Mutiscale Models of Materials: Linking Microstructure and Macroscopic Behavior

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Acknowledgements

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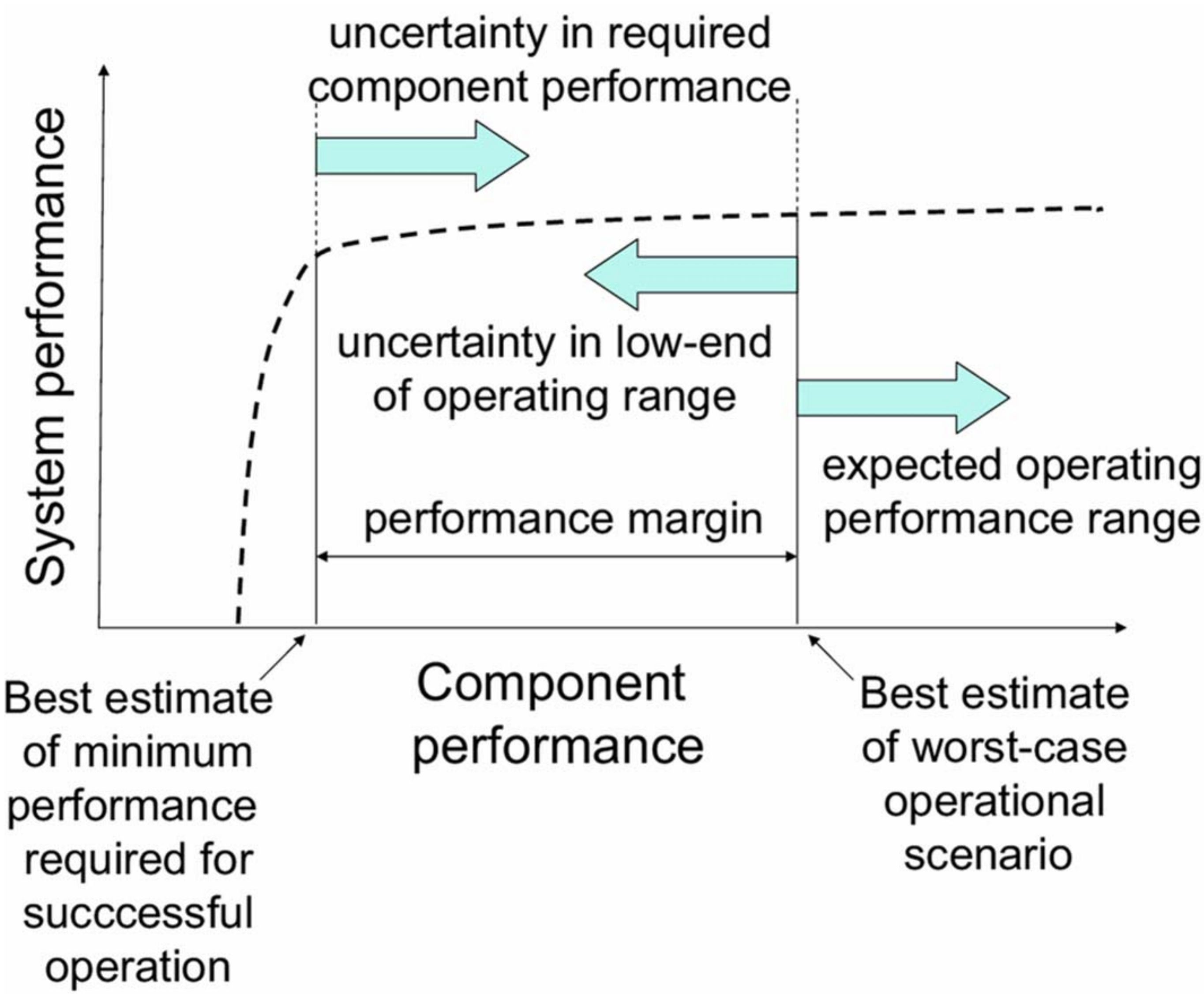
DoE Advanced Simulation & Computing (ASC)
Academic Strategic Alliance Program (ASAP)

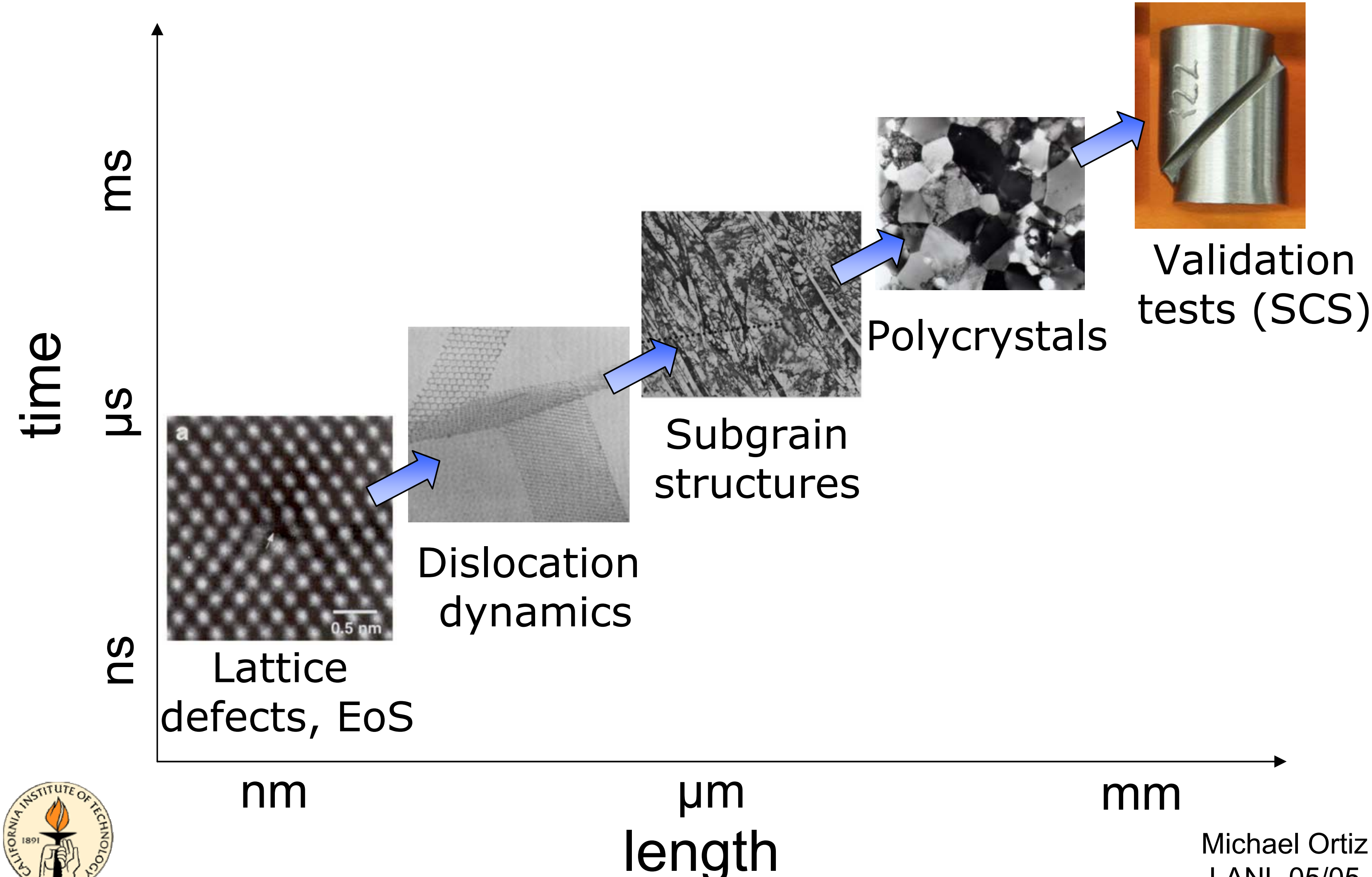
Introduction – The QMU framework



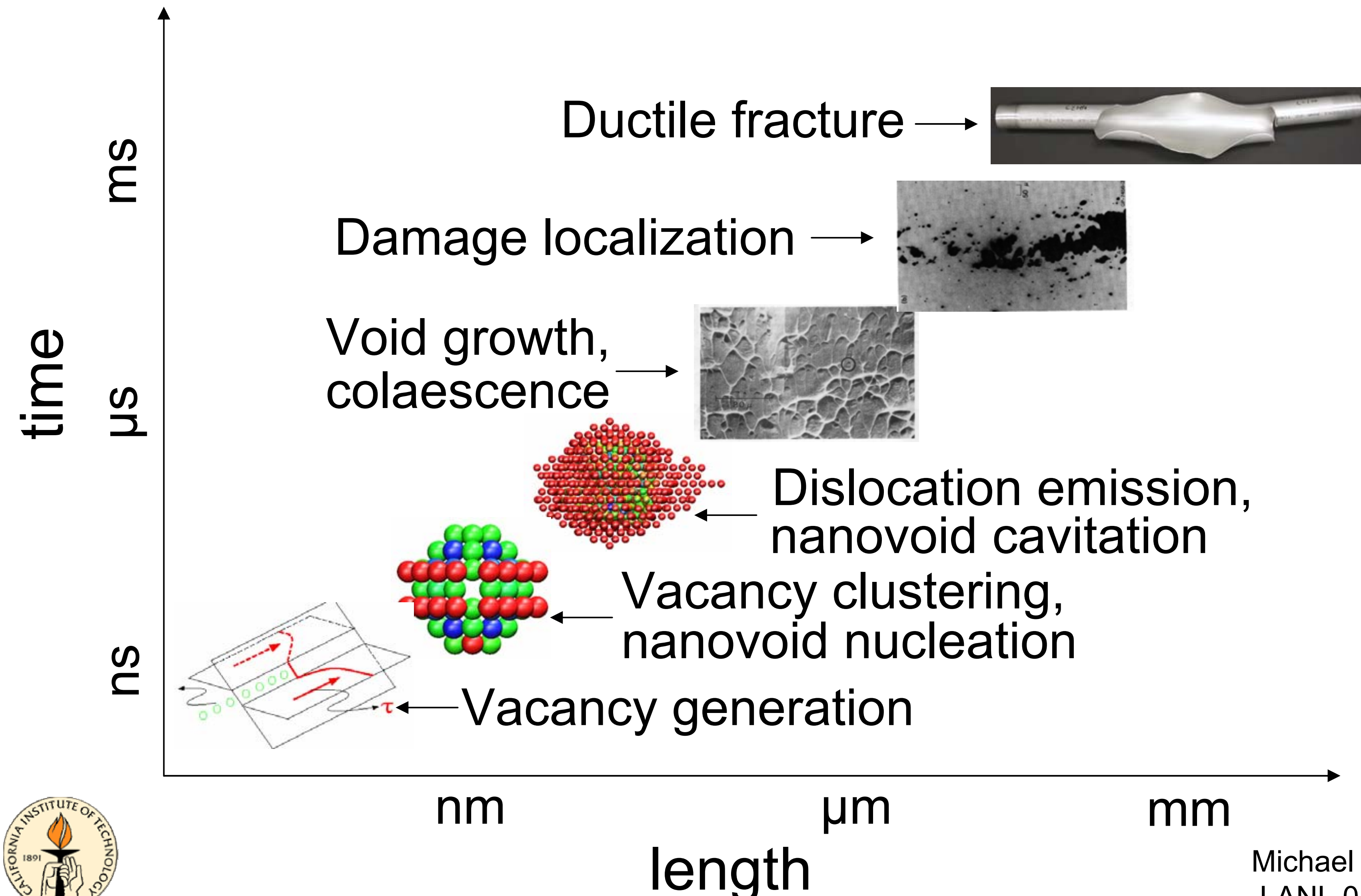
Introduction – Multiscale Modeling

- Multiscale modeling paradigm: Reduce/eliminate uncertainty and empiricism in the simulation of complex engineering systems.
- Ultimate goal: Parameter-free (first-principles) predictive simulation.
- Material behavior occurs on multiple length scales; the underlying physics changes from scale to scale.
- Physics provides governing equations at each scale. Bridging of length scales is largely a mathematical/computational problem.

Strength – Multiscale modeling

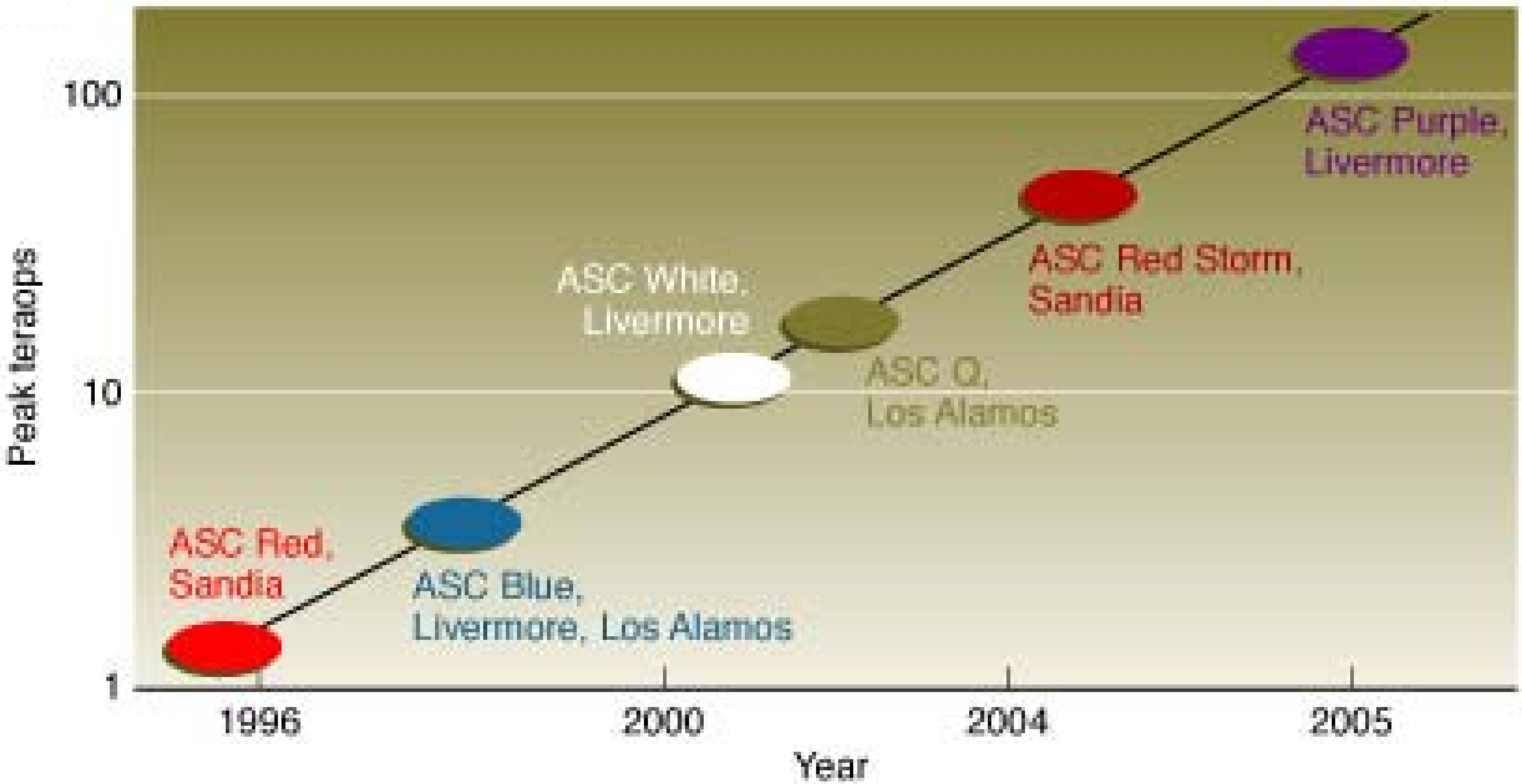


Spall – Lengthscale hierarchy



Direct multiscale computing – Outlook

ASC computing systems roadmap



- Computing power is growing rapidly, but…

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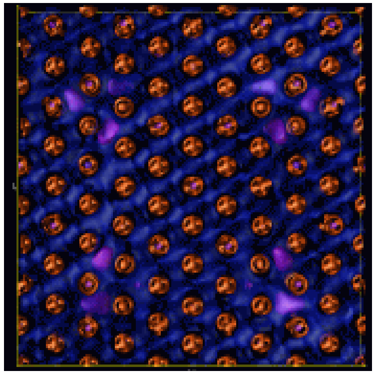
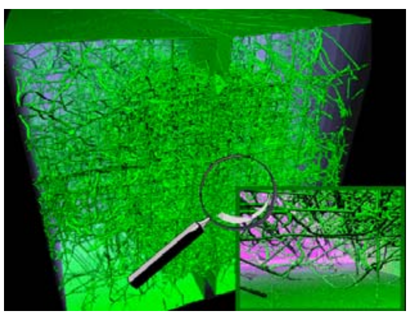
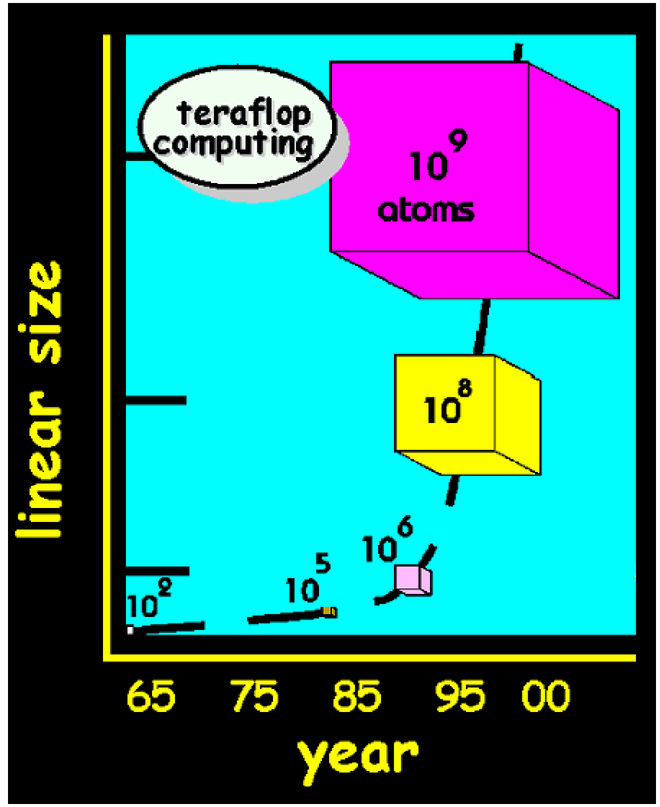
Direct multiscale computing – Outlook



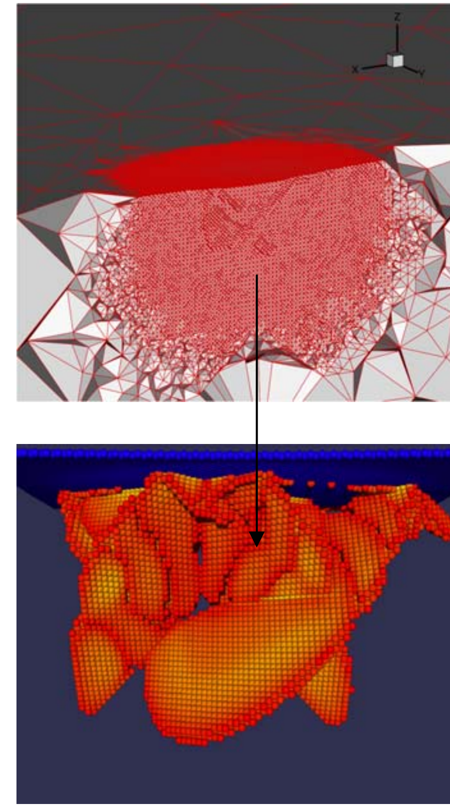
Ta quadrupole
(T. Arias ´00)



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



(Courtesy F.F. Abraham)

