Continuum Models of Dislocation Dynamics and Dislocation Structures

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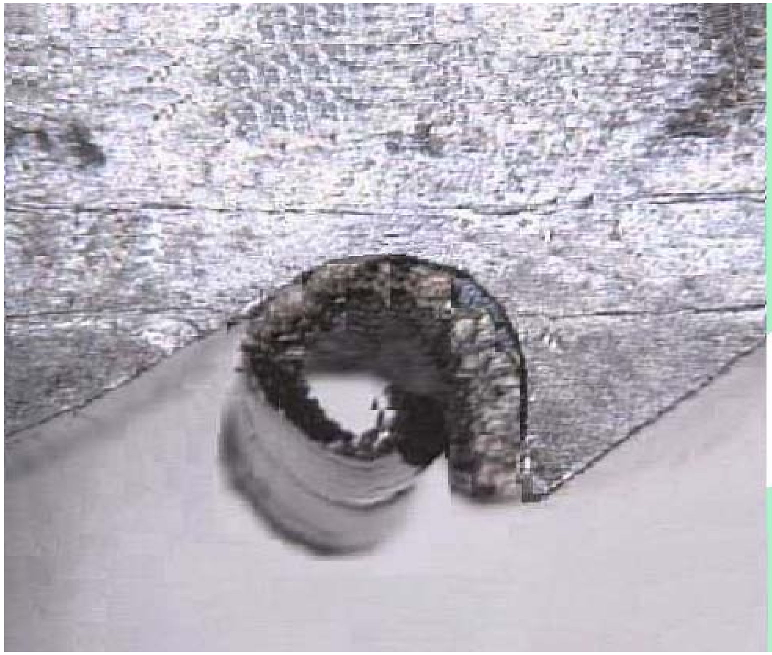
Outline

- The case for multiscale simulation
- The case for multiscale modeling
- The lengthscale hierarchy of polycrystalline metals
- The quasicontinuum method
- Phase-field dislocation dynamics
- Subgrid models of martensite
- Subgrid models of dislocation structures

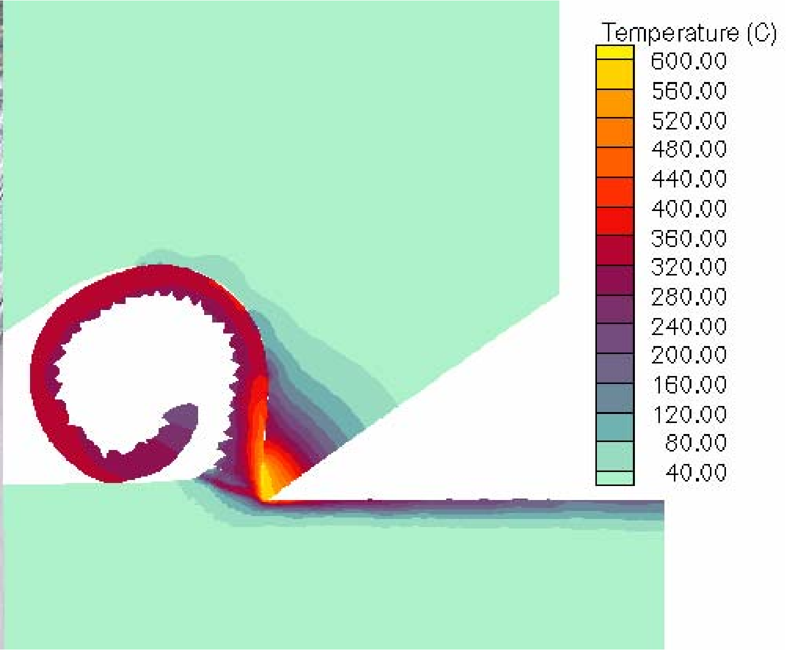
Machining – Experimental Validation

Chip Morphology Validation

(Courtesy of Third Wave Systems Inc)



(Courtesy of IWH, Switzerland)

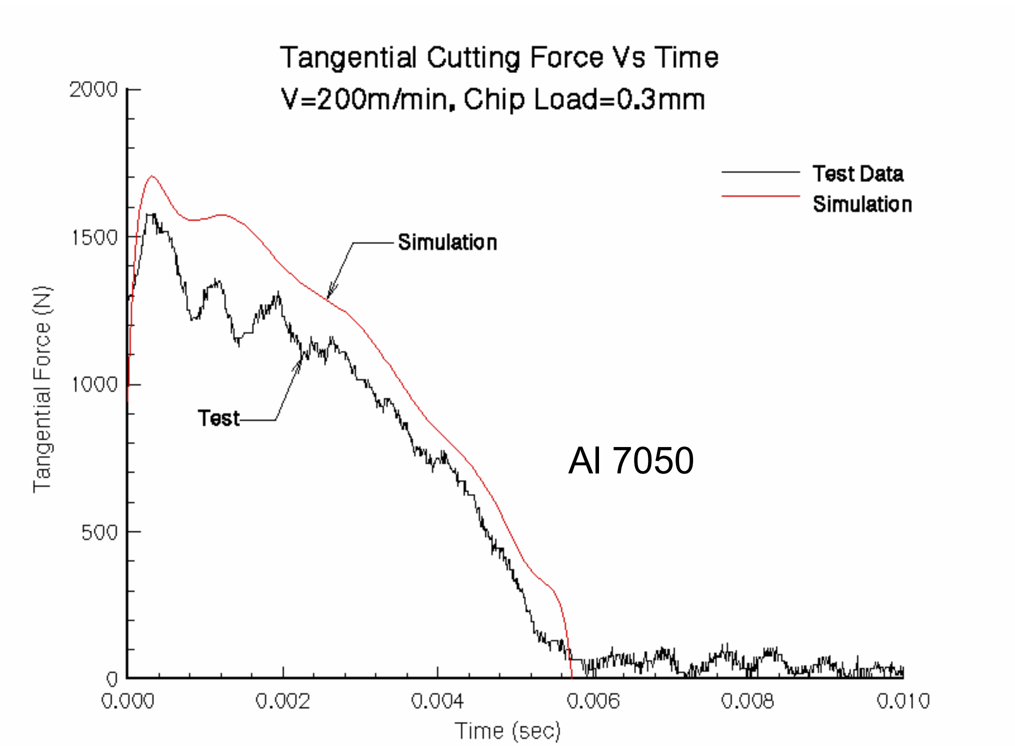


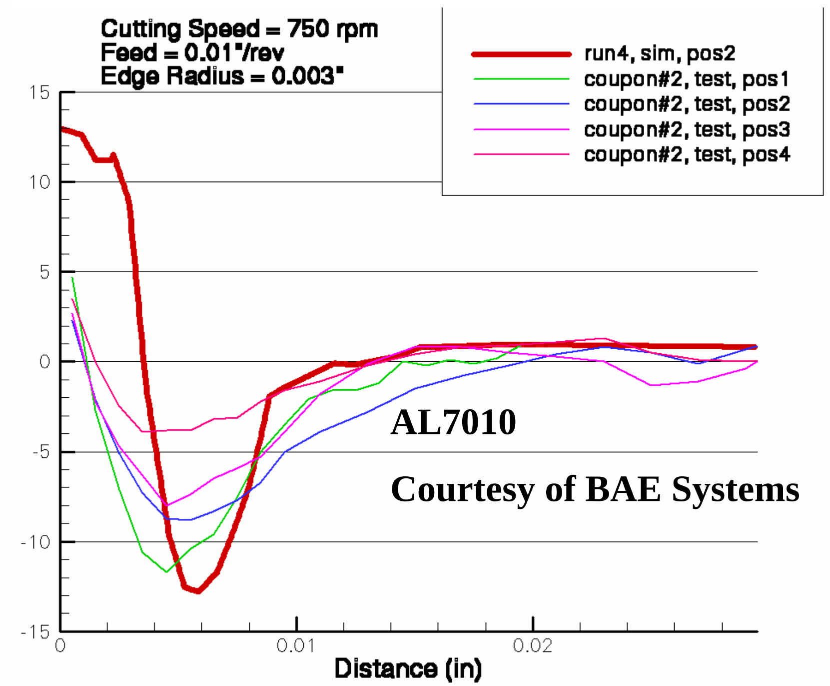
FE simulation

(Marusich and Ortiz, IJNME ´95)

Machining – Experimental Validation

(Courtesy of Third Wave Systems Inc)





Cutting Force Validation

Residual Stress Validation

- General trends predicted, but discrepancies remain!

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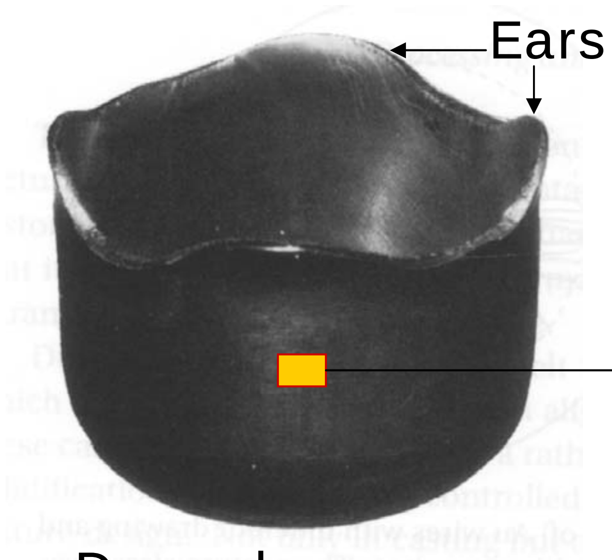
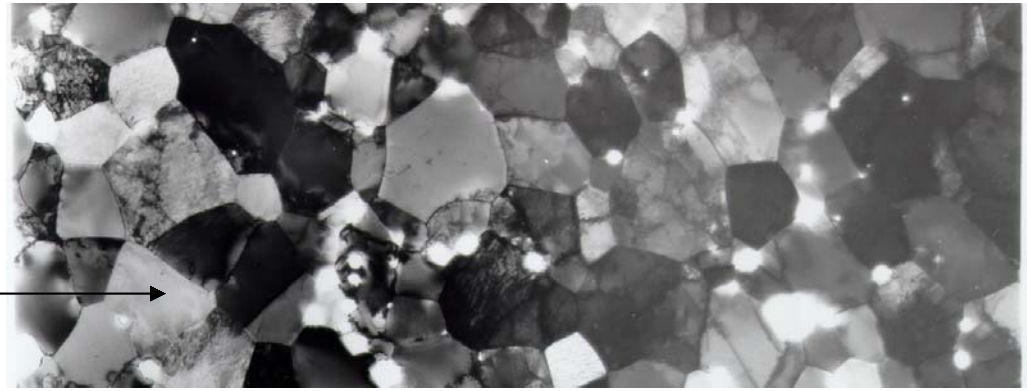
Validation and Verification

- Fidelity of simulation codes is critically limited by uncertainties in engineering (empirical) material models
- 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*
- Need to reduce uncertainty in engineering constitutive models for codes to be predictive!

Limitations of empirical models



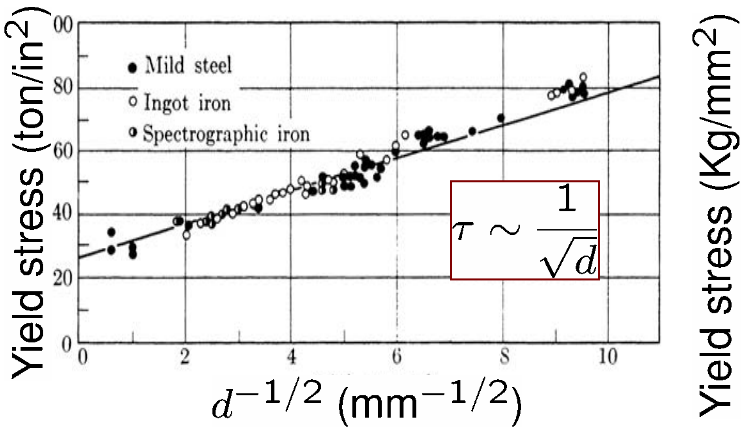
Deep-drawn cup



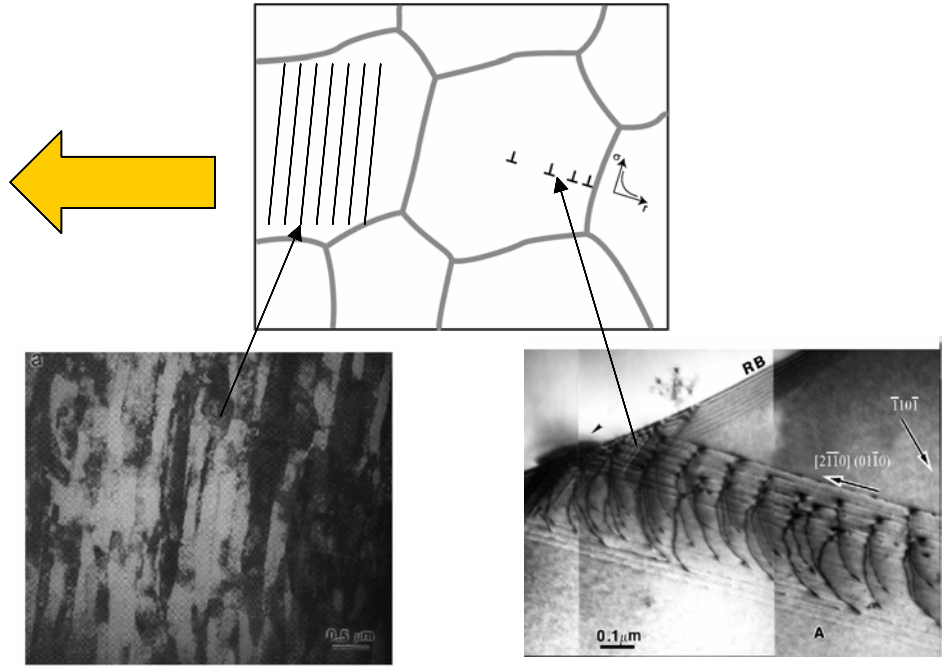
Grain structure of polycrystalline W
(Courtesy of Clyde Briant)

- 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.

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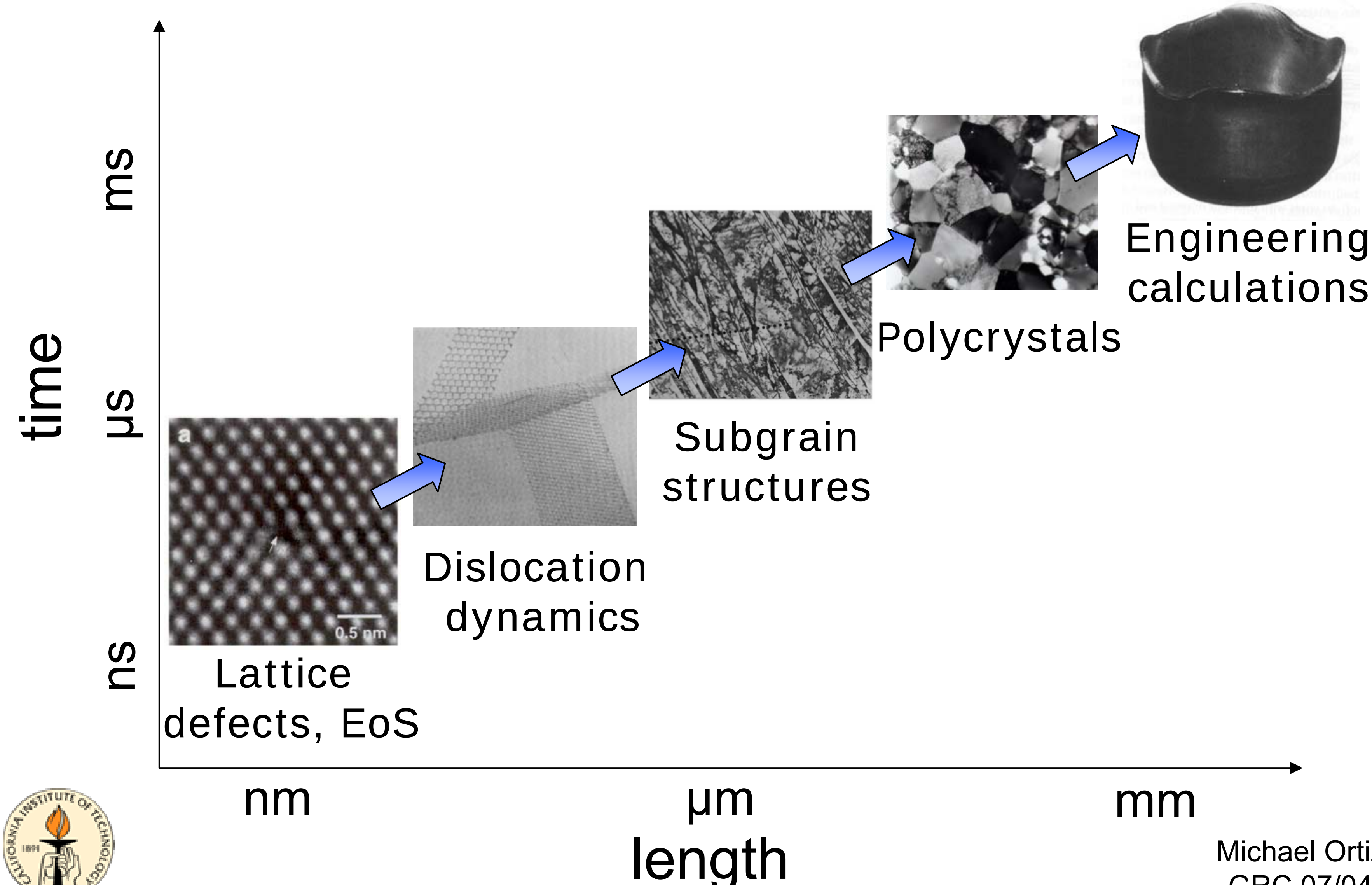
The case for multiscale computing

- 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, concurrent multiscale computing:
  - *Model physics at first-principles level, fine lengthscales*
  - *Compute on multiple lengthscales simultaneously*
  - *Fully resolve the fine scales*
- Bypasses the need to model at coarse lengthscales

Metal plasticity - Multiscale modeling



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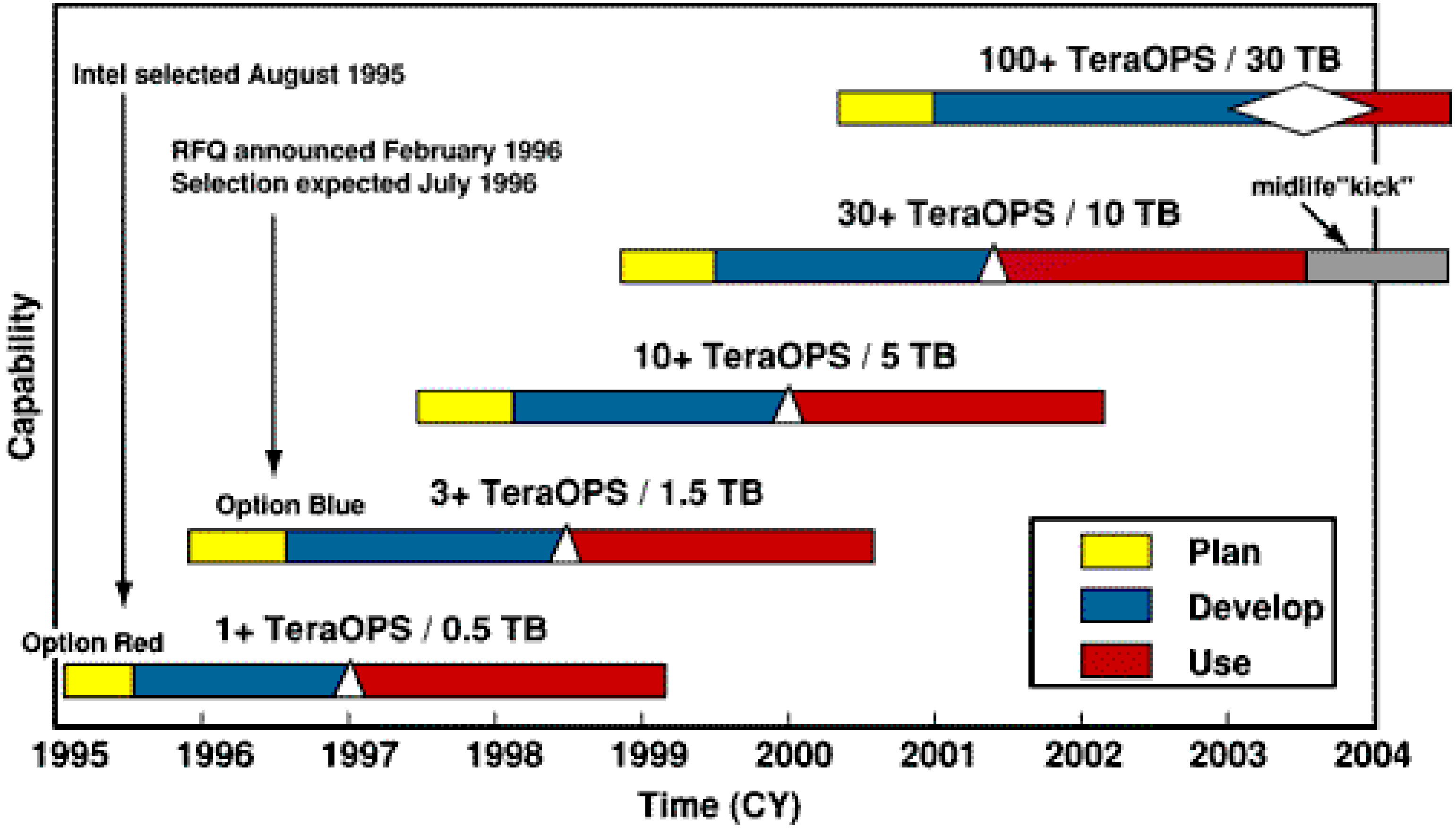
Multiscale computing - Feasibility

ASCI computing systems roadmap



- Computing power is growing rapidly, but...

