Variational Problems in Mechanics and the Link between Microstructure and Macroscopic Behavior

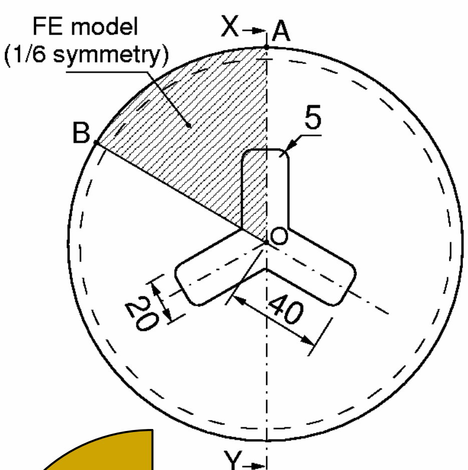
M. Ortiz
California Institute of Technology

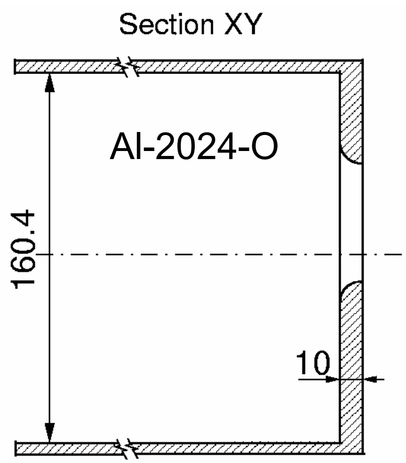
5th International Conference on Industrial and Applied Mathematics
Sydney, Australia
July 7-11, 2003

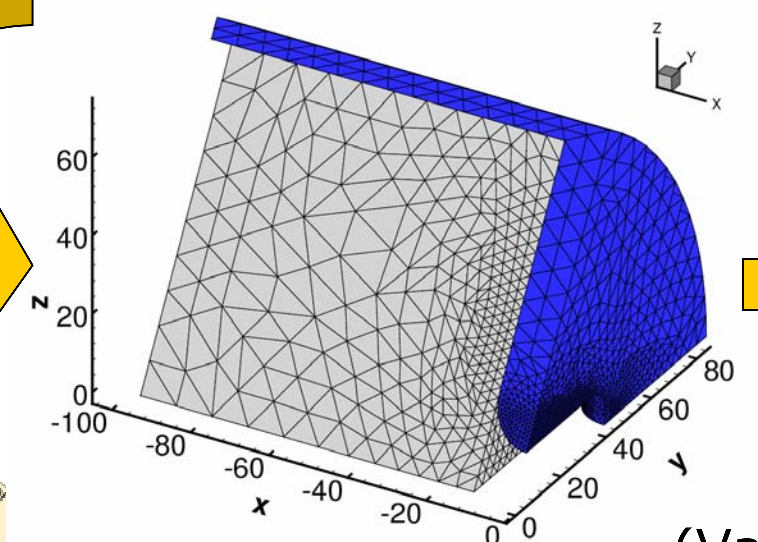
Introduction

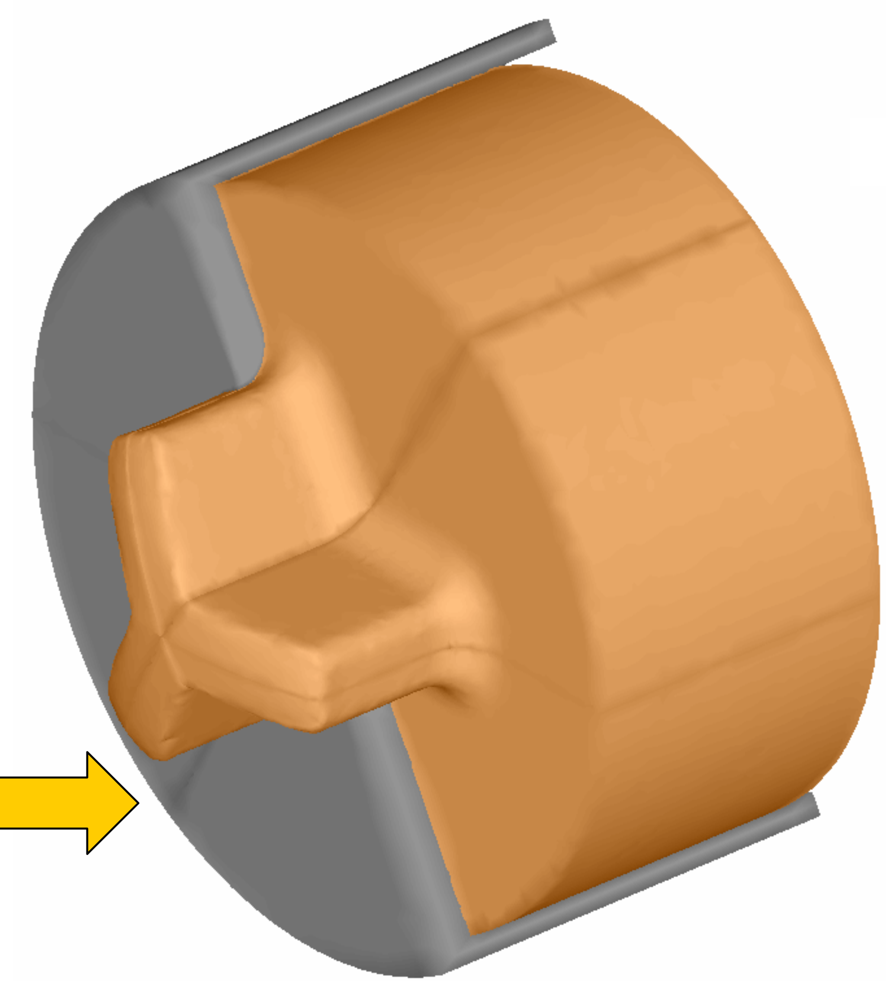
- The case for multiscale modeling in material science and computational mechanics
- How can microstructure, scaling and size effects be built into large-scale numerical calculations?
- Is brute-force raw computational power enough?
- A marriage of convenience: Mixed numerical and analytical multiscale (subgrid) models
- A case study in inelasticity: Metal plasticity
- How can multiscale methods be applied to inelastic, dissipative, hysteretic systems?

Manufacturing Processes - Extrusion





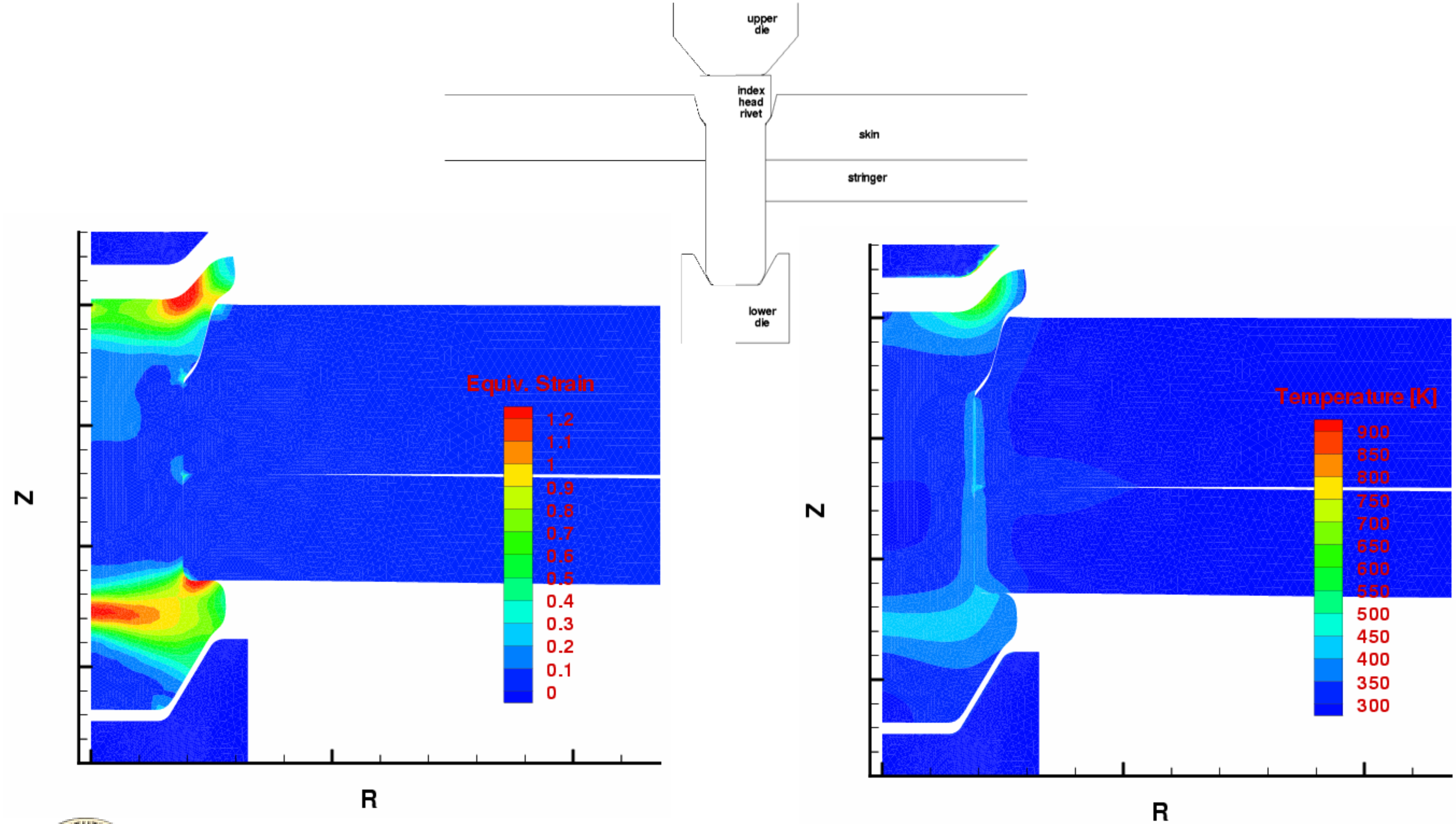




(Vallellano and Ortiz ´00)

Michael Ortiz
ICIAM 07/03

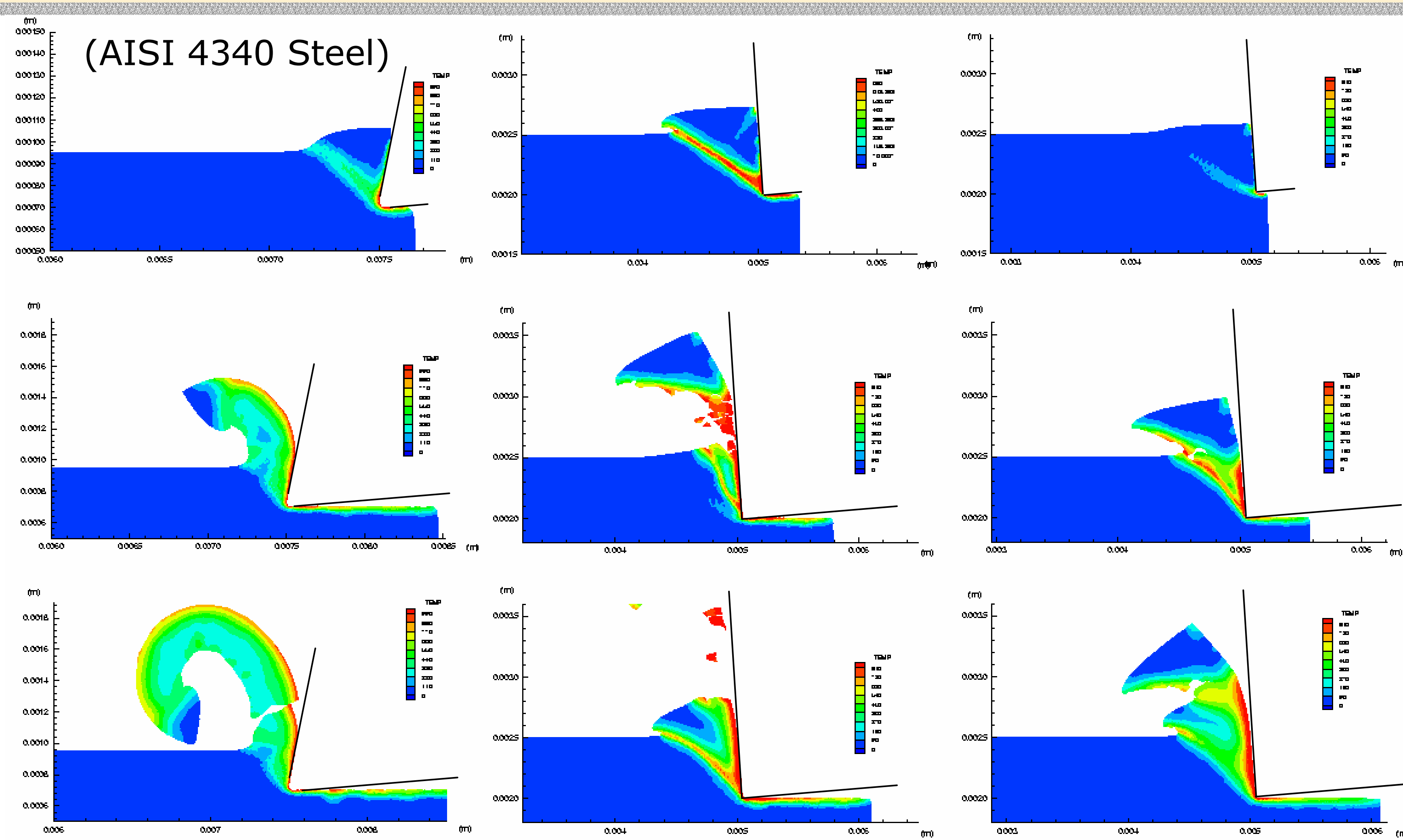
Manufacturing Processes - Riveting



(Repetto, Radovitzky and Ortiz ´99)