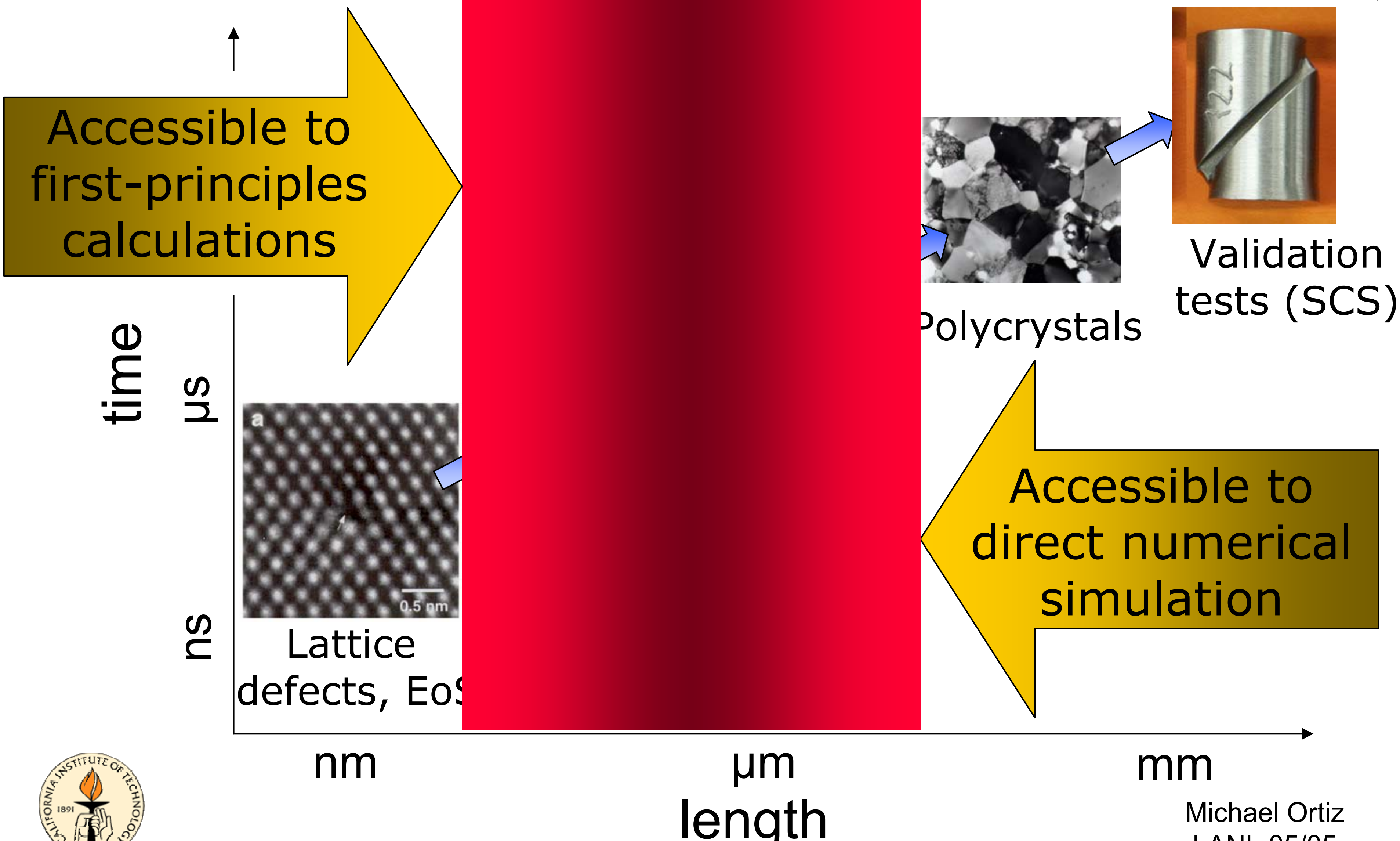


Au nanoindentation
(Knap and Ortiz ´03)

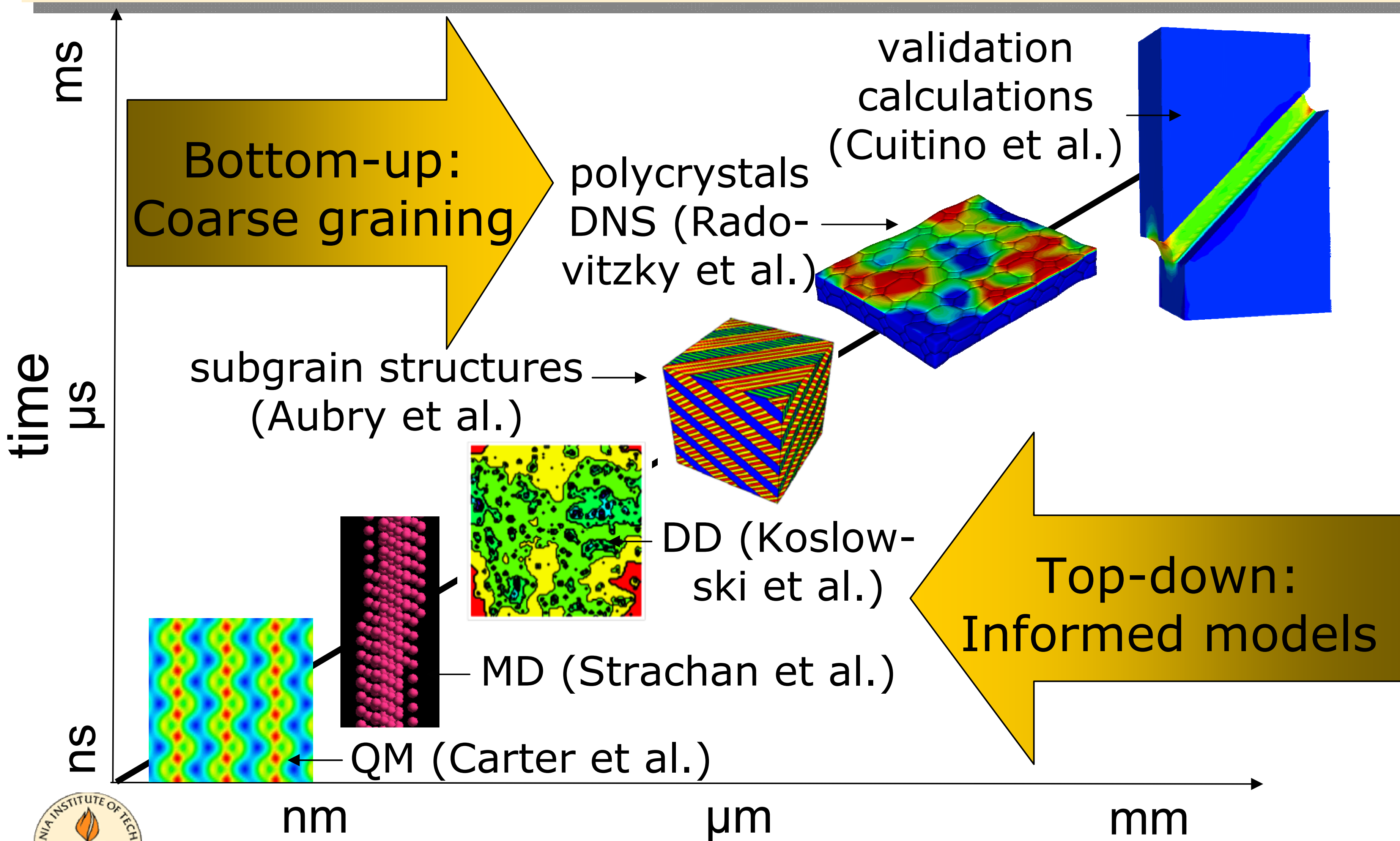
- Computing power is growing rapidly, but

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

Direct multiscale computing – Outlook



Multiscale modeling – Strength



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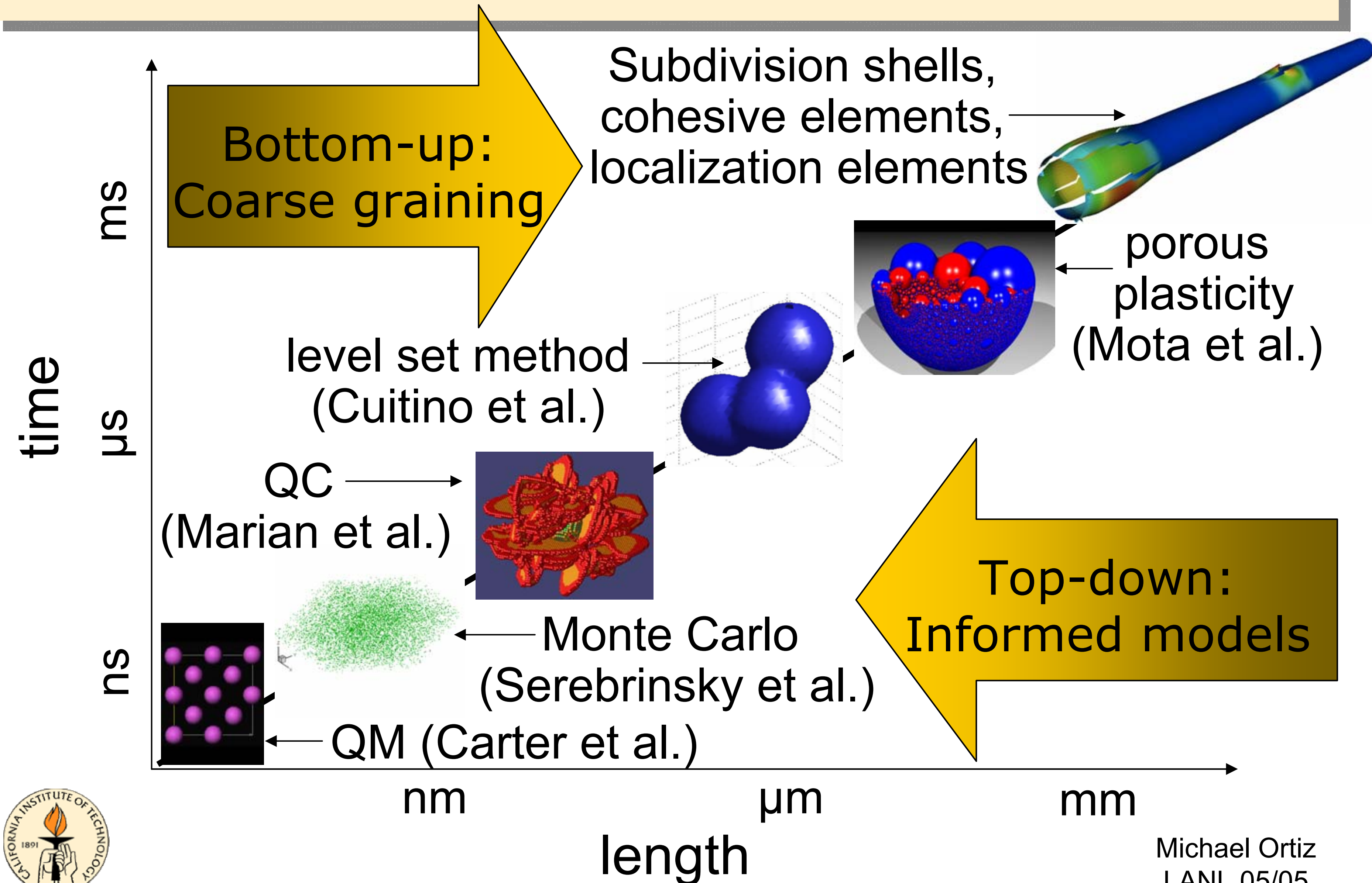
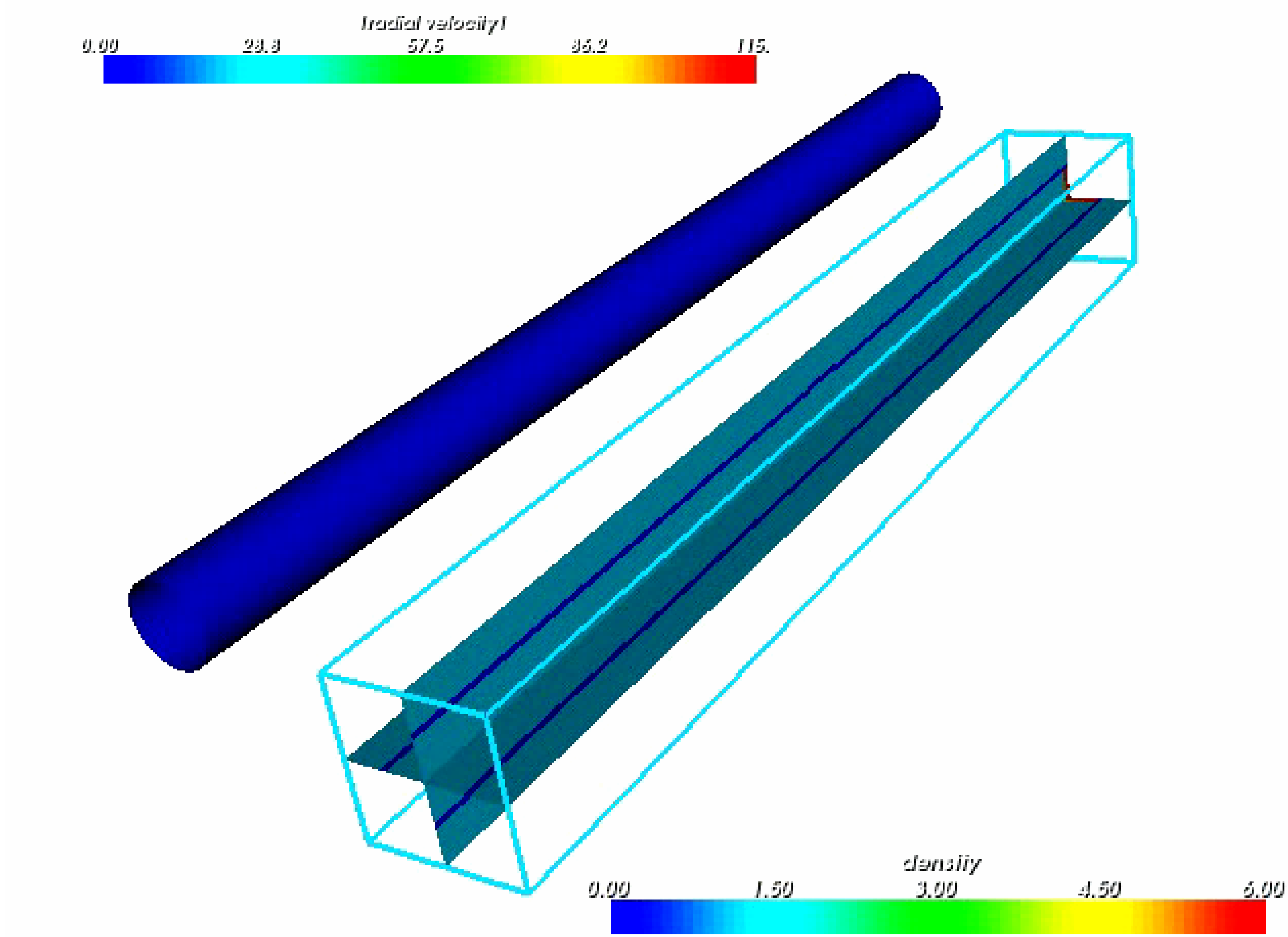
Multiscale modeling – Spall

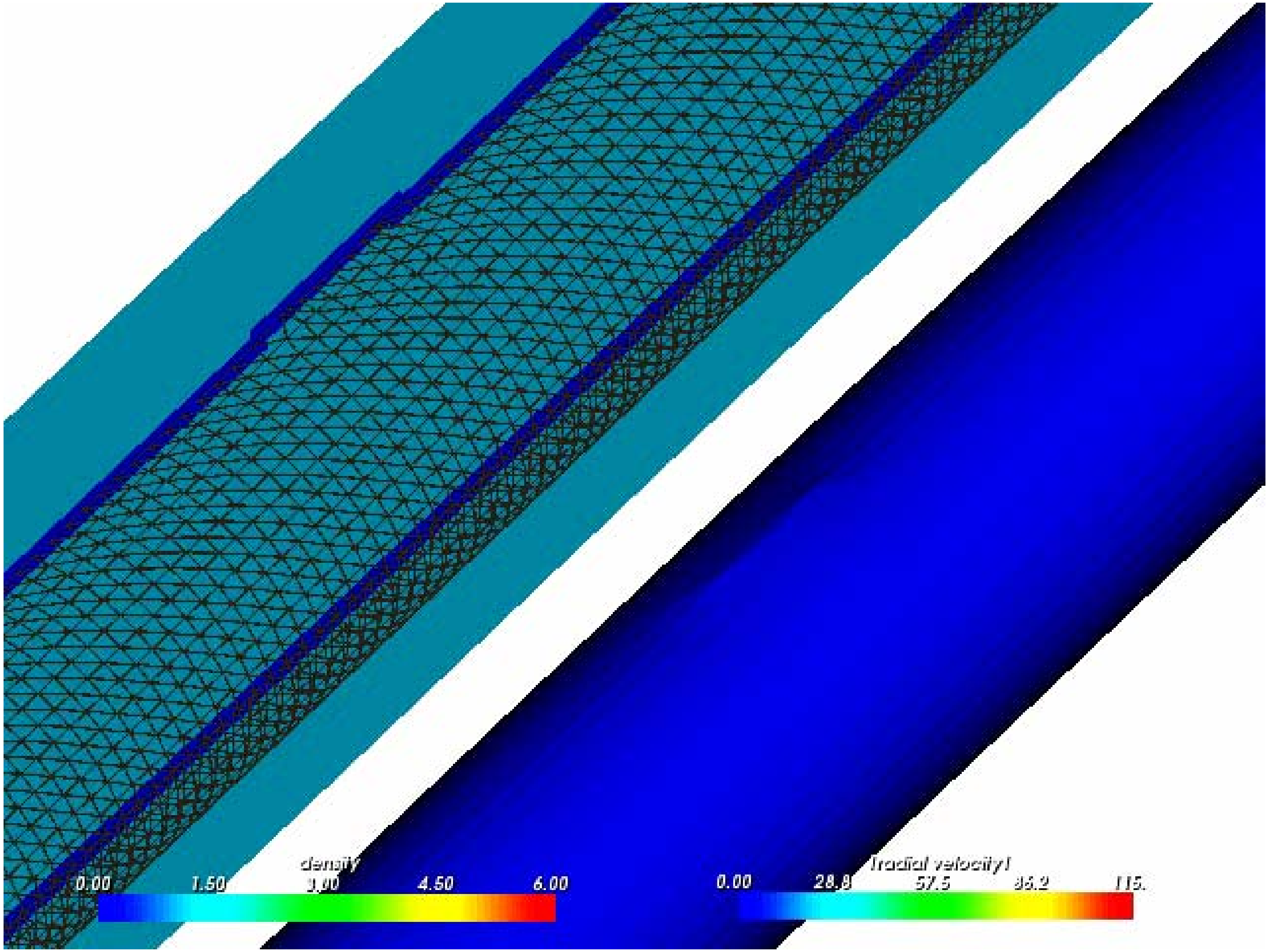


Ductile fracture - Engineering capability



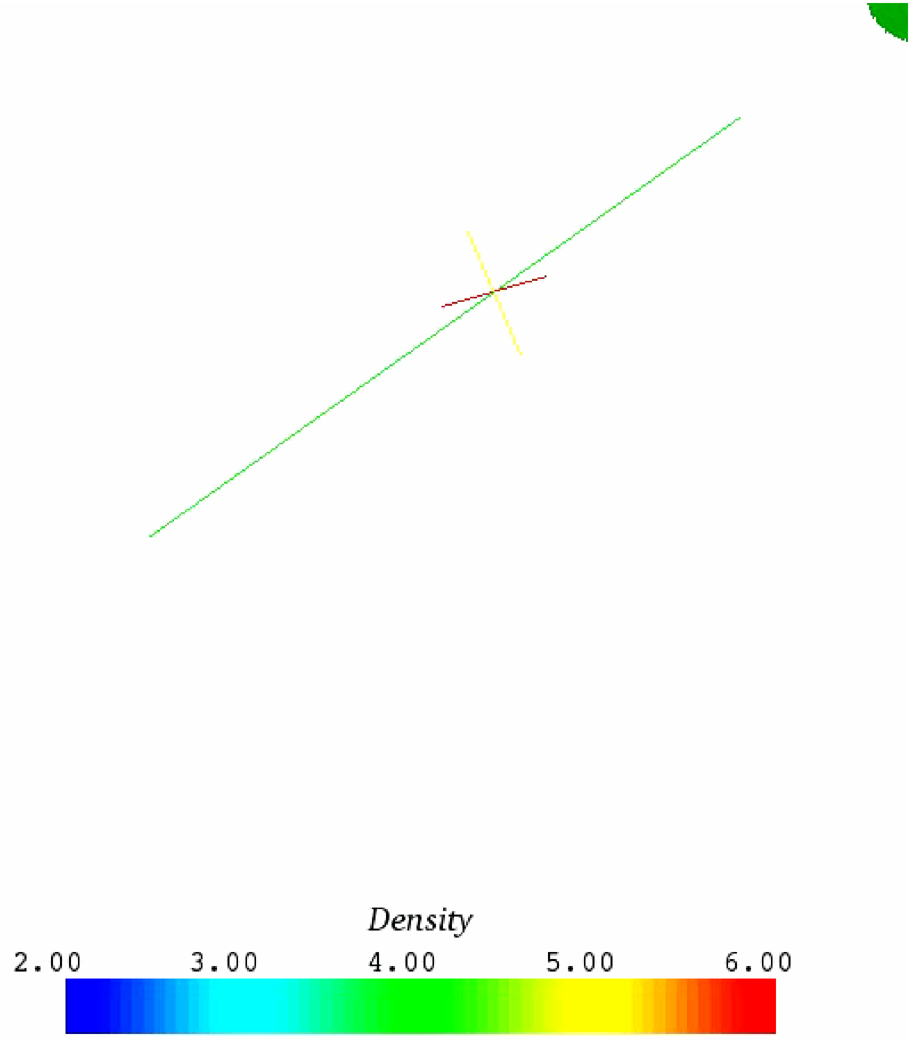
(Cirak et al., 2004)

