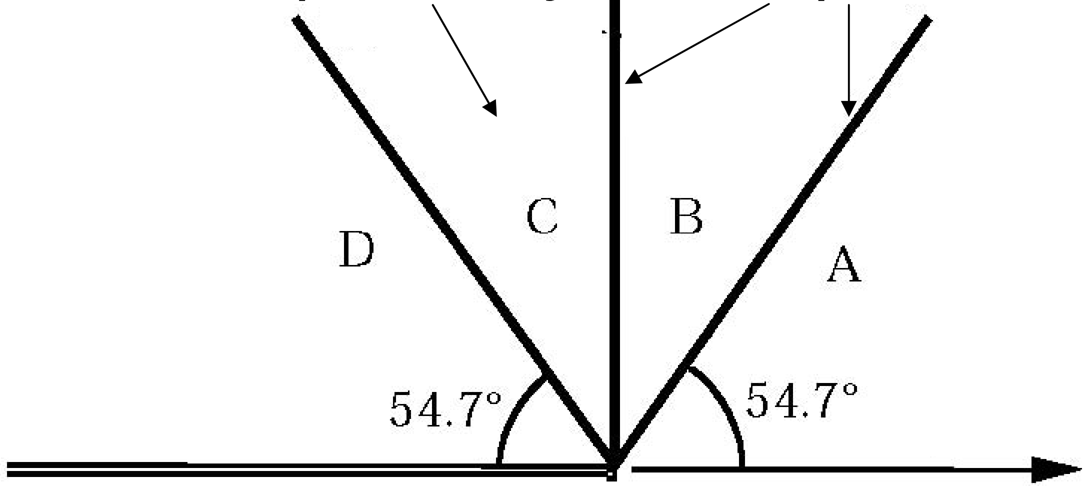
Lemma *Let $\mathcal{S}$ be a complete set of slip systems. For any $\beta \in \mathbb{R}^{3\times3}$ and any $\epsilon > 0$ there is a laminate ν (of finite order) such that*