Michael Ortiz
ICIAM 07/03

Manufacturing Processes - Machining



Cutting speed = 20 m/s | Cutting speed = 20 m/s | Cutting speed = 10 m/s

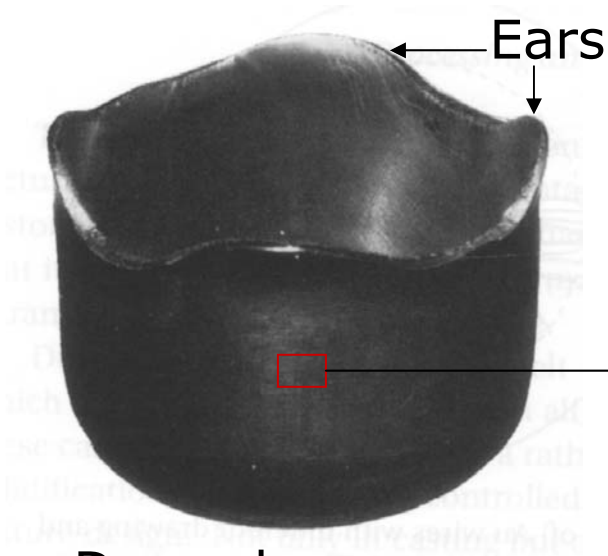
(Marusich and Ortiz, IJNME ´95)

Michael Ortiz
ICIAM 07/03

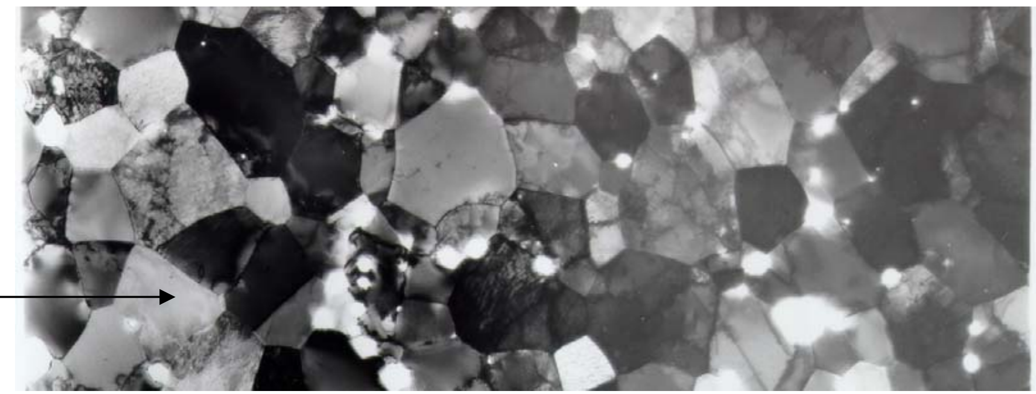
Validation and Verification

- Fundamental building blocks of simulations:
  - *Finite elements + time stepping algorithms*
  - *Finite deformation plasticity + heat conduction*
  - *Brittle and ductile fracture and fragmentation*
  - *Contact mechanics, friction*
- Main sources of error and uncertainty
  - *Discretization errors (spatial + temporal)*
  - *Uncertainties in data:*
    - *Material properties*
    - *Model geometry*
    - *Loading and boundary conditions…*
  - *Empiricism of constitutive models*

Limitations of empirical models



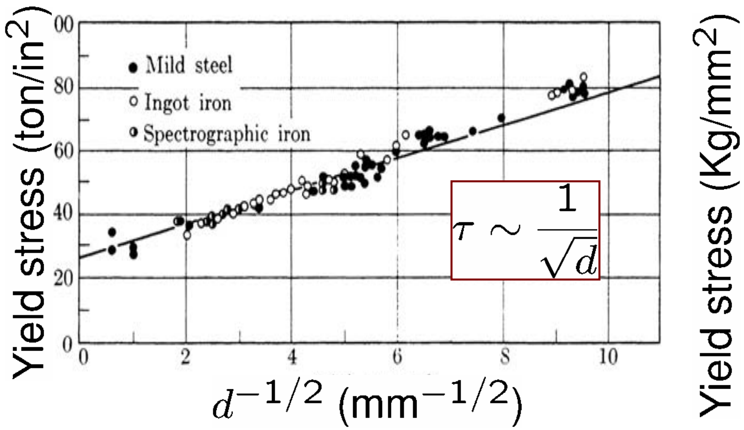
Deep-drawn cup



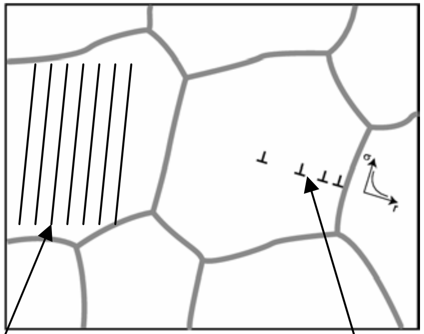
Grain structure of polycrystalline W
(Courtesy of Clyde Briant)

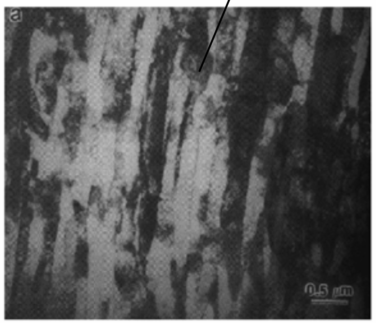
- Conventional engineering plasticity models fail to predict earing in deep drawing
- Prediction of earing requires consideration of polycrystalline structure, texture development

Limitations of empirical models

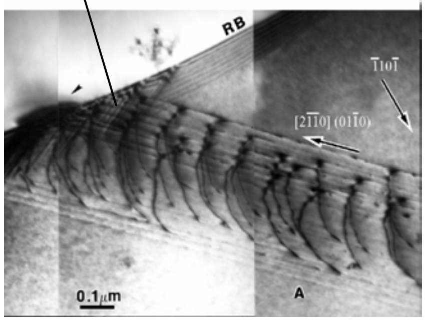


Hall-Petch scaling
(NJ Petch,
J. Iron and Steel Inst.,
174, 1953, pp. 25-28.)





Lamellar structure
in shocked Ta
(MA Meyers et al ´95)



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

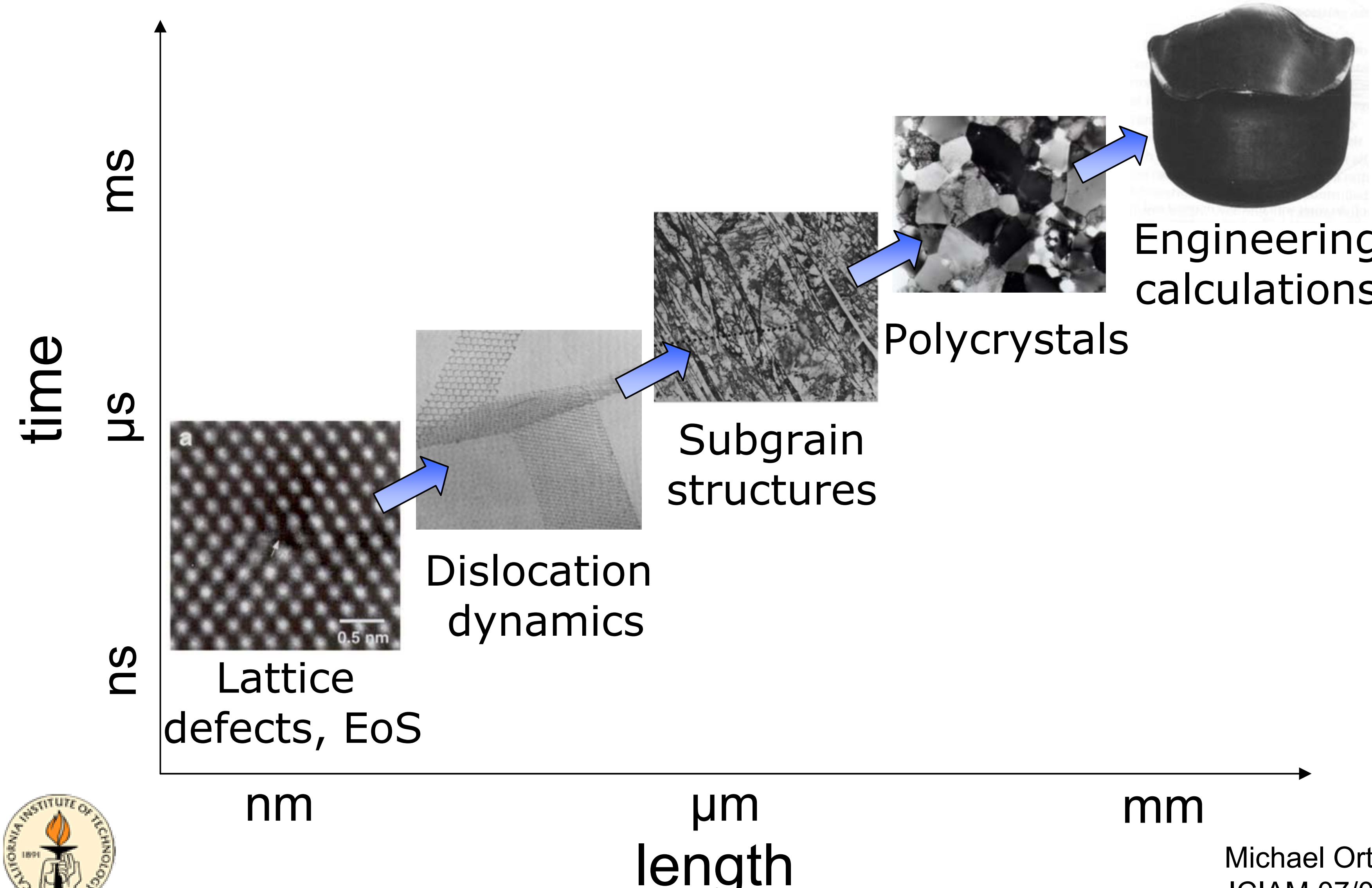
- Conventional plasticity models fail to predict scaling, size effects.