Ductile fracture - Engineering capability



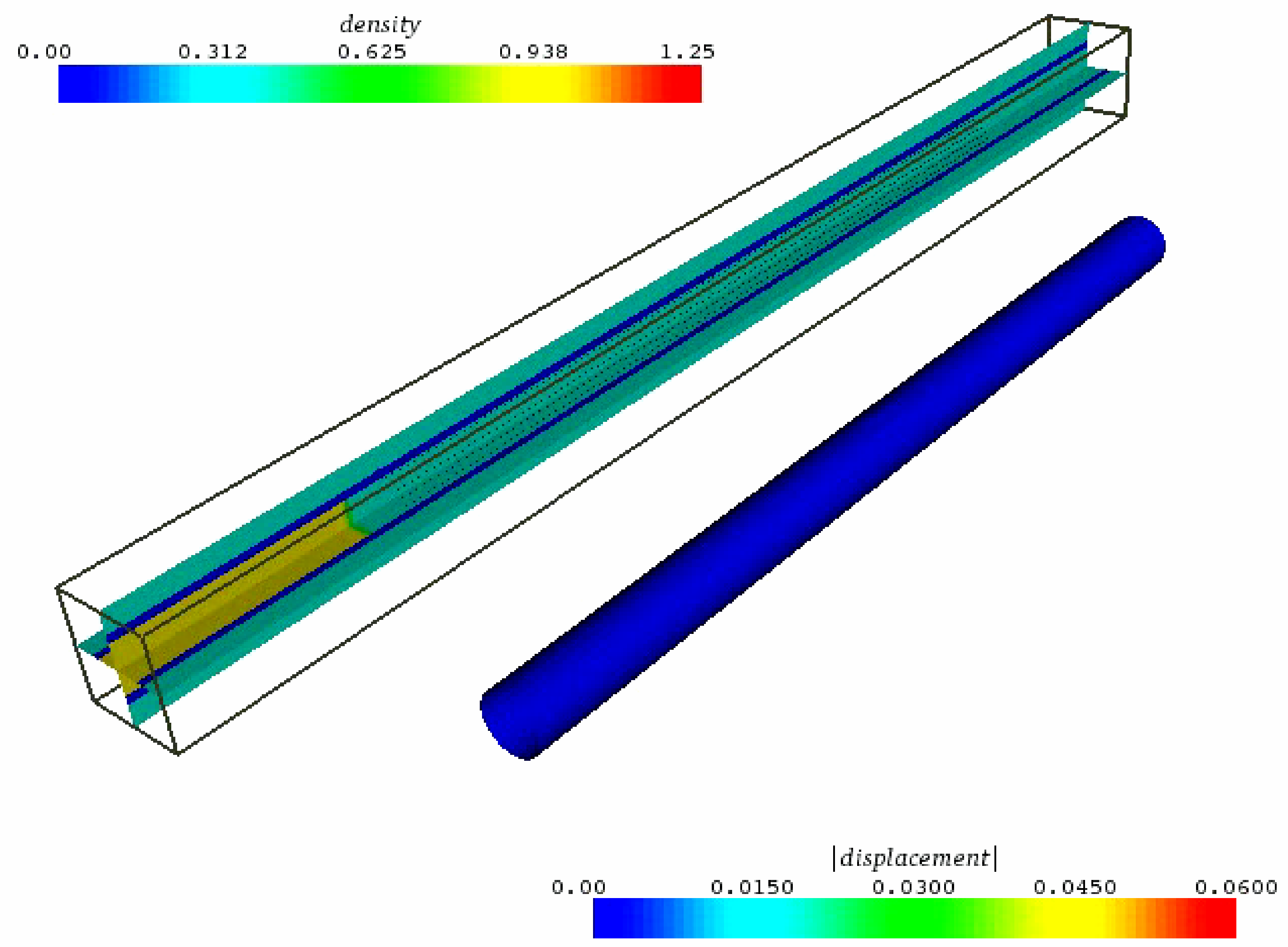
(Cirak et al., 2004)

Ductile fracture - Engineering capability



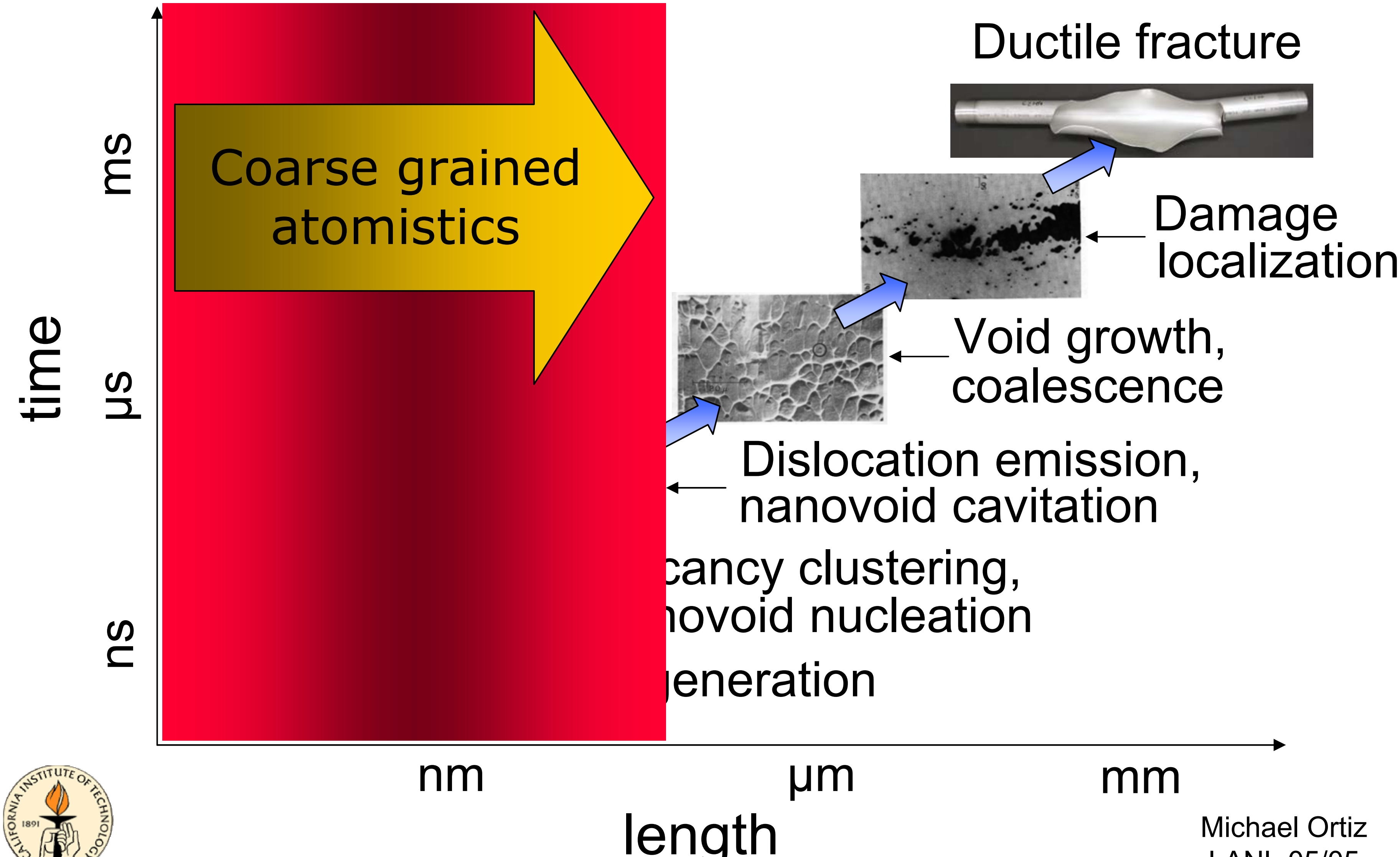
(Cirak et al., 2004)

Ductile fracture - Engineering capability



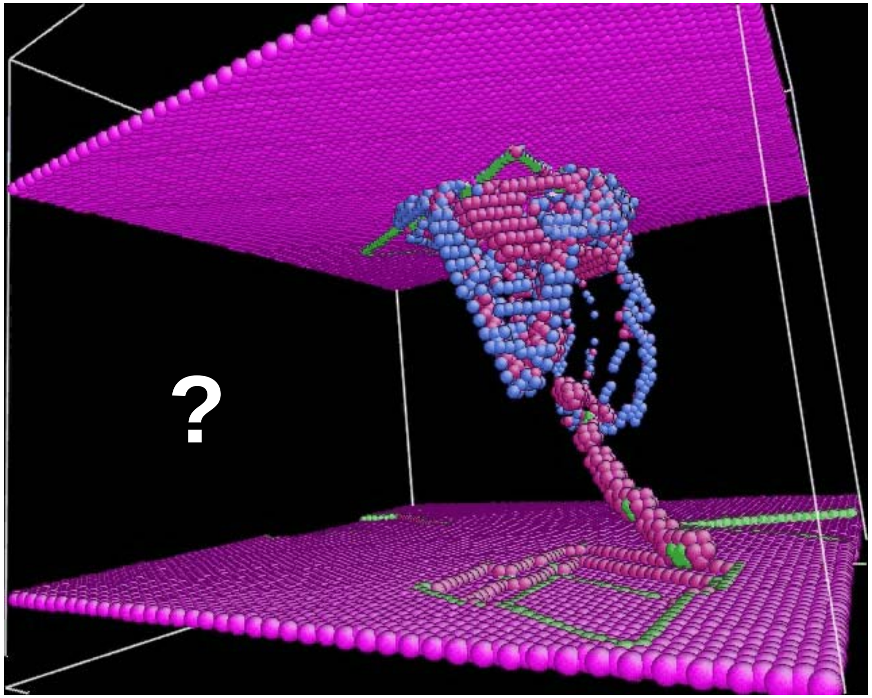
(Cirak et al., 2004)

Bottom-up – Quasicontinuum



The case for Quasicontinuum

Au (111) nanoindentation



Li, J., K.J. Van Vliet, T. Zhu, S. Yip, S. Suresh, "Atomistic mechanisms governing elastic limit and incipient plasticity in crystals", *Nature*, **418**, (2002), 307.

- Early stages of indentation mediated by a defects → Need atomistics
- But elastic (long range) field important → large cells
- Indenter sizes ~ 70 nm, film thickness ~ 1 μm → large cells
- The vast majority of atoms in MD calculations move according to smooth elastic fields → MD wasteful!
- Mixed continuum/ atomistic description.

The Quasicontinuum method

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

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

- Total energy:

$$E(\boldsymbol{q}), \quad \boldsymbol{q} \in X = \mathbb{R}^N$$

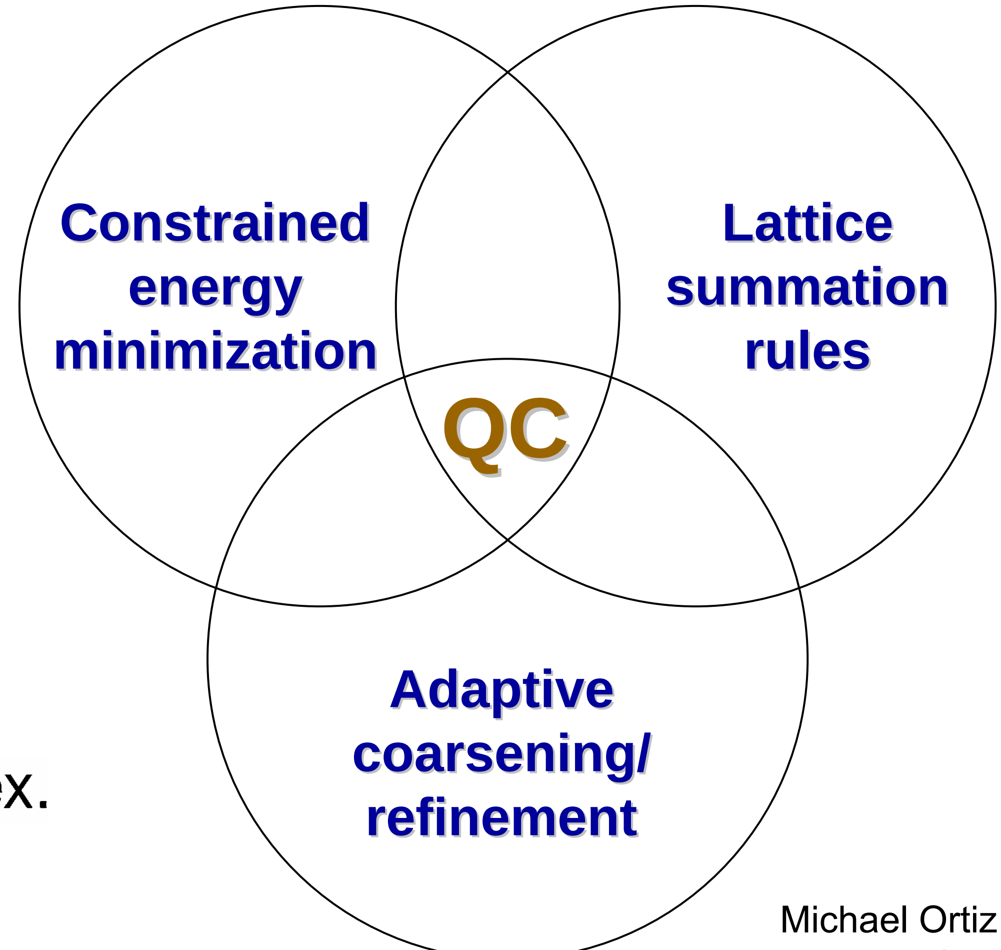
- Problem:

$$\inf_{\boldsymbol{q} \in X} E(\boldsymbol{q})$$

- Difficulties:

i) N very large $\sim 10^{23}$

ii) $E(\boldsymbol{q})$ highly nonconvex.



Quasicontinuum – Reduction

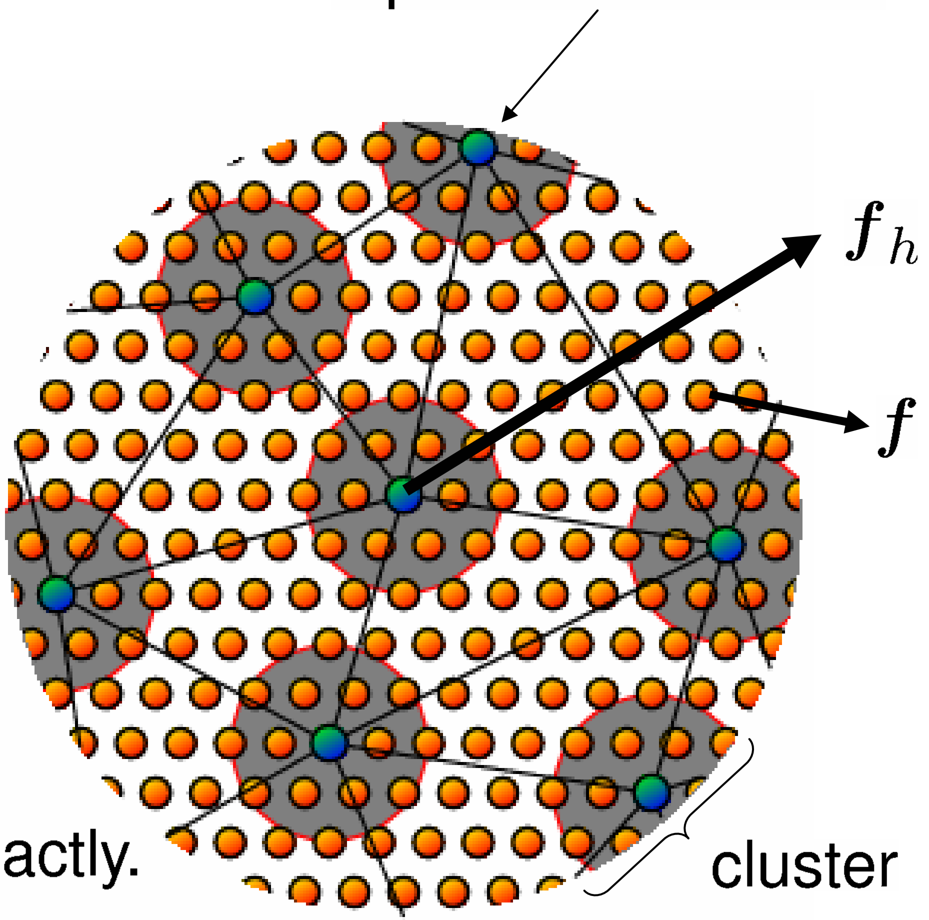
- Reduced problem:

$$\inf_{\boldsymbol{q}\in X_h} E(\boldsymbol{q})$$

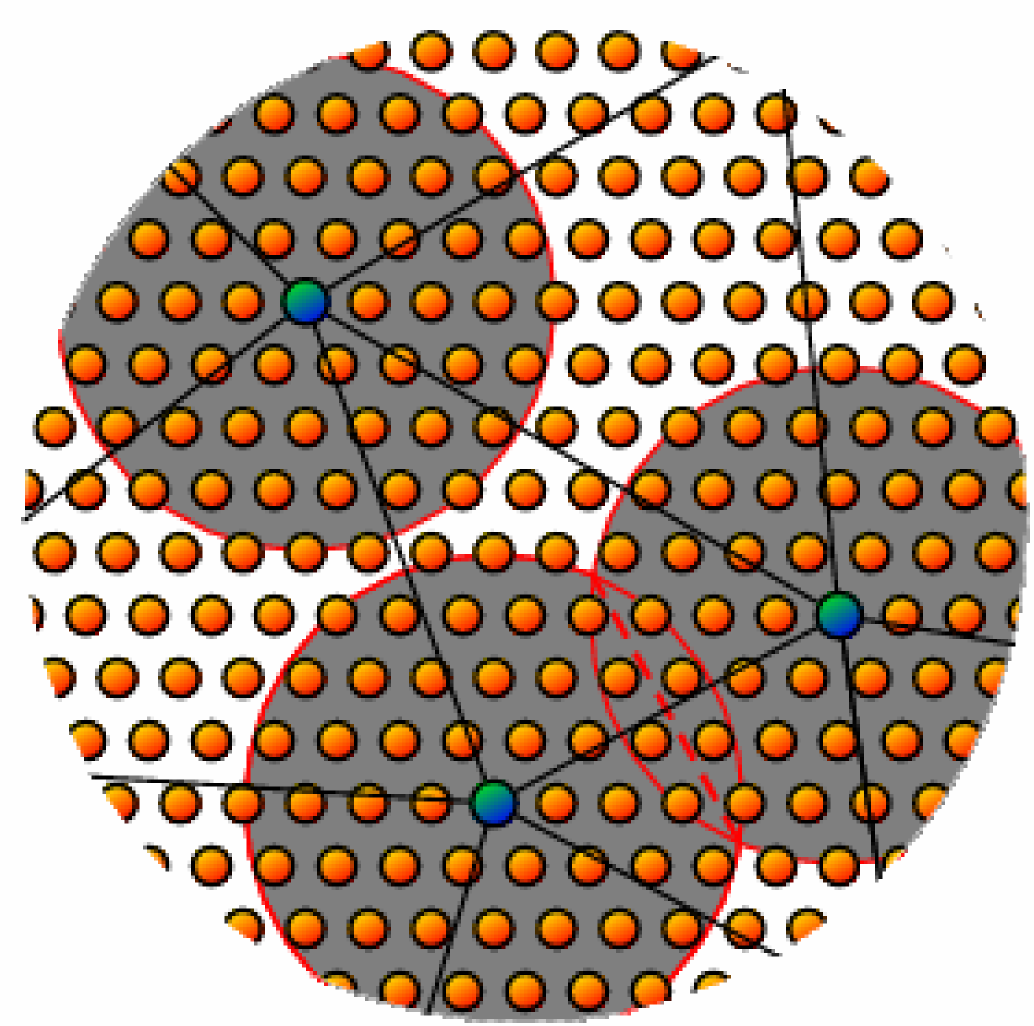
- Cluster summation rule:

$$S_h = \sum_{\boldsymbol{l}_h\in\mathcal{L}_h} n_h(\boldsymbol{l}_h) \sum_{\boldsymbol{l}\in\mathcal{C}(\boldsymbol{l}_h)} f(\boldsymbol{l}),$$

- $n_h(\boldsymbol{l}_h)$ chosen such that basis functions summed exactly.