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

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

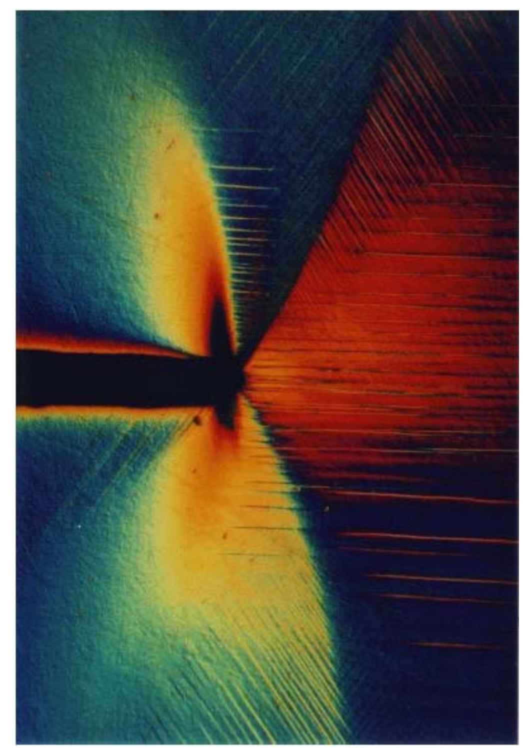
Standard model – Relaxation

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

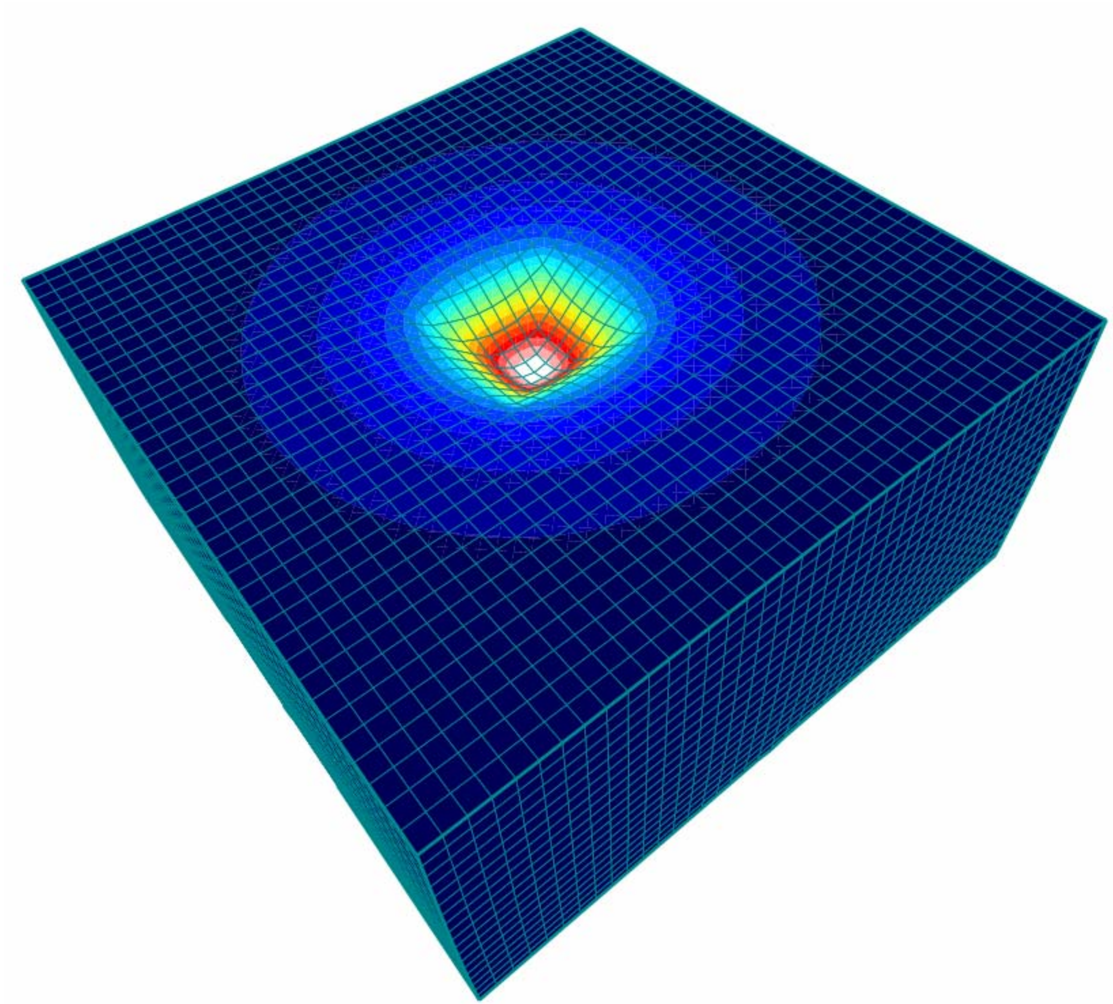


(Rice, *Mech. Mat*., 1987)

(Crone and Shield, *JMPS*, 2002) →



Relaxation and computation

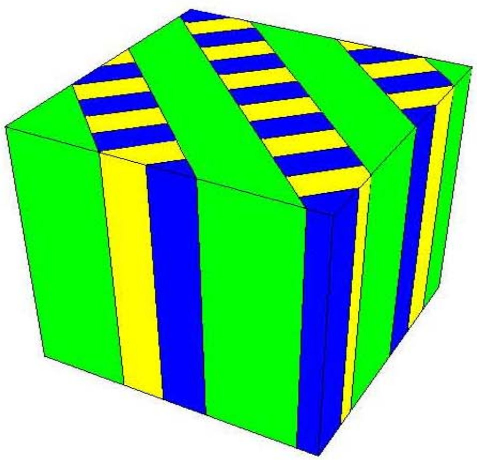


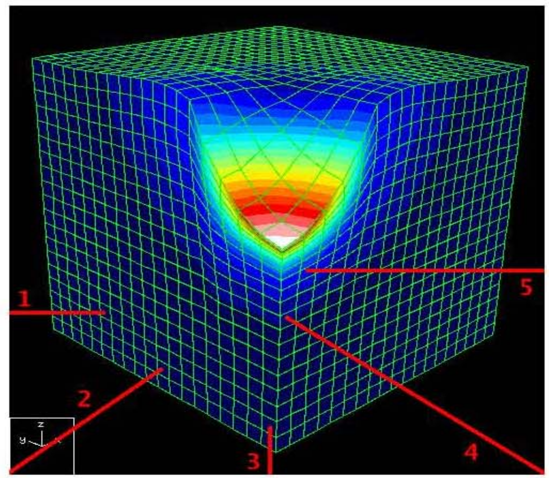
Indentation of [001] surface of FCC crystal

(Hauret and Ortiz, 2005)