Michael Ortiz
ICIAM 07/03

The case for multiscale modeling

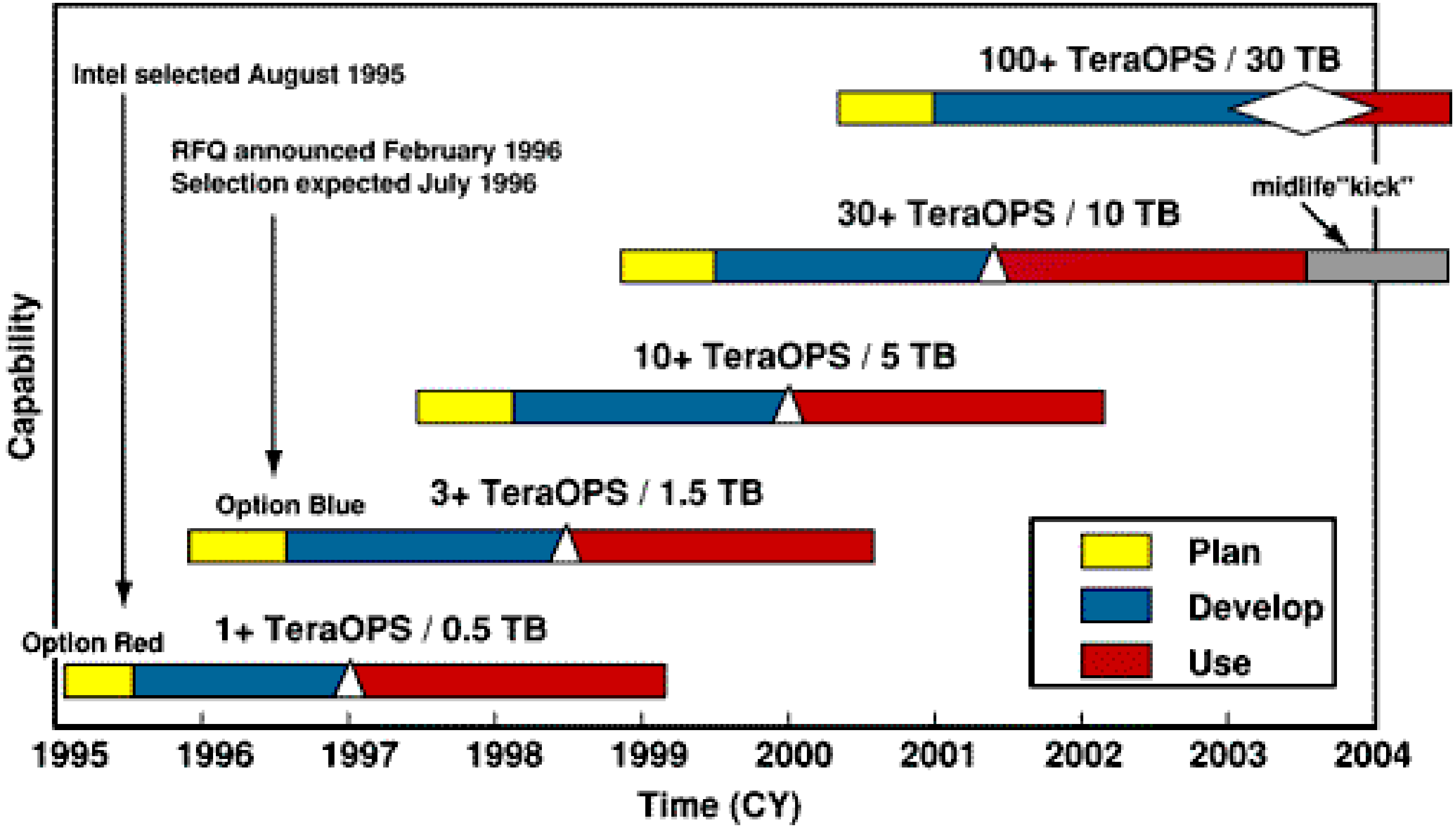
- Empirical models fail because they do not properly account for microstructure
- The empirical approach does not provide a systematic means of eliminating uncertainty from material models
- Instead, multiscale modeling:
  - *Identify relevant mechanisms at all lengthscales*
  - *Bridge lengthscales by:*
    - *Building models of effective behavior*
    - *Computing material parameters from first principles*
- Methods:
  - *Computational: Direct multiscale computing*
  - *Analytical: Methods of the calculus of variations*
  - *Mixed: Unresolved calculations + subgrid models*

Metal plasticity - Multiscale modeling



Direct multiscale computing - Outlook

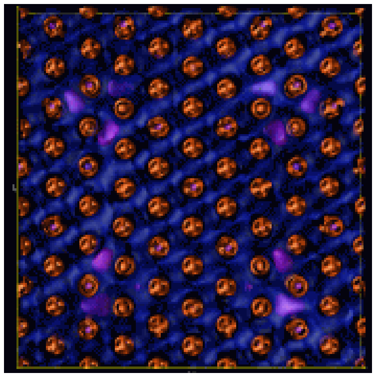
ASCI computing systems roadmap



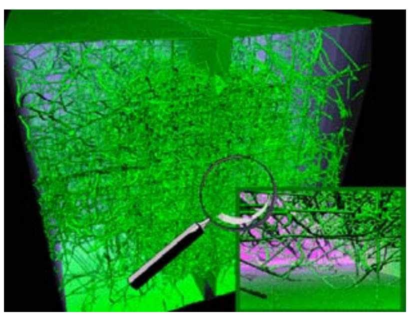
- Computing power is growing rapidly, but…

Michael Ortiz
ICIAM 07/03

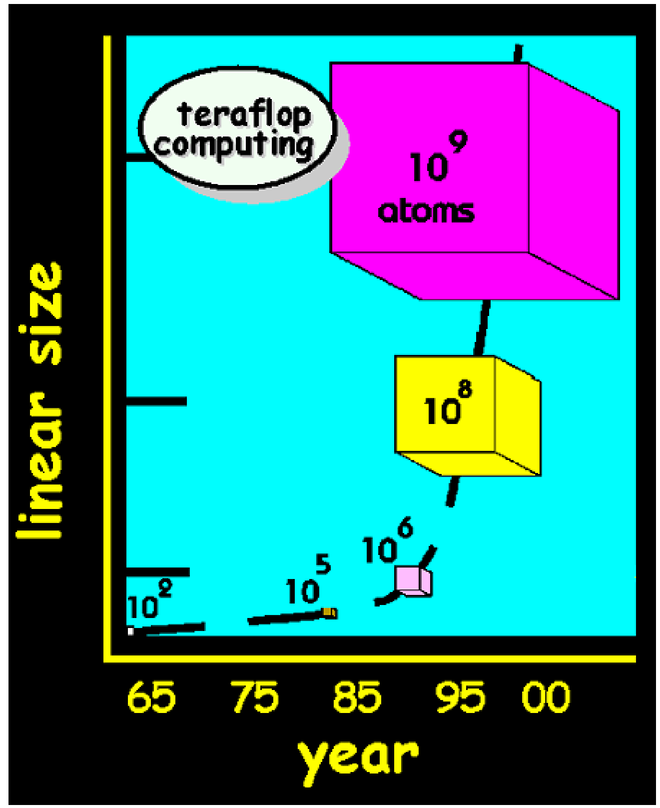
Direct multiscale computing – Bottom up



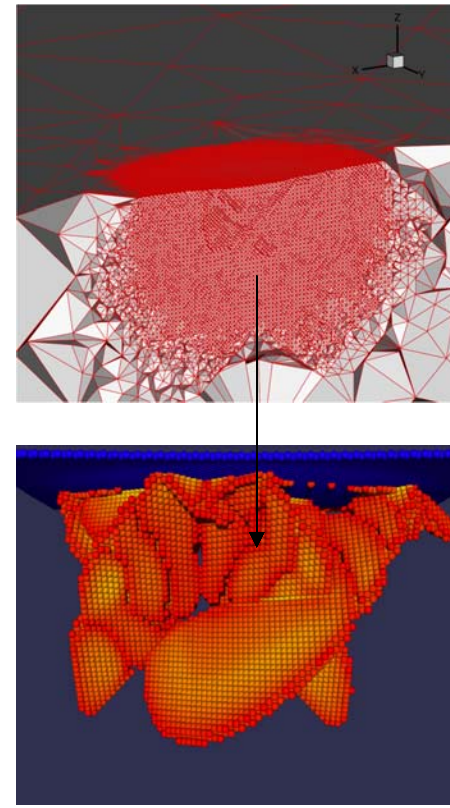
Ta quadrupole
(T. Arias ´00)



FCC ductile fracture
(F.F. Abraham ´03)



(Courtesy F.F. Abraham)

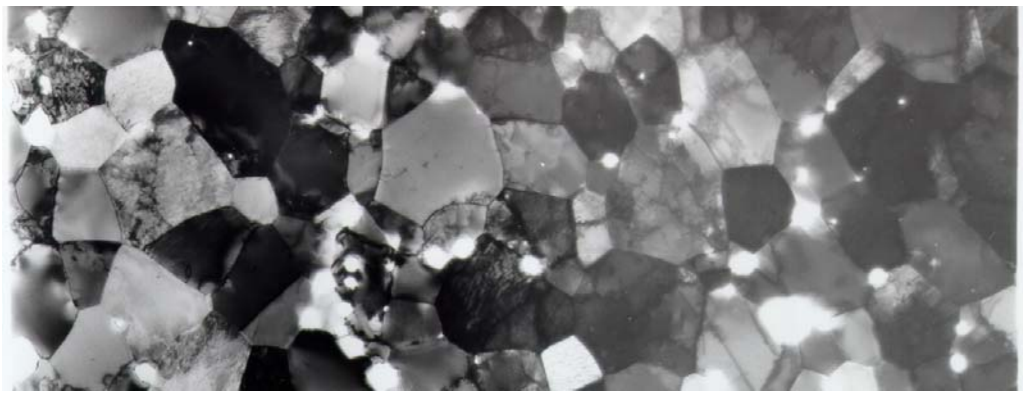


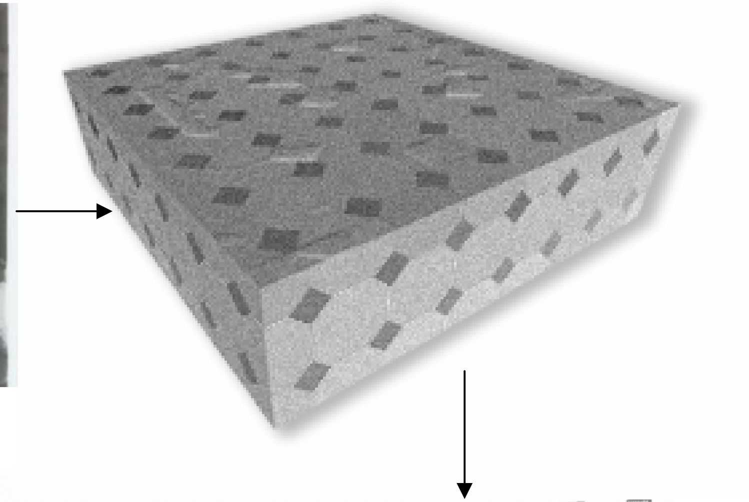
Au nanoindentation
(Knap and Ortiz ´03)

- Computing power is growing rapidly, but

  <u>$10^9 << 10^{23}$</u>

Direct multiscale computing – Top down

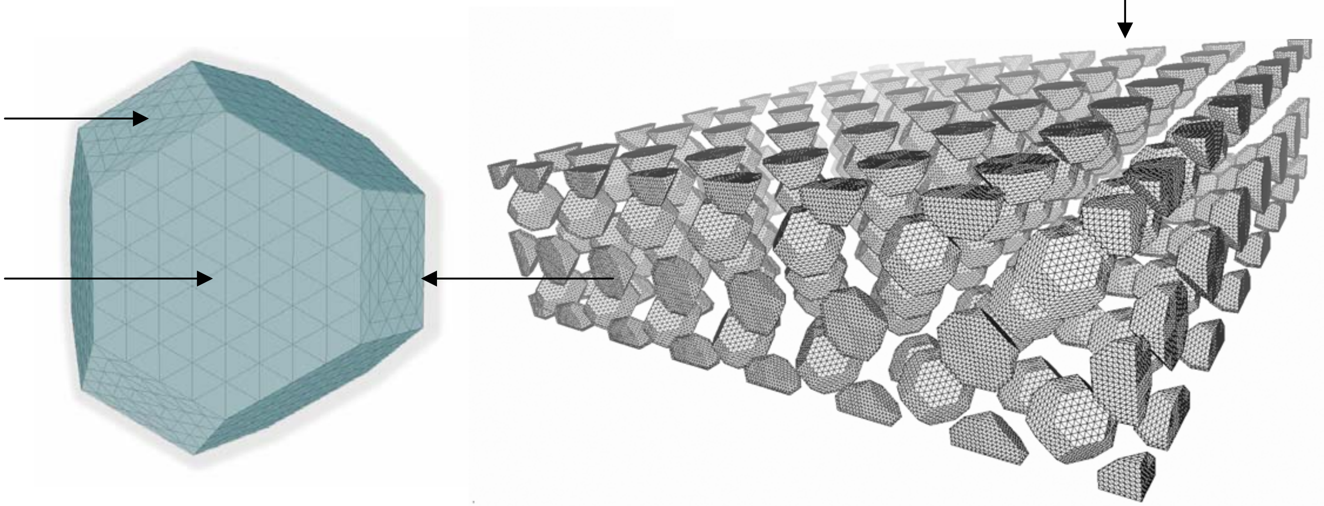




Polycrystalline W (Courtesy of C. Briant)