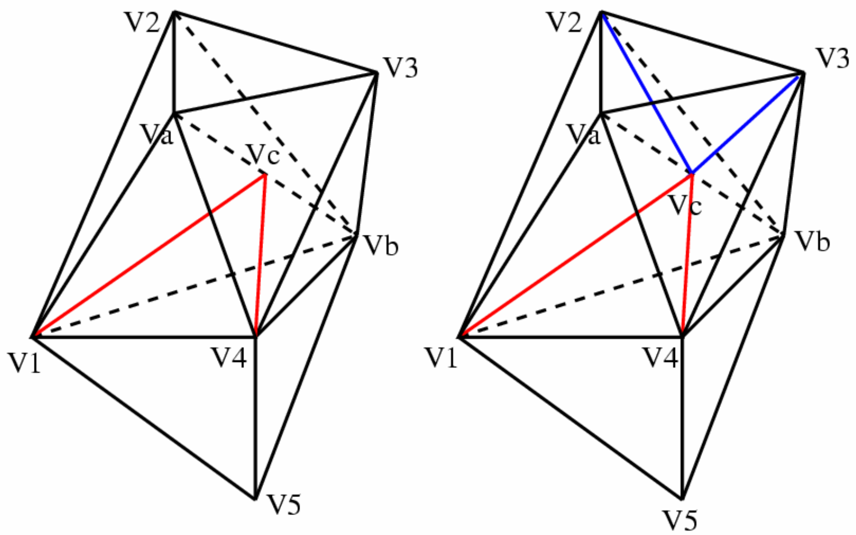
Quasicontinuum – Cluster sums



Merging of clusters near atomistic limit

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)

- TOL chosen s. t. dislocations have atomistic core.

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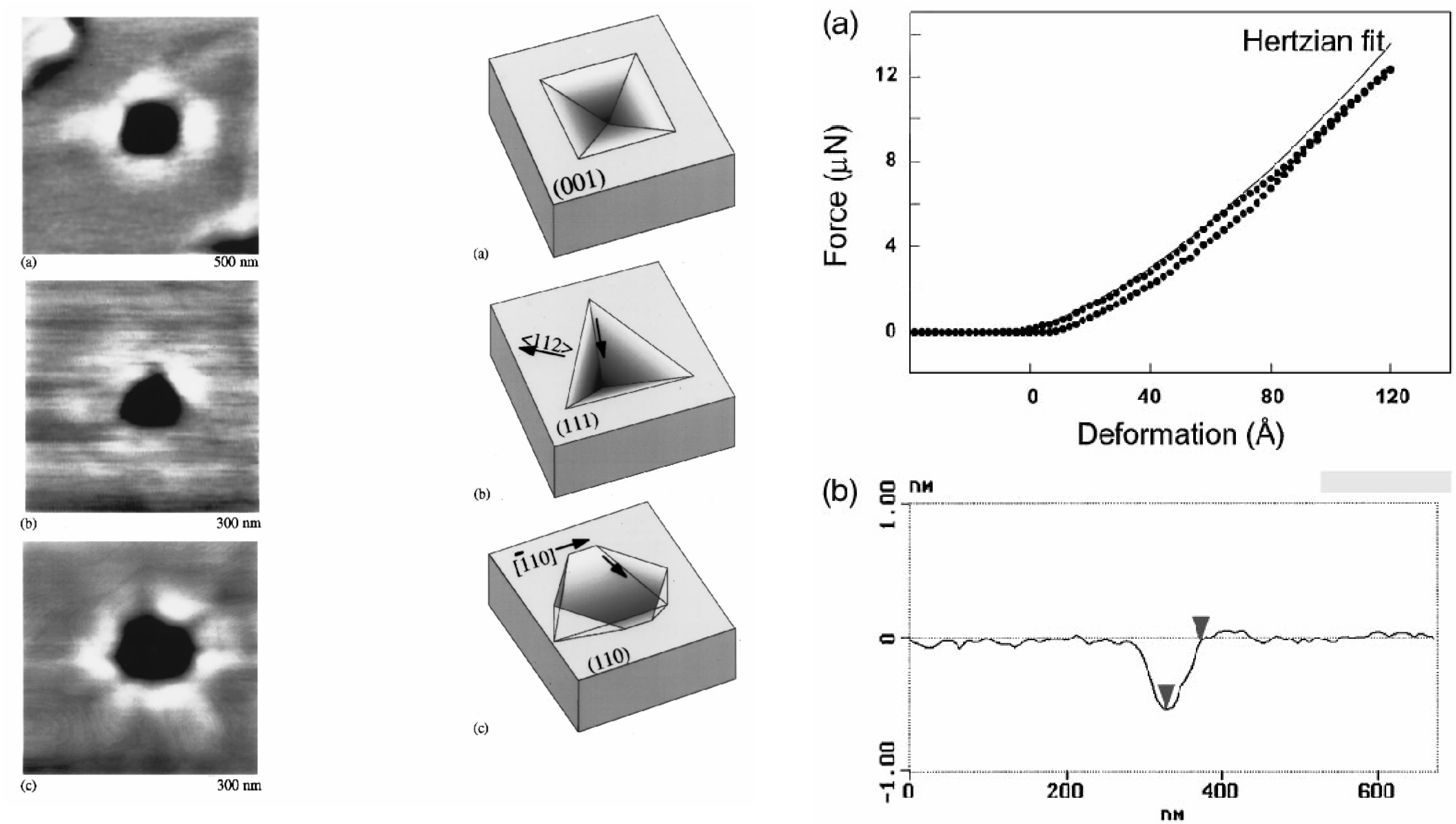
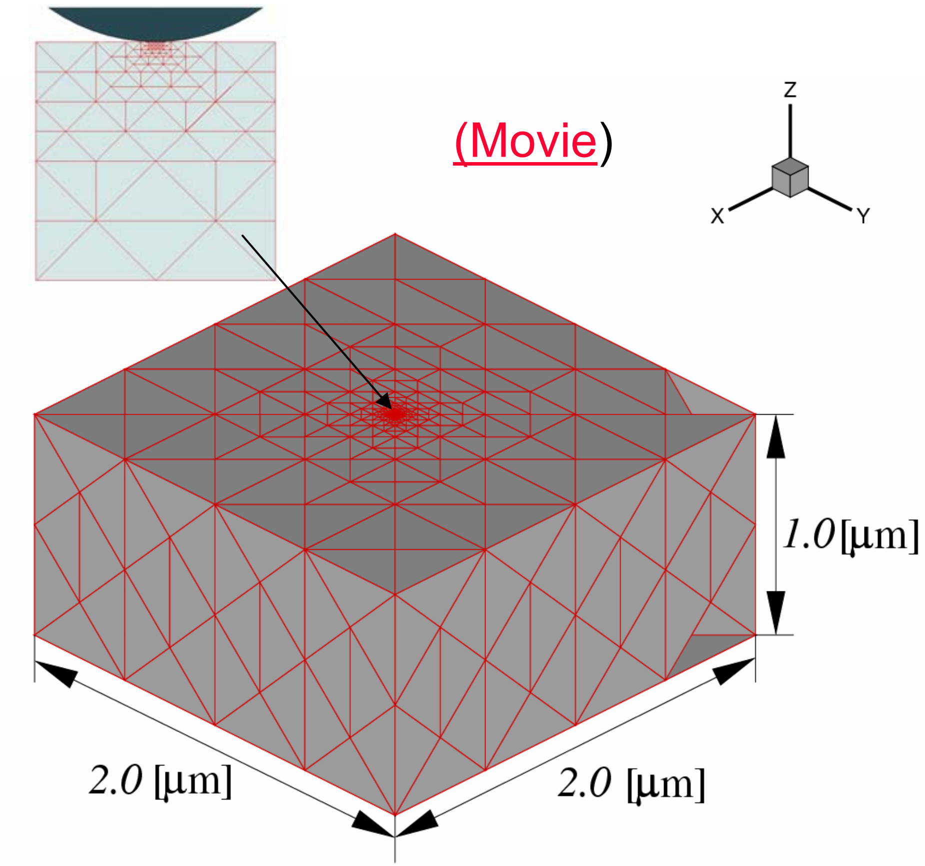
Nanoindentation of [001] Au



(Kiely and Houston, Phys. Rev. B, 1998)

QC - Nanoindentation of [001] Au

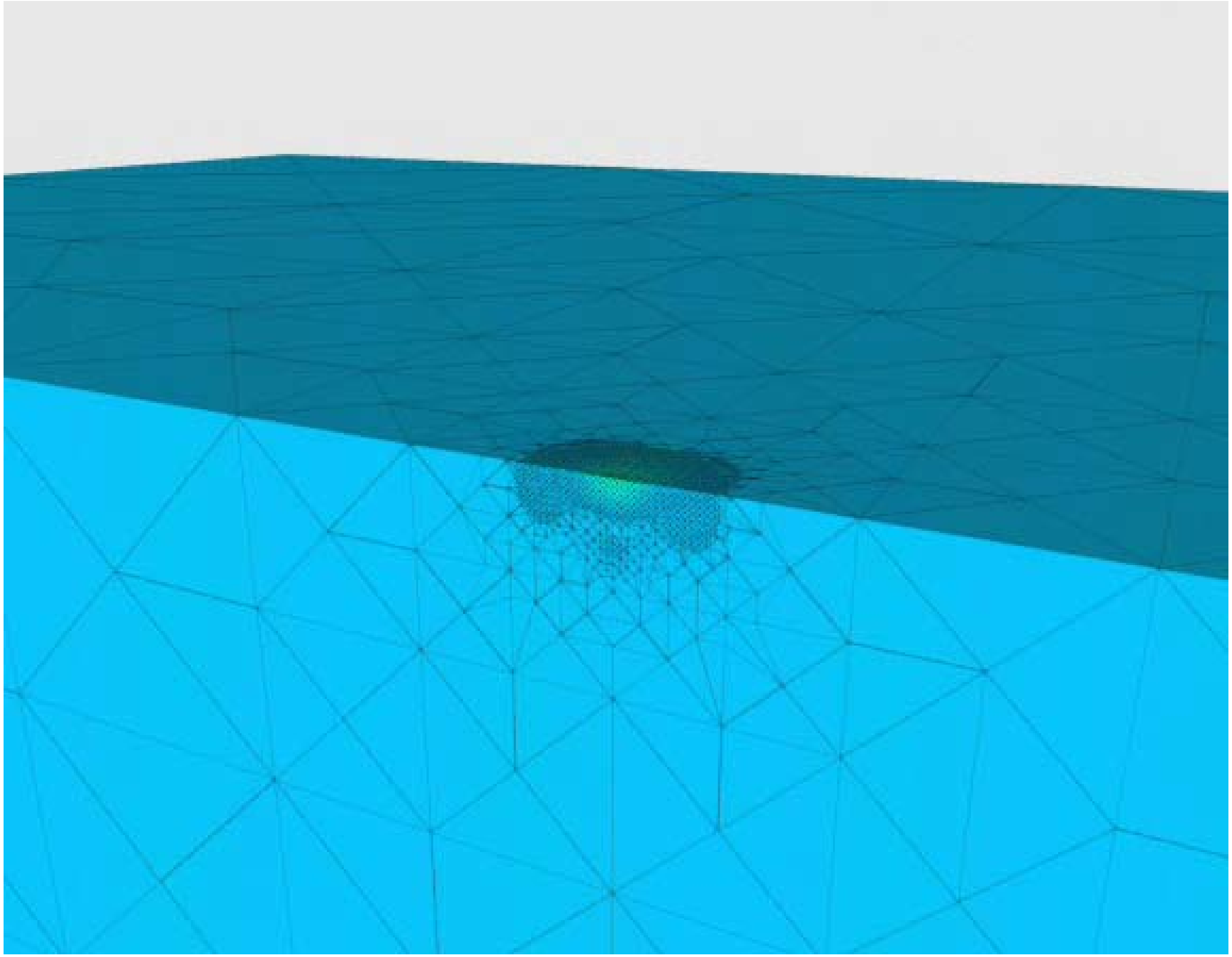


Detail of initial computational mesh

- 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

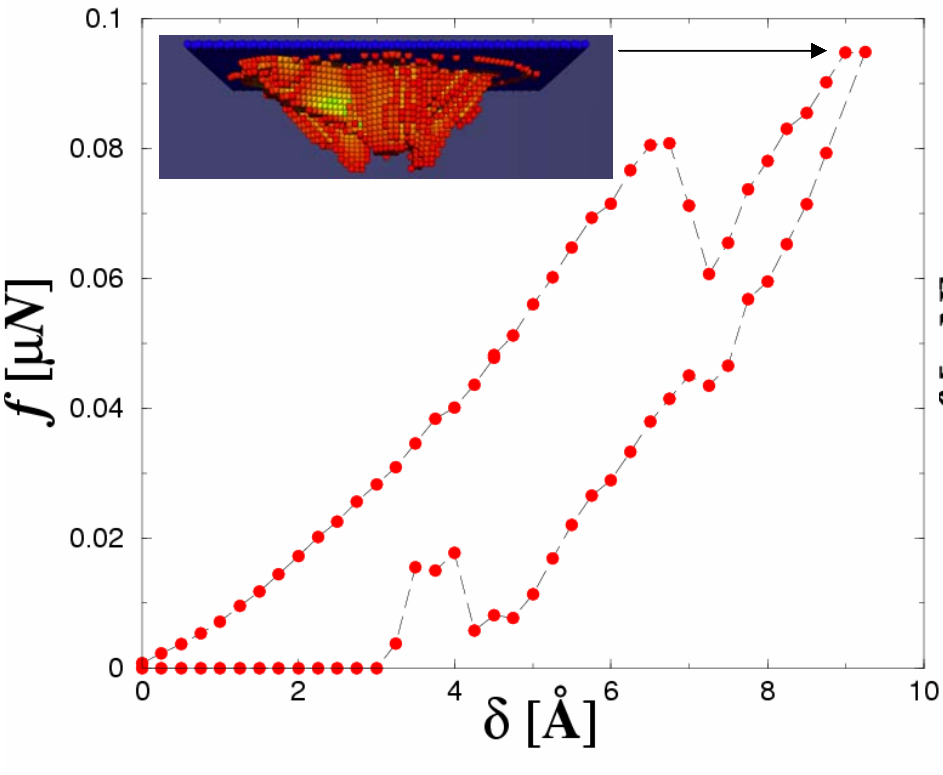
(Knap and Ortiz, *PRL* **90** 2002-226102)

QC - Nanoindentation of [001] Au

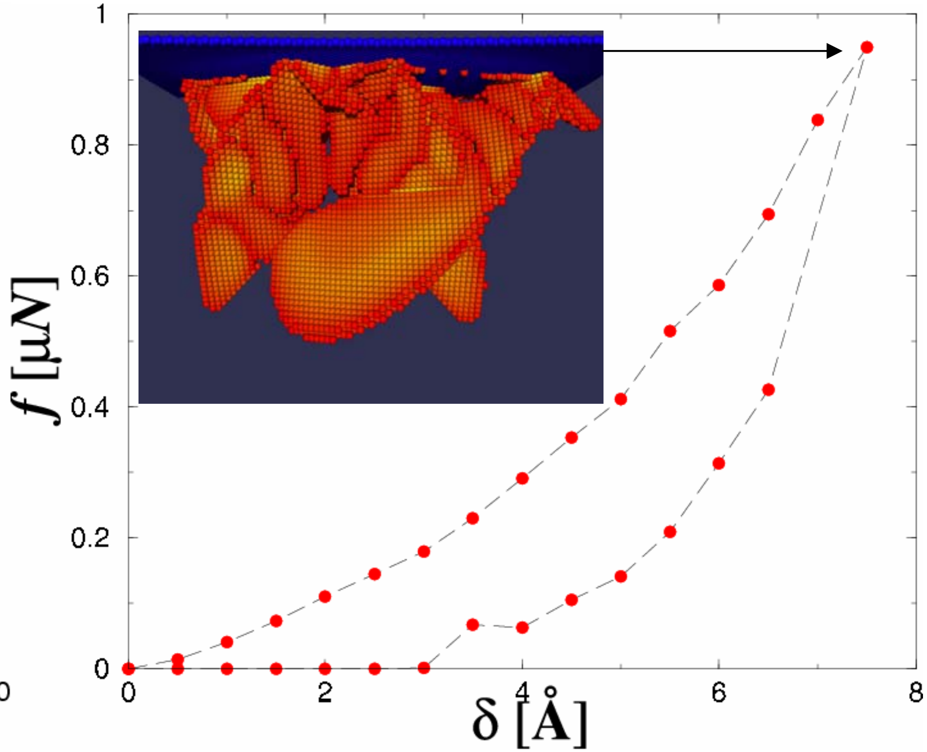


(Knap and Ortiz, *PRL* **90** 2002-226102)

QC - Nanoindentation of [001] Au

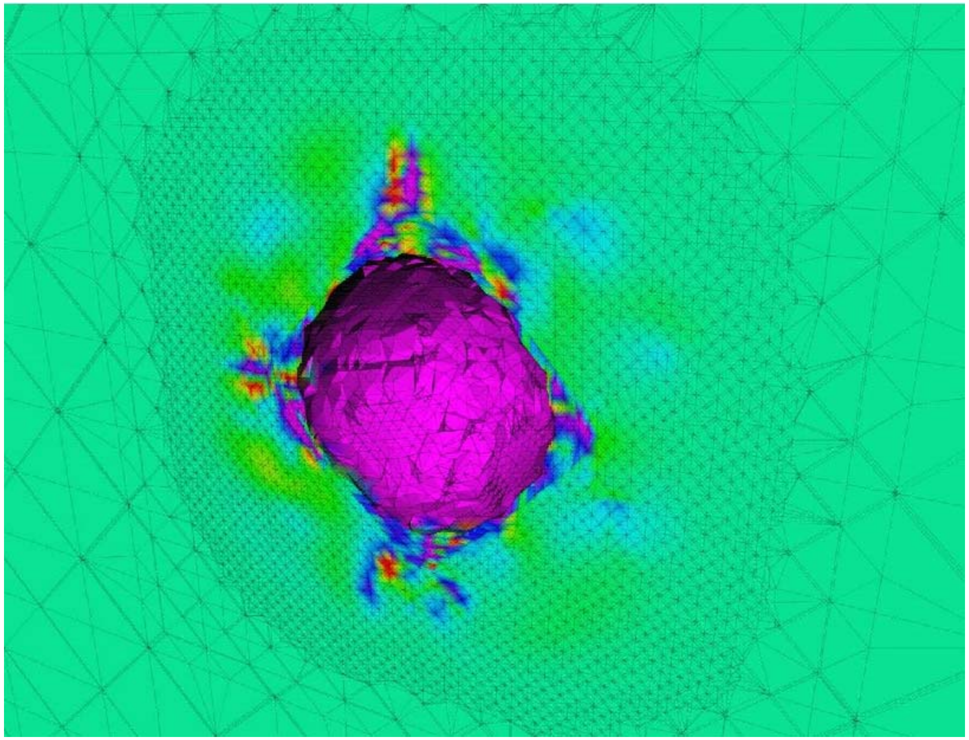


7 nm indenter,
depth = 0.92 nm



70 nm indenter,
depth = 0.75 nm

QC - Nanovoid cavitation in Al

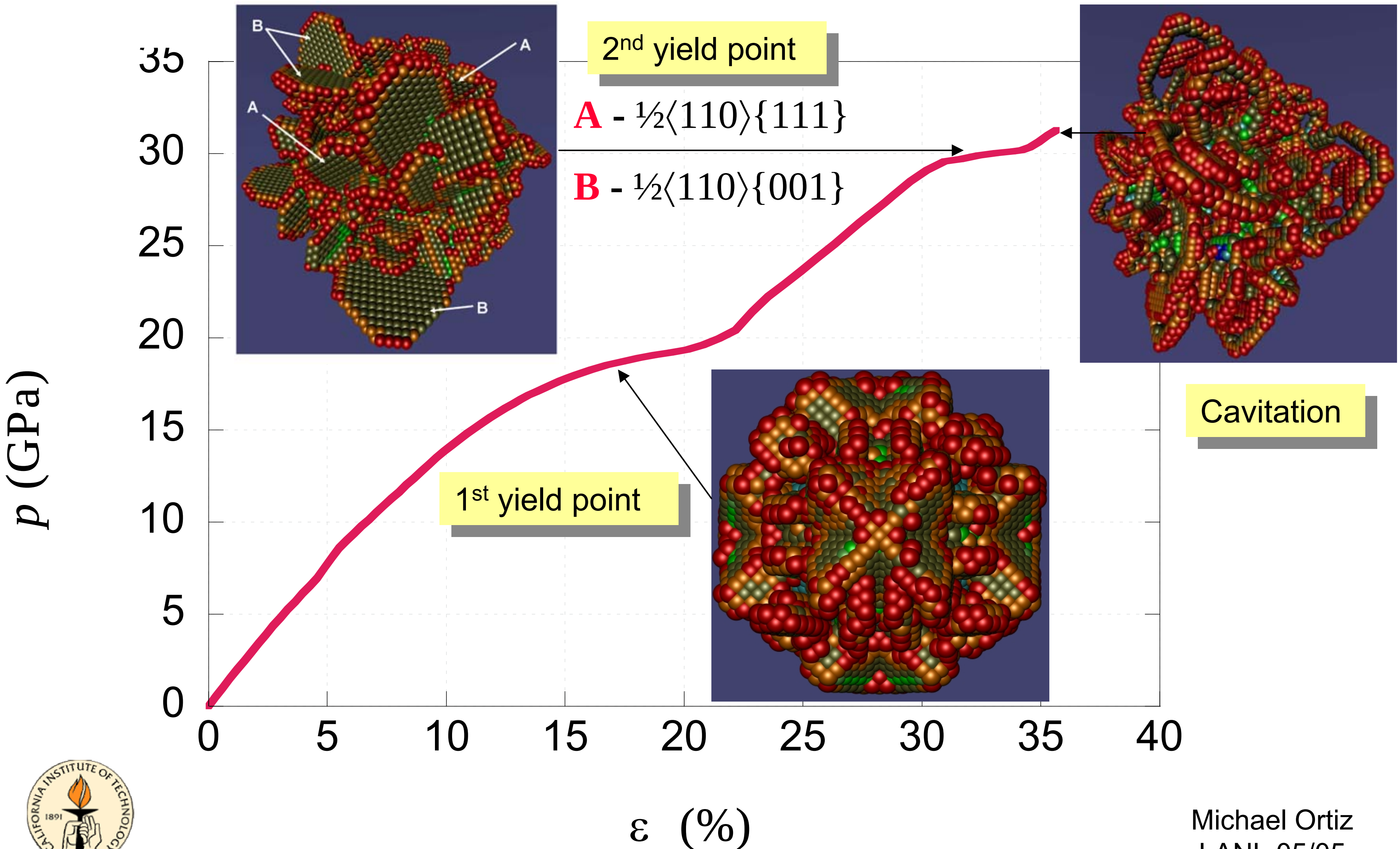


Close-up of internal void
and adapted mesh at ε_v=30.8%

- 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

QC calculations of nanovoid cavitation in EAM Al
(Marian, Knap and Ortiz, PRL ´04)