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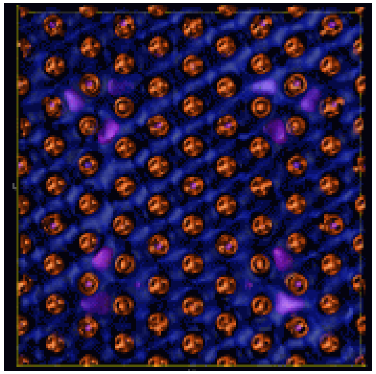
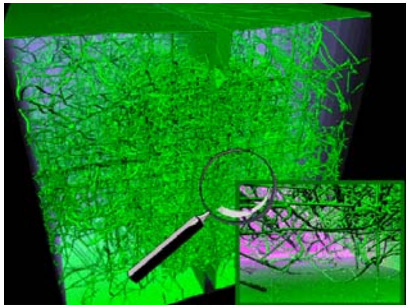
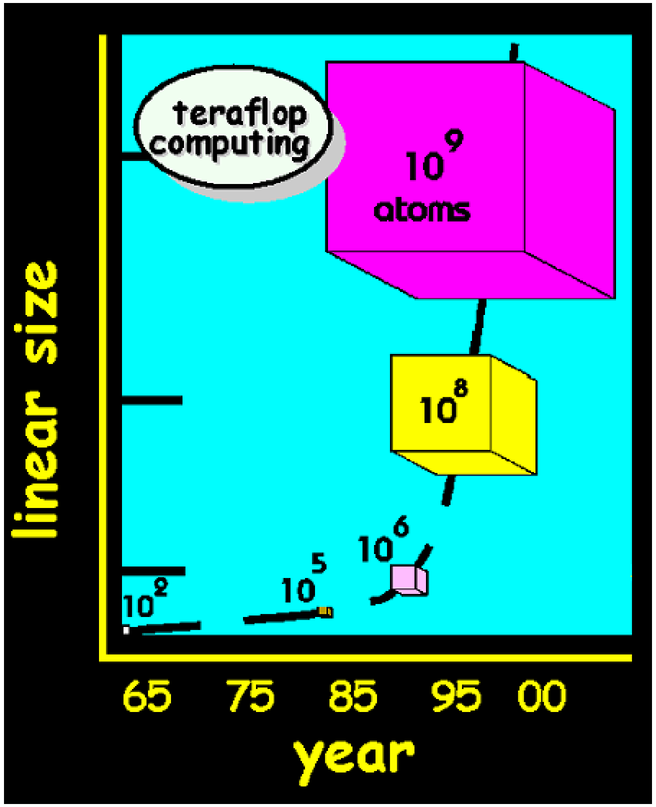
Multiscale computing – Feasibility



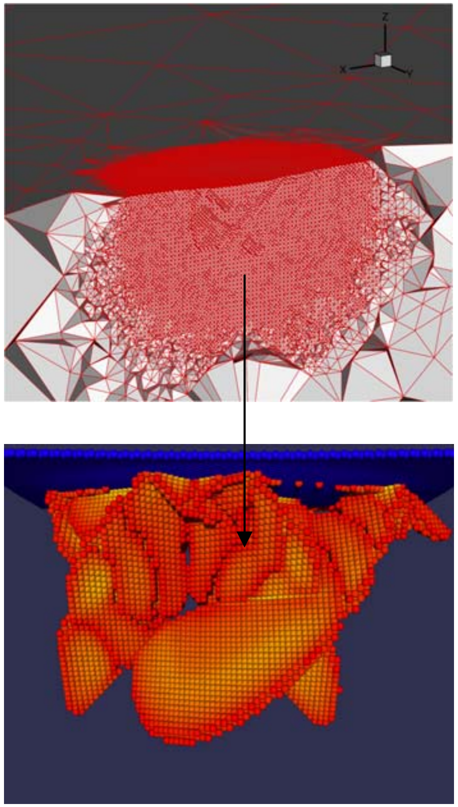
Ta quadrupole
(T. Arias ´00)



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



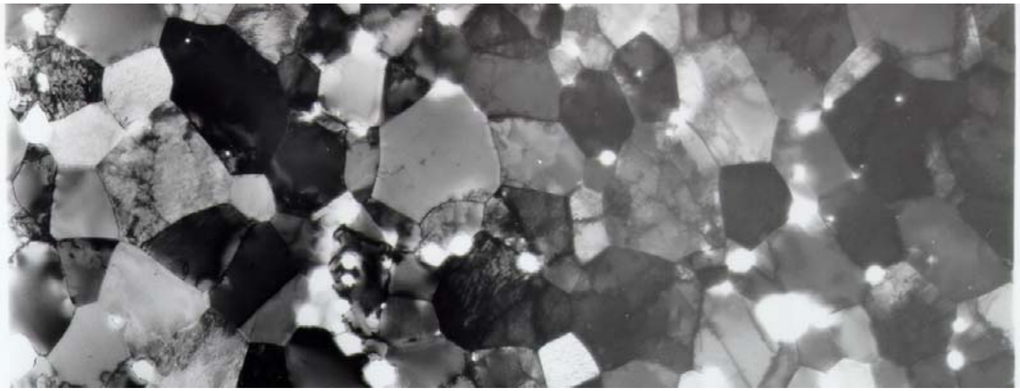
(Courtesy F.F. Abraham)



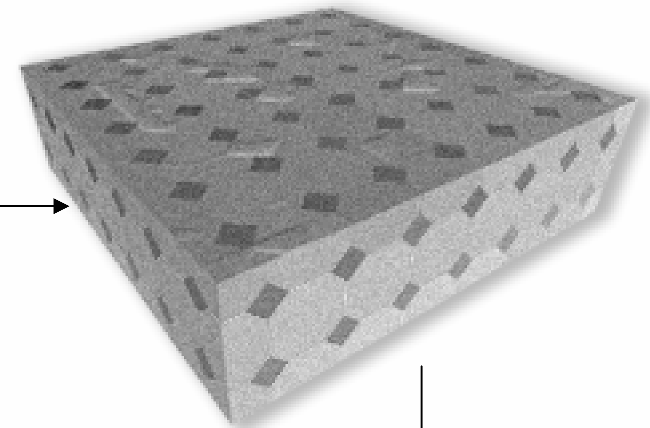
Au nanoindentation
(Knap and Ortiz ´03)

- Computing power is growing rapidly, but
  $10^9 << 10^{23}$

Multiscale computing – Feasibility

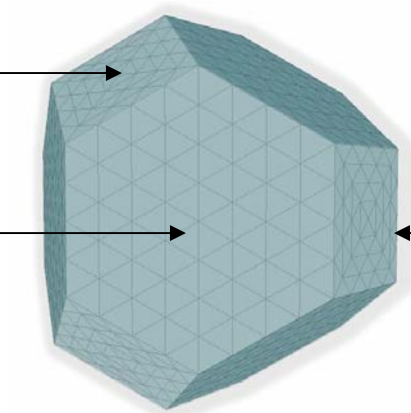


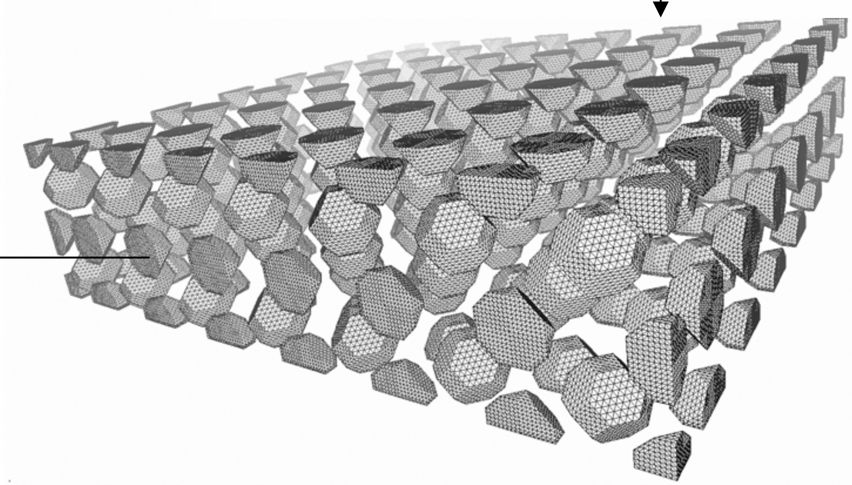
Polycrystalline W (Courtesy of C. Briant)



Grain-boundary sliding model

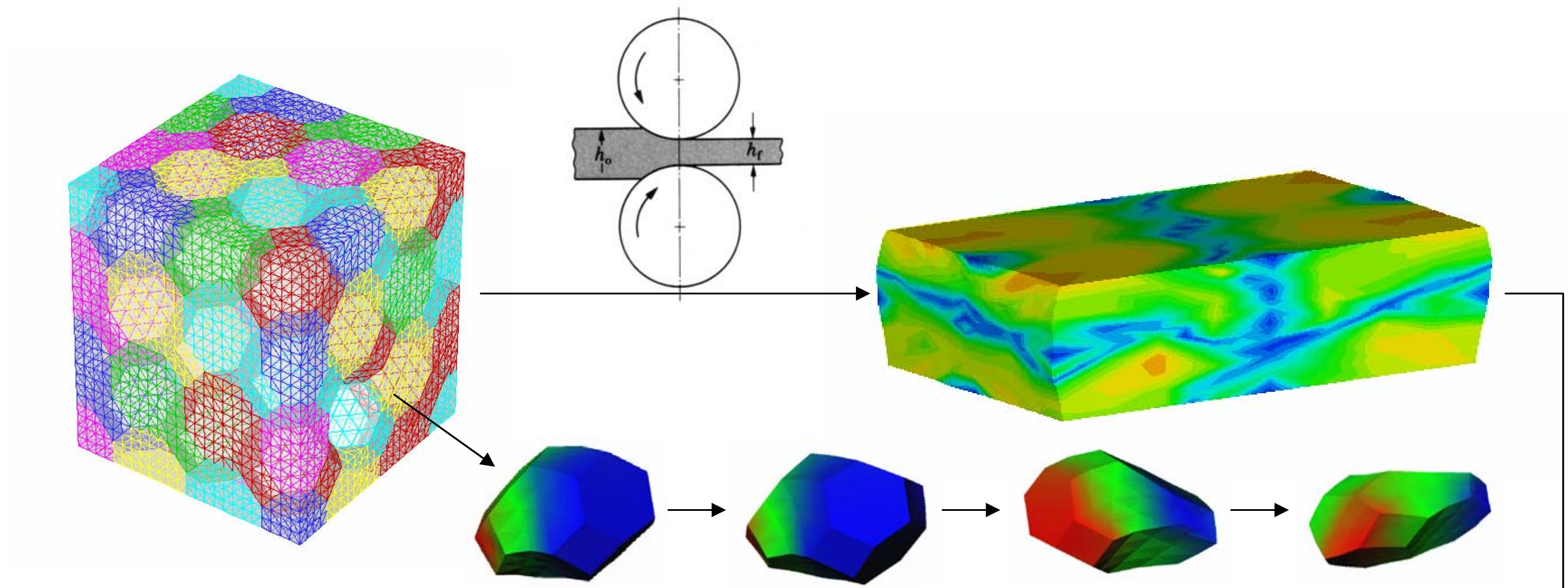
Single-crystal plasticity model





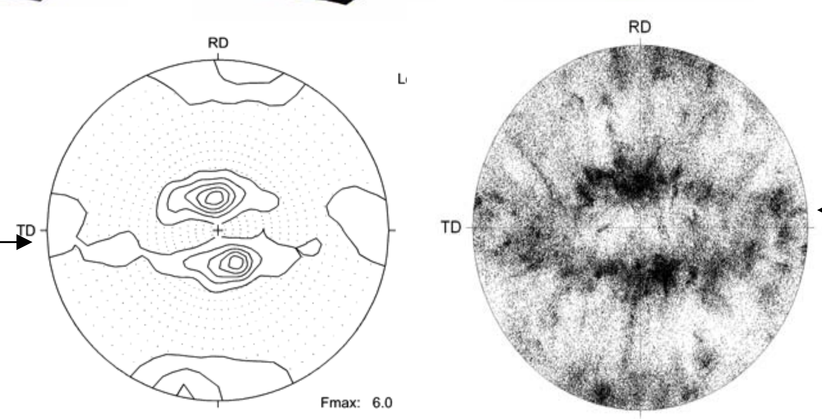
(A.M. Cuitiño and R. Radovitzky ´02)

Multiscale computing – Feasibility



Cold-rolled @ 42%
polycrystalline Ta

Experimental
cold-rolled texture

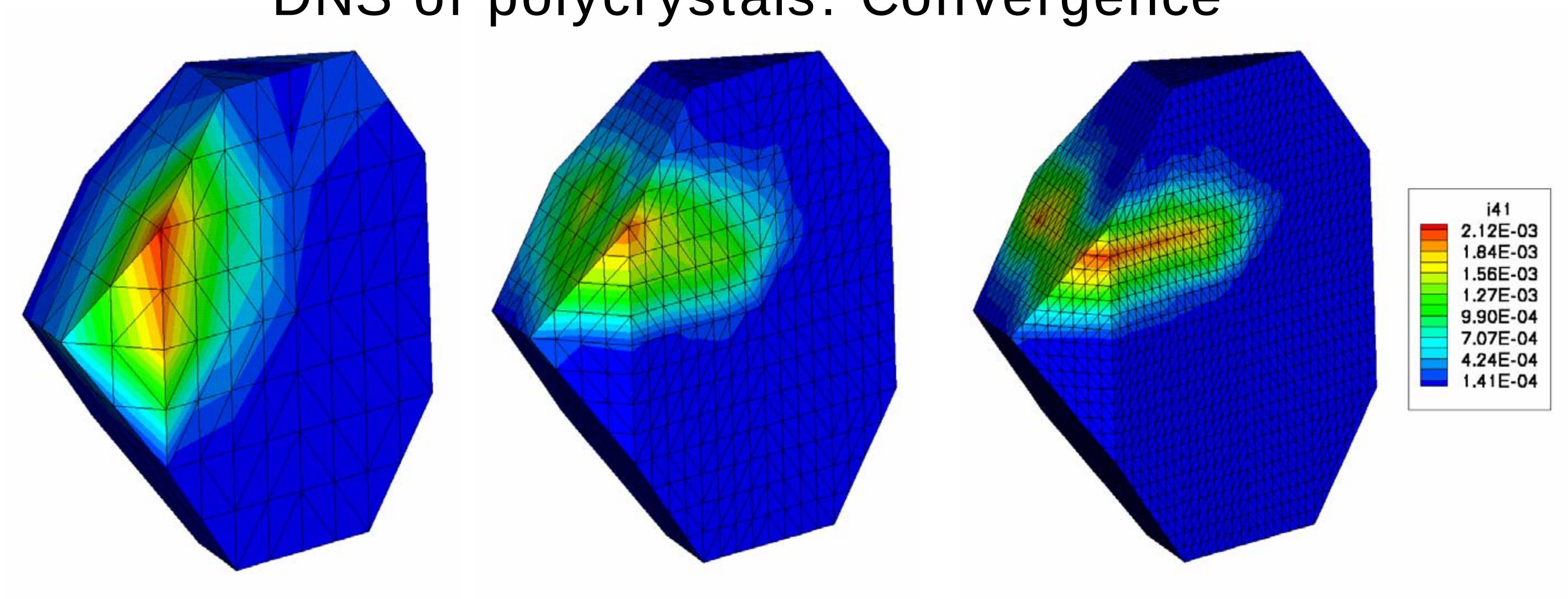


Pole
figure

(A.M. Cuitiño and R. Radovitzky ´03)

Multiscale computing – Feasibility

DNS of polycrystals: Convergence



Coarse mesh	Intermediate mesh	Fine mesh
192 elmts/grain	1536 elmts/grain	12288 el/grain

(A.M. Cuitiño and R. Radovitzky ´03)

- Numerical convergence extremely slow!

Multiscale computing - Feasibility

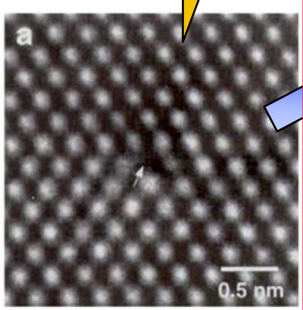
- ~ 10^9 elements at our disposal (10^6 elements/processor x 1000 processors)
- ~ 1000 elements/coordinate direction
- ~ 20 elements/grain/direction (8000 elements/grain)
- ~ 50 grains/direction (125K grains)
- ~ 2.5 mm specimen for 50 μm grains
- Not enough for complex engineering simulations!
- Subgrain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

Metal plasticity - Multiscale modeling

time

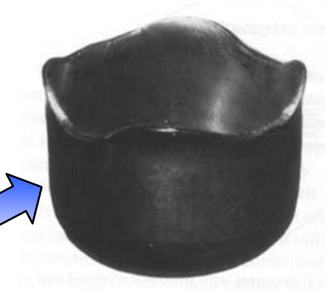
μs

ns



Lattice defects, EoS

s



Engineering calculations

Accessible to direct numerical simulation

nm

μm

length

mm

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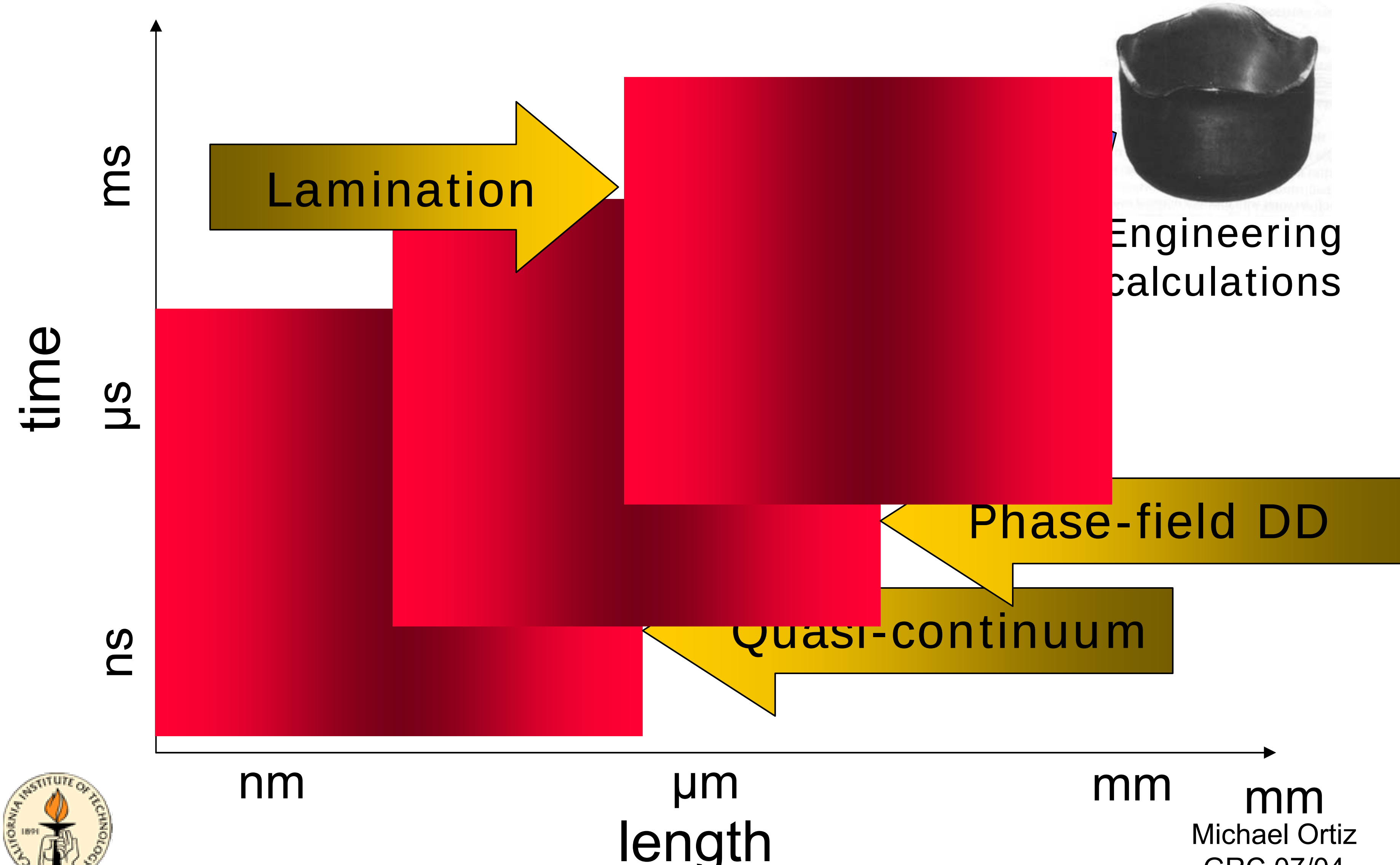
The case for multiscale modeling

- It is not possible to fully resolve material and deformation microstructures in complex engineering applications directly by brute force
- Instead, multiscale modeling:
  - *Identify relevant structures and mechanisms at all lengthscales*
  - *Bridge lengthscales by:*
    - *Building models of effective behavior (coarse graining)*
    - *Computing material parameters from first principles (parameter passing)*
- Approaches?