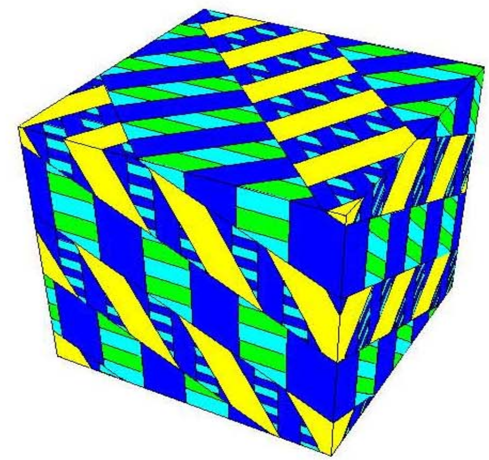
Relaxation and computation

rank 2/2, $|\gamma|_\infty = 0.0025$

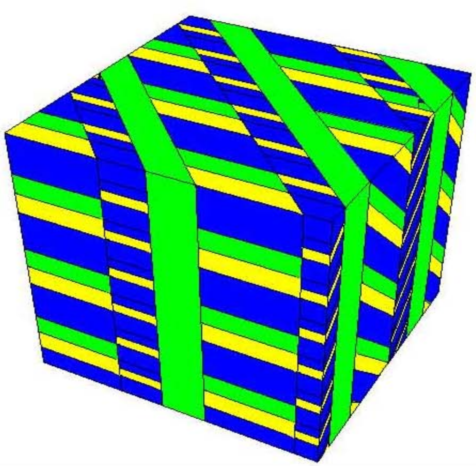




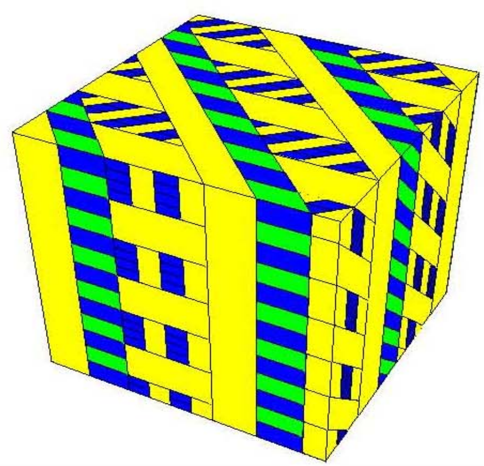
rank 4/14, $|\gamma|_\infty = 0.43$



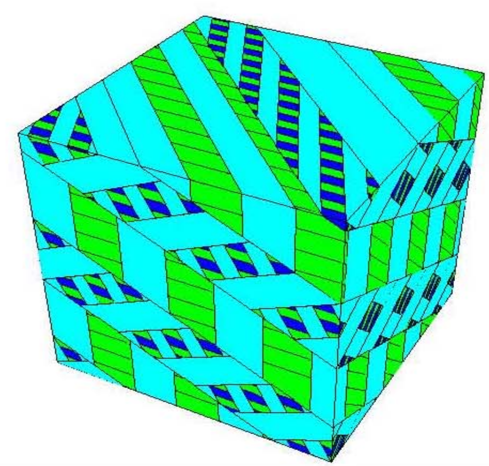