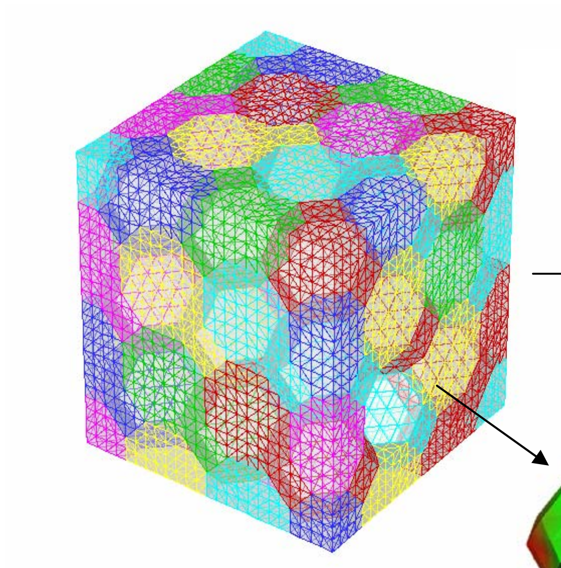
Grain-boundary sliding model

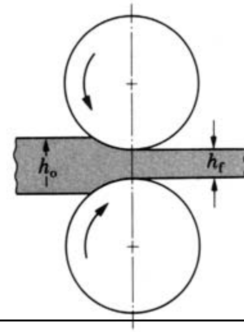
Single-crystal plasticity model

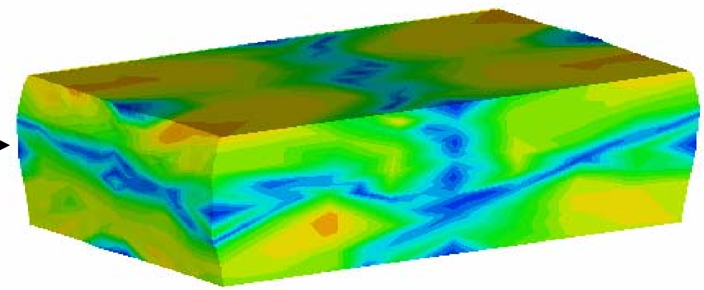


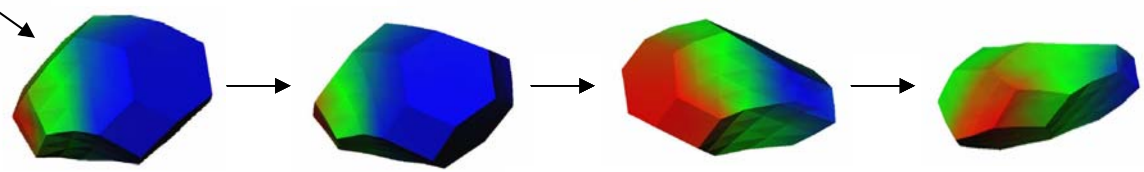
(A.M. Cuitiño and R. Radovitzky ´02)

Direct multiscale computing – Top down



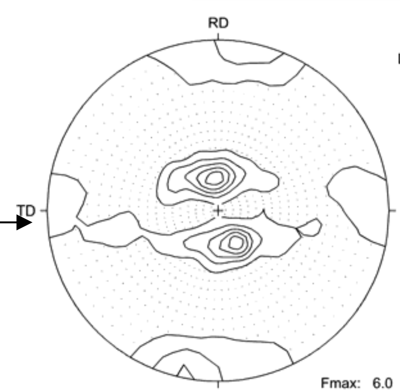


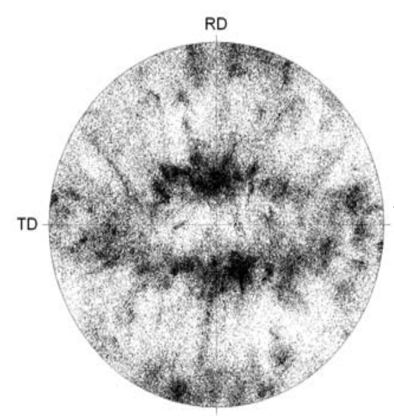




Cold-rolled @ 42%
polycrystalline Ta

Experimental
cold-rolled texture





Pole
figure

(A.M. Cuitiño and R. Radovitzky ´03)

Direct multiscale computing - Outlook

- ~ 10^9 elements at our disposal (10^6 elements/processor x 1000 processors)
- ~ 1000 elements/coordinate direction
- ~ 20 elements/grain/direction (8000 elements/grain)
- ~ 50 grains/direction (125K grains)
- ~ 2.5 mm specimen for 50 μm grains
- Not enough for complex engineering simulations!
- Subgrain scales still unresolved, require modeling!

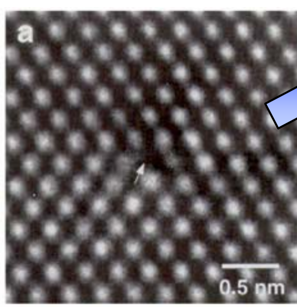
Metal plasticity - Multiscale modeling

Accessible to first-principles calculations

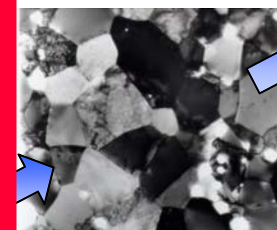
time

μs

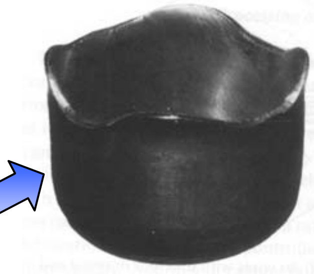
ns



Lattice defects, Eo



Polycrystals



Engineering calculations

Accessible to direct numerical simulation

nm

μm

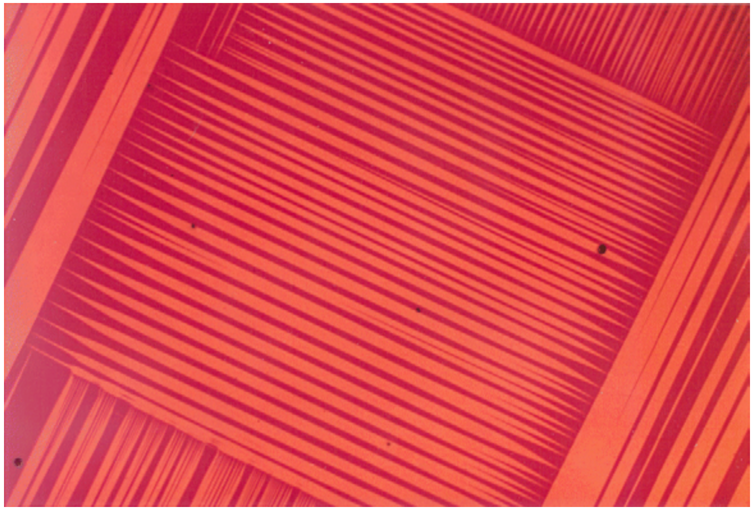
mm

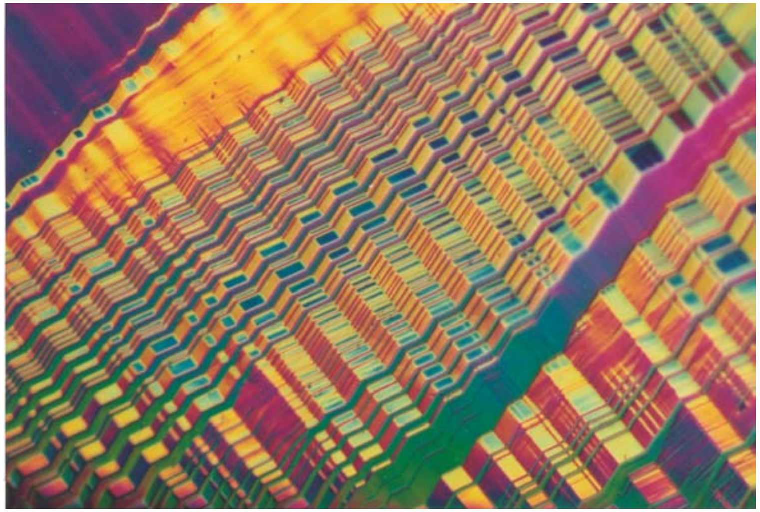
length

Michael Ortiz
ICIAM 07/03

Subgrid models – Relaxation methods

(Cu-Al-Ni, Chunhua Chu and Richard D. James)





- Use analytically-derived effective models to represent unresolved (sub-grid) phenomena
- Methods of the calculus of variations: relaxation, Γ-convergence, optimal scaling, homogeneization
- Model conservative system: Nonlinear elasticity

Nonlinear elasticity - Relaxation

- Nonlinear elasticity:

$$\inf_{y \in y_0 + W_0^{1,\infty}(\Omega)} \left\{ I(y) = \int_\Omega W(Dy)\, dx \right\}$$

- Functions $W(Dy)$ of interest have multi-well structure $\Rightarrow$ $I(y)$ lacks weak sequential lower-semi-continuity $\Rightarrow$ inifimum not attained in general.
- Direct numerical solutions based on $I(y)$ tend to exhibit exceedingly slow or no convergence.

Nonlinear elasticity - Relaxation

- Instead: Do numerics on the *relaxed* problem:

$$\inf_{y \in y_0 + W_0^{1,\infty}(\Omega)} \left\{ sc^- I(y) = \int_\Omega QW(Dy)\, dx \right\}$$

where $sc^- I$ is the lower semi-continuous envelop of I, and

$$QW(F) = \inf_{u \in W_0^{1,\infty}(E)} \frac{1}{|E|} \int_E W(F + Du)\, dx$$

is the *quasiconvex* envelop of W (independent of $E \subset \Omega$).

Nonlinear elasticity - Relaxation

Theorem. *Assume that* $I : X \to \bar{\mathbb{R}}$ *is coercive. Then:*

(i) $sc^- I$ *is coercive and lower semicontinuous.*

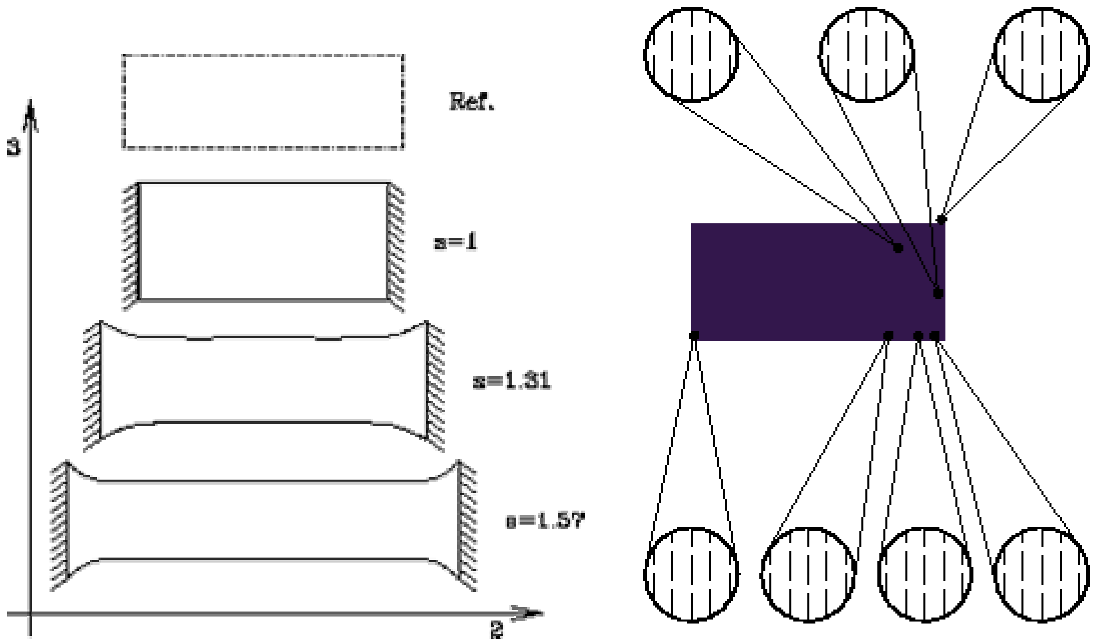
(ii) $sc^- I$ *has a minimum point in* X.

(iii) $\min_{y \in X} sc^- I(y) = \inf_{y \in X} I(y)$.

(iv) Every cluster point of a minimizing sequence of I *is a minimum point of* $sc^- I$ *in* X.

(v) If, in addition, X *is first-countable, then every minimum point of* $sc^- I$ *is the limit of a minimizing sequence of* I *in* X.