Multiscale modeling - Approaches



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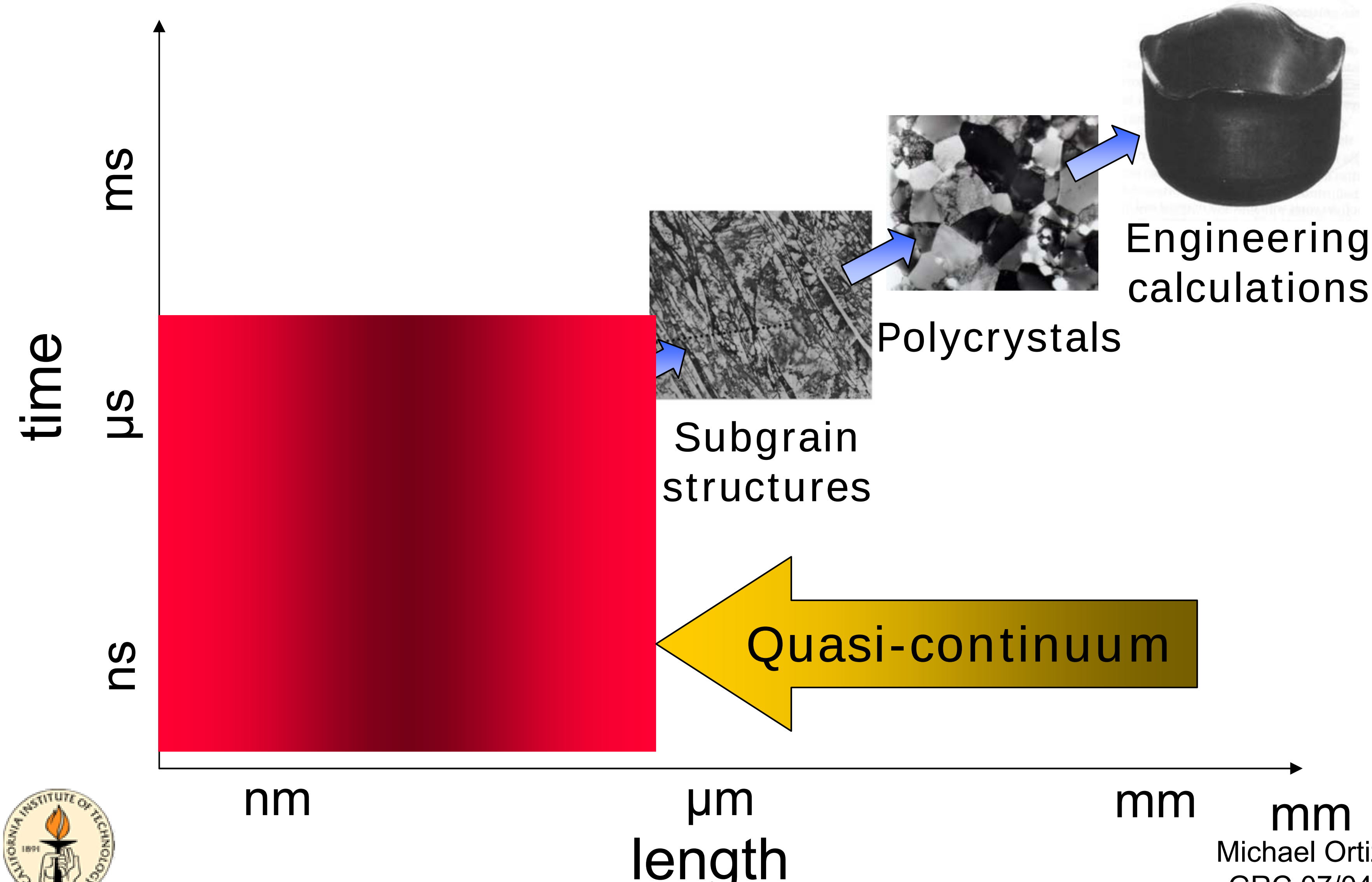
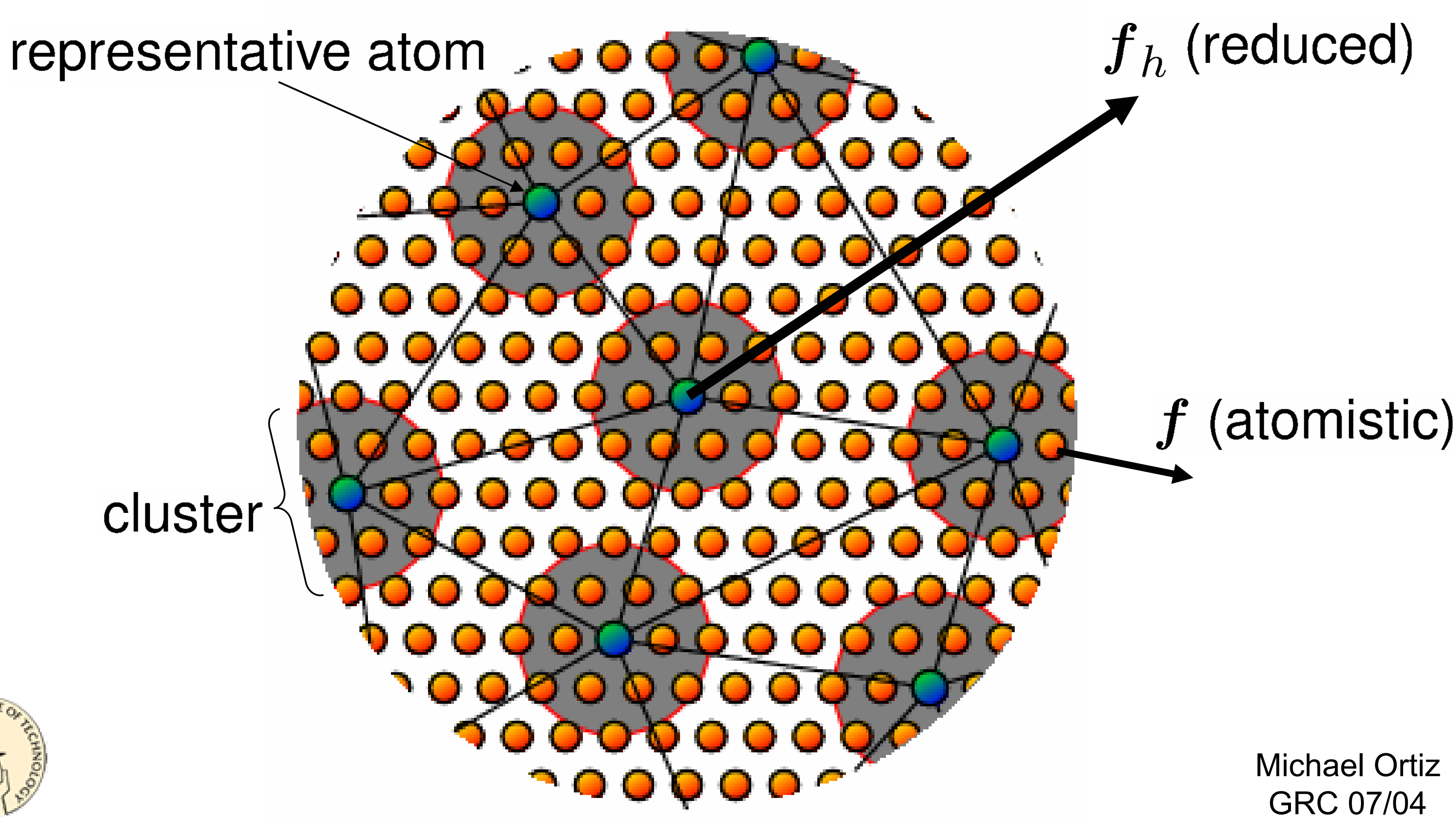
Multiscale modeling - Approaches



Quasicontinuum - Reduction

Tadmor, Ortiz and Phillips, *Phil. Mag. A*, **76** (1996) 1529.

Knap and Ortiz, *J. Mech. Phys. Solids*, **49** (2001) 1899.



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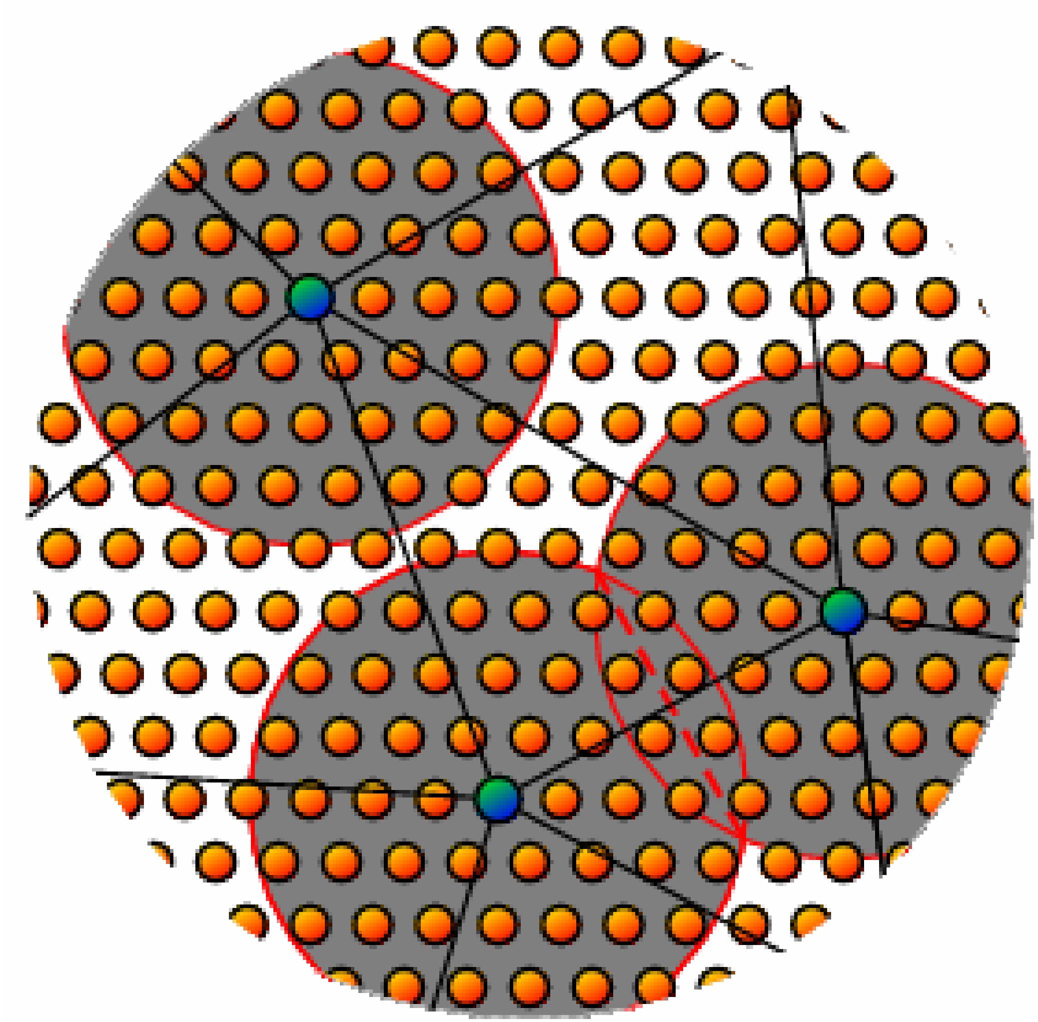
Quasicontinuum – Cluster sums



Merging of clusters near atomistic limit

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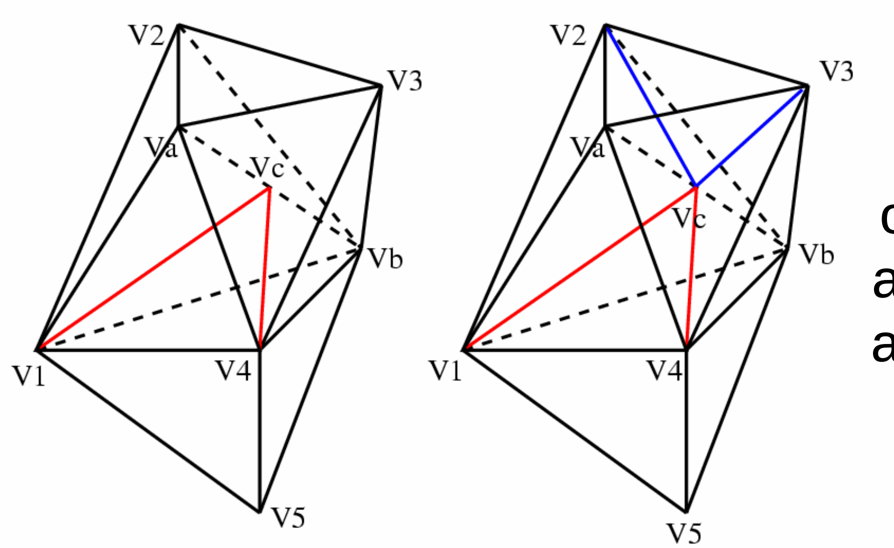
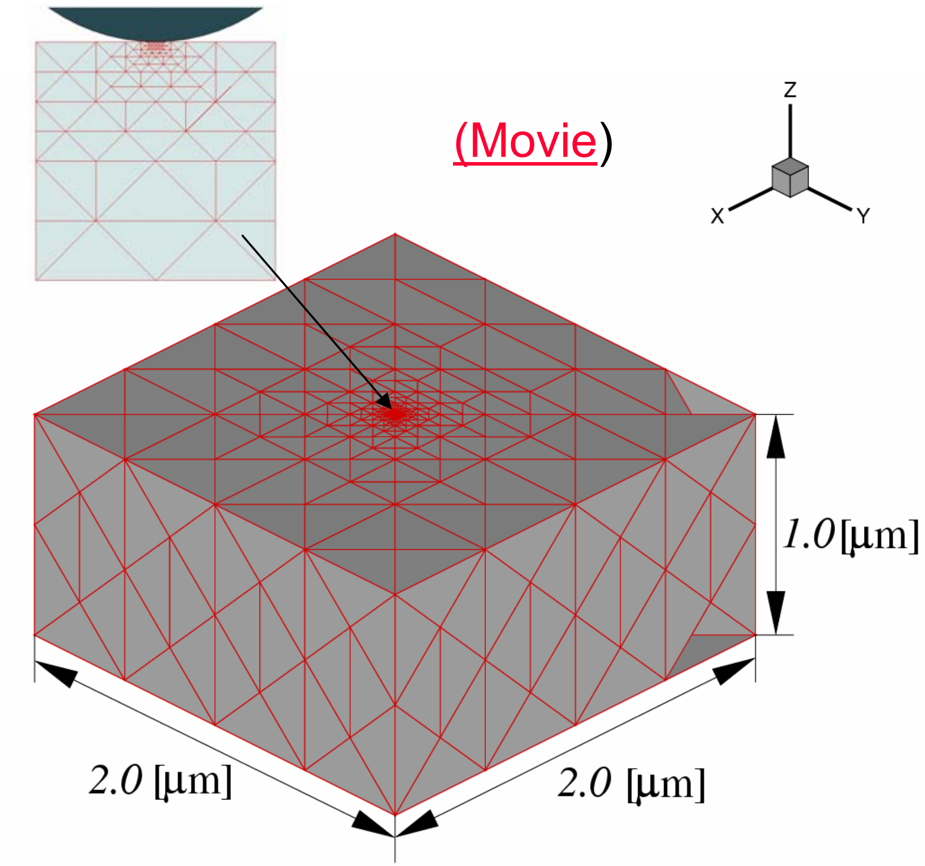
Quasicontinuum - Adaptivity

- $\boldsymbol{E}(K) \equiv$ Lagrangian strain in simplex K
- Refinement criterion: *Bisect* K if $|\boldsymbol{E}(K)| \geq \text{TOL}\dfrac{b}{h(K)}$



Longest-edge bisection of tetrahedron (1,4,a,b) along longest edge (a,b) and of ring of tetrahedra incident on (a,b)

QC - Nanoindentation of [001] Au

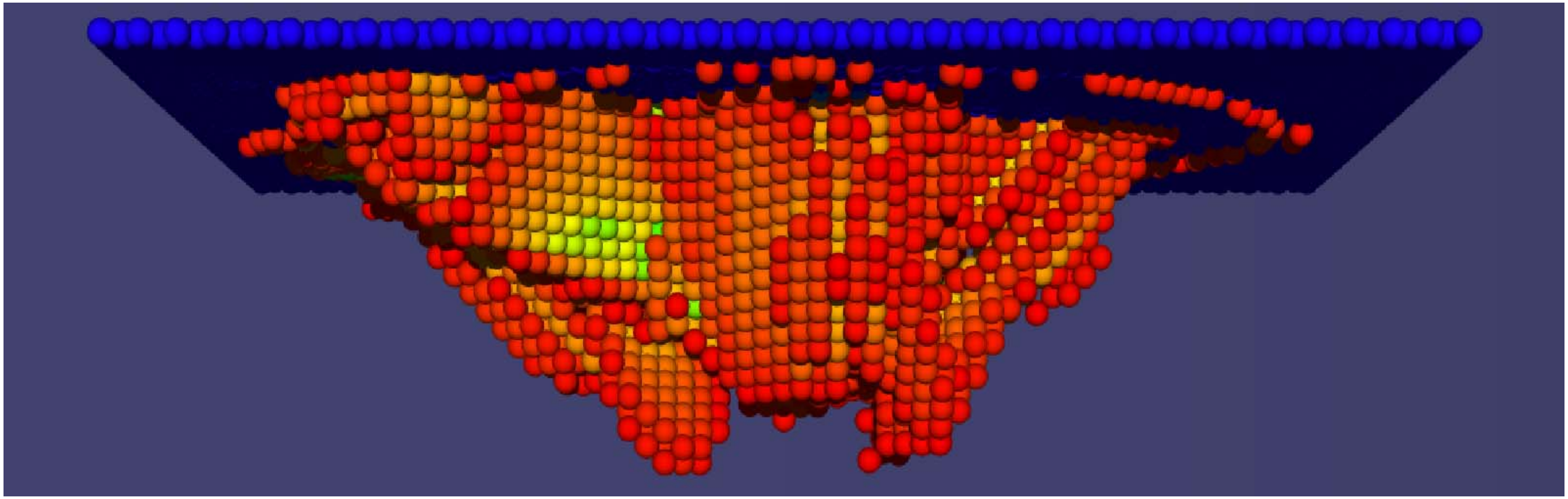


- Nanoindentation of [001] Au, 2x2x1 micrometers
- Spherical indenter, R=7 and 70 nm
- Johnson EAM potential
- Total number of atoms ~ 0.25 10^12
- Initial number of nodes ~ 10,000
- Final number of nodes ~ 100,000