rank 4/12, $|\gamma|_\infty = 0.02$



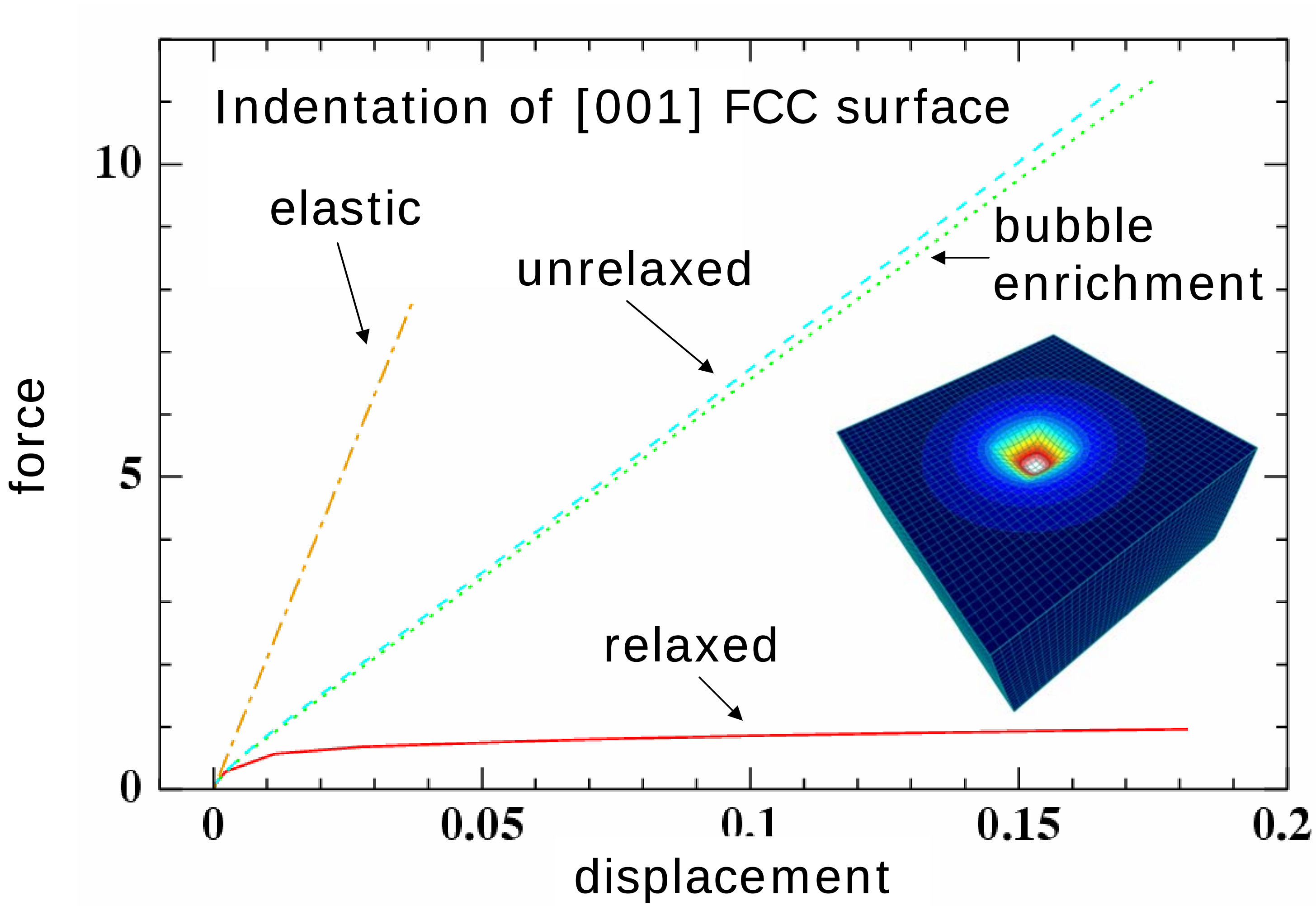
rank 4/6, $|\gamma|_\infty = 0.026$



rank 4/16, $|\gamma|_\infty = 0.21$

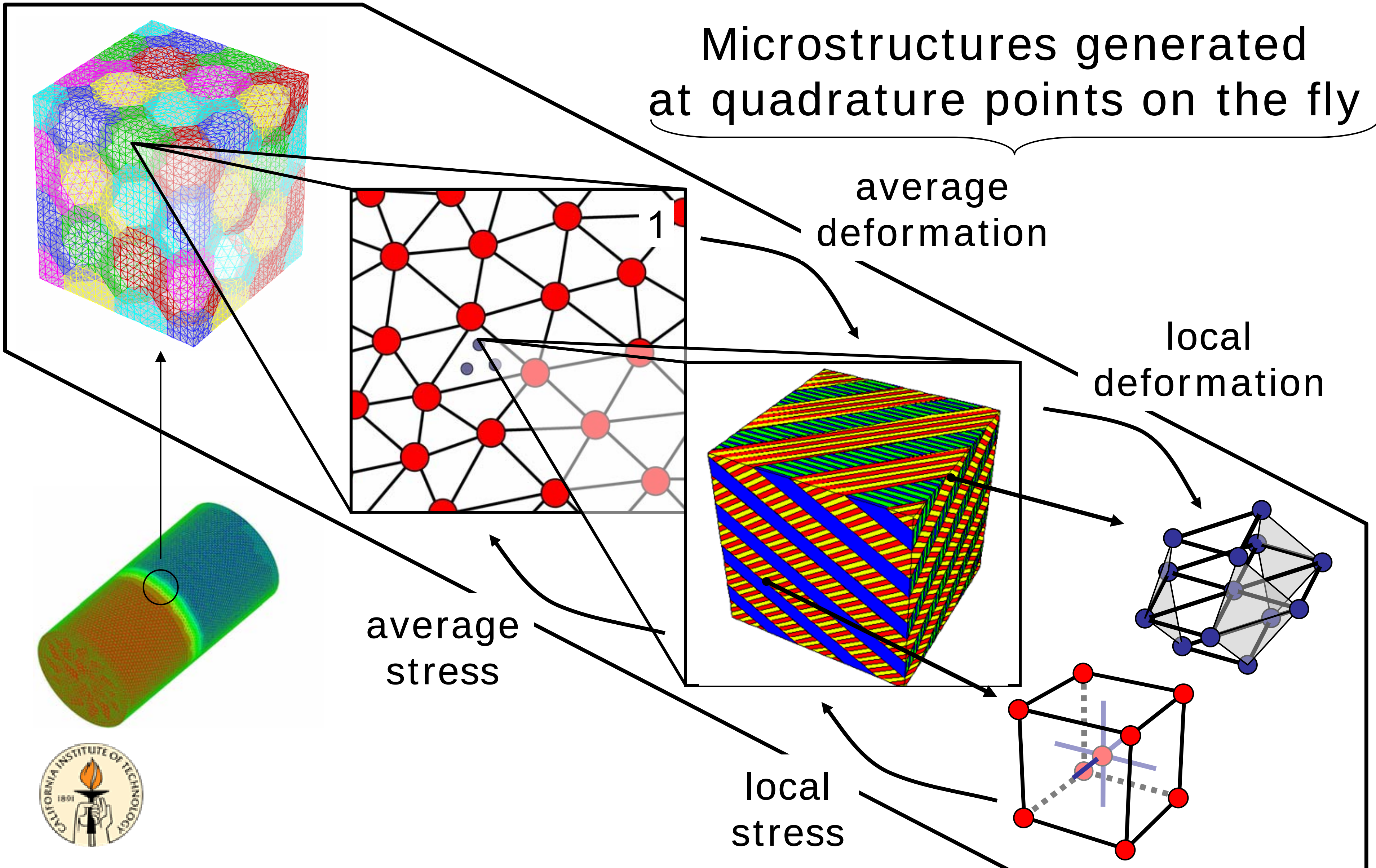


Relaxation and computation



(Hauret and Ortiz, 2005)