Example – Nematic elastomers



(Courtesy of de Simone and Dolzmann)

Central region of sample at moderate stretch (Courtesy of Kunder and Finkelmann)

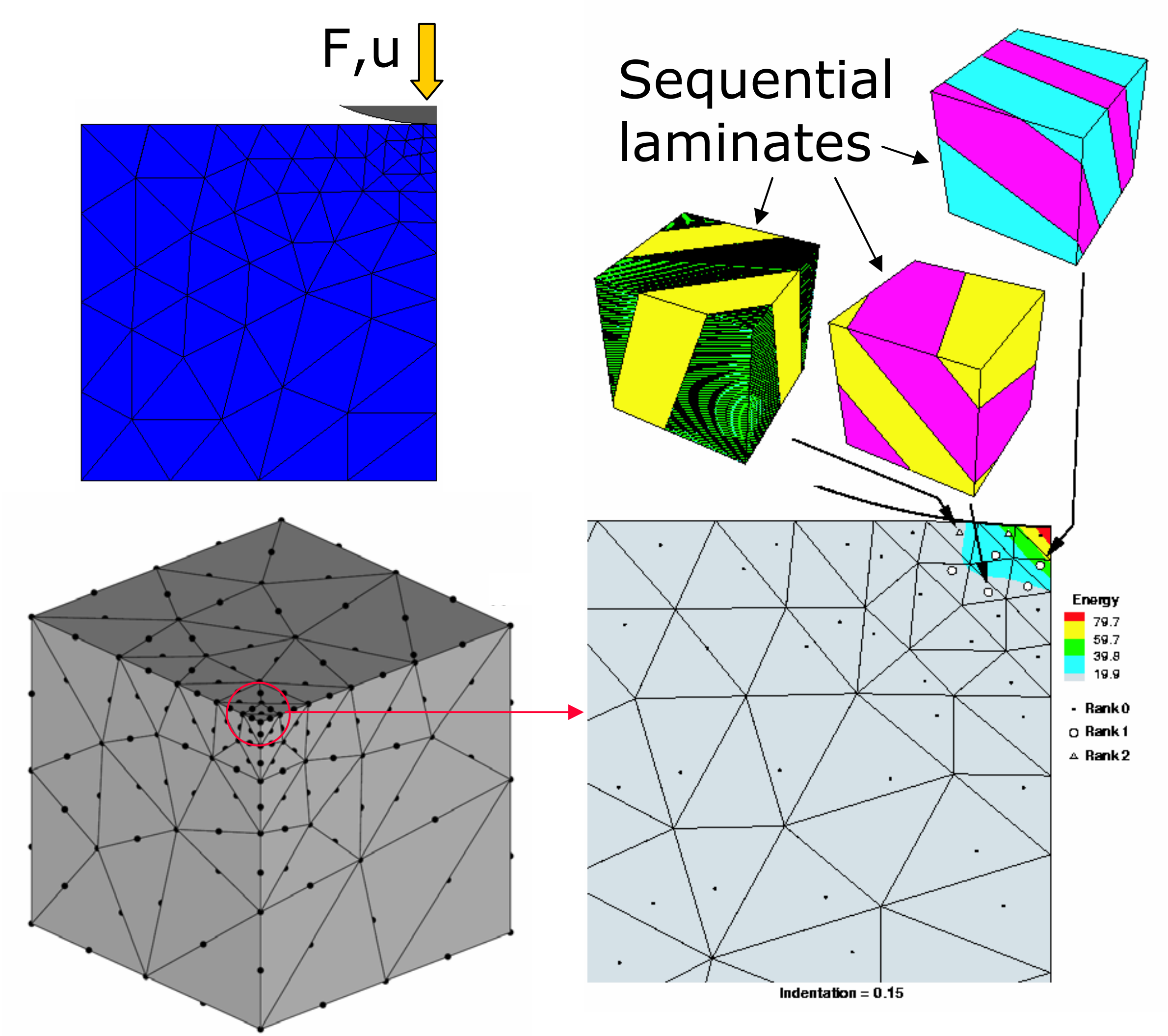
$$W(F, n) = A\,\mathrm{tr}(FF^T) - B\,||F^T n||^2$$

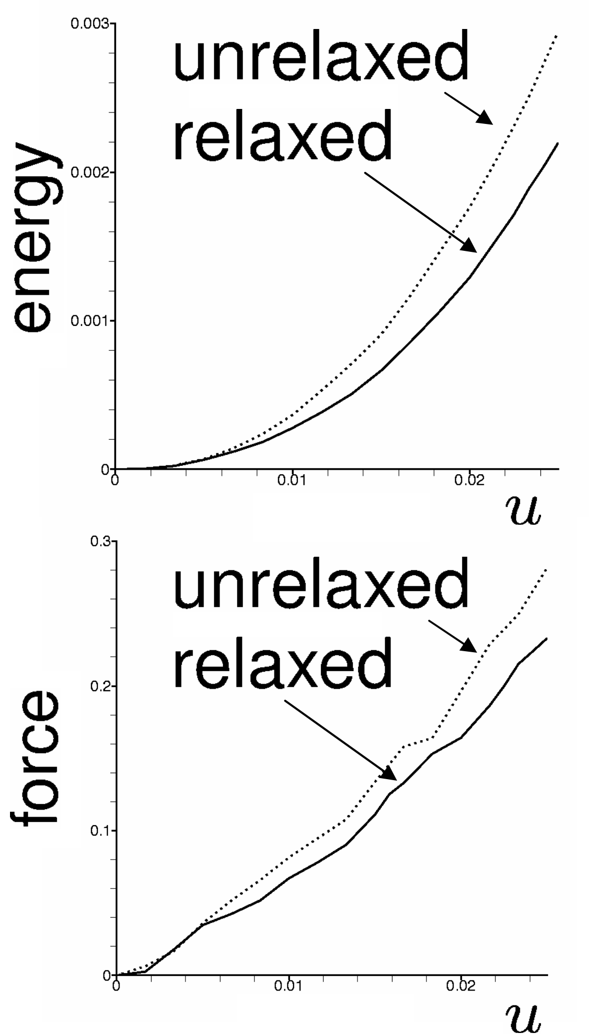
Blandon *et al.* ´93
De Simone and Dolzmann ´00
De Simone and Dolzmann ´02

Nonlinear elasticity - Relaxation

- Relaxed problem exhibits easy-to-compute regular solutions
- Sub-grid microstructural information is recovered locally from the solution of the relaxed problem
- But: Quasiconvex envelops are known explicitly in very few cases
- Instead: Consider easy-to-generate special microstructures, such as sequential laminates
  - *Off-line (Dolzmann ´99; Dolzmann & Walkington ´00)*
  - *Concurrently with the calculations (Aubry et al. ´03)*

Example - Indentation of Cu-Al-Ni



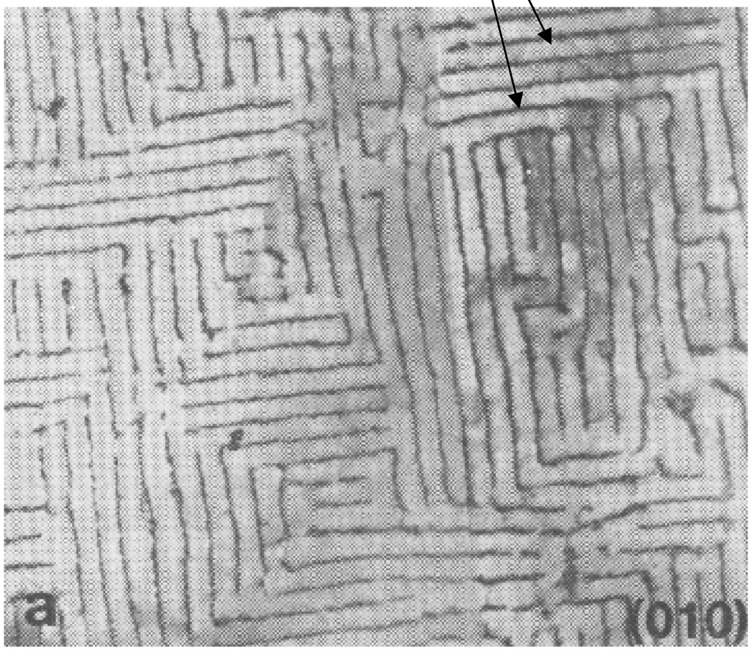


(Aubry, Fago and Ortiz ´03)

Michael Ortiz
ICIAM 07/03

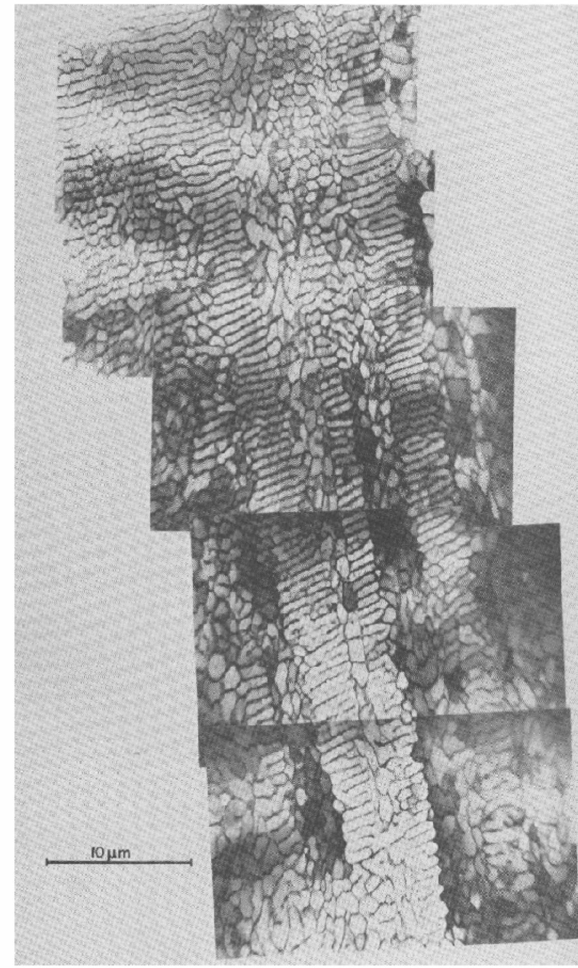
Crystal plasticity - Microstructures

Dipolar dislocation walls

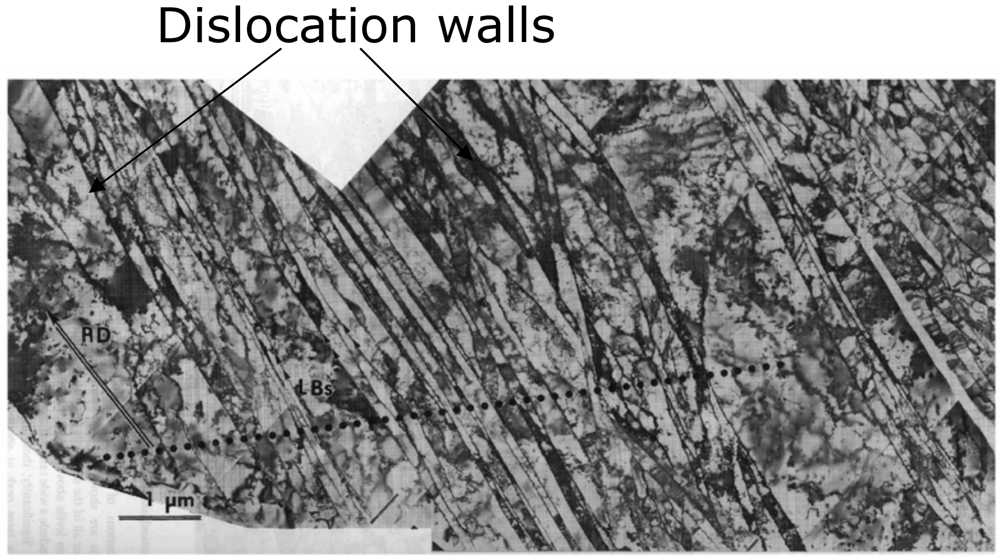


Labyrinth structure in fatigued copper single crystal
(Jin and Winter ´84)

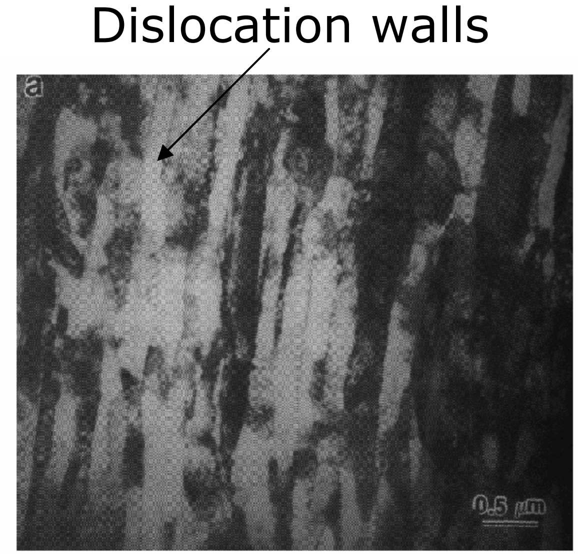
Nested bands in copper single crystal fatigued to saturation
(Ramussen and Pedersen ´80)



Crystal plasticity - Microstructures



Lamellar dislocation structure
in 90% cold-rolled Ta
(Hughes and Hansen ´97)