Detail of initial computational mesh

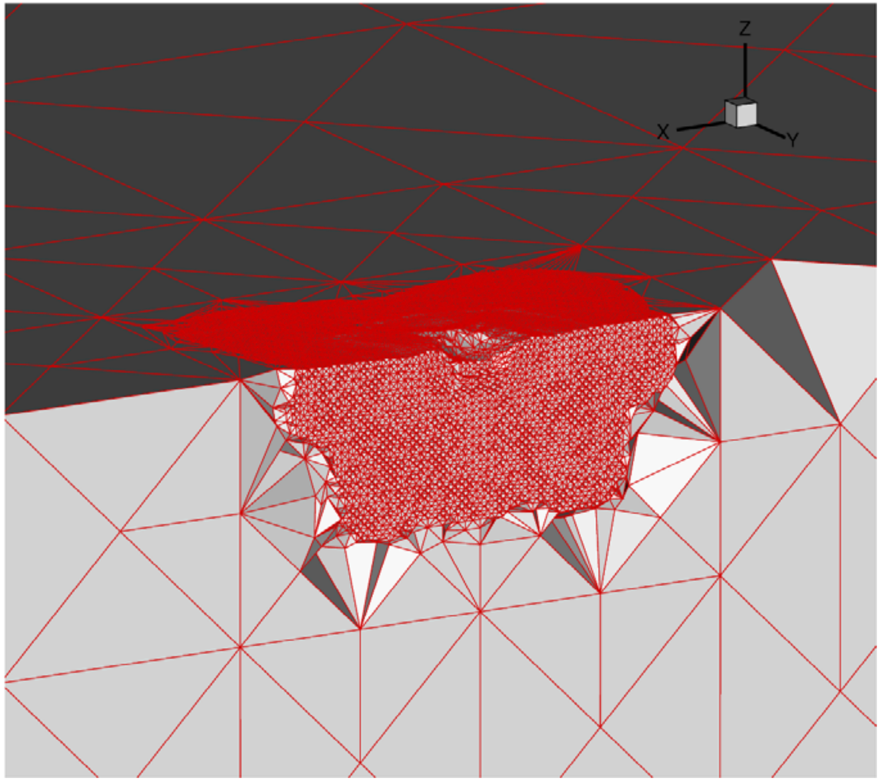
(Knap and Ortiz, *PRL* **90** 2002-226102)

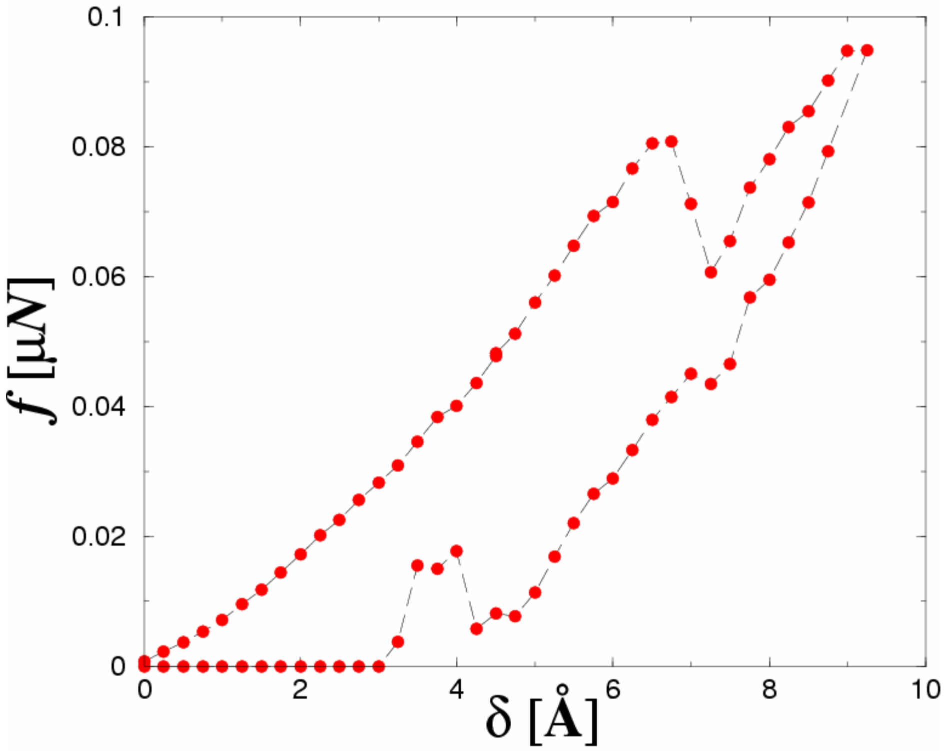
QC - Nanoindentation of [001] Au



7 nm indenter, depth = 0.92 nm

QC - Nanoindentation of [001] Au





7 nm indenter, depth = 0.92 nm

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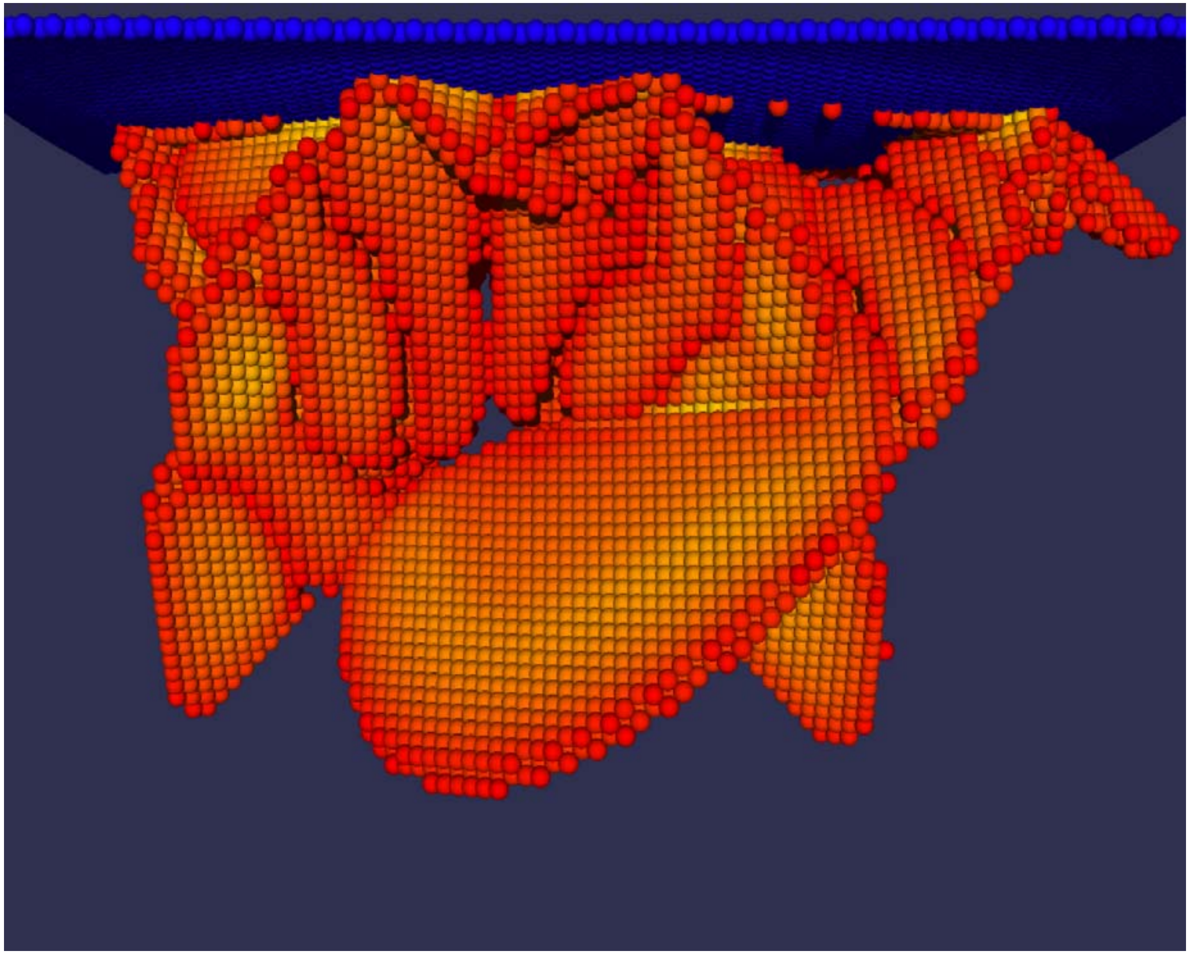
QC - Nanoindentation of [001] Au



70 nm indenter, depth = 0.75 nm

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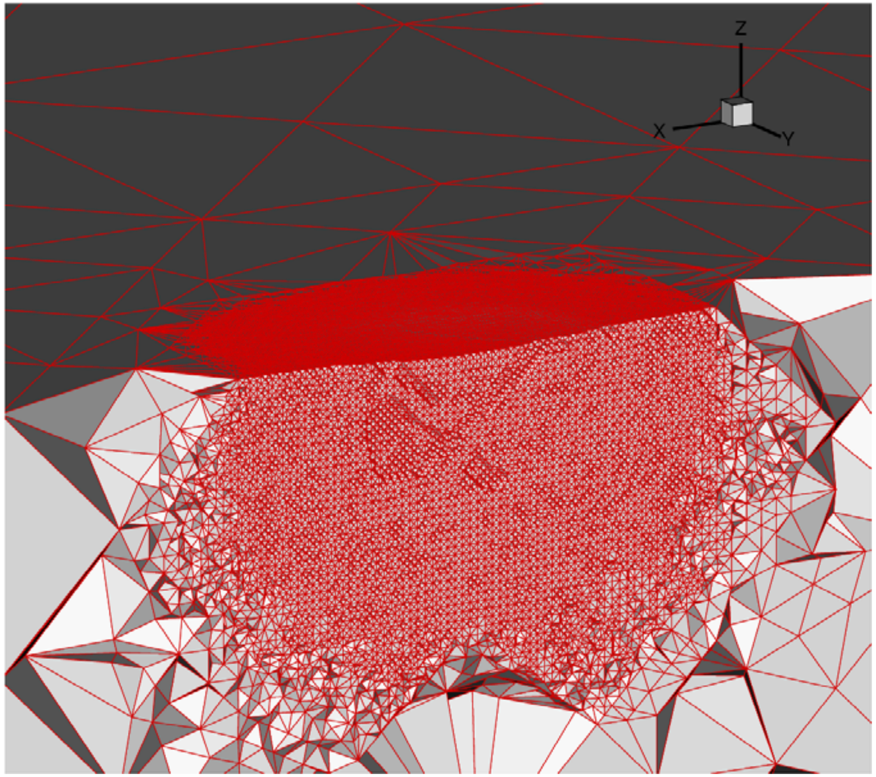
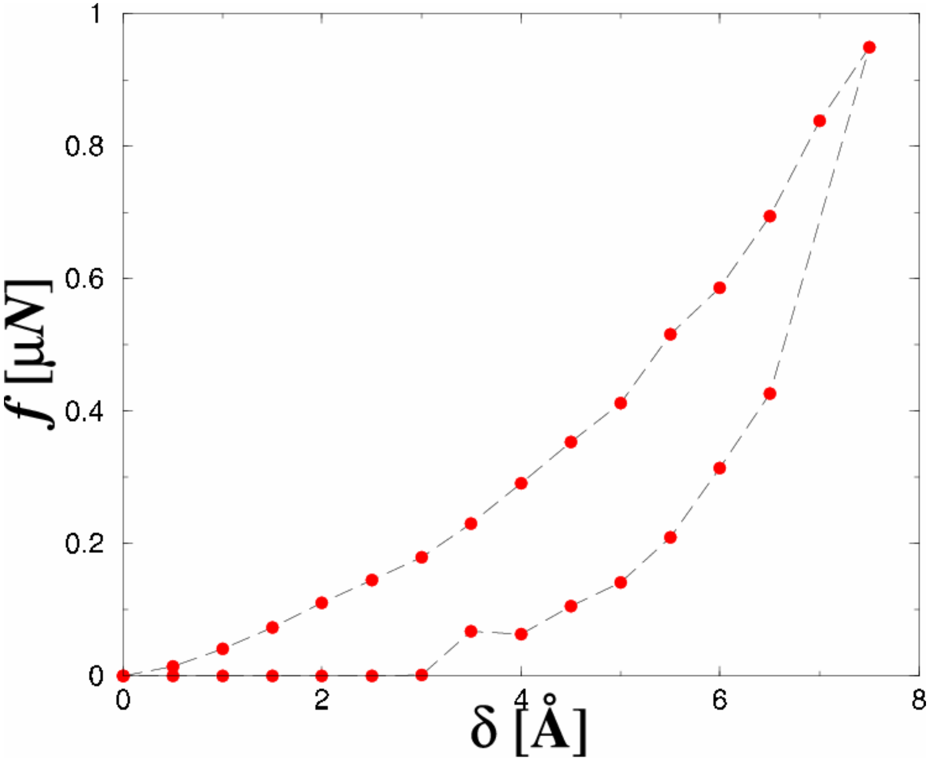
QC - Nanoindentation of [001] Au





70 nm indenter, depth = 0.75 nm

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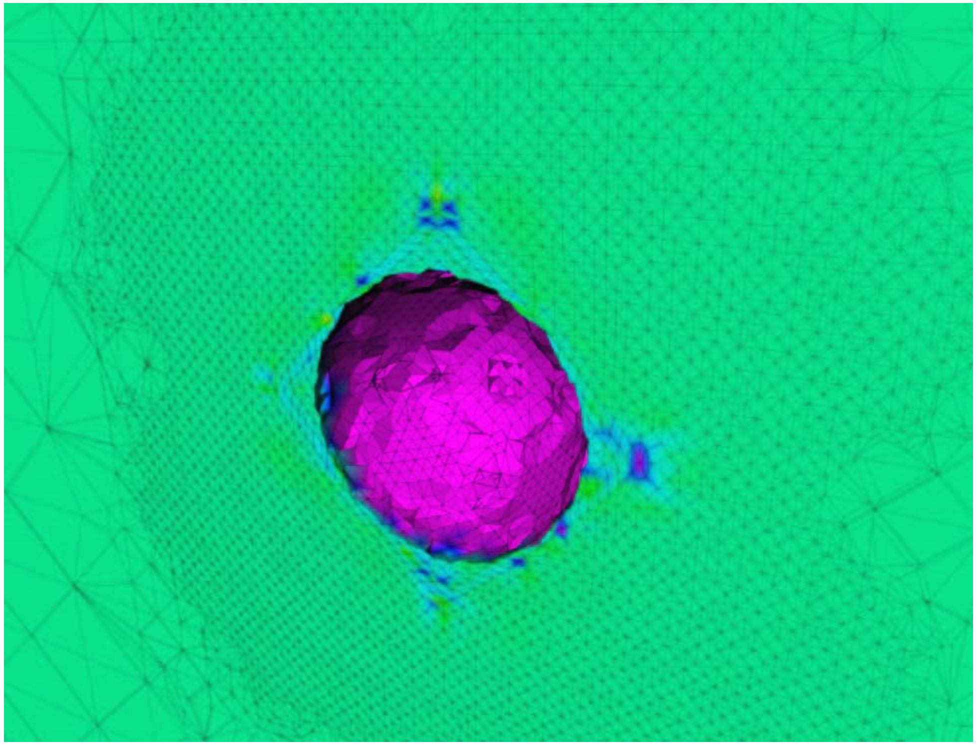
QC - Nanovoid cavitation in Al