Relaxation and computation



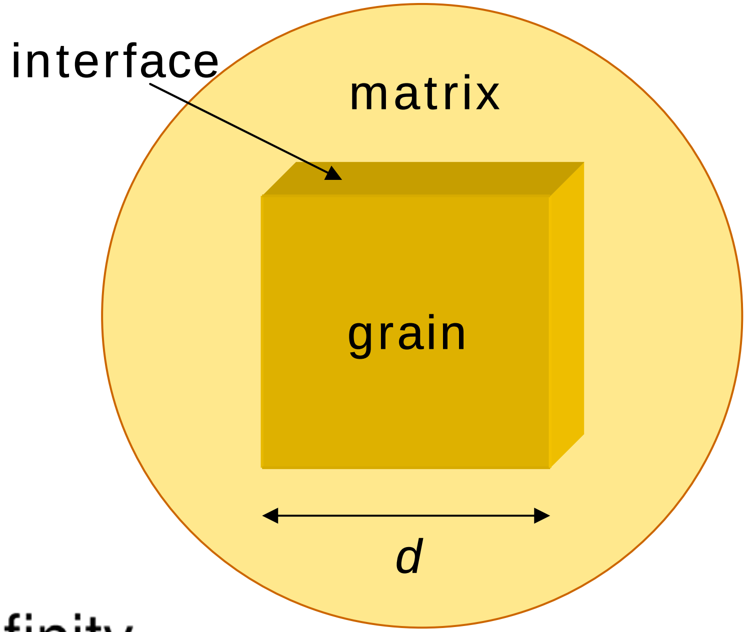
Model boundary-value problem

- Standard model: $E(u,\gamma) =$

$$\int_\Omega \left(\frac{1}{2}|\epsilon(u) - \bar{\epsilon}^p(\gamma)|^2 + W^p(\gamma) + (T/b)|\text{curl}\bar{\beta}^p(\gamma)|\right) dx$$

$$+\mu||u - \gamma\, x||^2_{H^{1/2}(\partial\Omega)}$$

- Assumptions:
  - $\ast$ $\Omega = [0,d]^3$, $d \equiv$ grain size.
  - $\ast$ Collinear double slip at 90°.
  - $\ast$ Scalar displacement u_3.
  - $\ast$ Shear strain γ prescribed at infinity.



Optimal scaling laws

Theorem (Conti and Ortiz, ARMA '05) *There are constants* c, c' *such that*

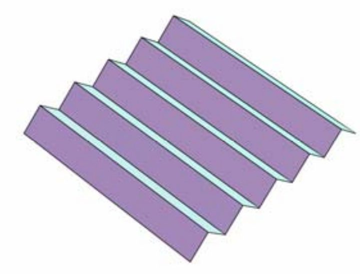
$$cE_0(T,\gamma,\tau_0,\mu,d) \leq \inf E \leq c' E_0(T,\gamma,\tau_0,\mu,d)$$

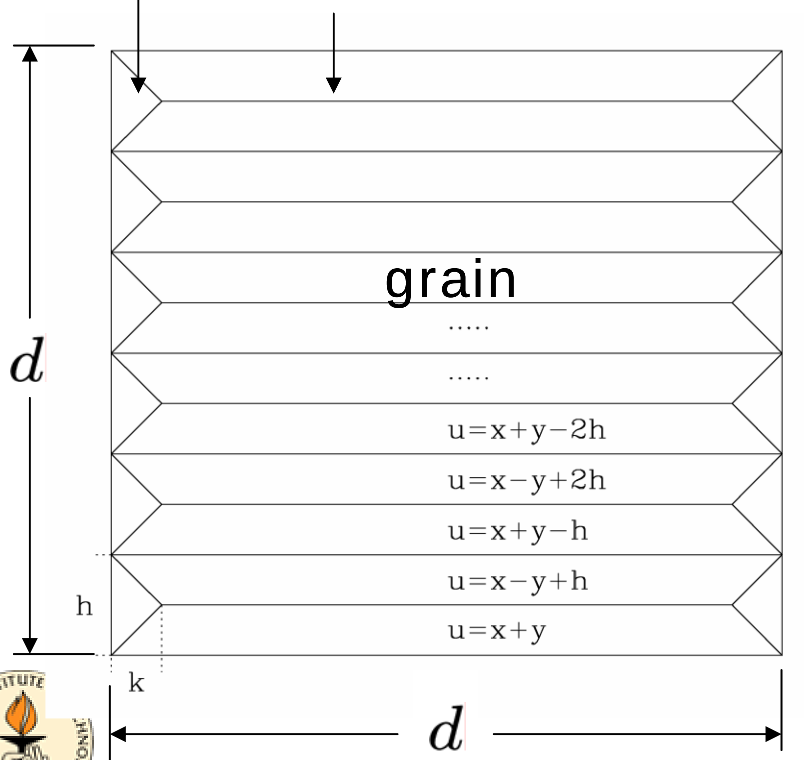
where $E_0(T,\gamma,\tau_0,\mu,d)\Big/G\gamma^2 d^3 =$