QC – Nanovoid cavitation in Al



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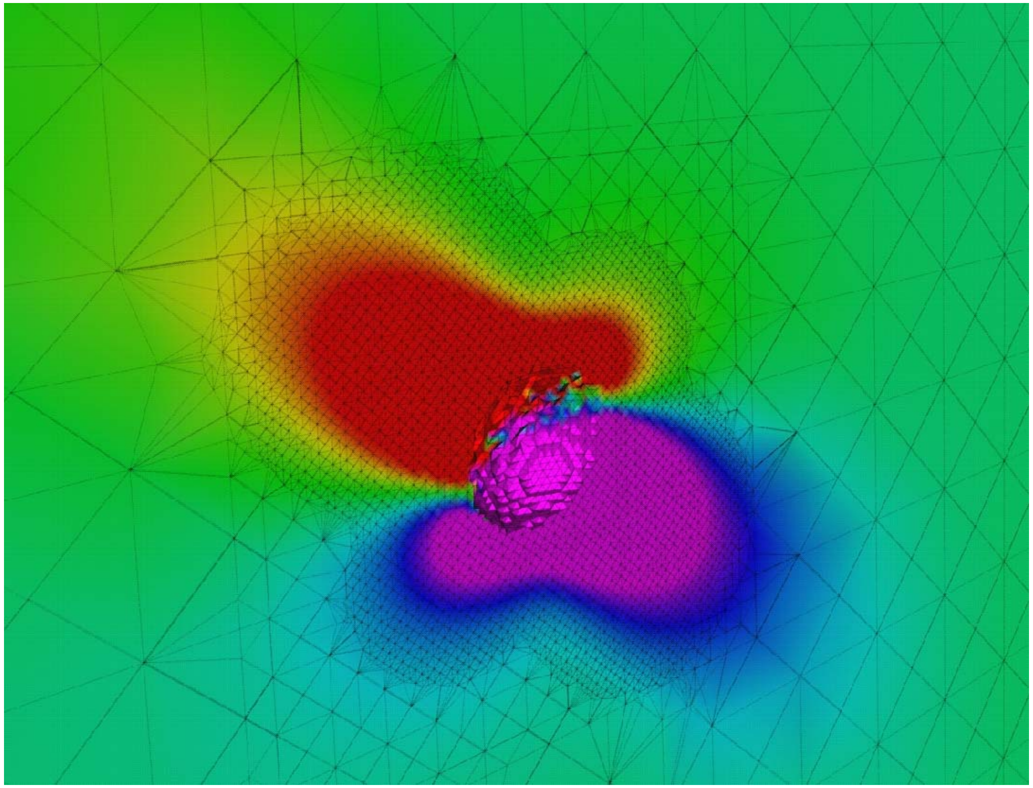
QC – Nanovoid shearing in Al

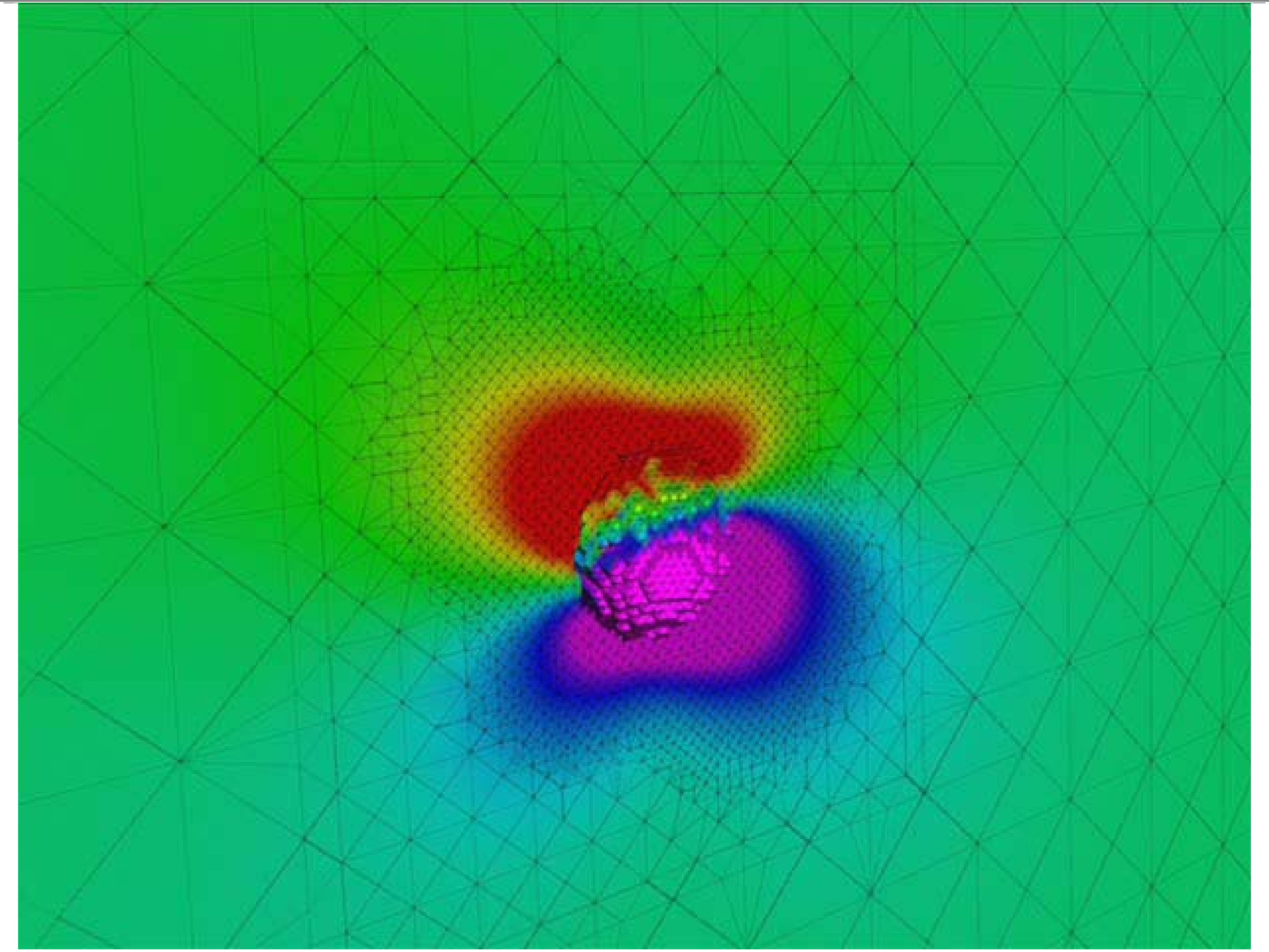


Close-up of internal void and adapted mesh at $\gamma = 12\%$

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

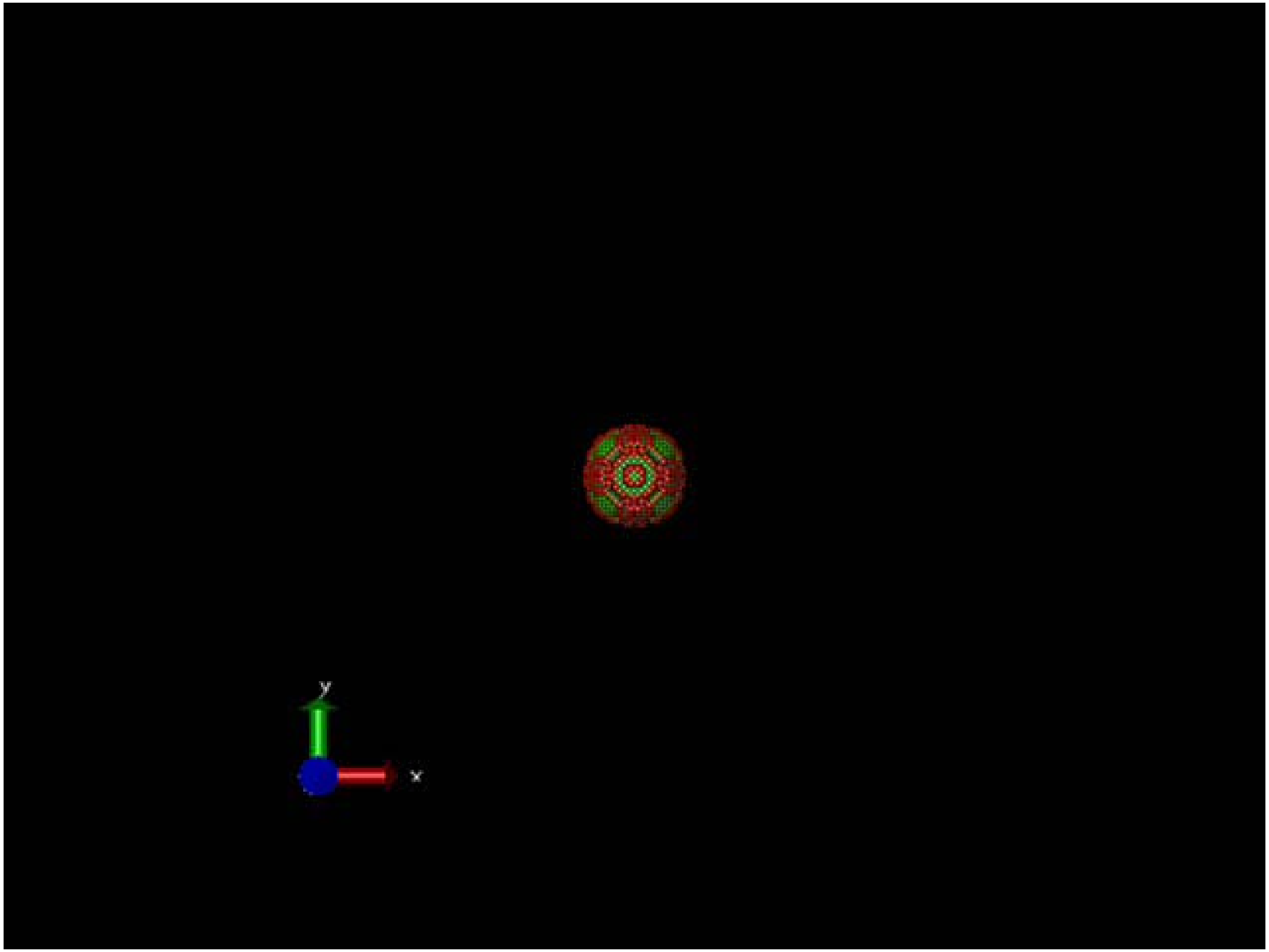
QC calculations of nanovoid shearing in EAM Al (J. Marian, J. Knap and M. Ortiz, '05)

QC – Nanovoid shearing in Al



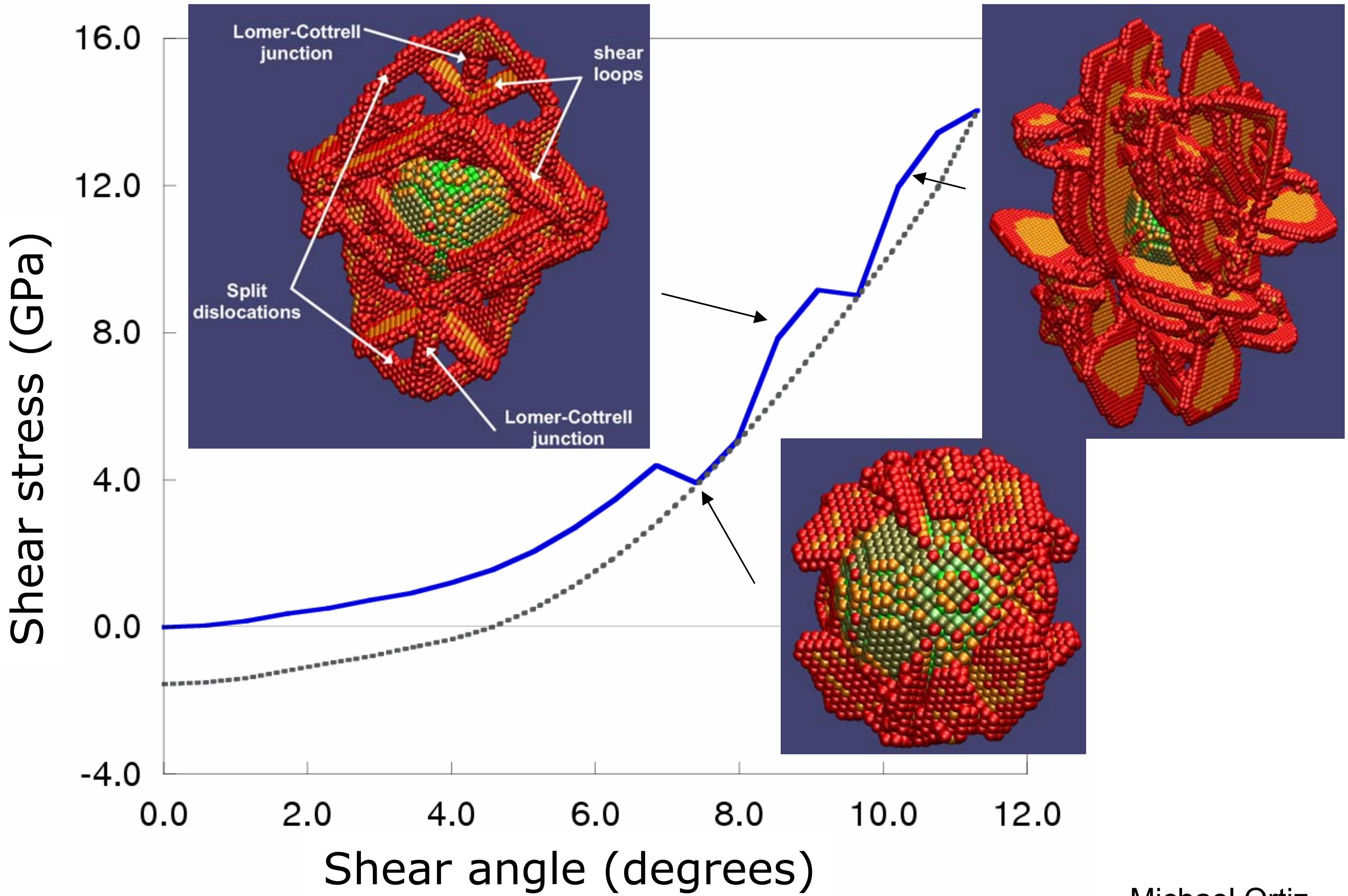
Evolution of adapted mesh

QC – Nanovoid shearing in Al



Evolution of dislocation structures

QC - Nanovoid cavitation in Al



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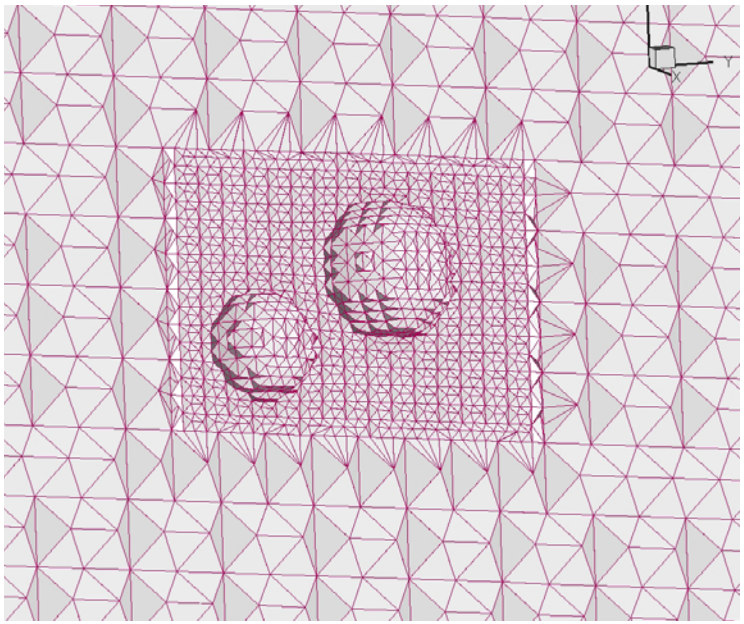
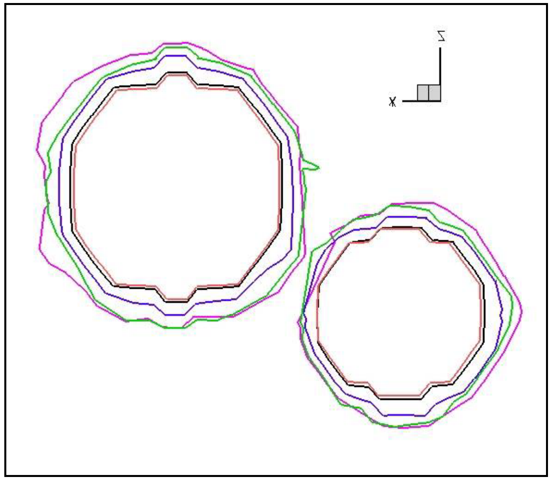
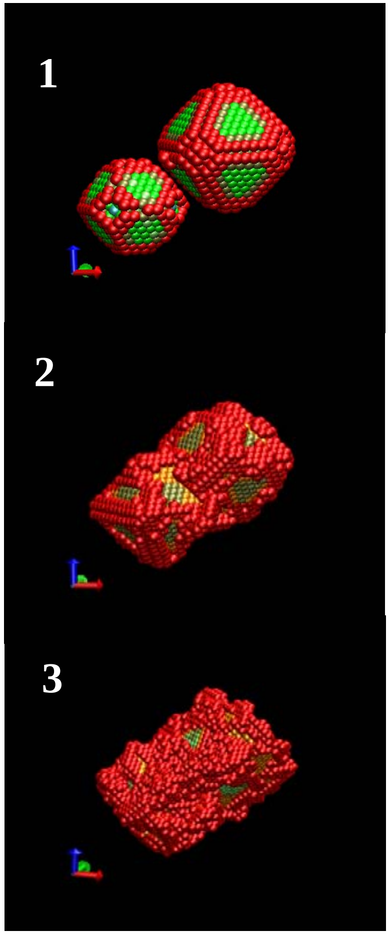
Nanovoid coalescence in Al