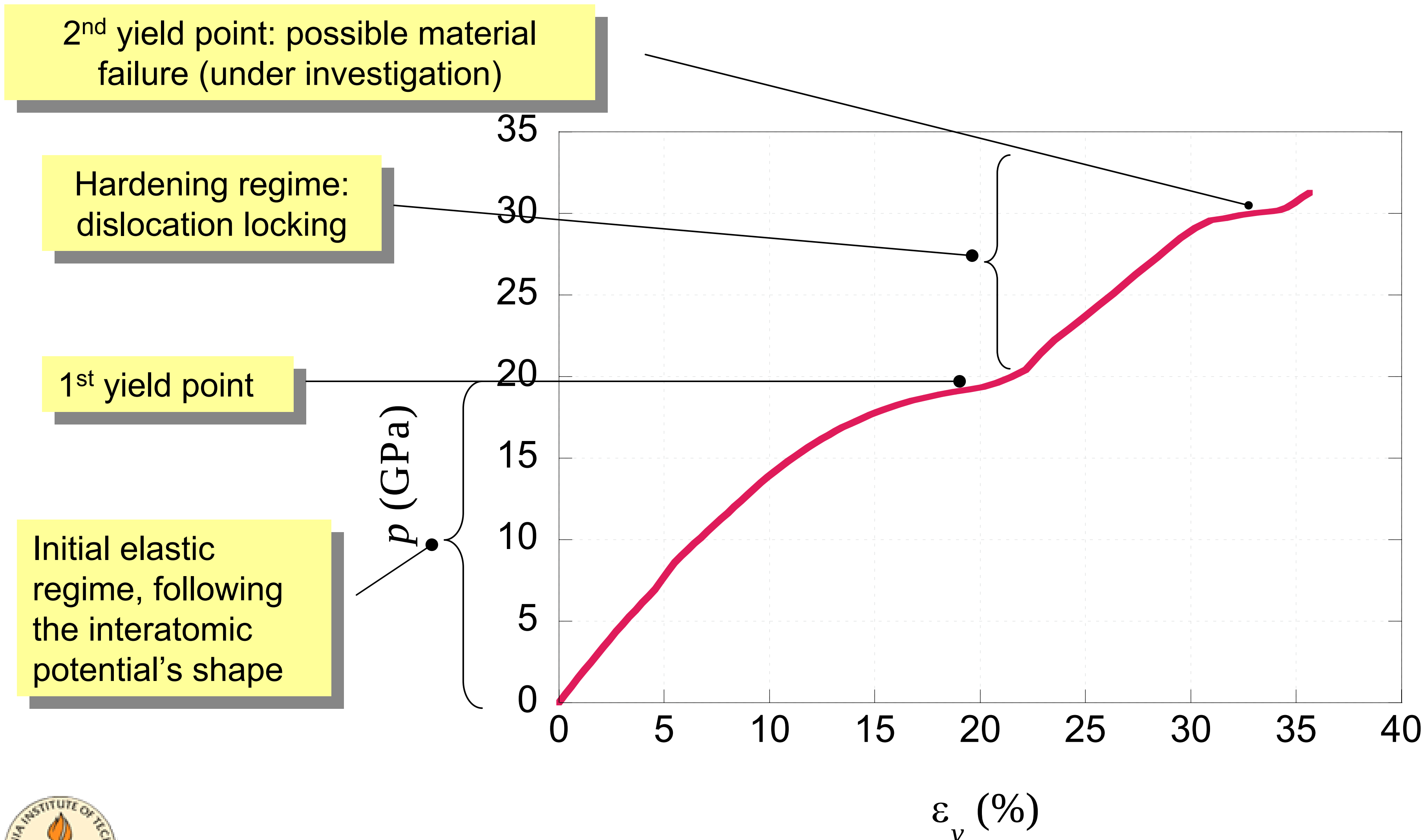


Close-up of internal void

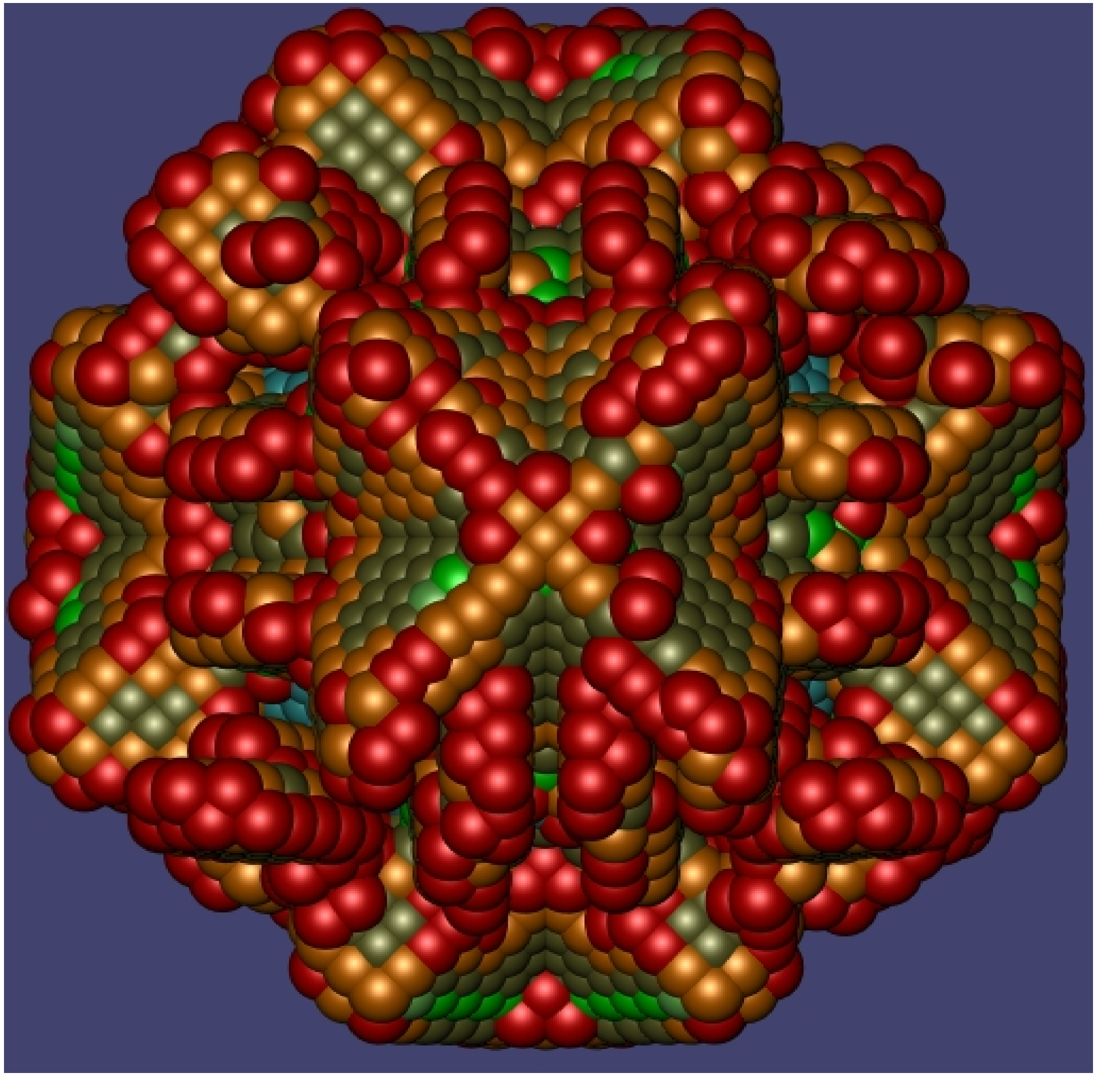
- 72x72x72 cell sample
- Initial radius R=2a
- Ercolessi and Adams (*Europhys. Lett.* **26**, 583, 1994) EAM potential.
- Total number of atoms ~16×10^6
- Initial number of nodes ~ 34,000

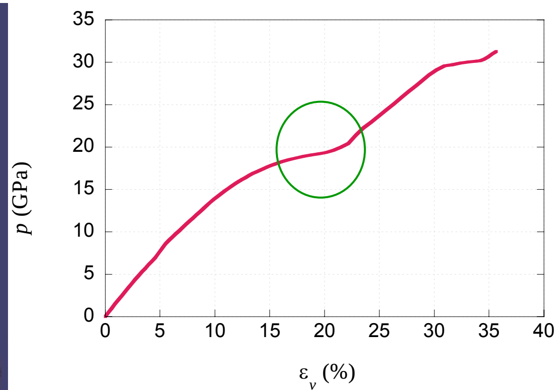
(Marian, Knap and Ortiz ´04)

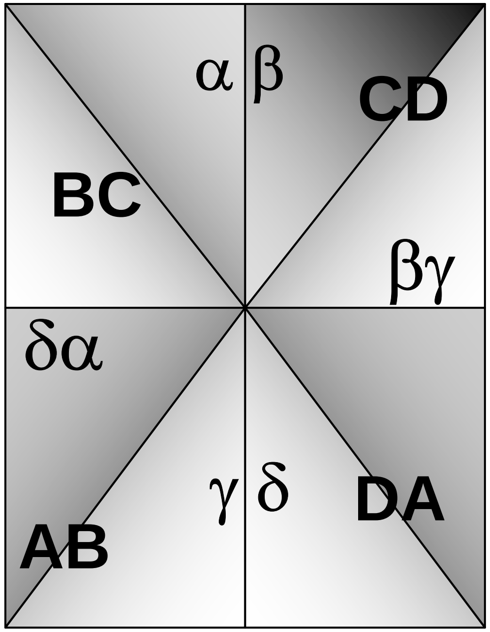
QC - Nanovoid cavitation in Al



QC - Nanovoid cavitation in Al







Dislocation structures, first yield point

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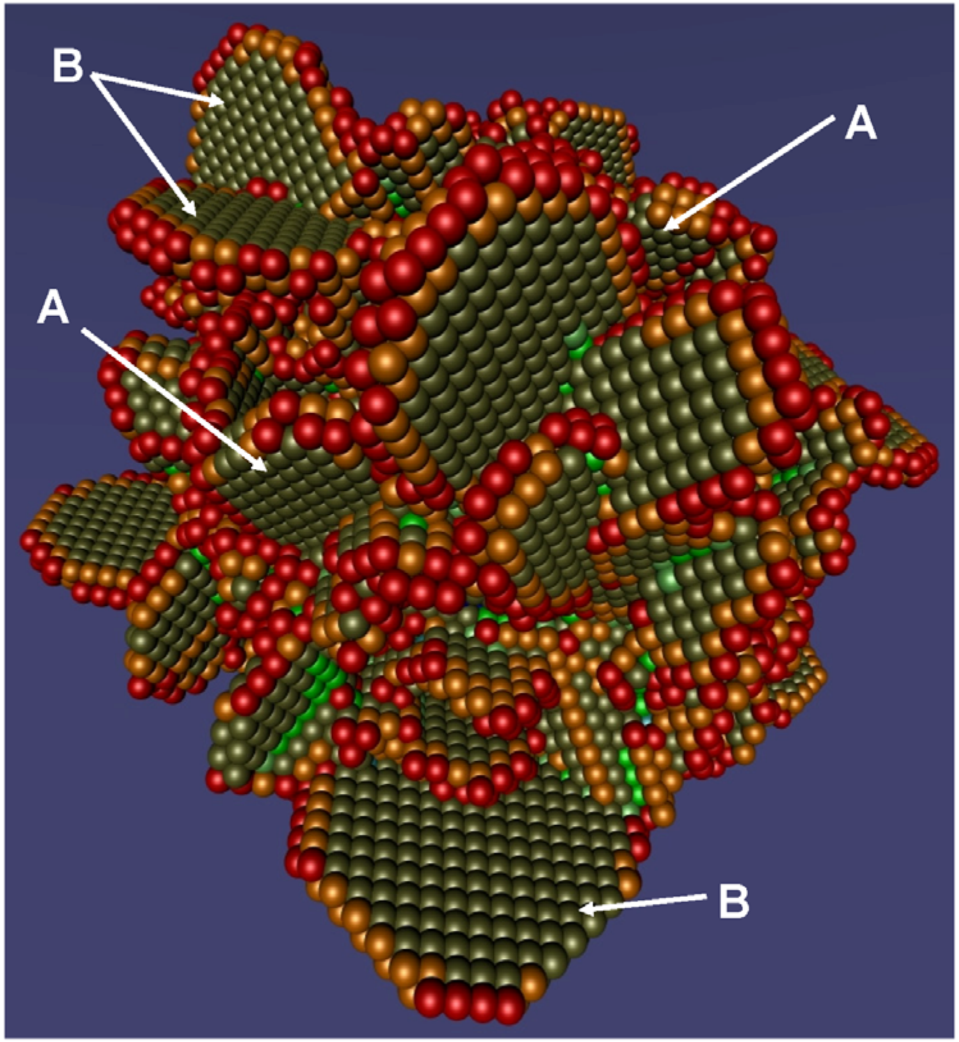
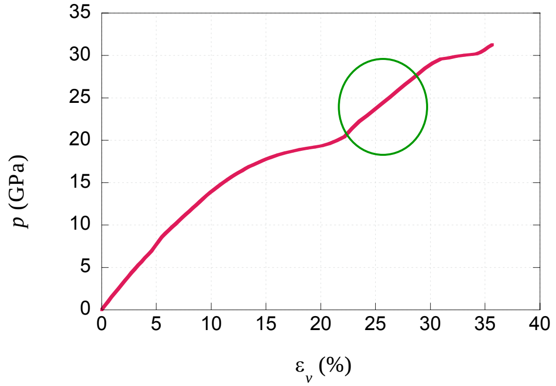
QC - Nanovoid cavitation in Al





Dislocation types:

A - *Conventional*
½⟨110⟩{111}

B - *Anomalous*
½⟨110⟩{001}

Dislocation structures, hardening stage

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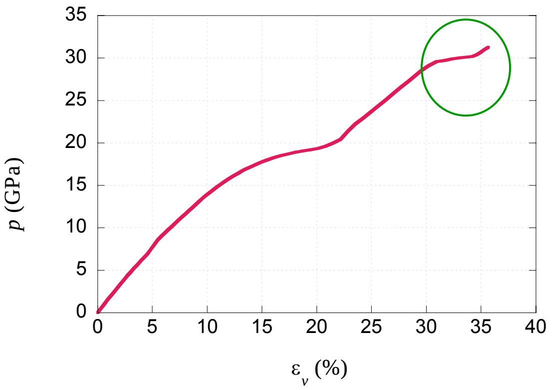
QC - Nanovoid cavitation in Al



Unconfined plastic flow carried by *conventional* ½⟨110⟩{111}

dislocations

Dislocation structures, second yield point

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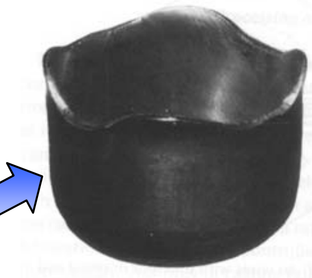
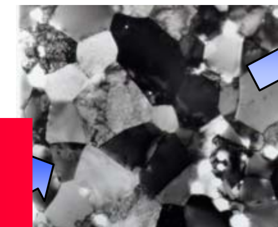
Quasicontinuum

- The Quasicontinuum method is an example of a multiscale method based on:
  - *Kinematic constraints (coarse-graining)*
  - *Clusters (sampling)*
  - *Adaptivity (spatially adapted resolution)*
- The Quasicontinuum method is an example of a *concurrent multiscale computing*: it resolves continuum and atomistic lengthscales concurrently during same calculation
- Challenges:
  - *Dynamics (internal reflections)*
  - *Finite temperature (heat conduction)*
  - *Transition to dislocation dynamics*

Multiscale modeling - Approaches

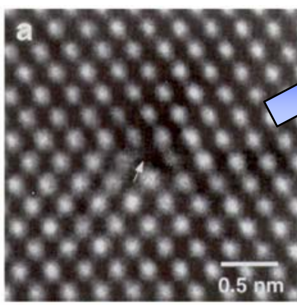


Engineering calculations



Polycrystals

Phase-field DD



Lattice defects, EoS

time: ns, μs, ms

length: nm, μm, mm, mm

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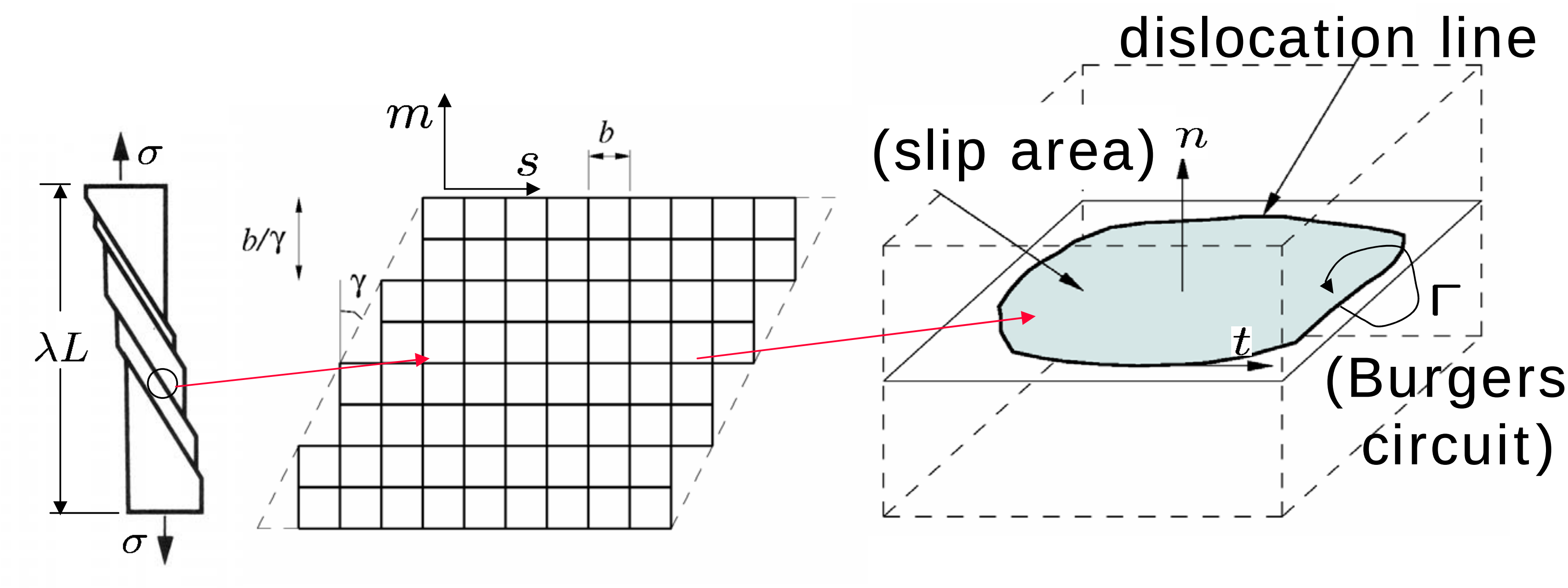
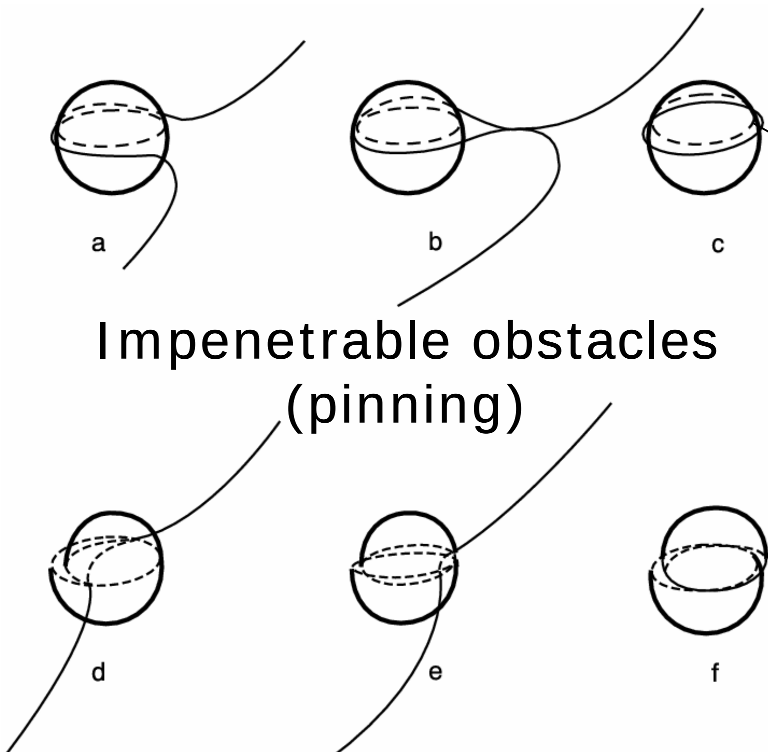
Phase-field dislocation dynamics



- Irreversible accommodation of shear deformation by crystallographic slip
- Volterra dislocation: $[\![u]\!] = b,$ on slip area

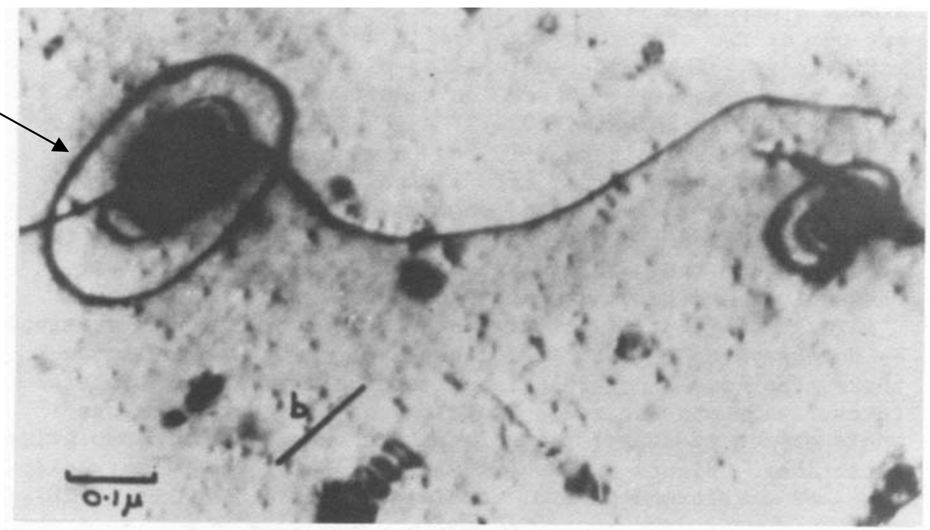
Phase-field dislocation dynamics

- Interaction with short-range obstacles:



Impenetrable obstacles
(pinning)

Obstacles of finite strength
(dissipative interaction)



(Humphreys and Hirsch '70)

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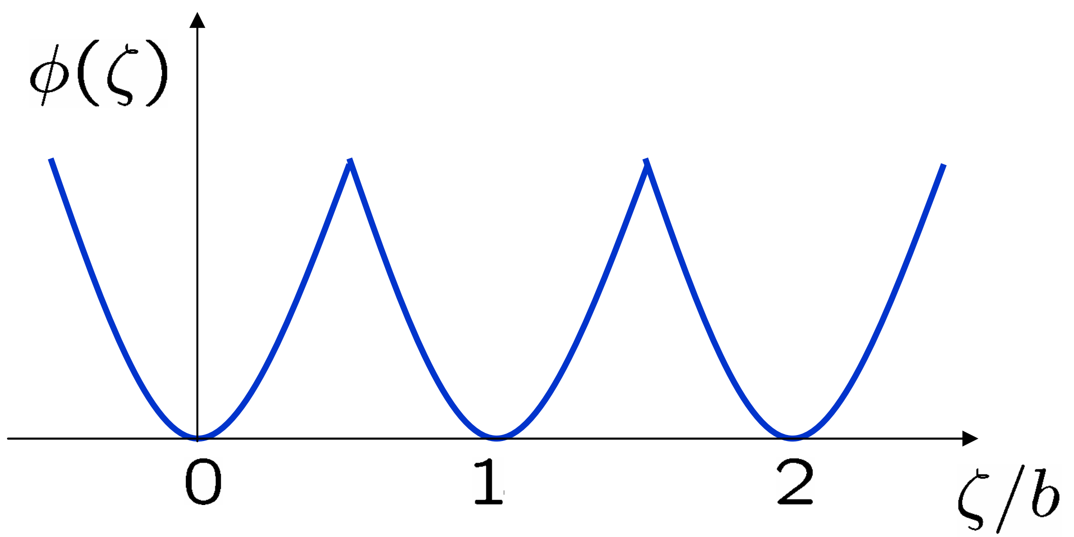
Phase-field dislocation dynamics

(Koslowski, Cuitiño and Ortiz, JMPS '02)