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

- 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:

$$W \equiv \frac{E_0}{d^3} \sim \tau_0 \gamma + \left(\frac{\mu T \gamma^3}{bd} \right)^{1/2}$$

- Yield stress:

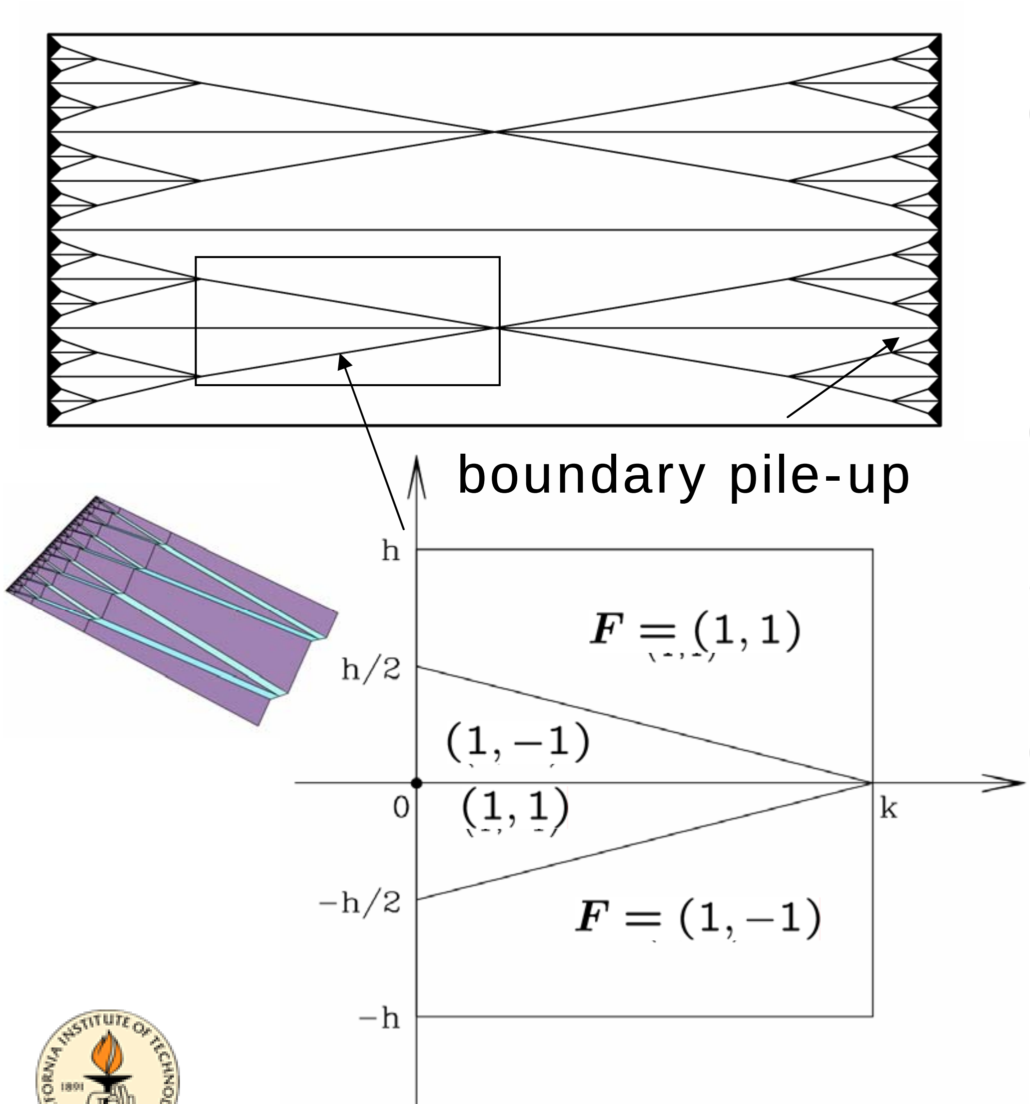
$$\tau \equiv \frac{\partial W}{\partial \gamma} \sim \tau_0 + \frac{1}{2} \left(\frac{\mu T \gamma}{bd} \right)^{1/2}$$