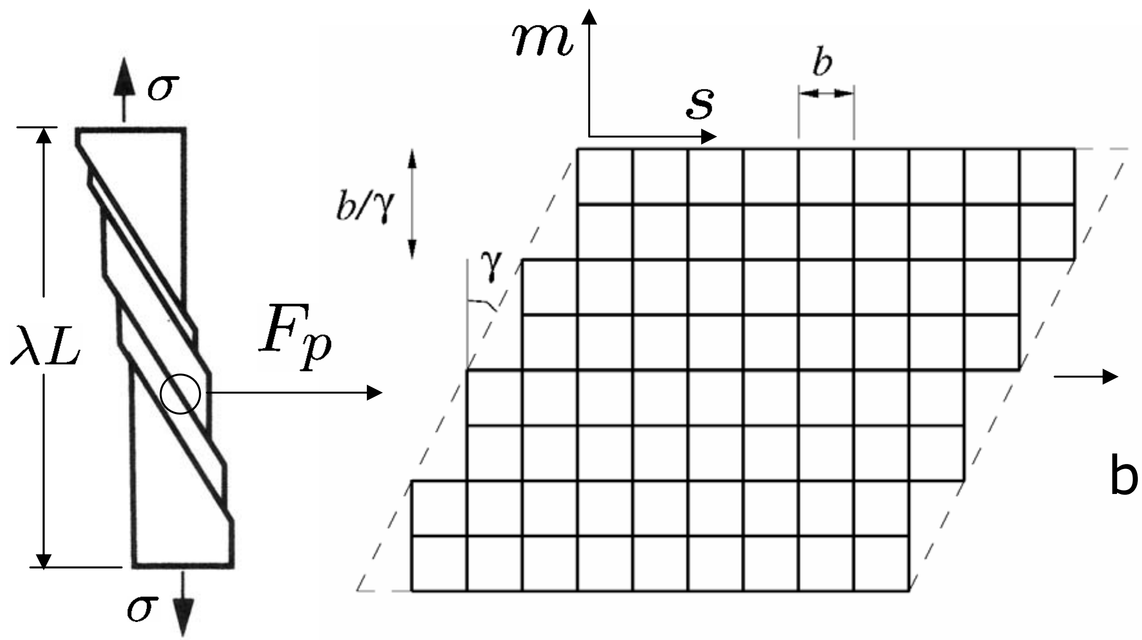
Lamellar structure
in shocked Ta
(Meyers et al ´95)

- Lamellar structures are universally found on the micron scale in highly-deformed crystals
- These microstructures are responsible for the soft behavior of crystals and for size effects

Crystal plasticity - Microstructures

- For conservative systems, there is a clear connection between microstructure and non-attainment
- Difficulties in applying program to plasticity:
  - *Plasticity involves both energetics and kinetics*
  - *Plasticity exhibits strong scaling and size effects*
  - *No general analytical method for relaxing functionals*
- Difficulties are overcome by:
  - *Incremental variational formulation (Ortiz and Repetto ´99; Ortiz and Stainier ´00; Mielke ´00)*
  - *Non-local energies (Ortiz and Repetto ´99; Mielke and Müller ´03)*
  - *Numerical relaxation (Dolzmann ´99; Dolzmann and Walkington ´00; Aubry, Fago and Ortiz ´03)*

Crystal plasticity - BVP



Irreversible accommodation of shear deformation by crystallographic slip

$$\inf_{y \in y_0 + W_0^{1,\infty}(\Omega)} \left\{ I(y) = \int_\Omega A(Dy\, F_p^{-1}, \gamma)\, dx \right\}$$

Pointwise: $F_p = I + \gamma\, s \otimes m, \quad (s, m) \in \{\text{finite set}\}$

$$\dot{\gamma} = \partial_\tau \psi(\tau)$$

$$\tau = -\partial_\gamma A(Dy\, F_p^{-1}, \gamma)$$

Crystal plasticity - BVP

- Crystal plasticity involves both energetics and kinetics
- The variational structure of the BVP is not clear from the outset…
- …but it can be revealed by recourse to time discretization (Ortiz and Repetto ´99, Ortiz and Stainier ´00, Mielke ´00)

Crystal plasticity – Variational problem

- Discretize time: $t_0, \ldots, t_n, t_{n+1}, \ldots$
- Define incremental strain energy density (Ortiz and Repetto '99; Ortiz and Stainier '99):

$$W_n(F_{n+1}) = \inf_{\text{paths}} \int_{t_n}^{t_{n+1}} \partial_F A \cdot \dot{F} \, dt$$

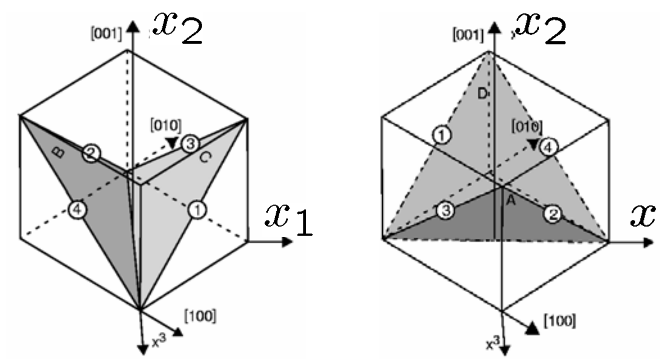
- Incremental variational problem:

$$\inf_{y_{n+1} \in y_0 + W_0^{1,\infty}(\Omega)} \left\{ I_n(y_{n+1}) = \int_\Omega W_n(D y_{n+1}) \, dx \right\}$$

- Incremental problem is formally identical to non-linear elasticity problem!

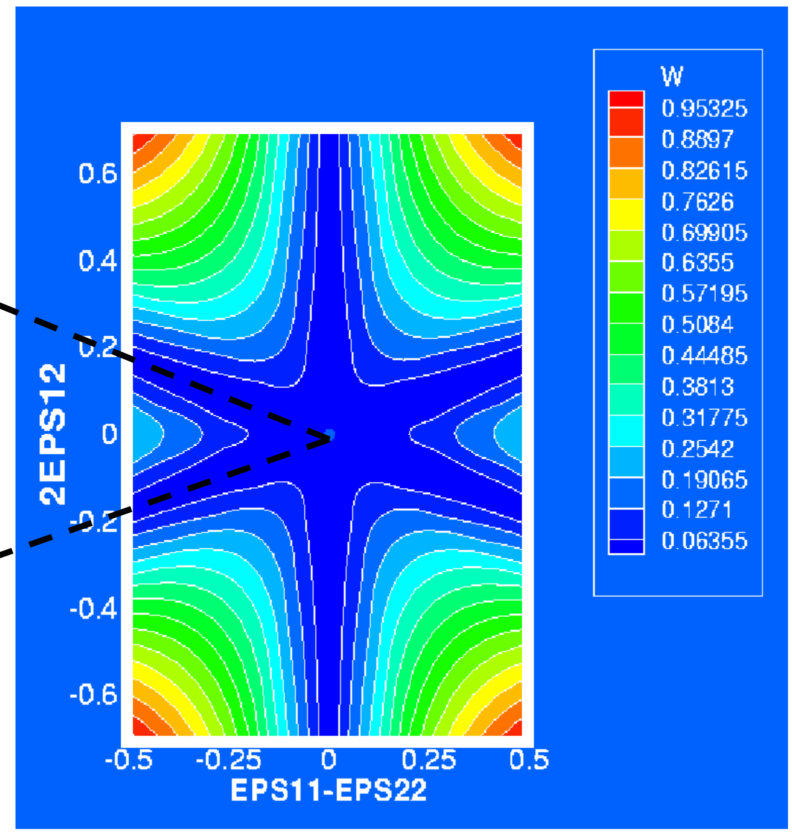
Crystal plasticity – Non-attaiment

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



$$F \in SO(3) \times (I + \gamma s \otimes m)$$

(Single slip)



$W_n(F)$

- $W_n(F)$ non-convex!

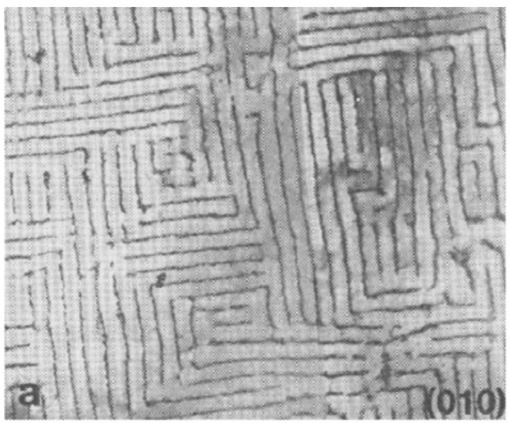
Michael Ortiz
ICIAM 07/03

Crystal plasticity - Relaxation

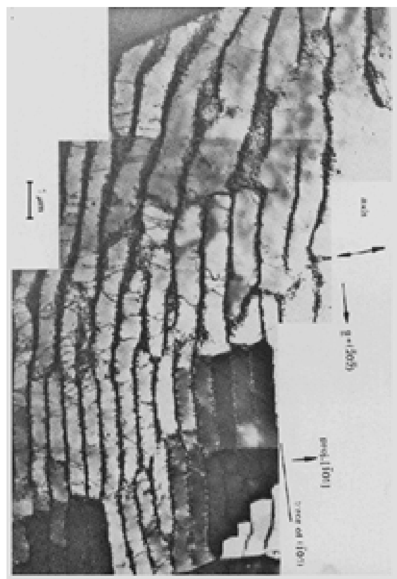
- Crystal plasticity has an incremental variational structure
- Incremental energy functional lacks lower semicontinuity
- Observed microstructures are a manifestation of non-attainment
- Numerical implementation: Relax incremental energy functional
- Fall-back position: Consider special microstructures, e.g., sequential laminates

Validation – Fatigued copper

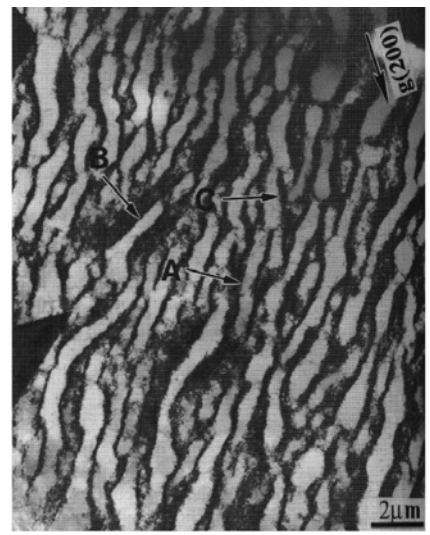
- Problem (Ortiz and Repetto '97): Find all laminates such that $F \in SO(3) \times (I + \gamma s \otimes m)$, $(s, m) \in$ finite set.



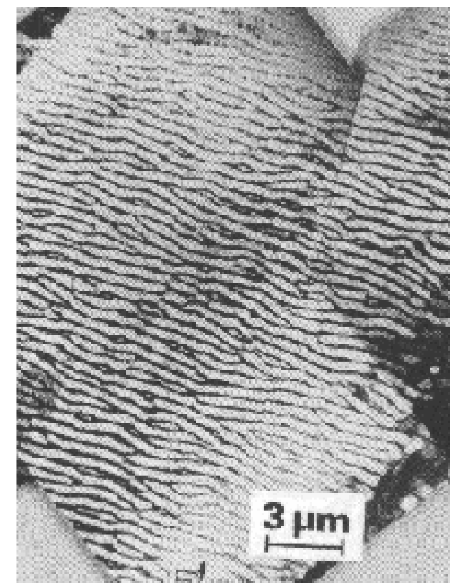
(100) walls
(Jin and Winter ´84)



(101) walls
(Wang and Mughrabi ´84)