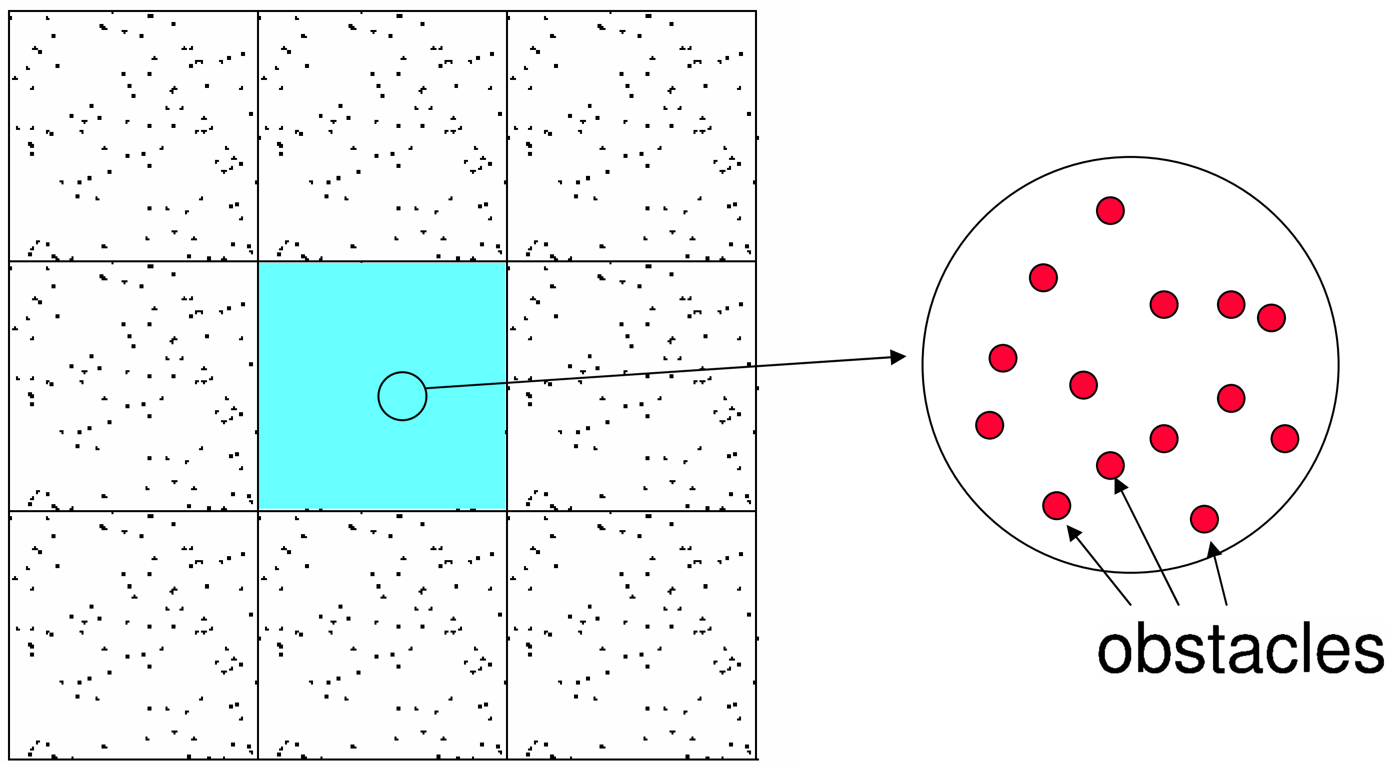
- Assumption: The energy is of the form

$$E(u) = \underbrace{\int \frac{1}{2} c_{ijkl} u_{i,j} u_{k,l} dx}_{\text{Elastic energy}} + \underbrace{\int_S \phi([\![u]\!]) dS}_{\text{Peierls energy}}$$

- Piecewise-quadratic Peierls potential:

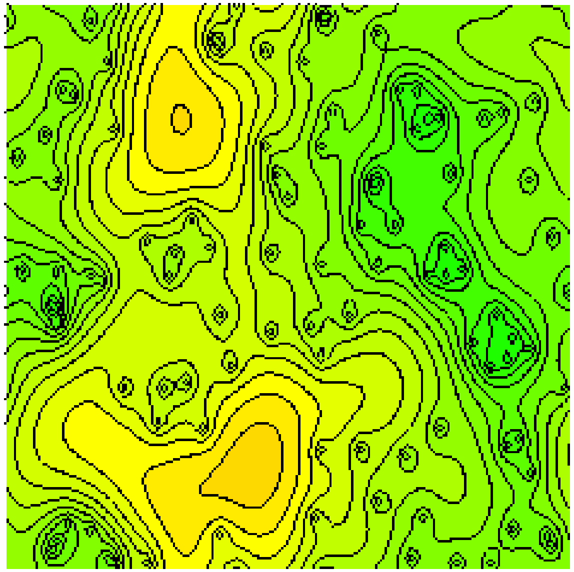


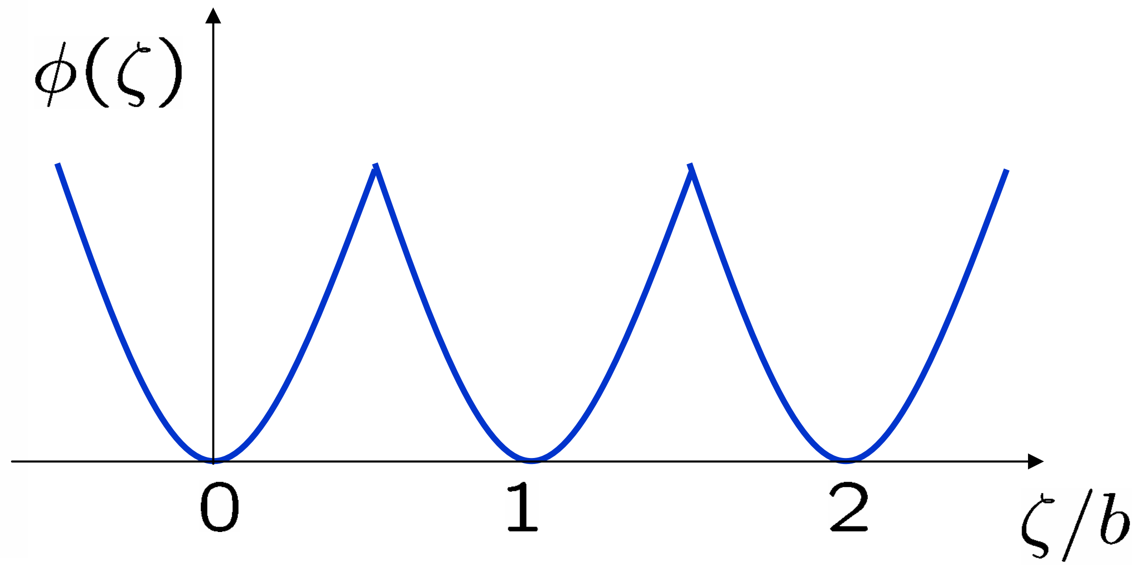
Phase-field dislocation dynamics



- Problem: Minimize energy $E(u)$ subject to:
  - Interaction with obstacles (pinning or dissipative)
  - Applied shear stress

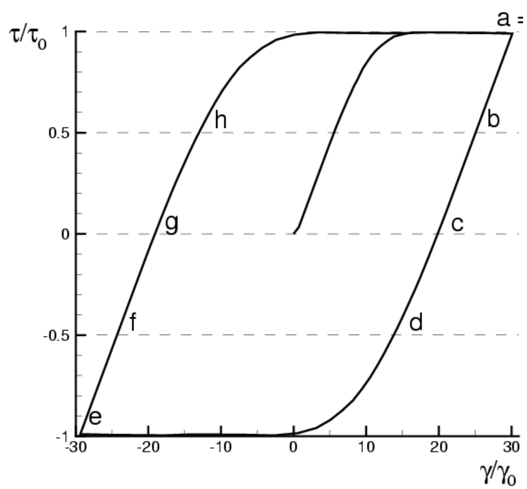
Phase-field dislocation dynamics



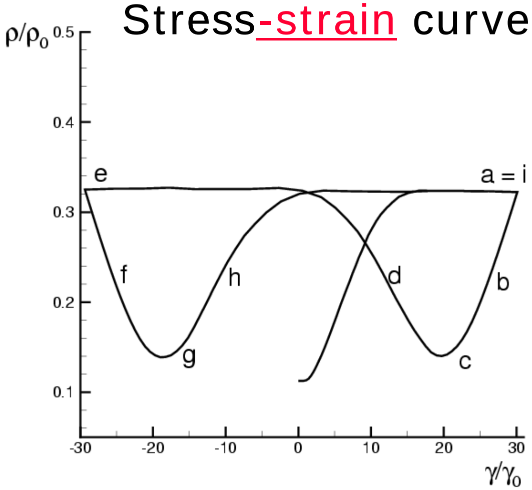


- Phase field $\xi(x)$: Counts (signed) crossings of dislocations over $x \equiv$ Peierls energy well, or *phase*
- Pinning case can be solved analytically.
- Penetrable obstacle case can be reduced to determining value of phase field on obstacles.

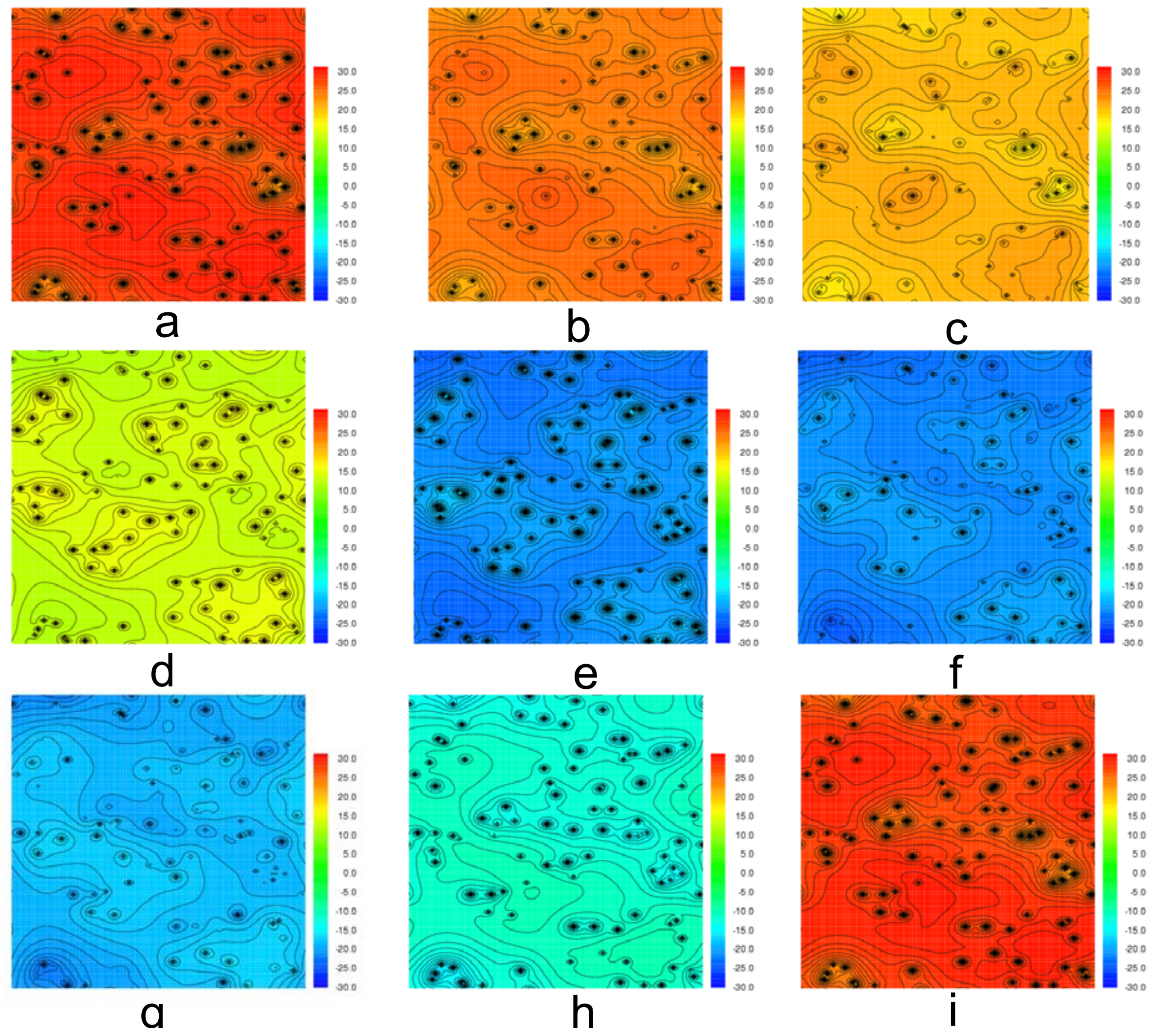
Phase-field dislocation dynamics



Stress-strain curve



Dislocation density



(Movie)

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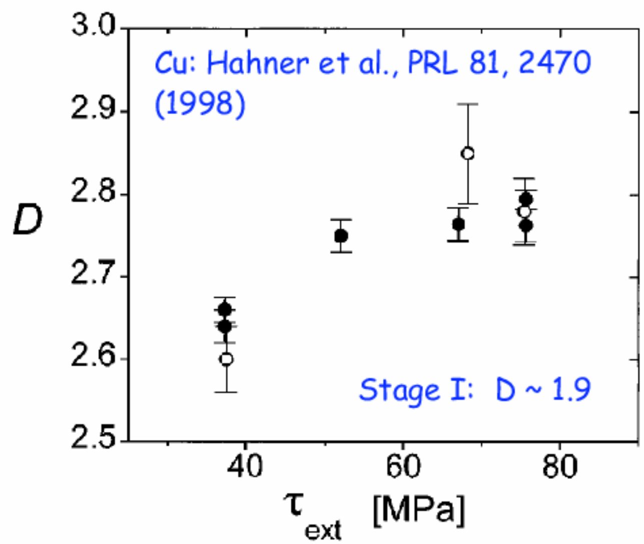
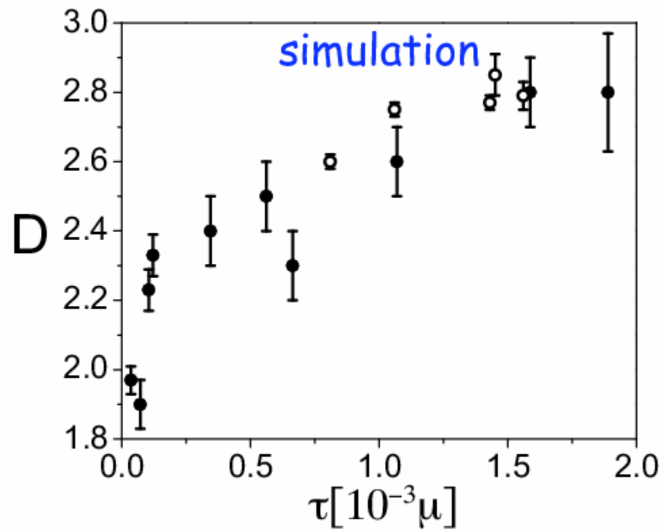
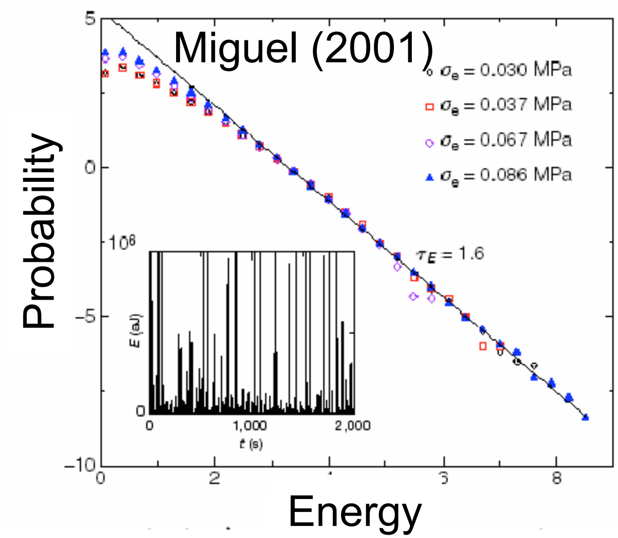
Phase-field dislocation dynamics

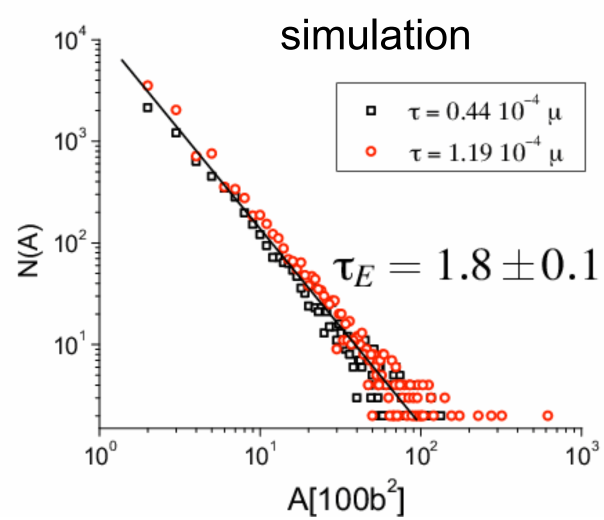
Fractal dimension





Avalanches





Koslowski, Le Sar and Thompson ’04

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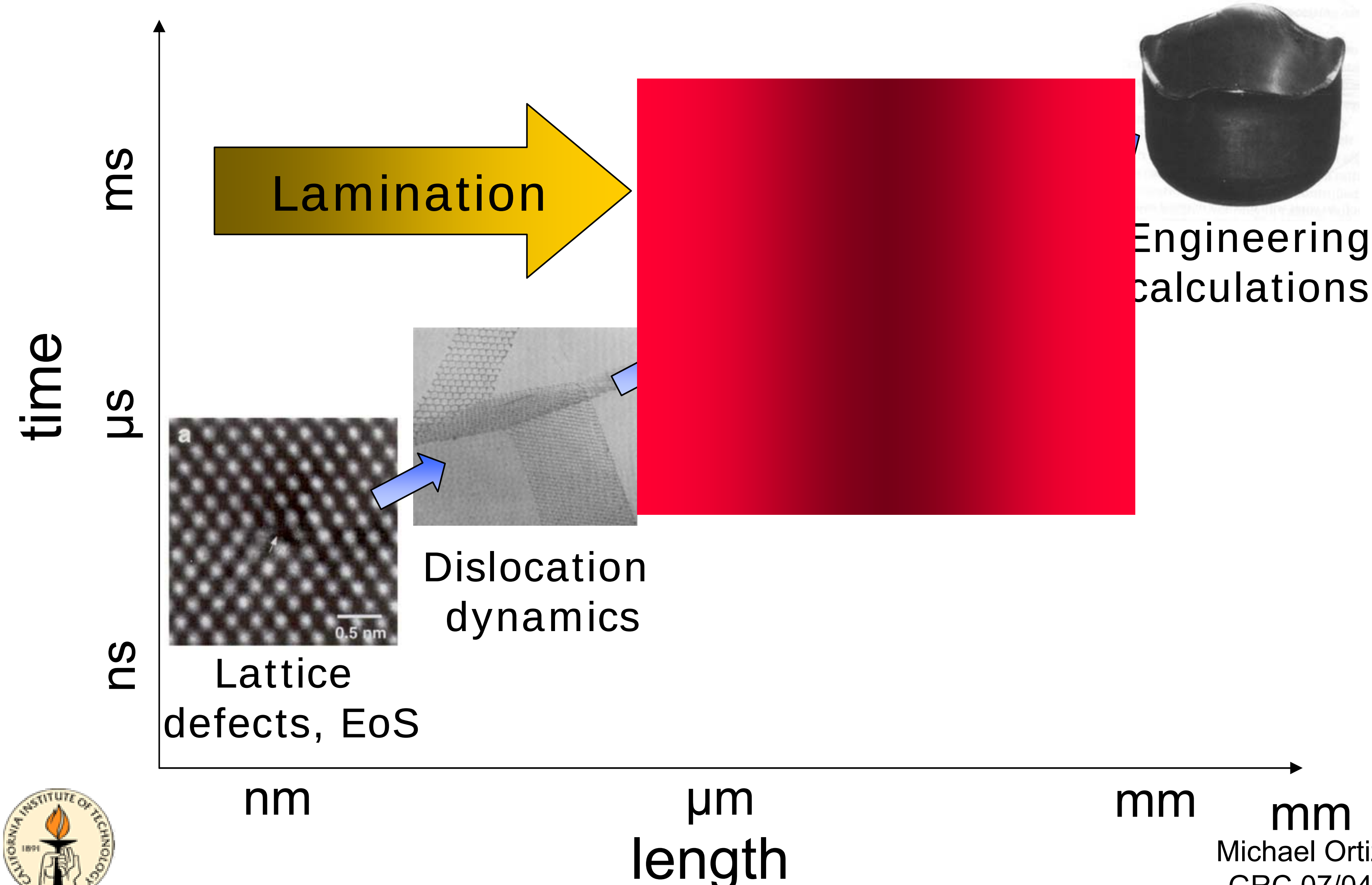
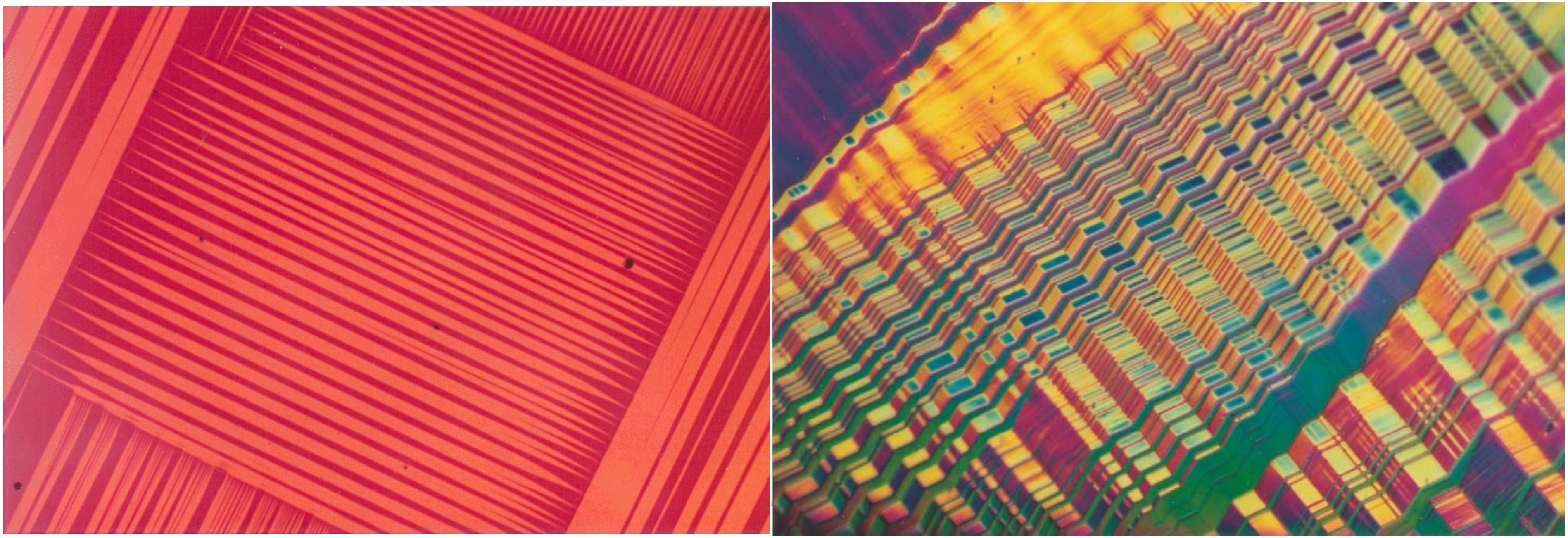
Phase-field dislocation dynamics