parabolic hardening + Hall-Petch scaling

- Lamellar width:

$$l \sim \left(\frac{\mu T d}{\mu \gamma b} \right)^{1/2}$$

Optimal scaling – Branching construction



- Energy:

$$W \sim \tau_0 \gamma + G \left(\frac{T\gamma^2}{Gbd} \right)^{2/3}$$

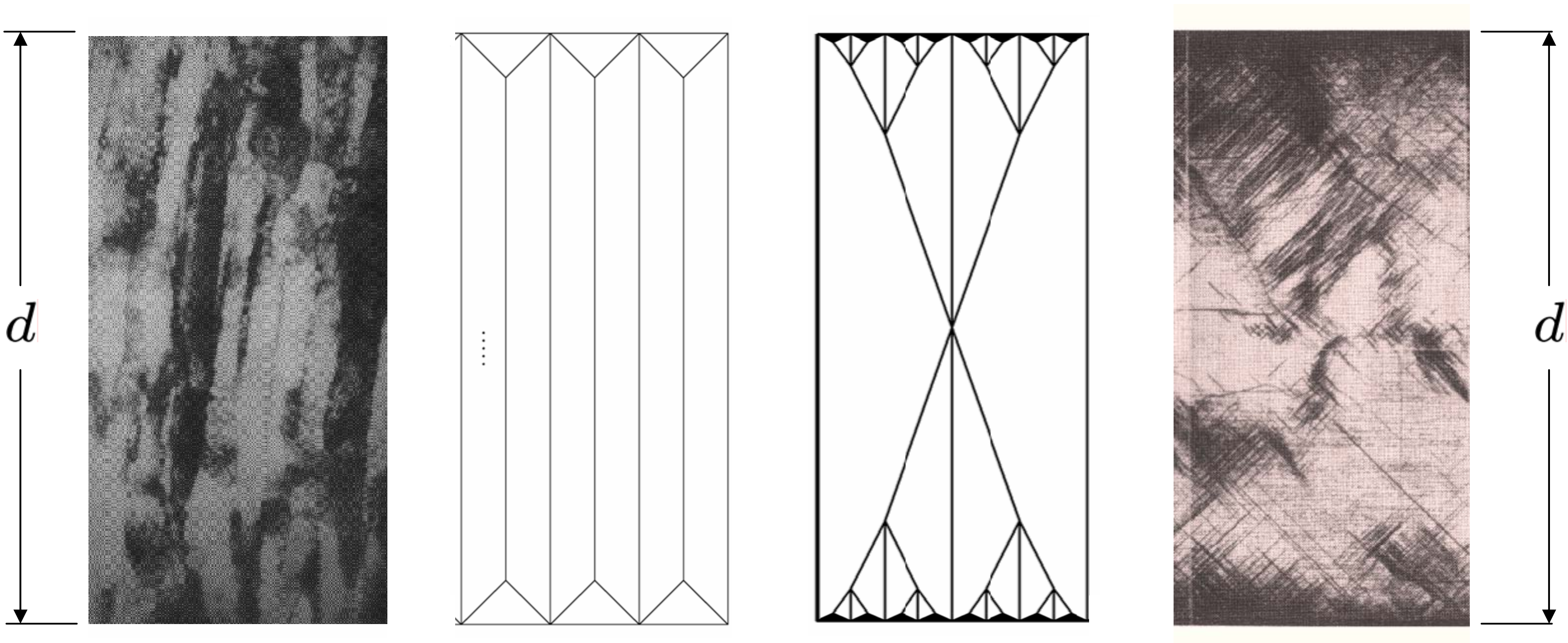
- Yield stress:

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

- Microstructure size:

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

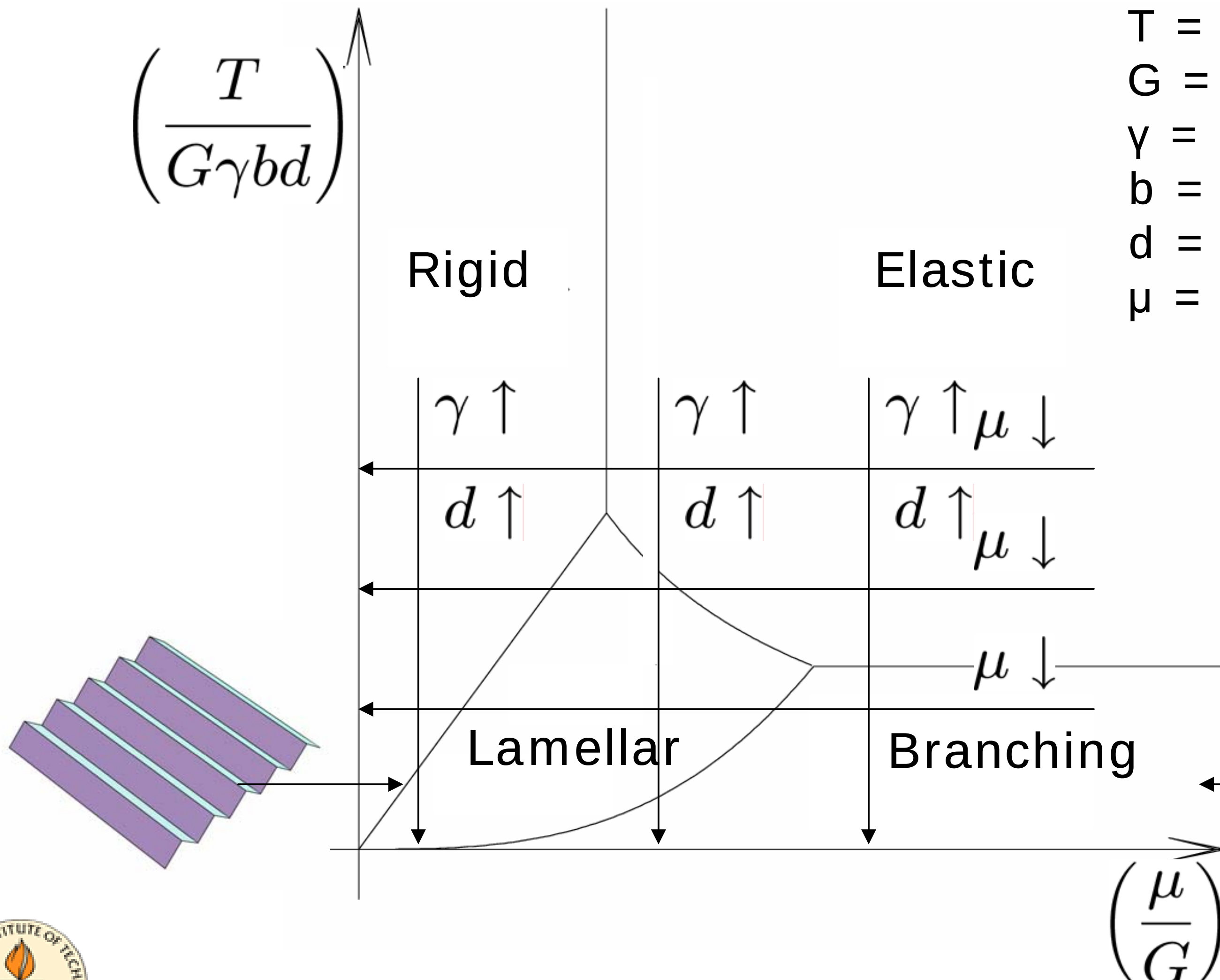
Optimal scaling – Microstructures

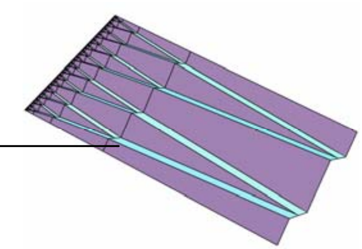


Shocked Ta (Meyers et al ´95) | Laminate $\tau \sim d^{-1/2}$ | Branching $\tau \sim d^{-2/3}$ | LiF impact (Meir and Clifton´86)

Dislocation structures corresponding to the lamination and branching constructions

Optimal scaling – Phase diagram





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

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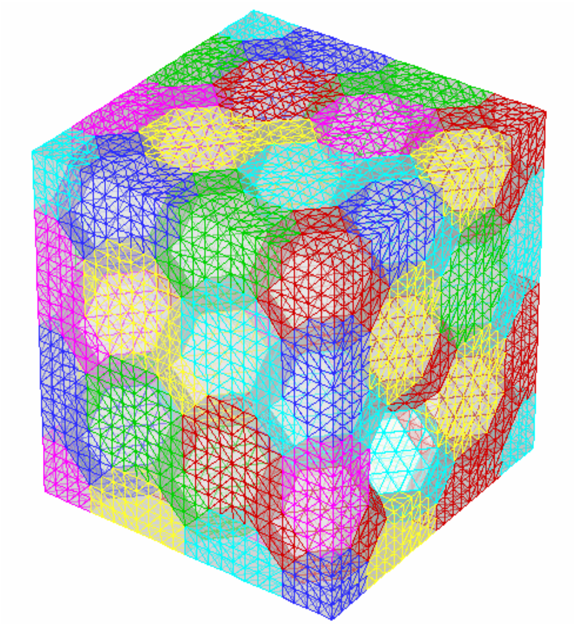
Non-locality and computation



Wrong picture!

- Effective behavior of each grain: $E(u|_{\partial\Omega}, \Omega)$, not a functional a gradient type.
- Need 'whole grain' elements! (open at present).