- **2 Spherical** (5 and 4-nm) **voids** under tri-axial tension





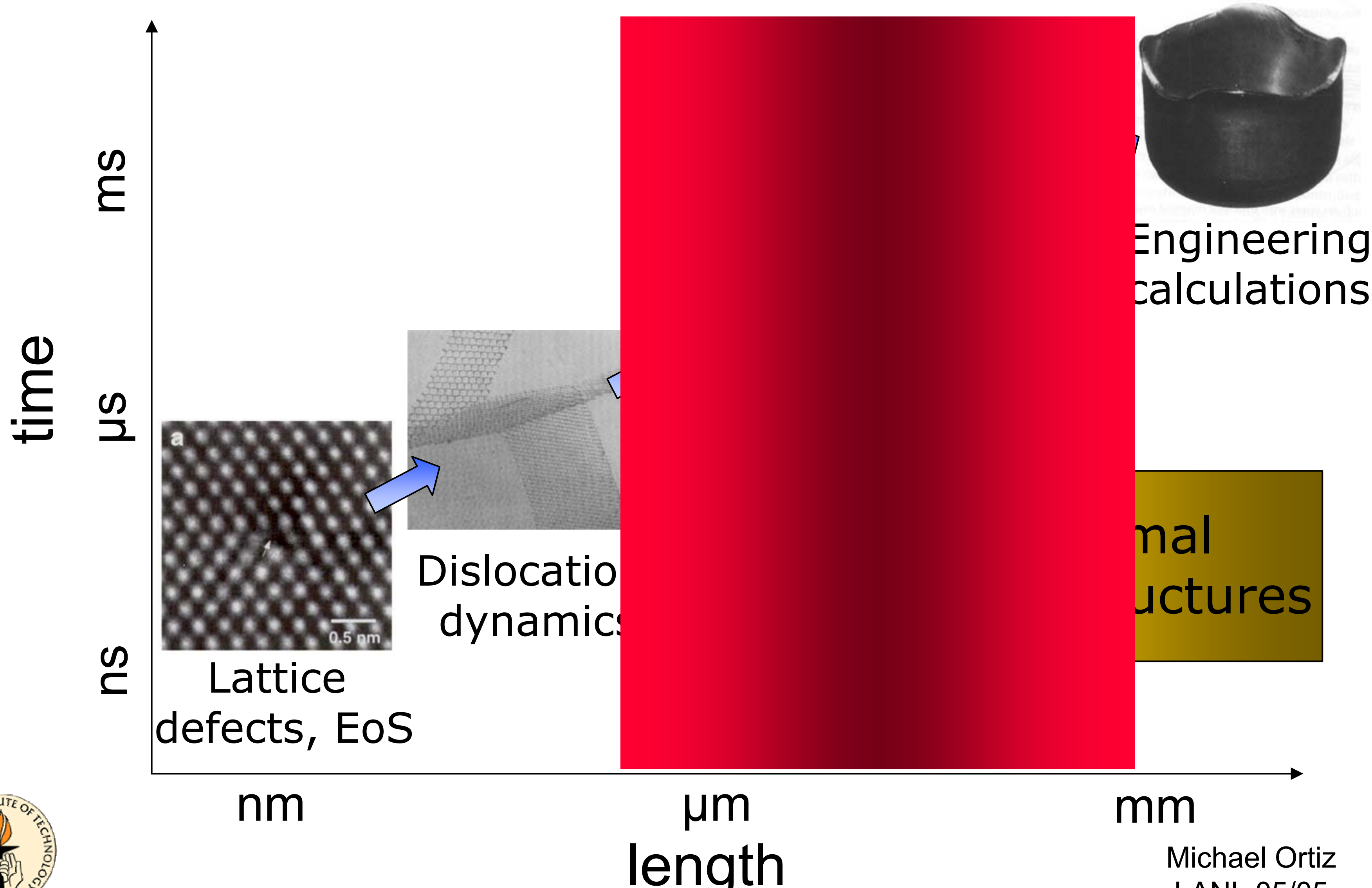
- Symmetry-breaking conditions
- Cavitation occurs at ~8 GPa (as opposed to 19 GPa for a single void)

(J. Marian, J. Knap and M. Ortiz, 2005)

Quasicontinuum – Outlook

- The Quasicontinuum method is an example of a bottom-up multiscale method based on:
  - *Coarse-graining (kinematic constraints)*
  - *Sampling (clusters)*
  - *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*

Top-down – Relaxation



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Framework – Calculus of variations

Problem. *For* $F : X \to \bar{\mathbb{R}}$, *find:*

$$\begin{cases} m_X(F) = \inf\limits_{u \in X} F(u) \\ M_X(F) = \{u \in X, \text{ s. t. } F(u) = m_X(X)\} \end{cases}$$

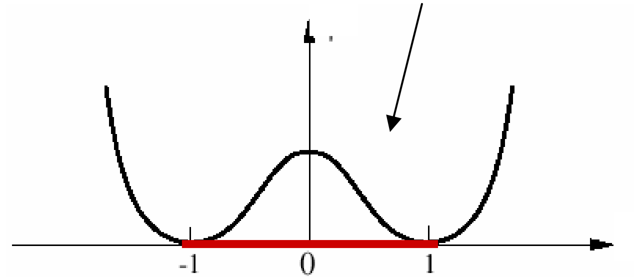
Theorem. *Let* $F : X \to \bar{\mathbb{R}}$ *be lower-semicontinuous and coercive. Then* F *has a minimum point in* X. *If, in addition,* F *is convex, then the minimizer is unique.*

- Many functions F of interest lack lower-semicontinuity $\Rightarrow$ inifimum not attained.
- Direct numerical solutions exhibit exceedingly slow or no convergence!

Lack of l.s.c. and microstructure

Example. $X = W_0^{1,\infty}([0,1])$,

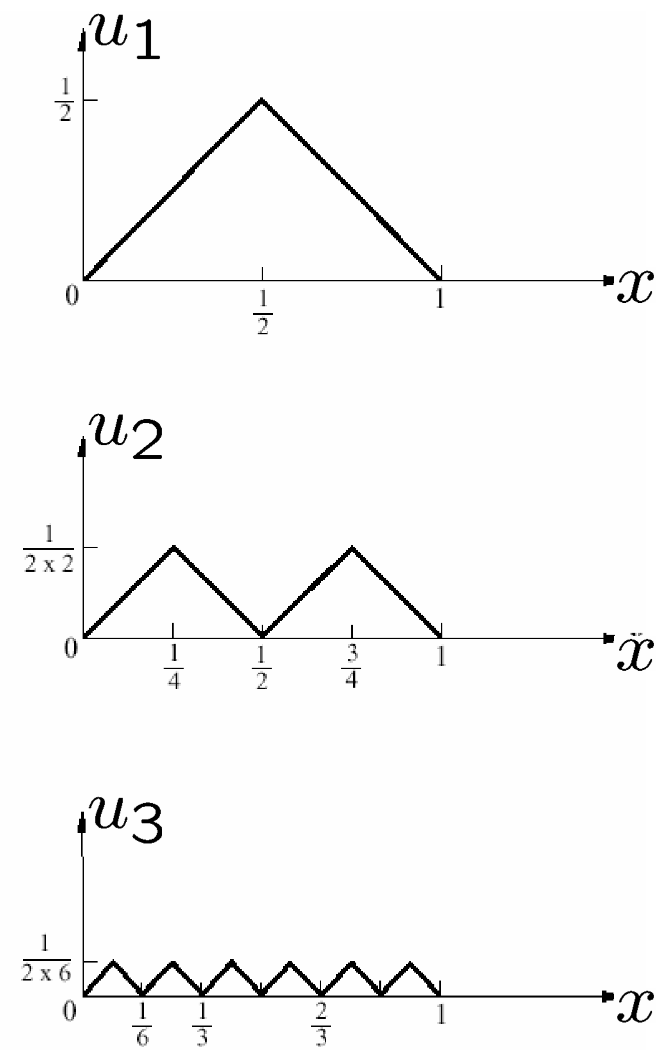
$$F(u) = \int_0^1 [u^2 + \underbrace{(u_x^2 - 1)^2}] \, dx$$



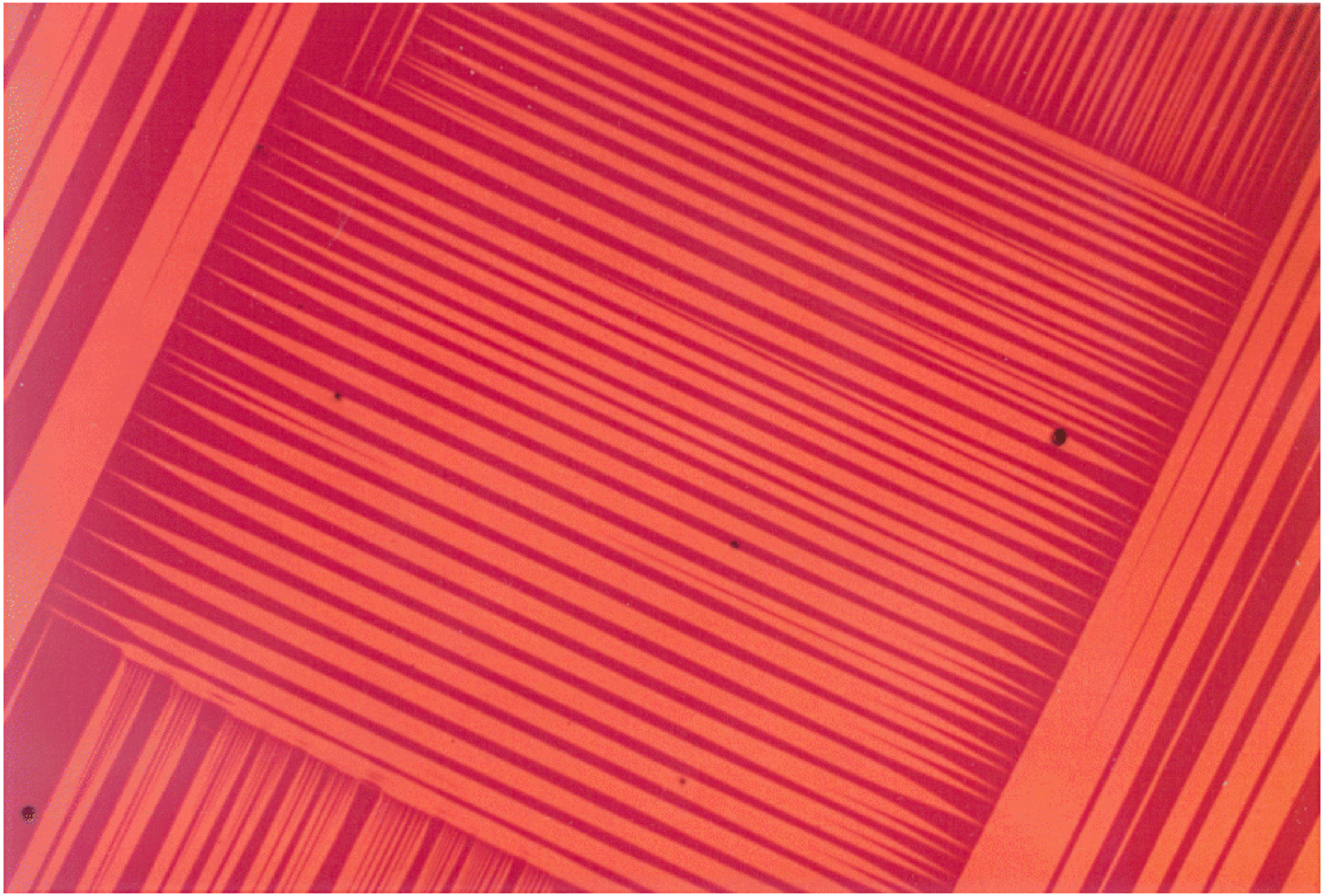
$$\exists u_j \rightharpoonup 0 \text{ in } W_0^{1,\infty}([0,1])$$