- Dislocation dynamics approaches rely on *analytical solutions* of linear elasticity to reduce the *dimensionality* of the problem from 3 (crystal) to 1 (dislocation lines): semi-inverse approach
- Phase-field dislocation dynamics with pairwise Peierls potential reduces dimensionality further, from 3 (crystal) to 0 (point obstacles)
- Challenges:
  - *Large three-dimensional ensembles*
  - *Atomistic dislocation cores*
  - *Dislocation reactions, junctions*

Multiscale modeling - Approaches



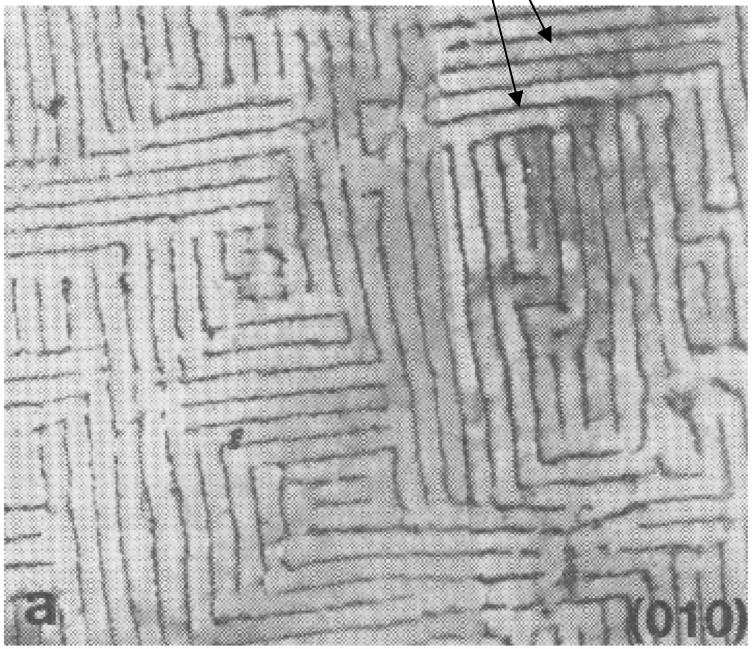
Twinning - Microstructures



(Cu-Al-Ni, C. Chu and R. D. James)

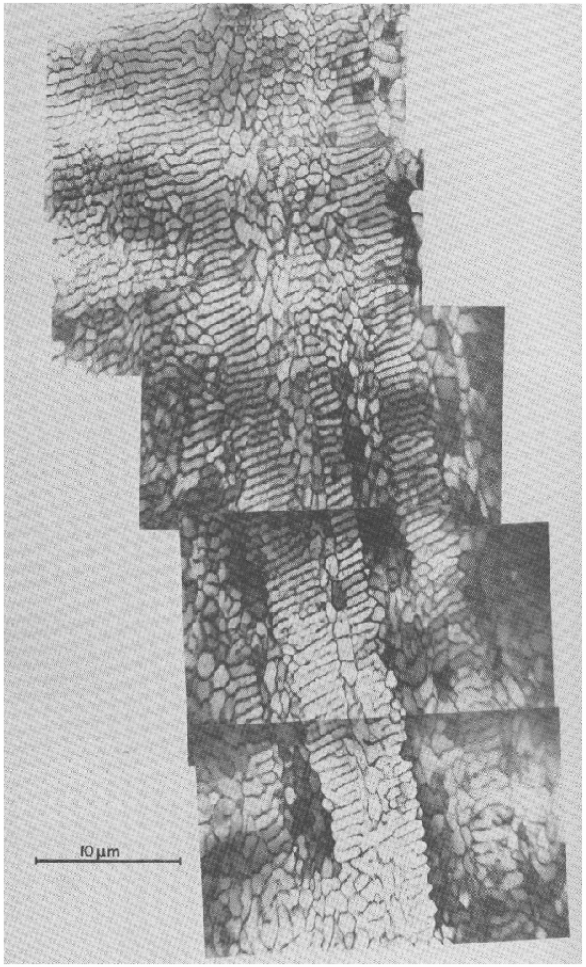
Crystal plasticity - Microstructures

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)



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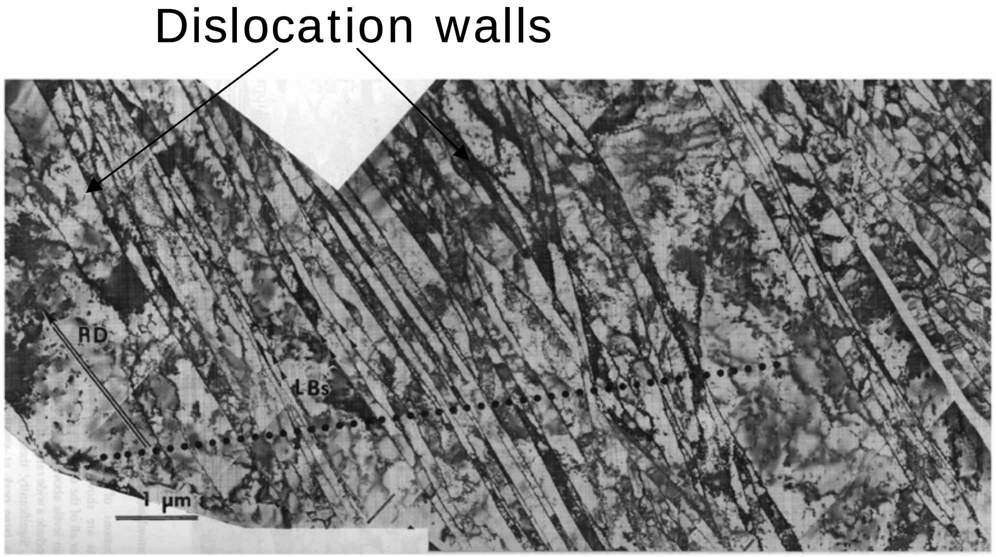
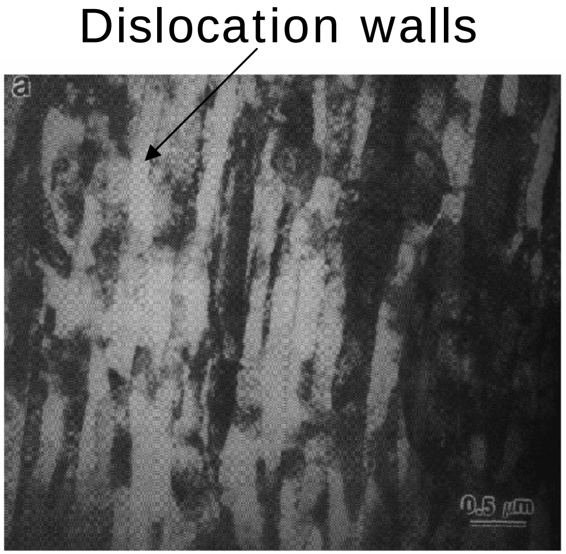
Crystal plasticity - Microstructures



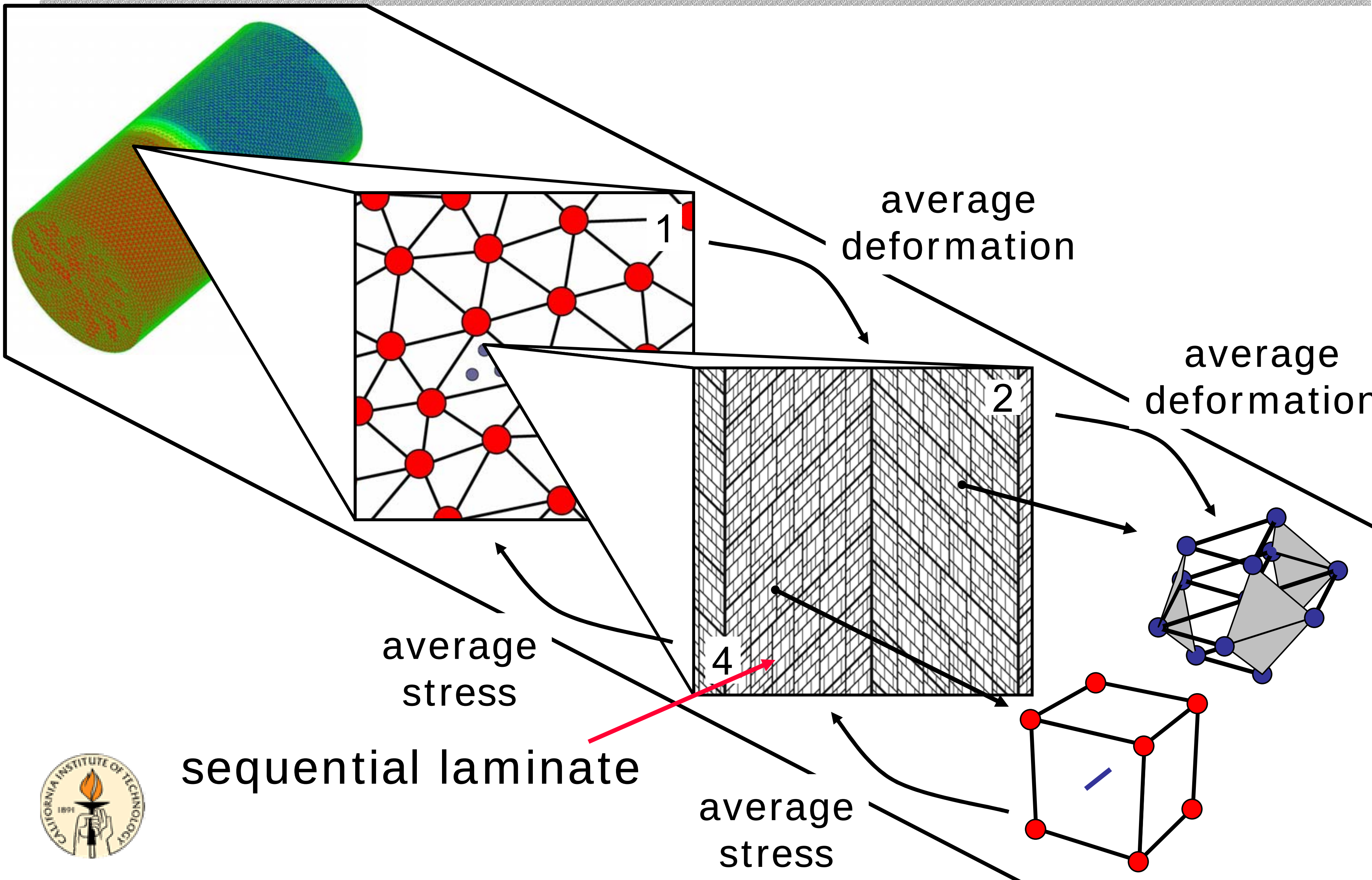
Lamellar dislocation structure
in 90% cold-rolled Ta
(Hughes and Hansen ´97)



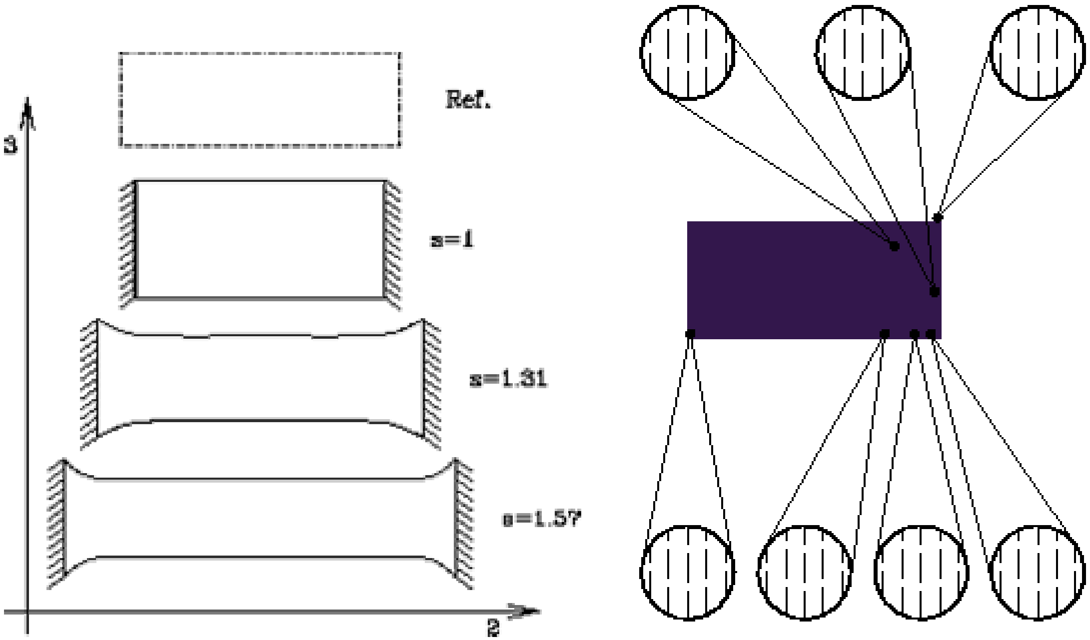
Lamellar structure
in shocked Ta
(Meyers et al ´95)

- 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

Microstructures – Sequential lamination



Nematic elastomers - Lamination



(Courtesy of de Simone and Dolzmann)

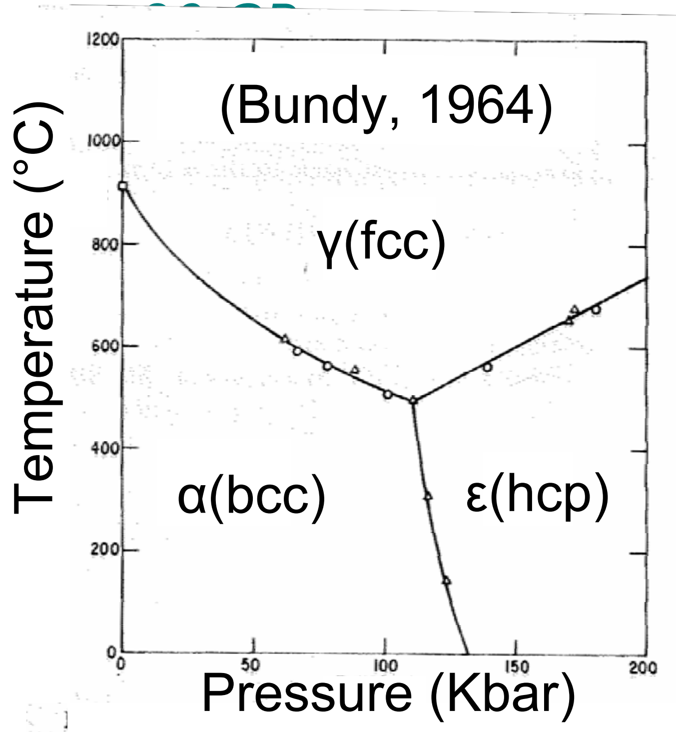
$$W(F,n) = A\,\mathrm{tr}(FF^T) - B\,||F^T n||^2$$

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

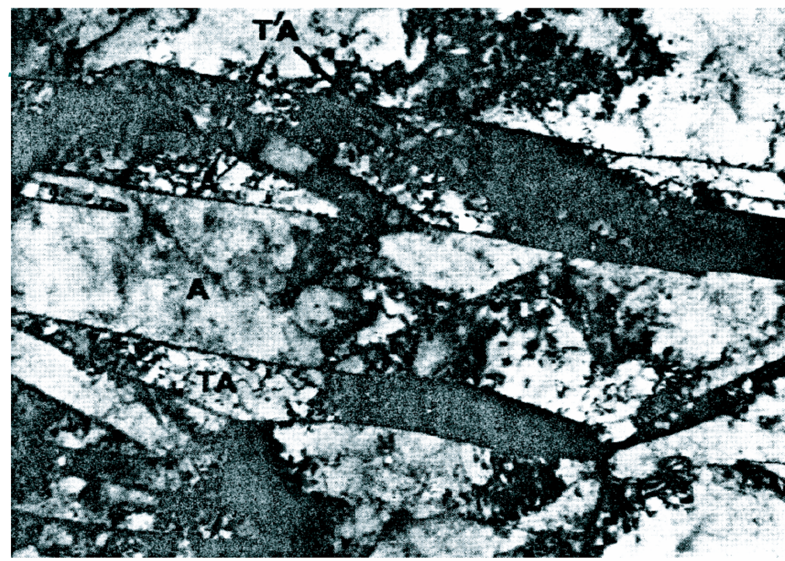
Blandon *et al.* ´93
De Simone and Dolzmann ´00
De Simone and Dolzmann ´02

Solid/solid transitions in iron

- Commonly observed solid/solid transitions in Fe:
  - *α(bcc) → ε(hcp) at p = 13 GPa, coexisting phases p <*