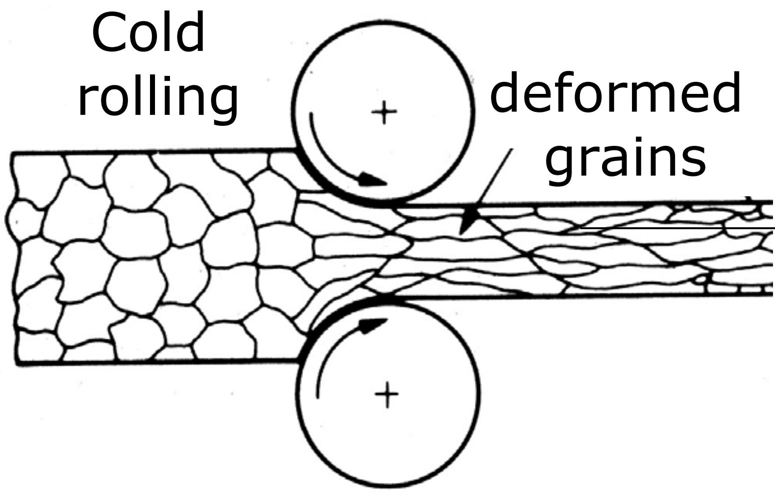


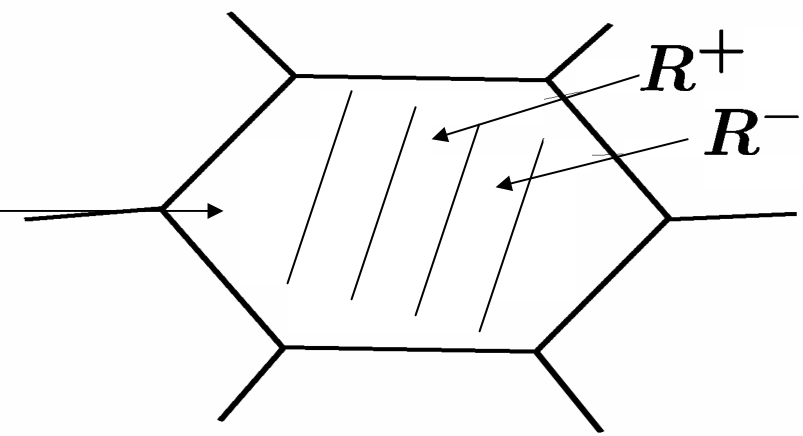
(111) walls
(Yumen ´89)

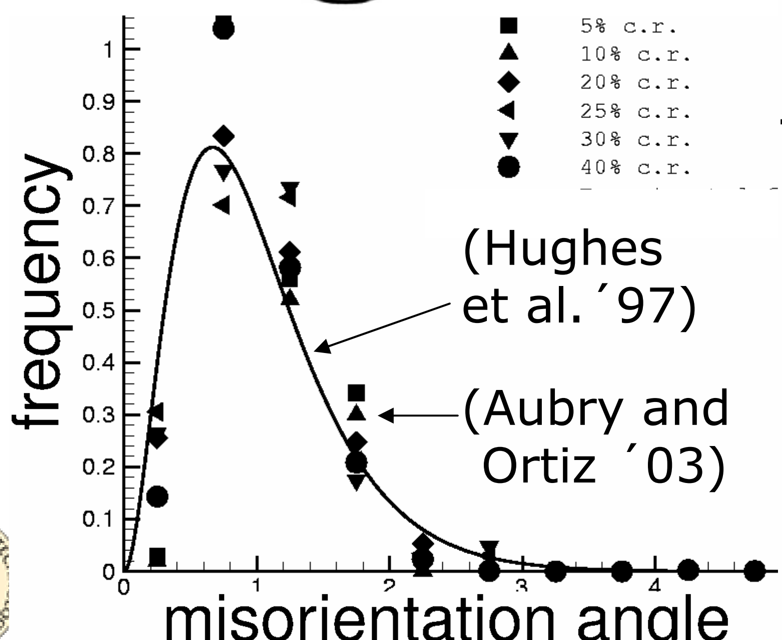


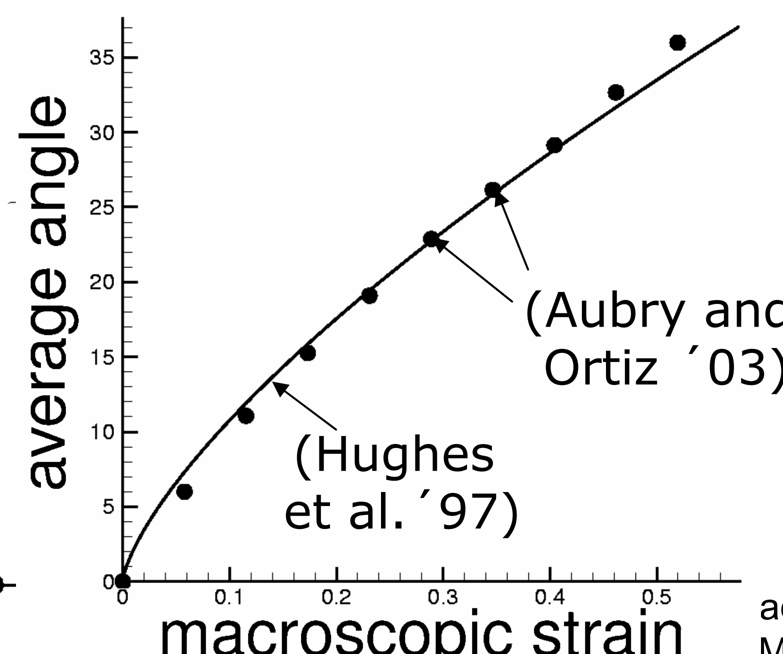
(131) walls
(Lepisto et al., 1986)

Validation – Misorientation angles





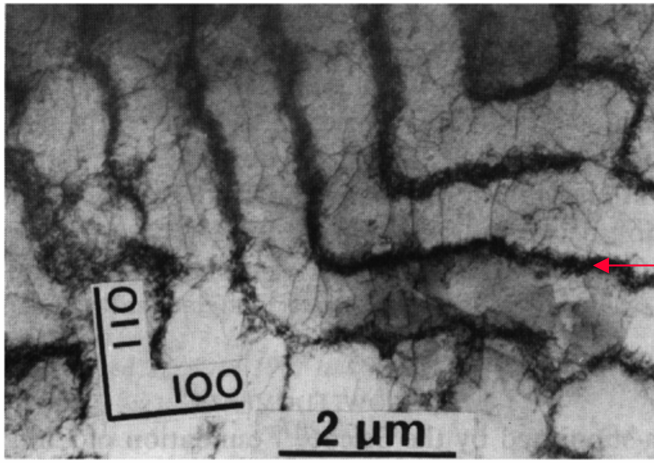




Crystal plasticity – Nonlocal extension

- Thus far the material description is local
- Local material models do not possess a characteristic length scale an cannot predict scaling relations such as the Hall-Petch effect
- In order to predict scaling relations we need to account for additional physics:
  - *Dislocation core energies*
  - *Dislocation wall energies*
- This renders the material description nonlocal…

Crystal plasticity – Nonlocal extension



Fatigued copper (Jin ´87)

Dislocation walls carry additional energy

- Nonlocal free energy:

$$I(y,\Omega) = \int_\Omega \left\{ A(Dy\, F_p^{-1}, \gamma) + (T/b)||\text{curl} F_p|| \right\} dx$$

- Energy density of a subset $E \subset \Omega$:

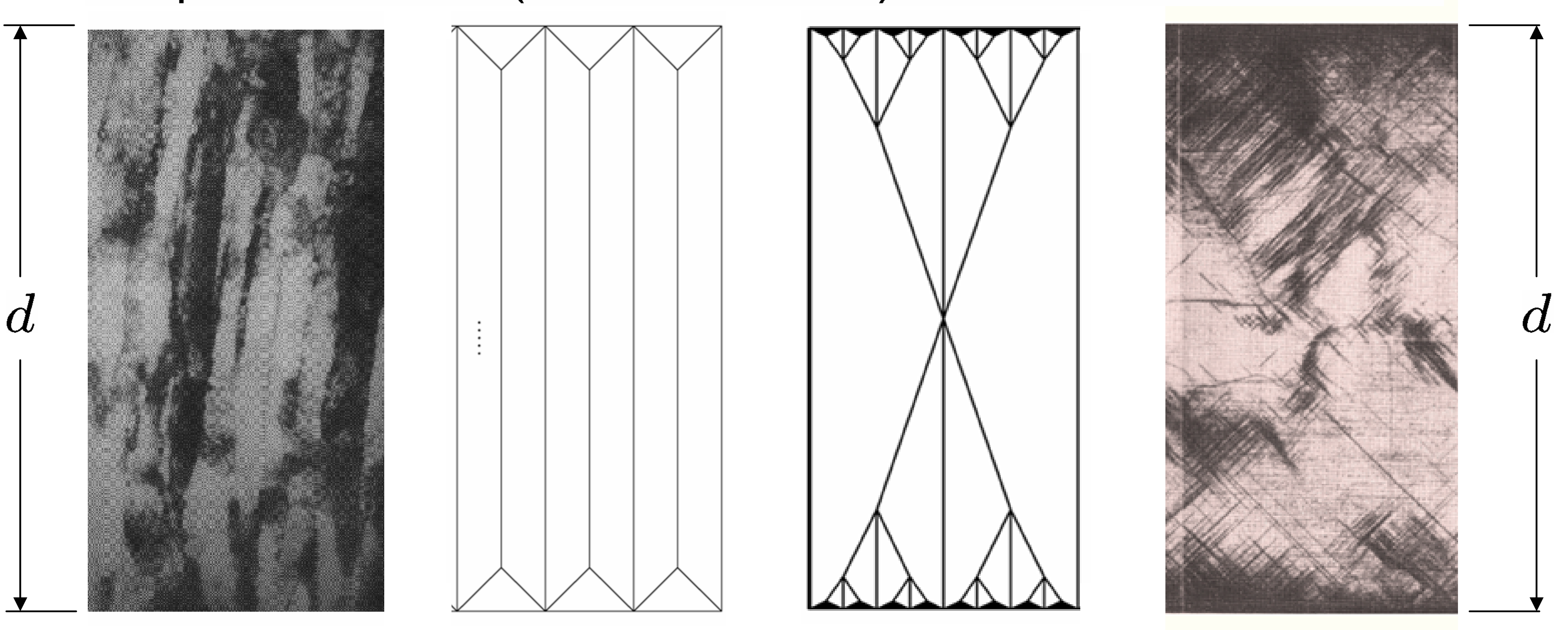
$$\frac{1}{|E|} \inf_{u \in W_0^{1,\infty}(E)} I_n(Fx + u, E) \;\rightarrow \text{depends on } E!$$

Crystal plasticity – Nonlocal extension

- Energy density depends on size, shape of domain.
- We can no longer defined a meaningful effective energy density
- Need to model entire domains at a time!
- Analytical tools:
  - *Optimal scaling (Kohn and Müller ´92, ´94; Conti ´00, ´03)*
  - *Young measures of micro-patterns (Alberti and Müller ´99)*
- Work in progress: `Grain elements'
  - *Each element represents one entire grain*
  - *Energy of grain depends on its size, shape and exhibits optimal scaling*

Crystal plasticity – Nonlocal extension

- Optimal scaling constructions for double slip, antiplane shear (Conti ’00, ’03)



Shocked Ta (Meyers et al ´95)

Laminate

$\tau_c \sim d^{-1/2}$

Branching

$\tau_c \sim d^{-2/3}$

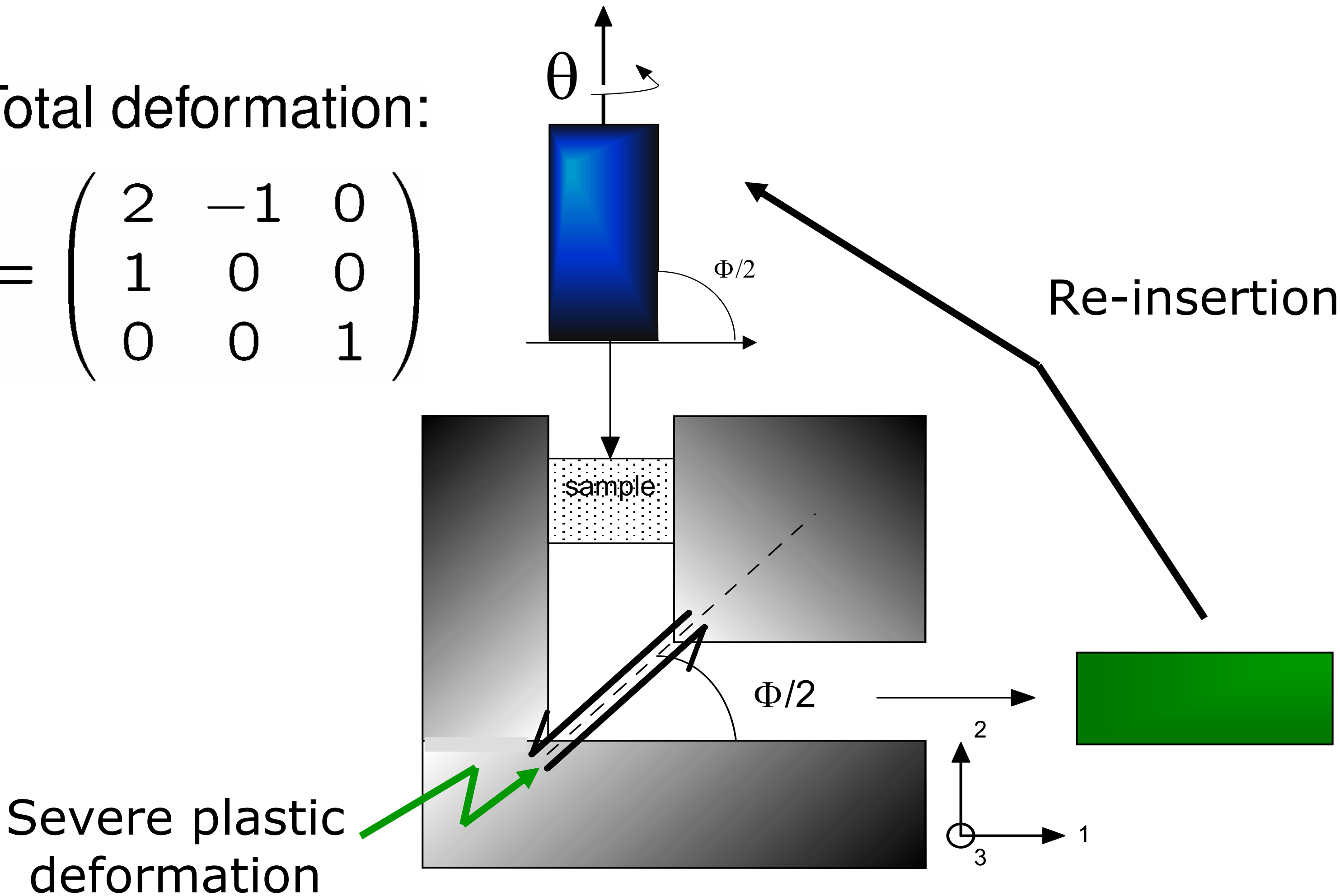
LiF impact (Meir and Clifton ´86)

Hall-Petch effect!