$$u_j \to 0 \text{ in } L^2([0,1])$$

$$\text{s. t. } F(u_j) \to 0 \leq F(0) = 1$$

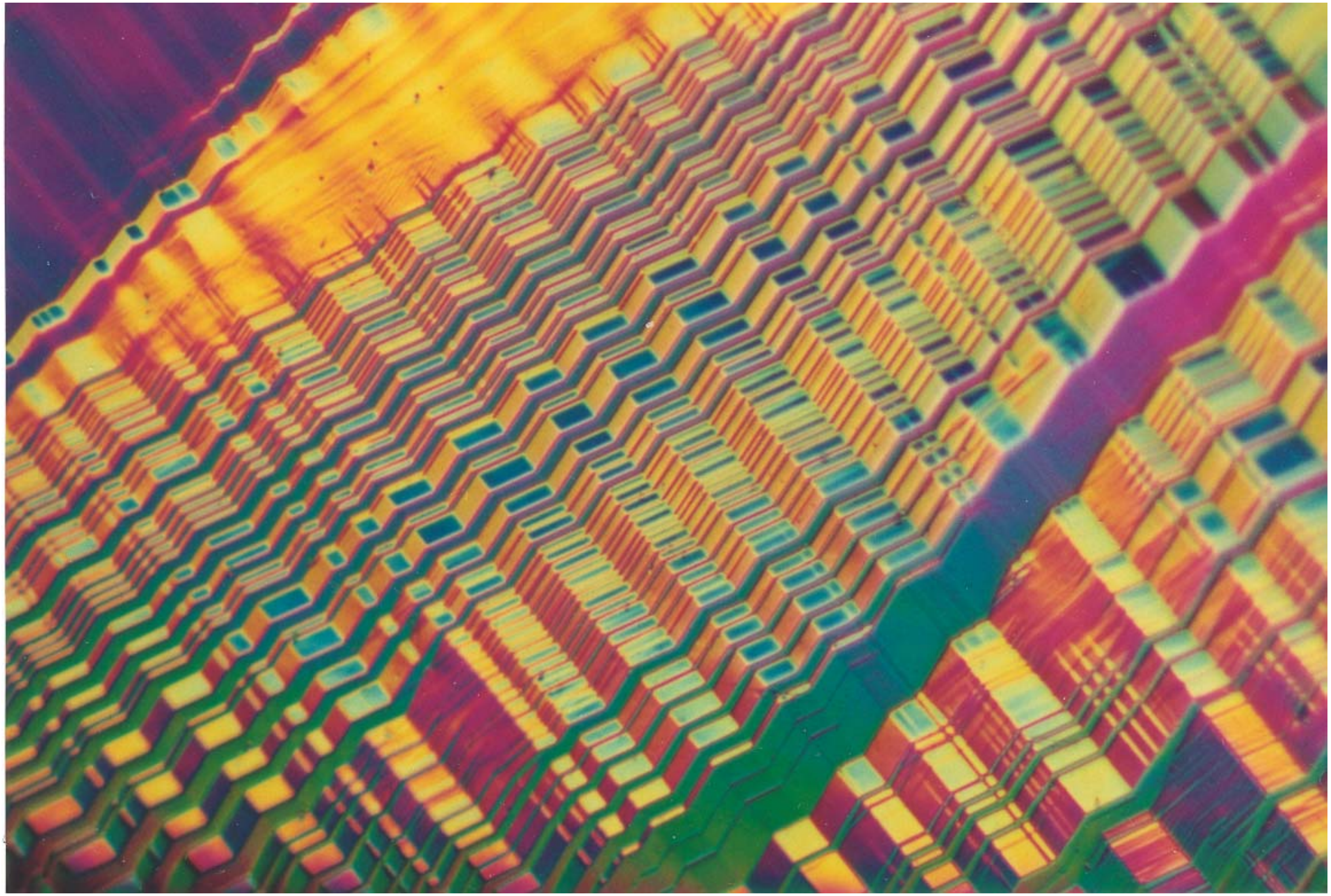


Microstructure of martensite in Cu-Al-Ni



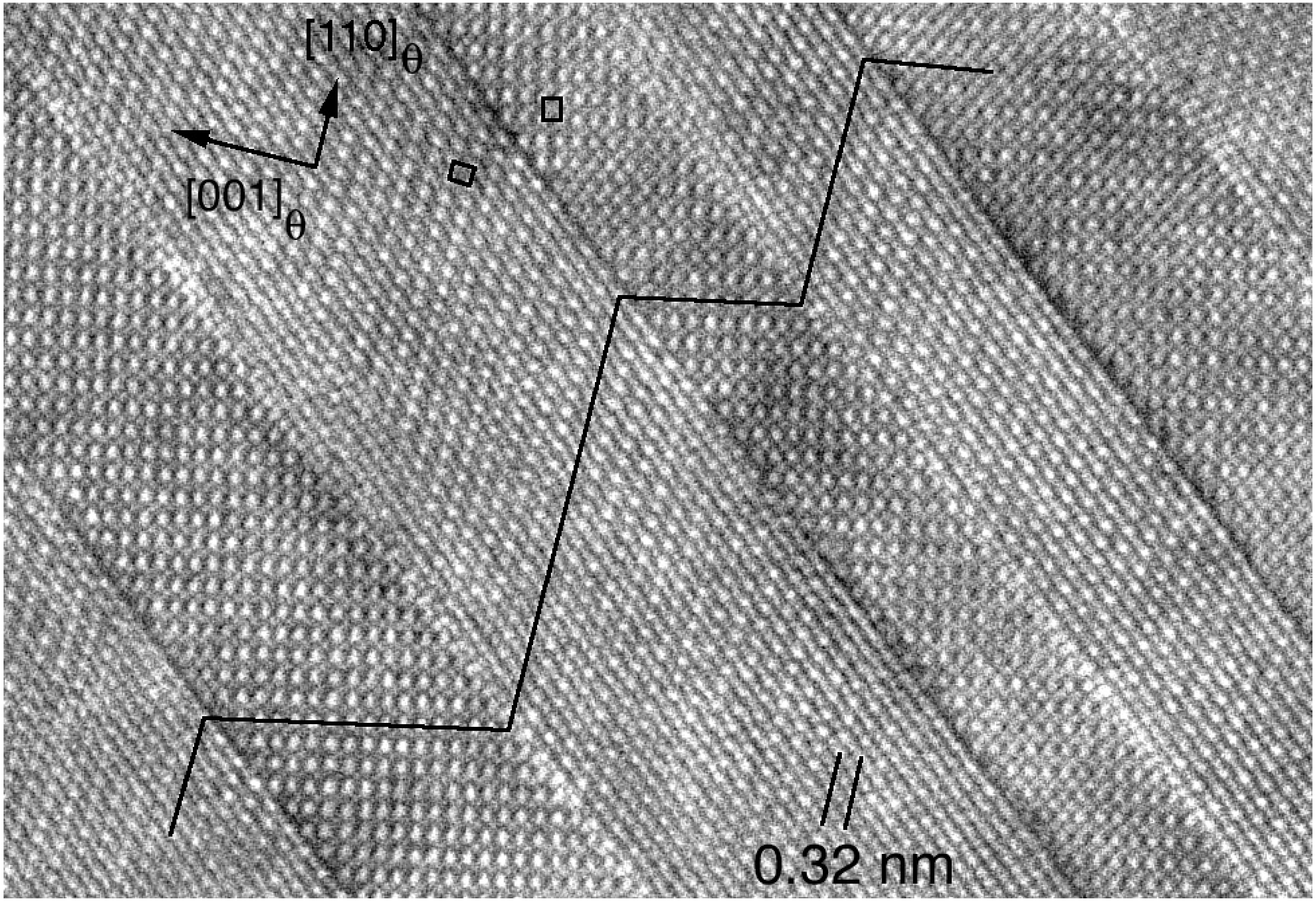
Cu-Al-Ni, C. Chu and R. D. James

Microstructure of martensite in Cu-Al-Ni



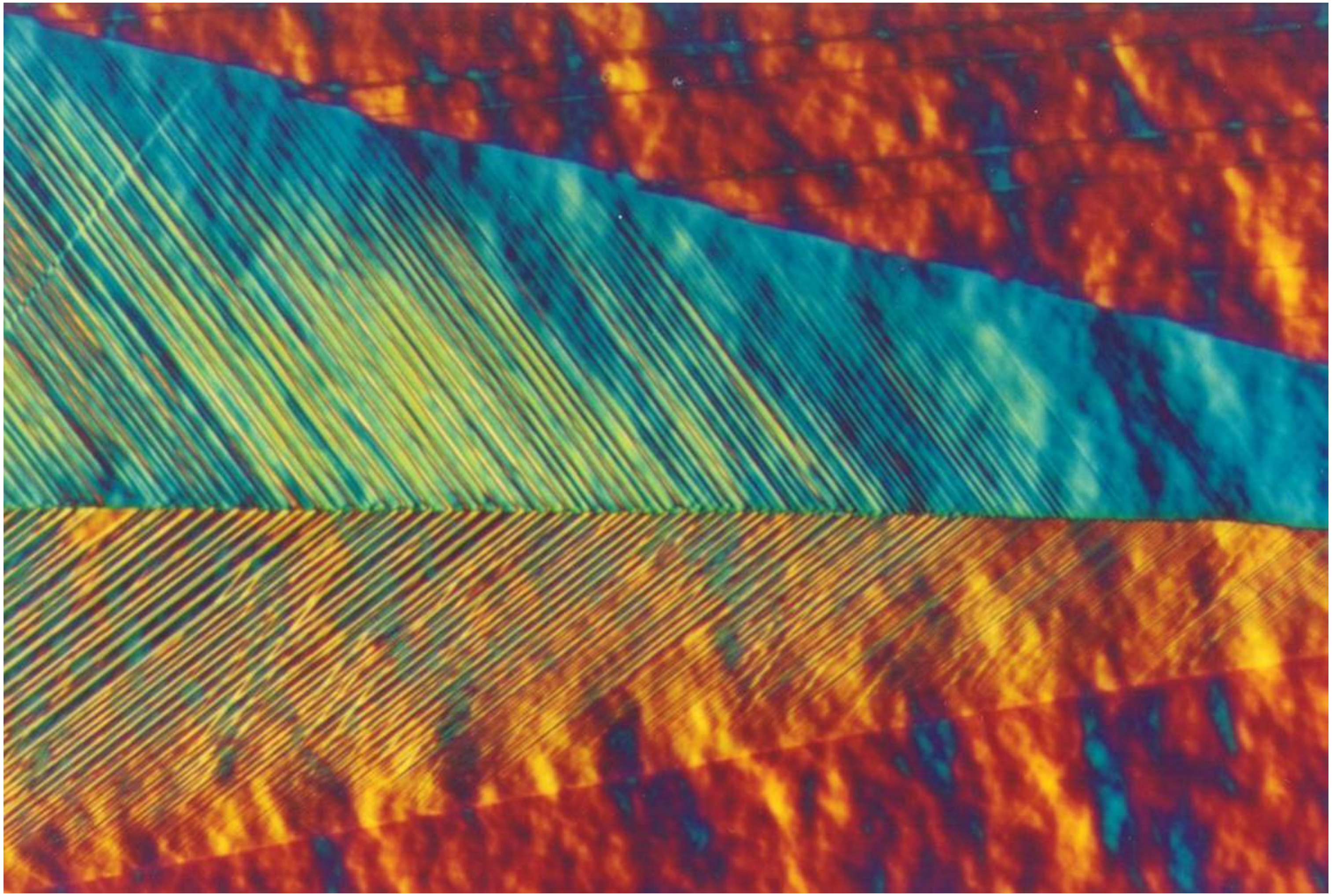
Cu-Al-Ni, C. Chu and R. D. James

Fine twins in Ni-Al



Ni-Al, Dominique Schryvers

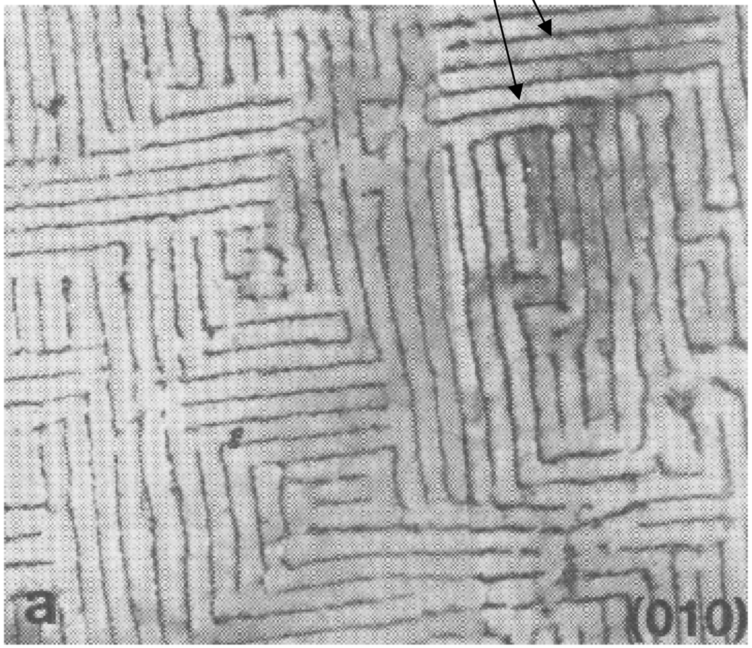
Wedge-like microstructure in Cu-Al-Ni



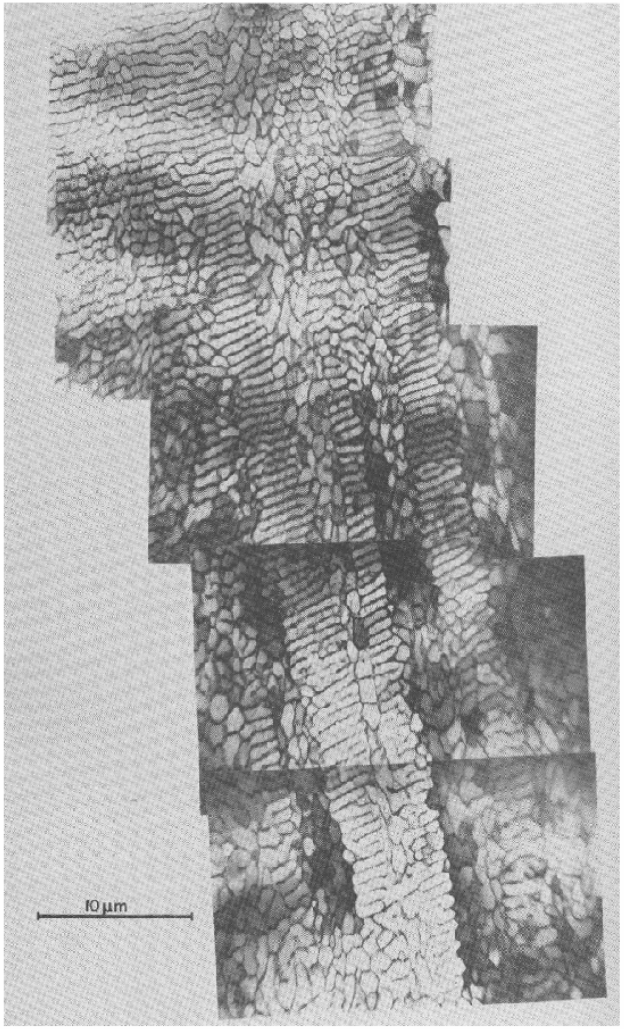
Cu-Al-Ni, C. Chu and R. D. James

Subgrain dislocation structures - Fatigue

Dipolar dislocation walls



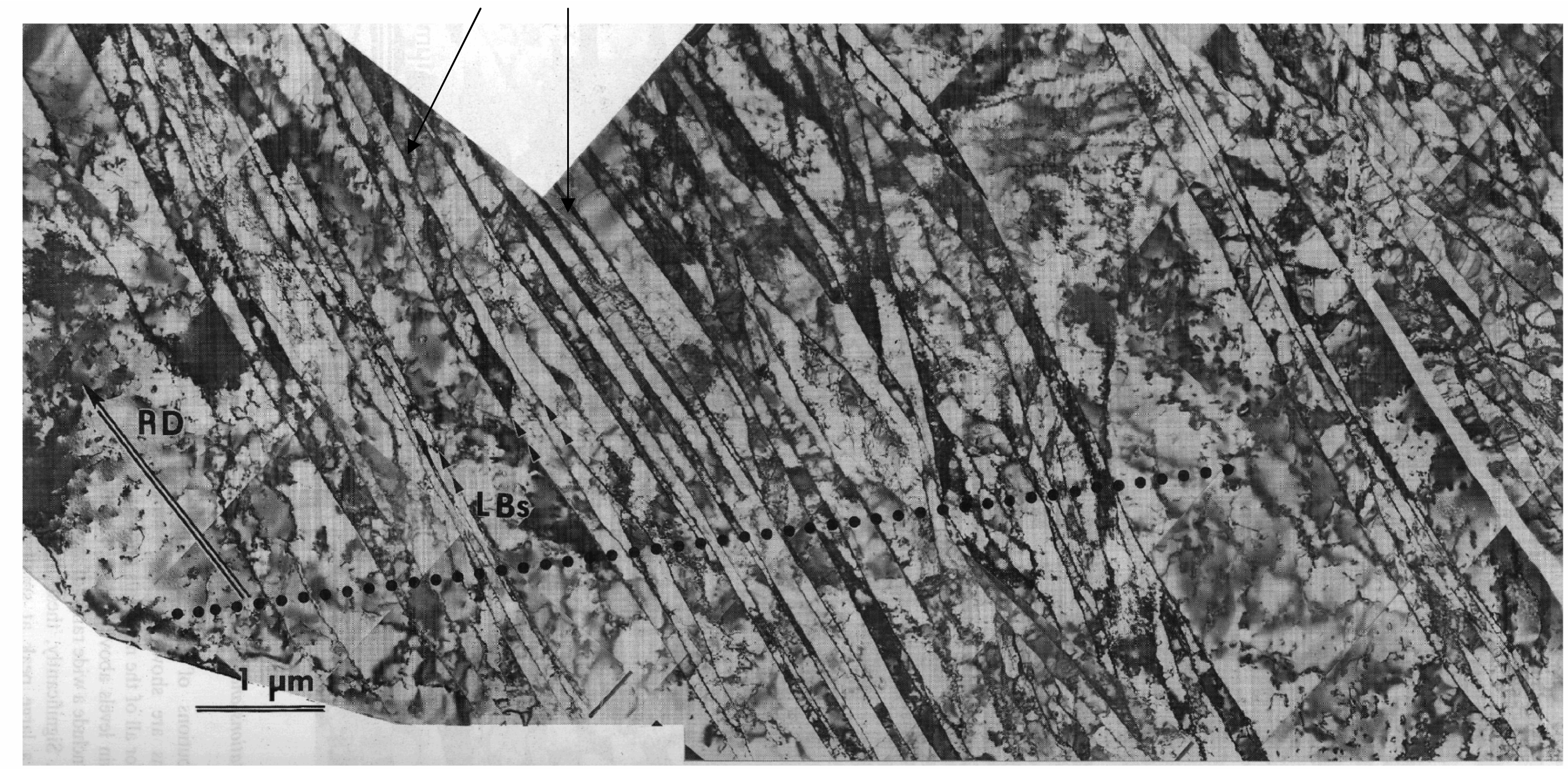
Labyrinth structure in fatigued copper single crystal (Jin and Winter, 1984)



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

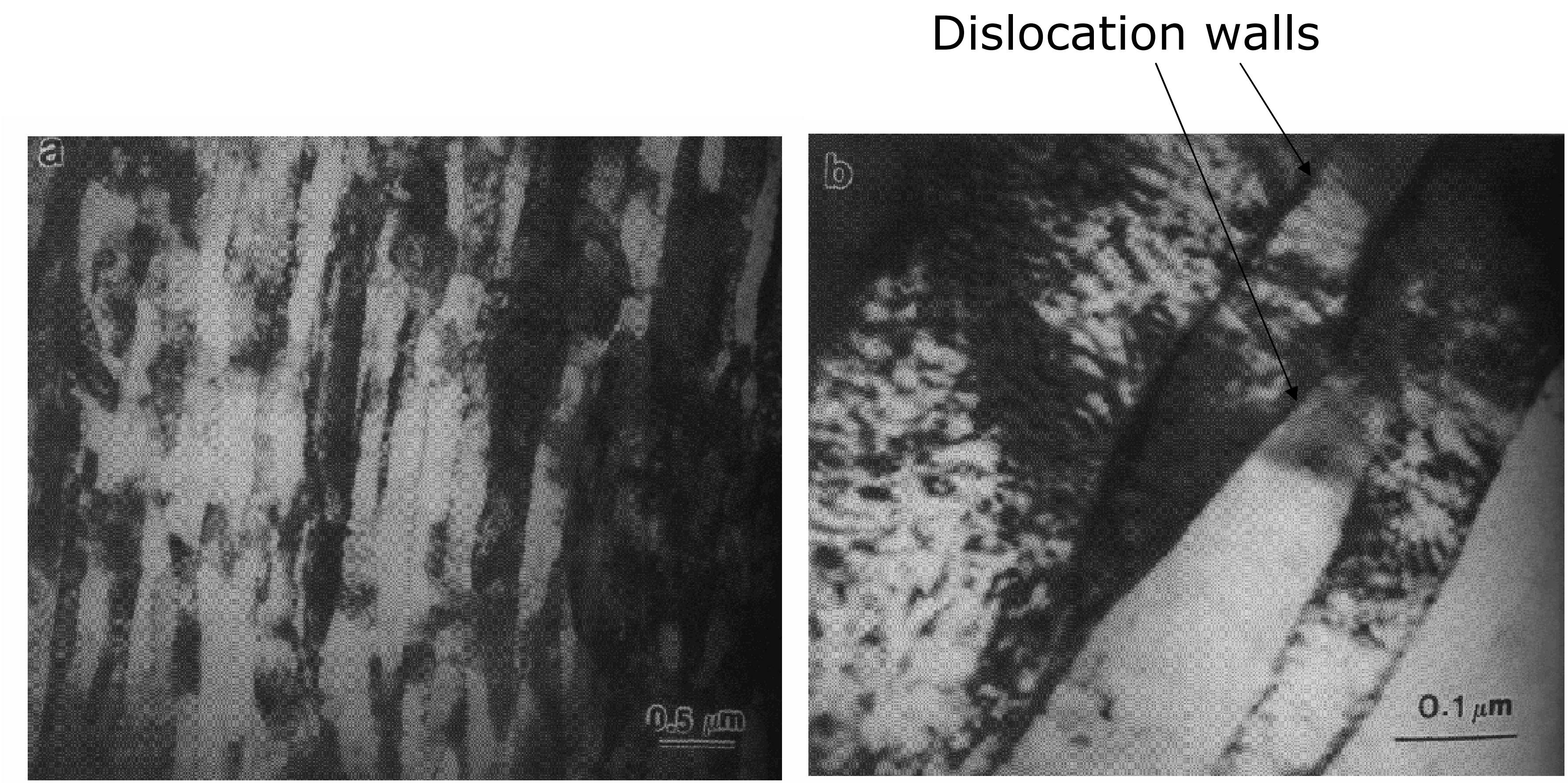
Subgrain dislocation structures - Static

Dislocation walls



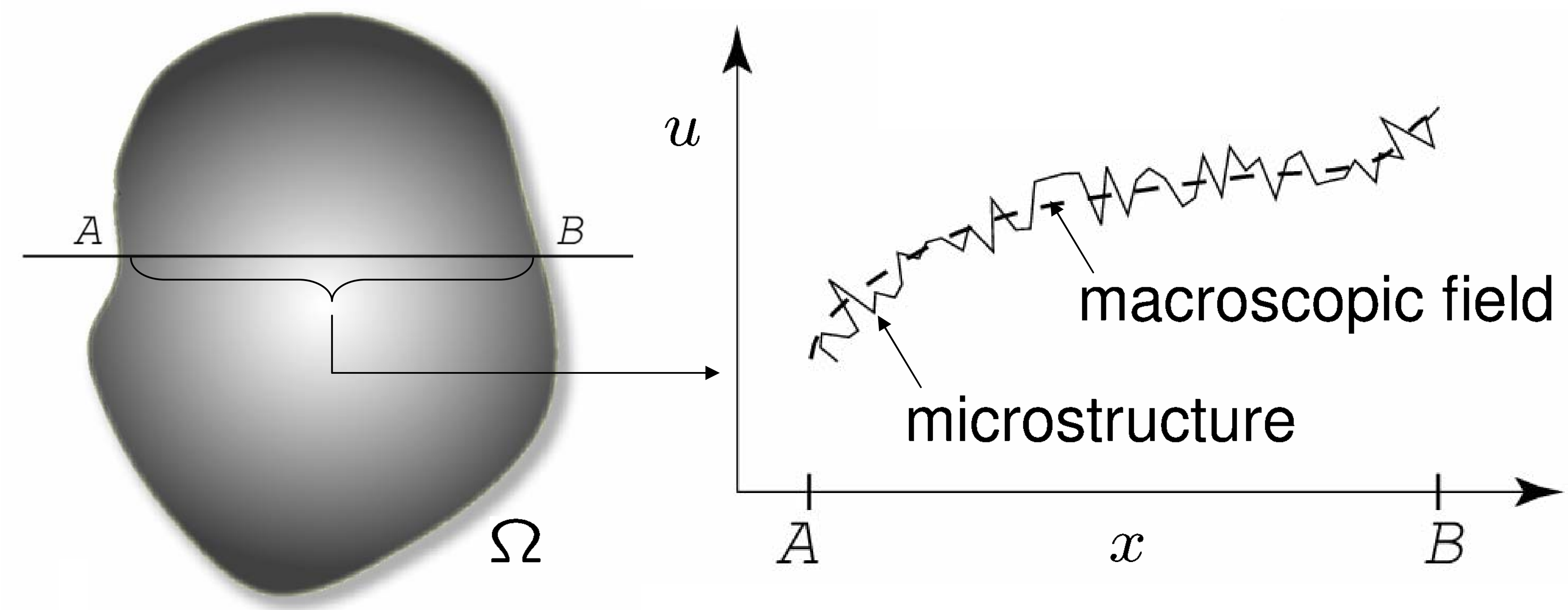
90% cold rolled Ta (Hughes and Hansen, 1997)

Subgrain dislocation structures - Shock



Shocked Ta (Meyers et al., 1995)

Relaxation



- Separation of scales, two coupled problems:
  - ***Relaxed problem***: *Well posed, determines macroscopic field, e.g., by finite-element analysis.*
  - ***Relaxation problem***: *Determines microstructure, effective energetics, at the* ***subgrid*** *level*

Relaxation

- Lower semicontinuous envelop:

  $sc^- F$ = Largest lsc function $\leq F$

- Relaxed problem: $m_X(F) = \inf_{u \in X} sc^- F(u)$

- Functions of integral form: $F(u) = \int_\Omega W(\nabla u)\, dx$

- Then: $sc^- F(u) = \int_\Omega QW(\nabla u)\, dx,$ where

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

is the *quasiconvex* envelop of W.

Relaxation

Theorem. *Let* $F : X \to \bar{\mathbb{R}}$ *be coercive. Then:*

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

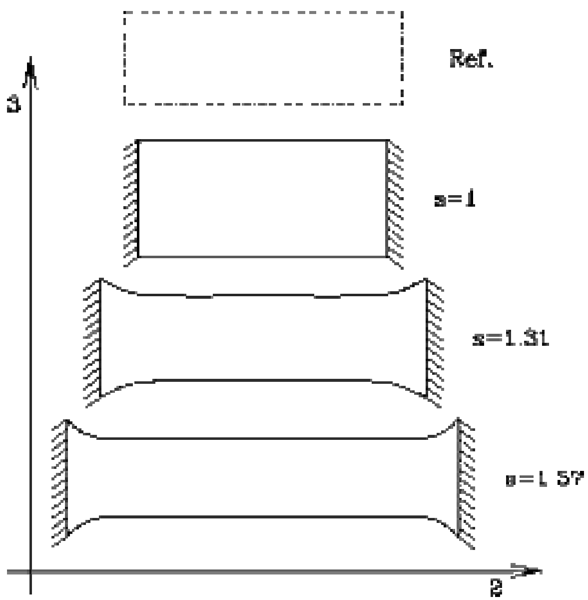
(ii) $sc^- F$ *has a minimum point in* X.

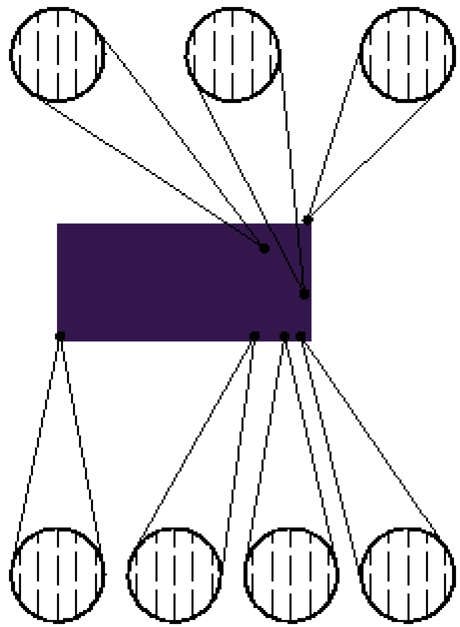
(iii) $\min_{u \in X} sc^- F(u) = \inf_{u \in X} F(u)$.