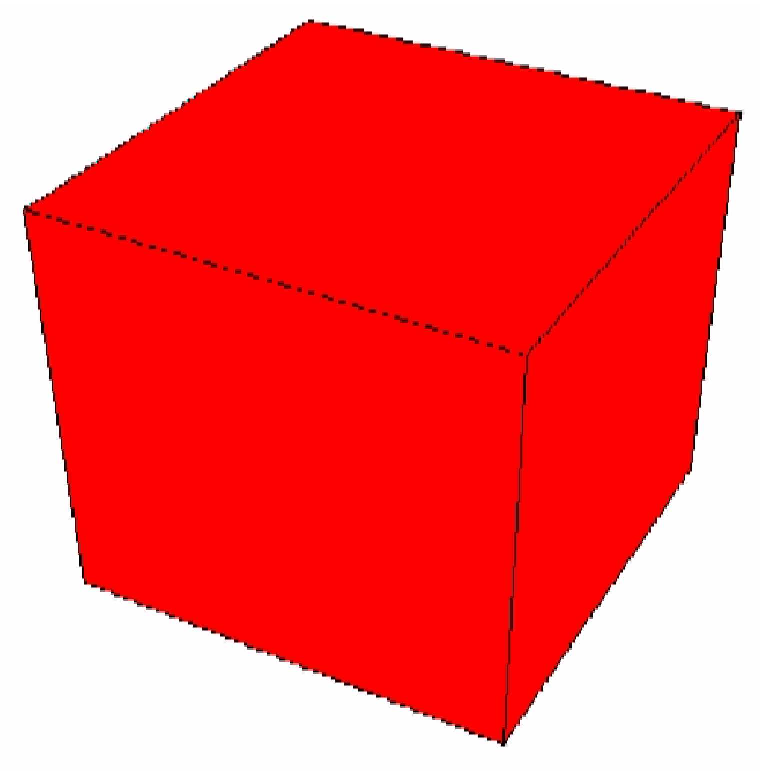
Phase diagram for Fe



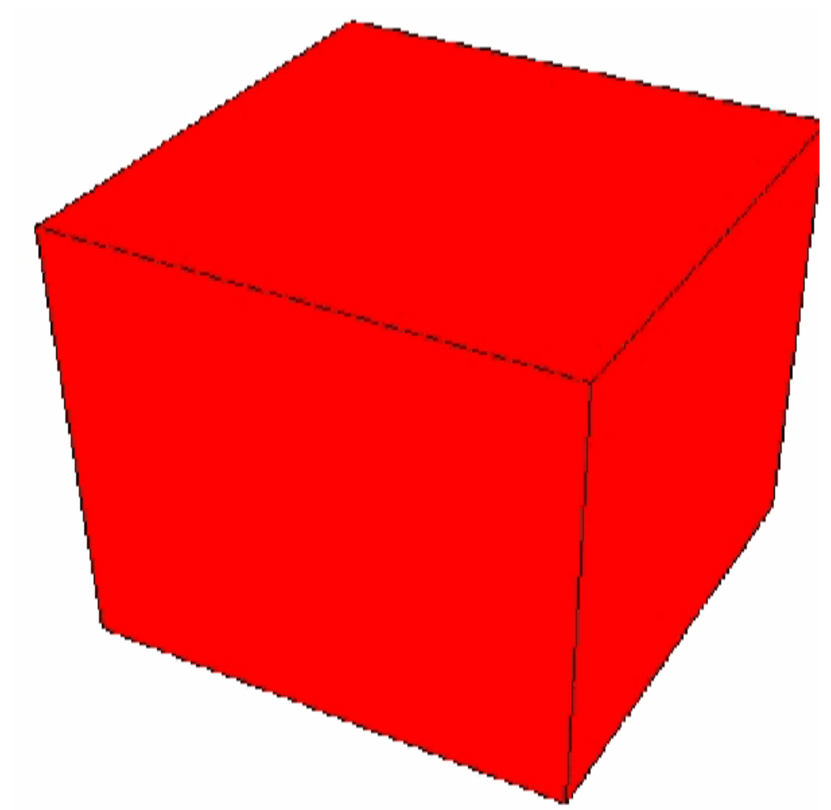
ε platelets in 0.1%C steel shocked to 20 GPa (Bowden and Kelly, 1967)

Phase transitions in Fe – Effect of shear

Hydrostatic Compression



Shear Compression



Initial model with 7 total variants (1 bcc/6 hcp)

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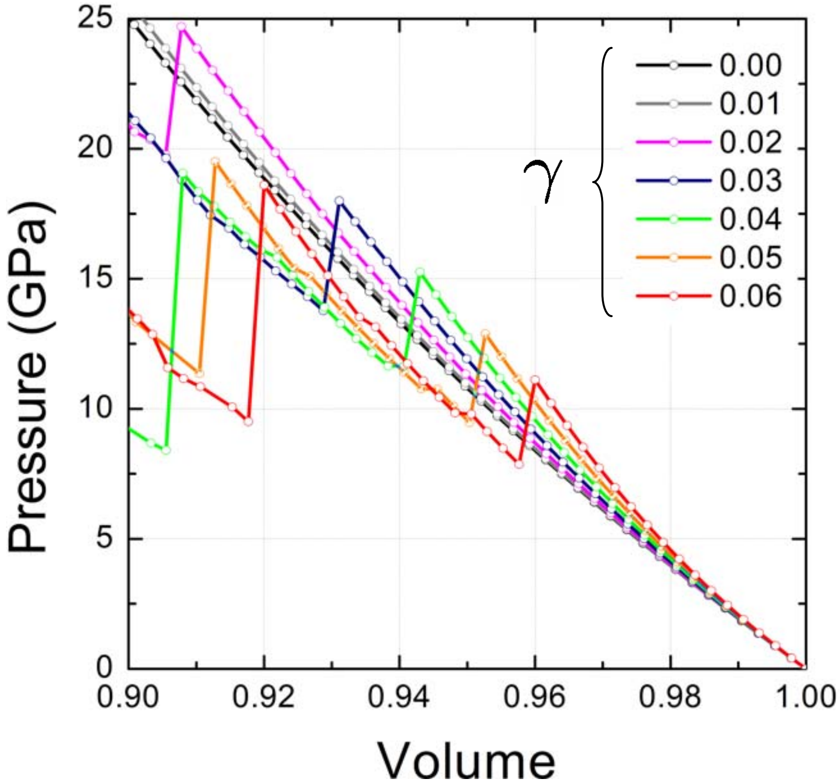
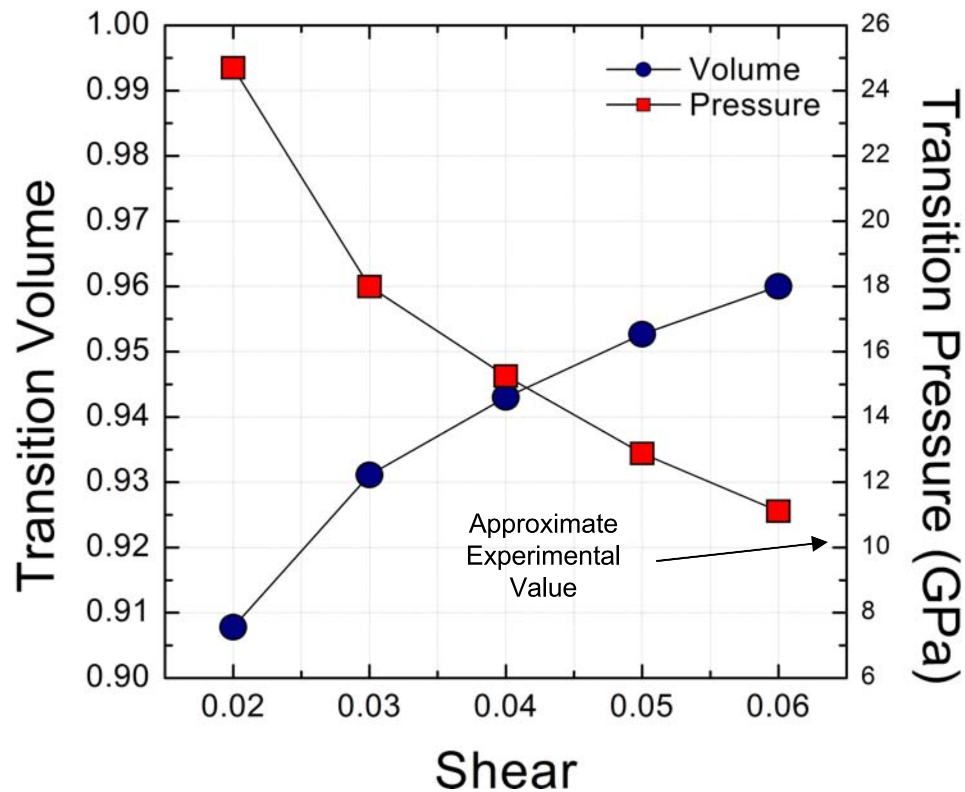
Phase transitions in Fe – Effect of shear





$$\boldsymbol{F} = \begin{pmatrix} 1 & \gamma & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix}$$

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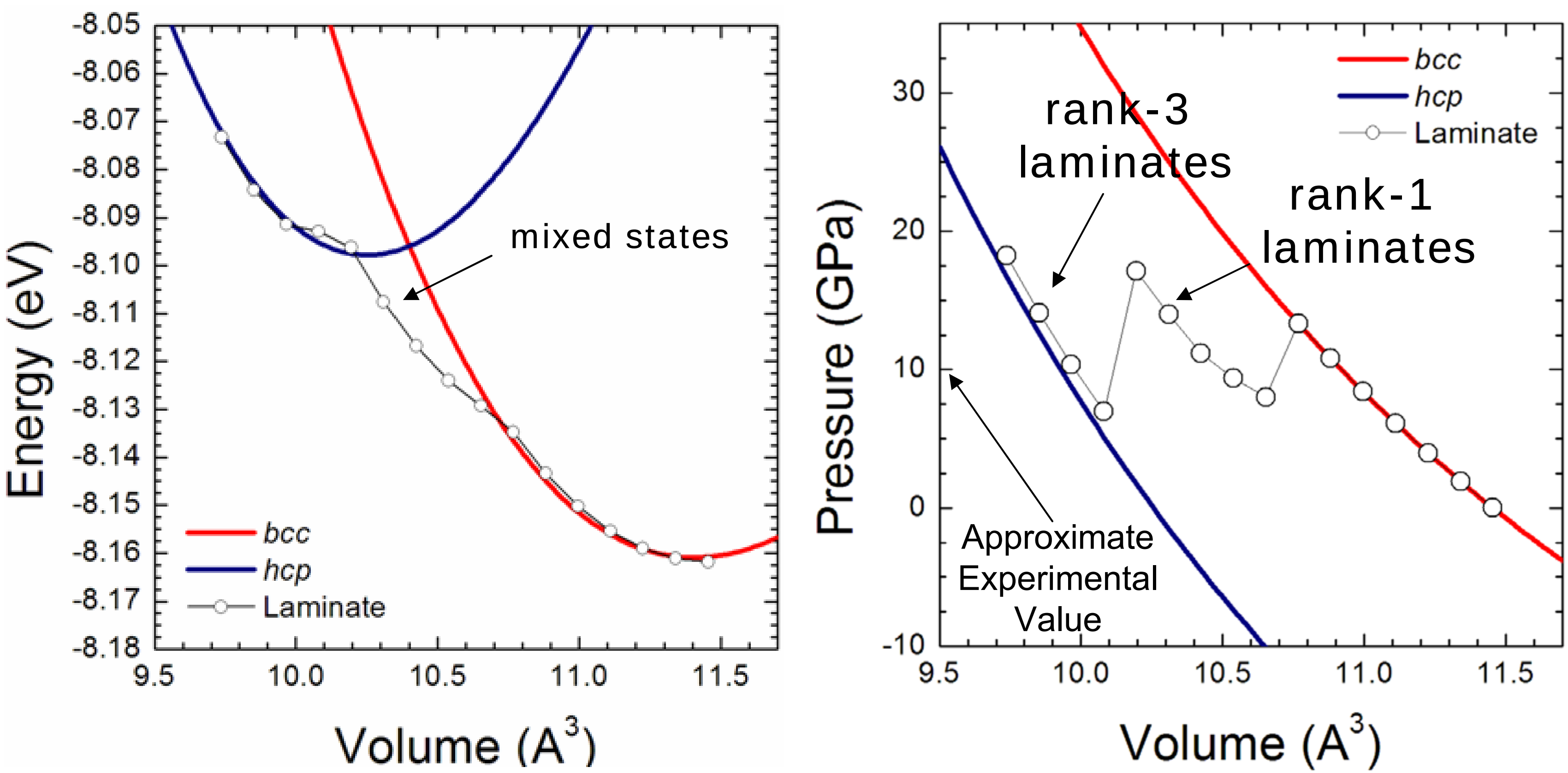
Phase transitions in Fe – Effect of shear



- Shear lowers bcc to hcp transition pressure.
- bcc to hcp transition path involves mixed states in the form of rank-1 and rank-3 laminates

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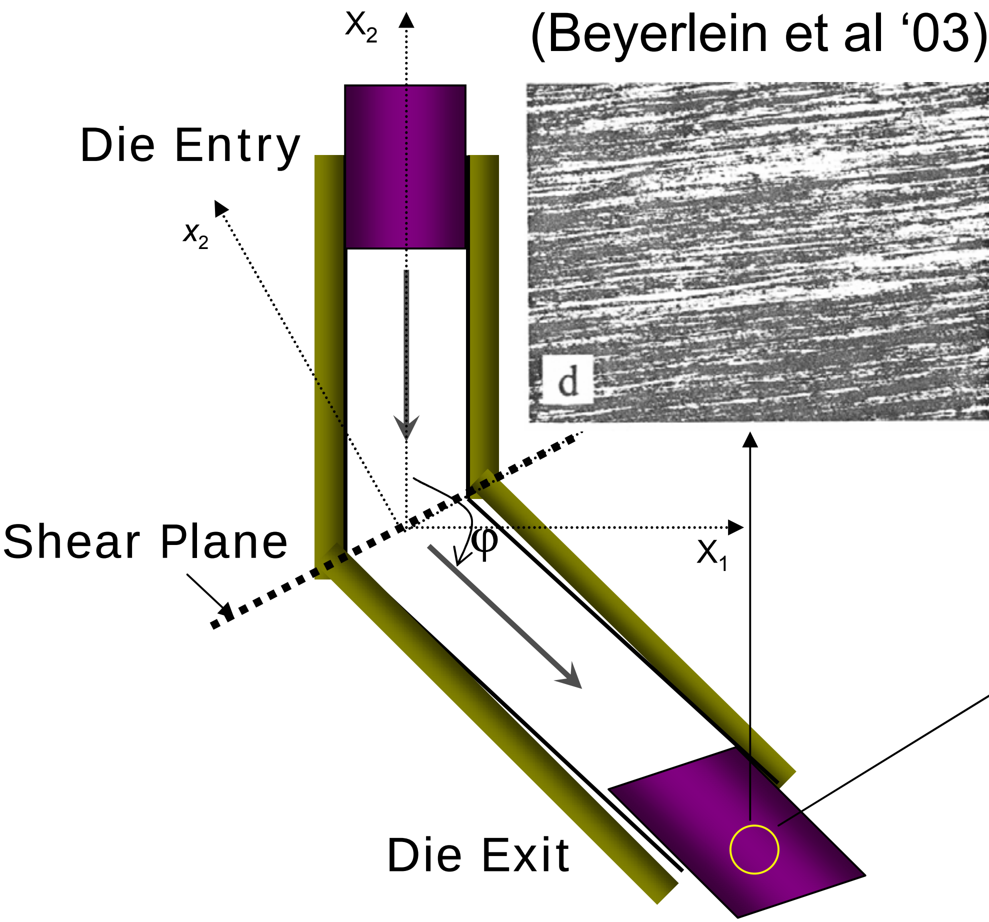
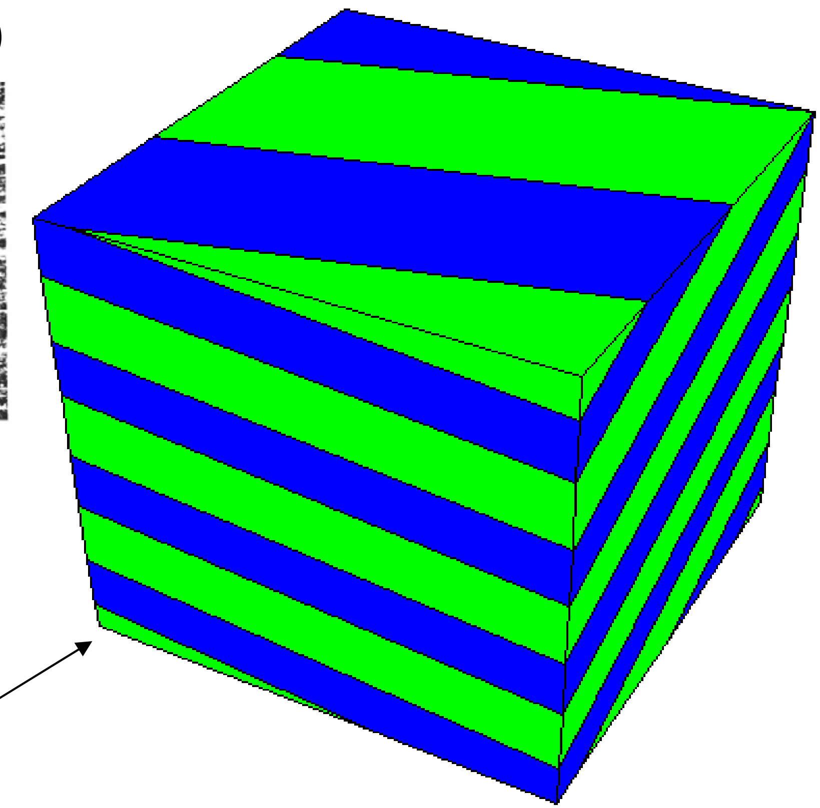
ECAP – Lamination



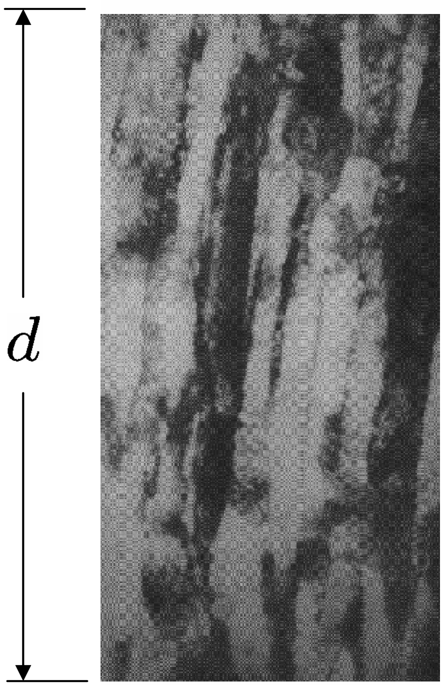


Evolution of microstructure
(sequential lamination)

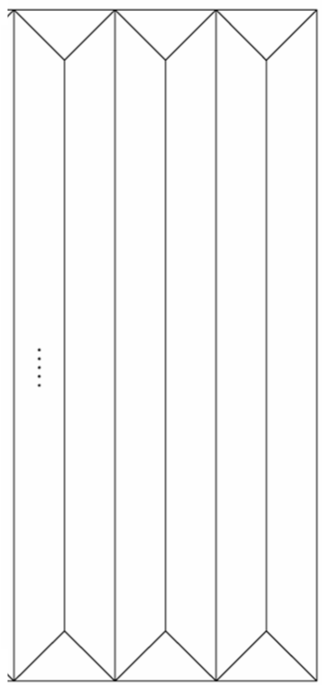
(Sivakumar and Ortiz ´03)

Crystal plasticity – size effects

- Optimal scaling constructions for double slip, antiplane shear (Conti and Ortiz '04)

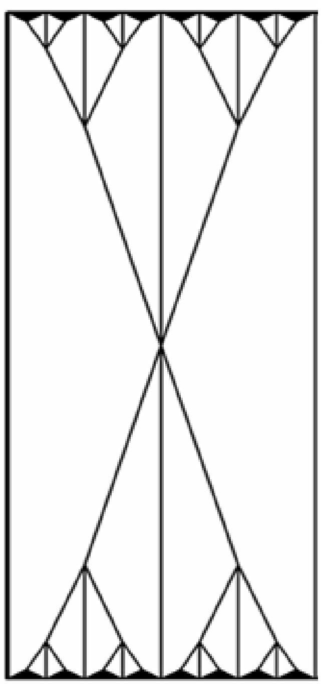


Shocked Ta
(Meyers et al ´95)



Laminate

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



Branching

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

LiF impact
(Meir and Clifton´86)

Hall-Petch effect!

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Subgrid microstructures - Lamination

- Sequential lamination supplies microstructures ‘on demand’ and is another example of concurrent multiscale computing
- Sub-grid microstructural information is recovered locally at the Gauss-point level
- But: Effective response is known explicitly in very few cases (e.g., nematic elastomers)
- 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)*

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 modeling at all lengthscales, including:
  - *subgrid models of microstructure (a la sequential lamination)*
  - *analytical methods, algorithms, for computing effective behavior, coarse graining*
  - *Kinetics, dynamics, rare events...*