Equal Angular Channel Extrusion

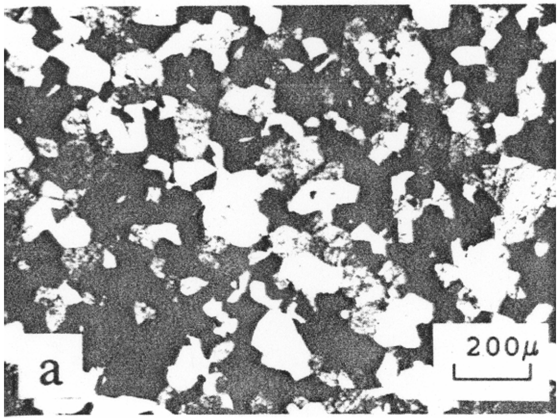
- Total deformation:

$$A = \begin{pmatrix} 2 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$



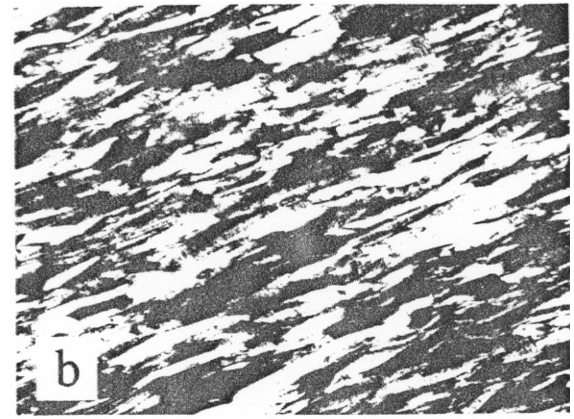
(Beyerlein, Lebensohn and Tome, LANL, 2003)

Case study - ECAE



Observed:
Equiaxed

Original

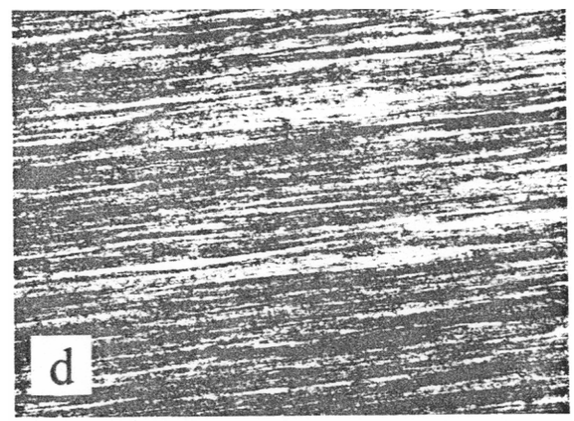


Observed:
~20º

1st pass

Observed:
~12º

2nd pass

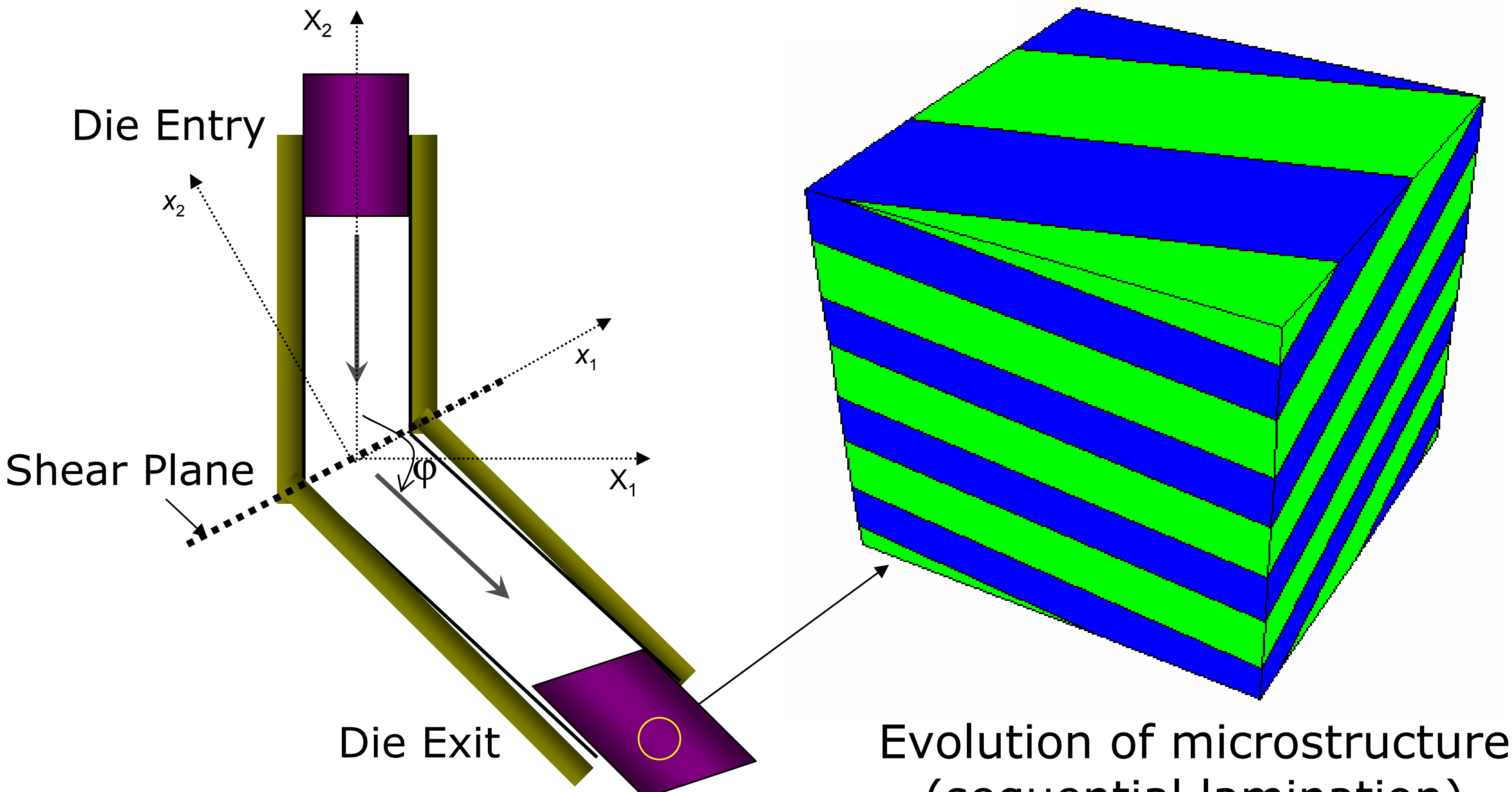


Observed:
~7º

3rd pass

(Beyerlein, Lebensohn and Tome, LANL, 2003)

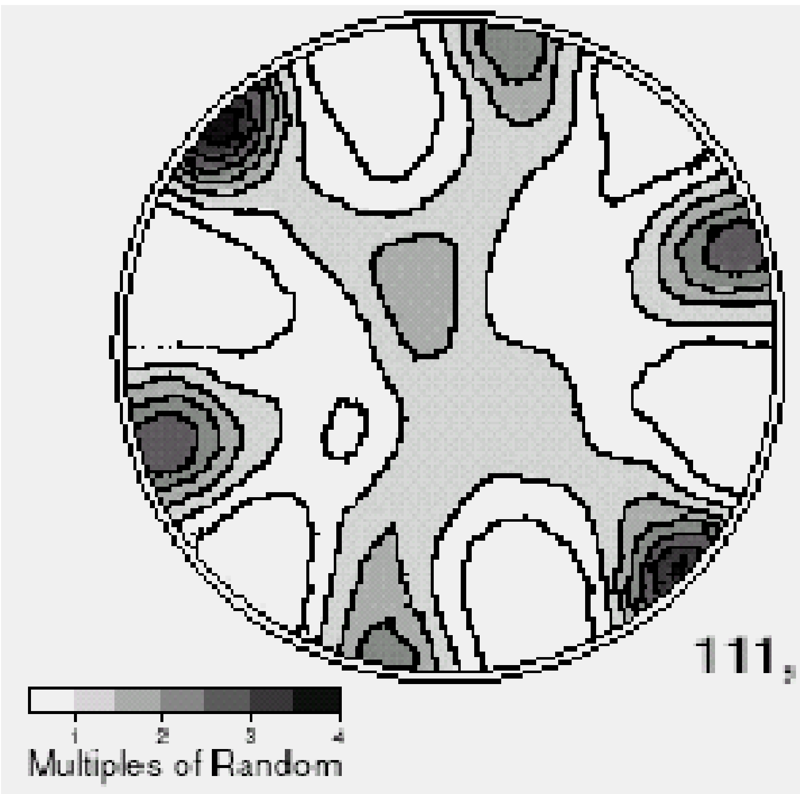
Case study - ECAE



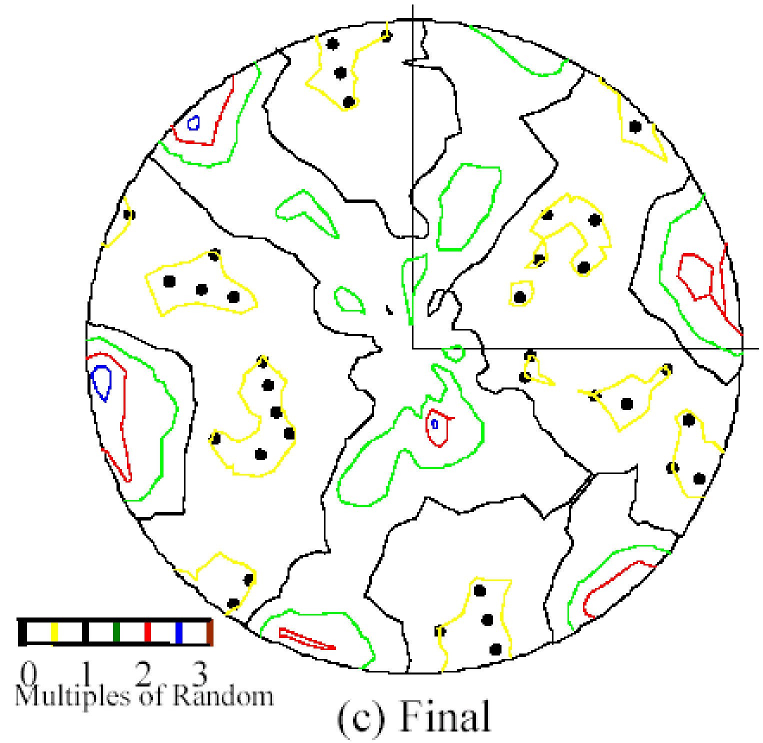
Evolution of microstructure
(sequential lamination)

(Sivakumar and Ortiz ´03)

Case study - ECAE



Experimental texture
(Vogel *et al.* ´03)



Computed texture
(Sivakumar and Ortiz ´03)

Michael Ortiz
ICIAM 07/03

Summary and conclusions

- The multiscale modeling paradigm provides a systematic means of eliminating empiricism and uncertainty from material models
- Present computing capacity is not sufficient to integrate entire multiscale hierarchies into large-scale engineering simulations
- There remains a need for subgrid models (as in other fields, e.g., turbulence)
- Inroads are being made in the application of calculus of variations to inelastic systems
- Many open questions remain (regularity of minimizers, convergence of incremental approach, relaxation of non-local functionals…)