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

(v) If, in addition, X *is first-countable, then every minimum point of* $sc^- F$ *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)

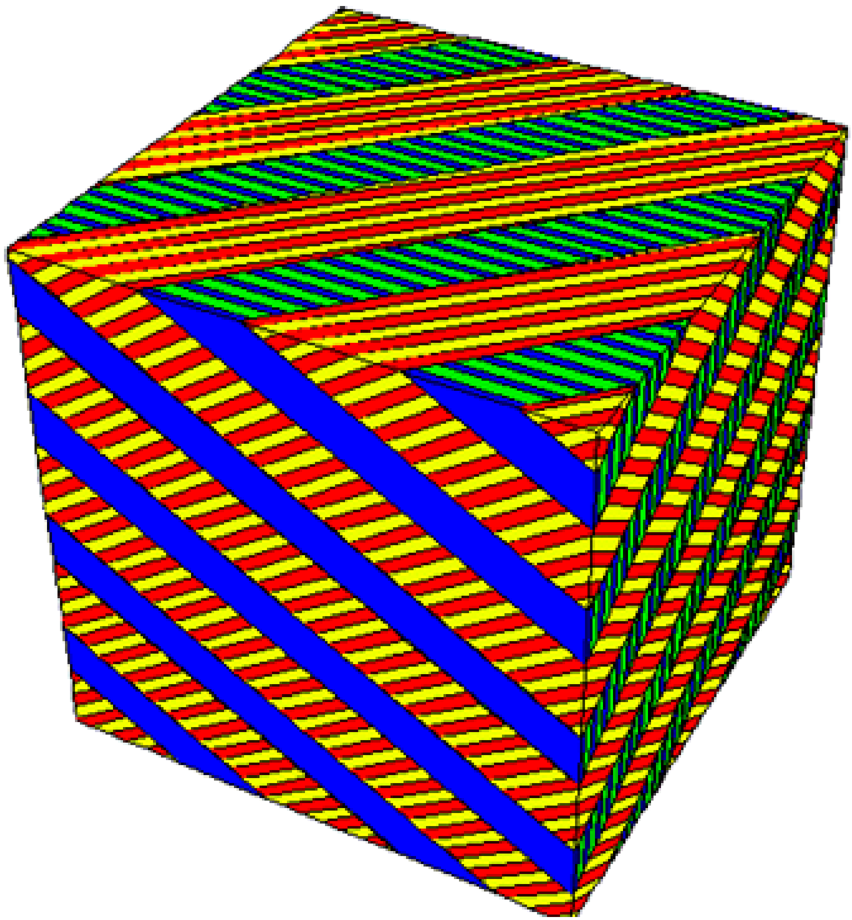
$$W(F,n) = A\,\mathrm{tr}(FF^T) - B\,||F^T n||^2$$

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

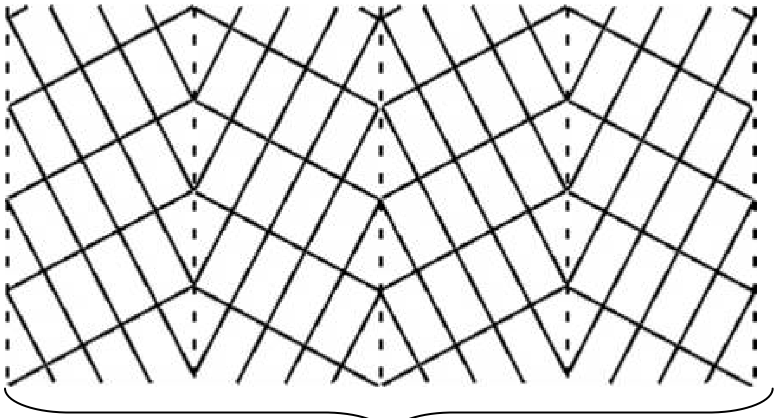
Relaxation

- 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)*

Relaxation – Sequential lamination



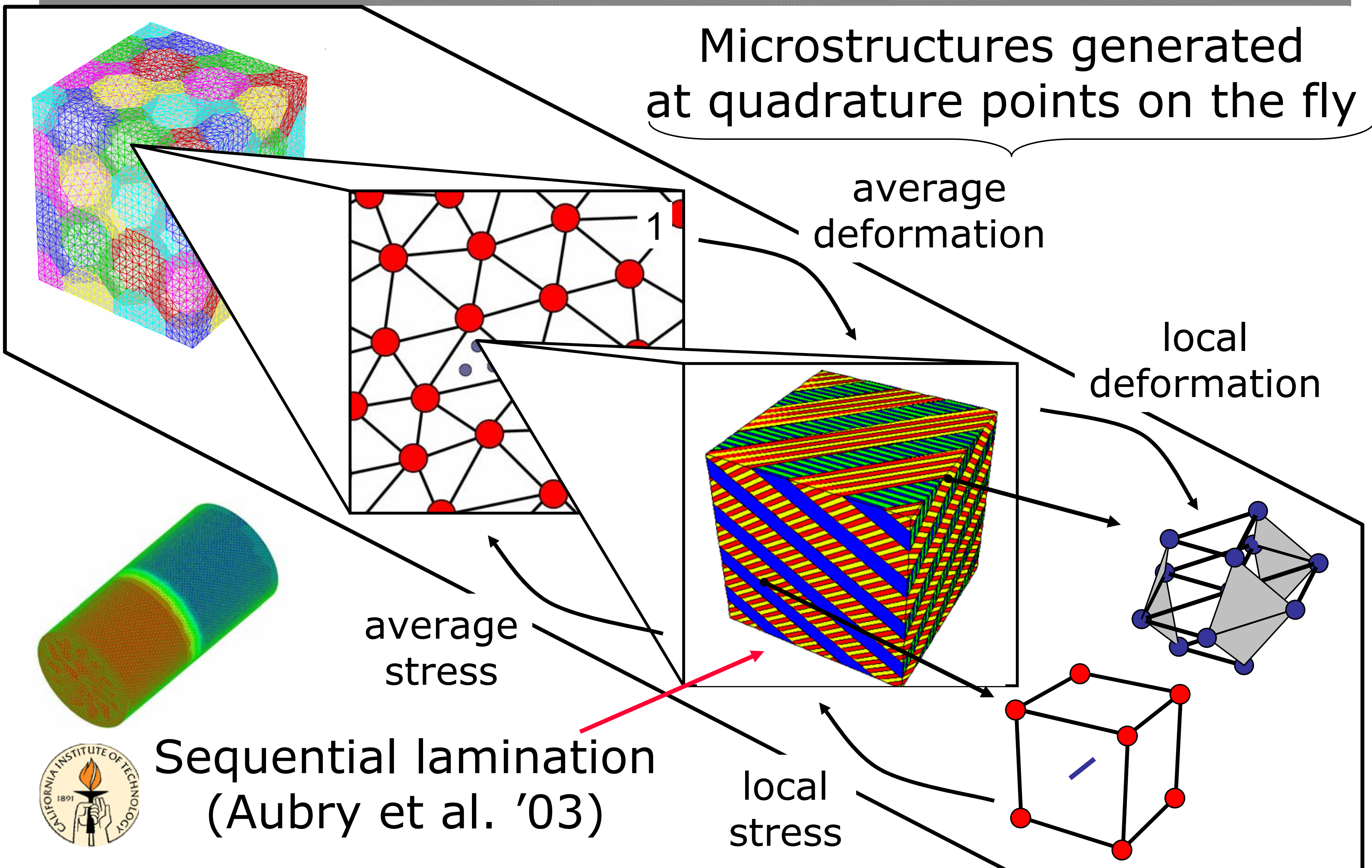
Rank-2 laminate



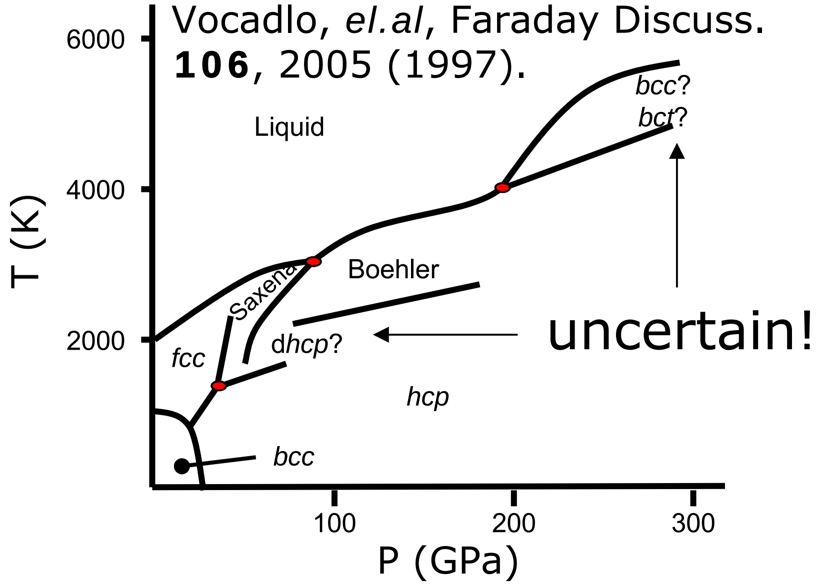
Coherent interfaces

- Compatibility.
- Equilibrium.
- Optimize:
  - i) Orientations.
  - ii) Volume fractions.

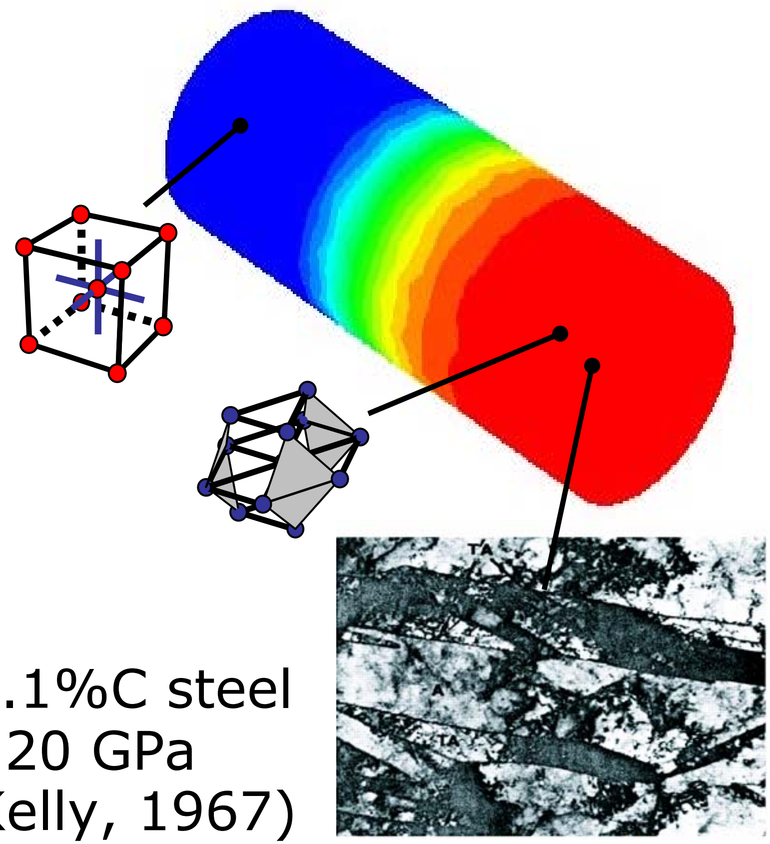
Relaxation – Concurrent multiscale



Phase transitions in Fe



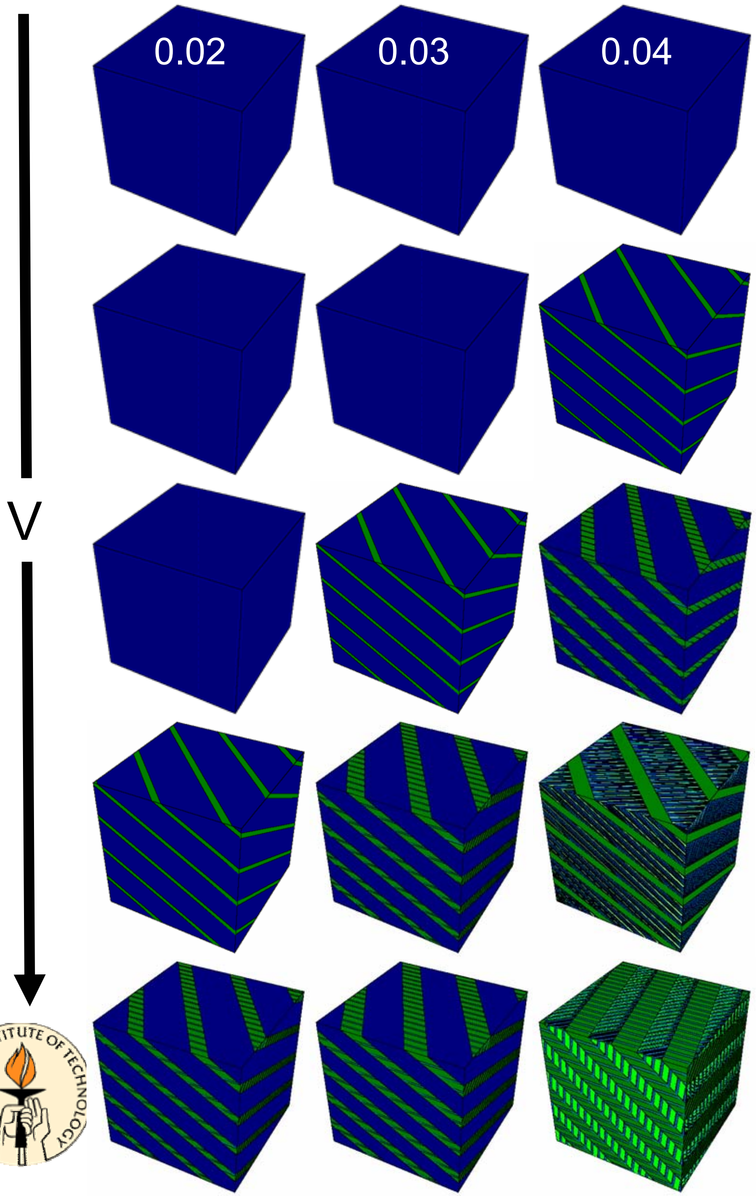
Strong shocks induce phase transitions involving complex microstructures

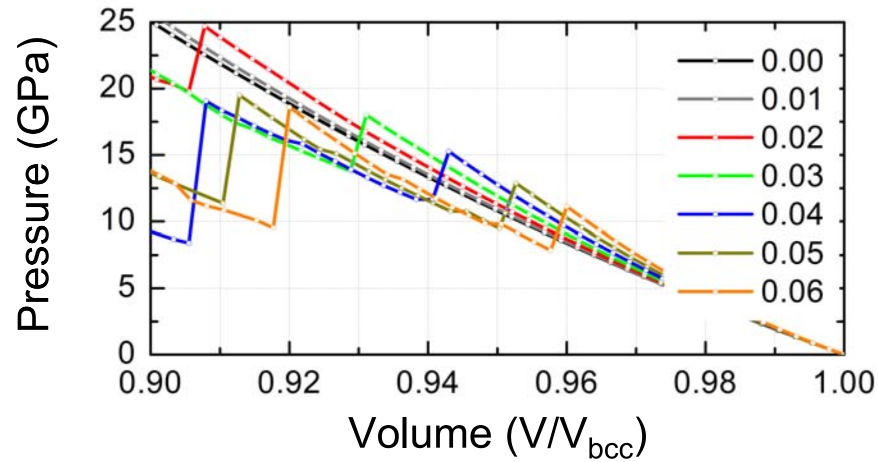


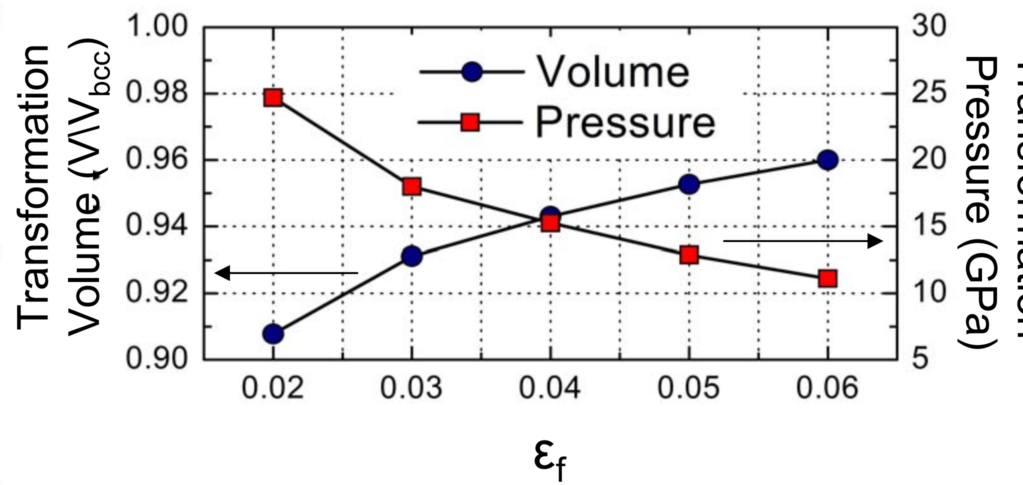
Ground state ferromagnetic *bcc* undergoes a *martensitic* phase transformation to non-magnetic *hcp* at ~10 GPa.

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

Phase transitions in Fe

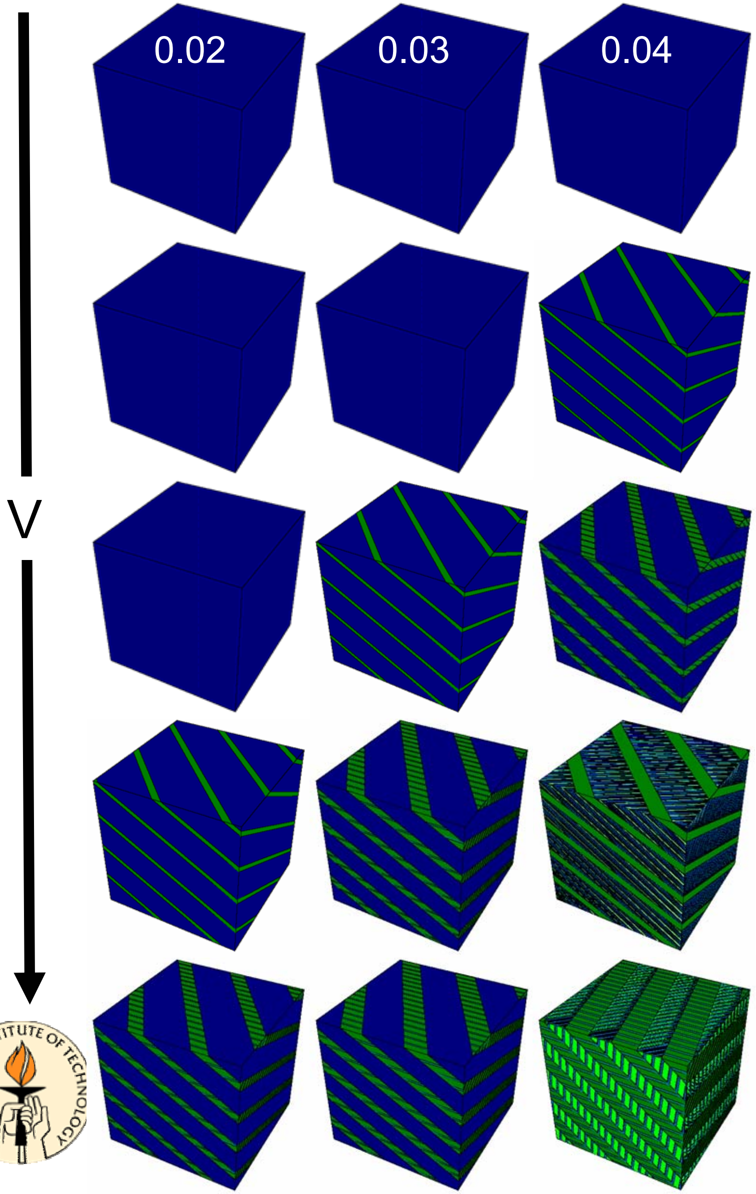


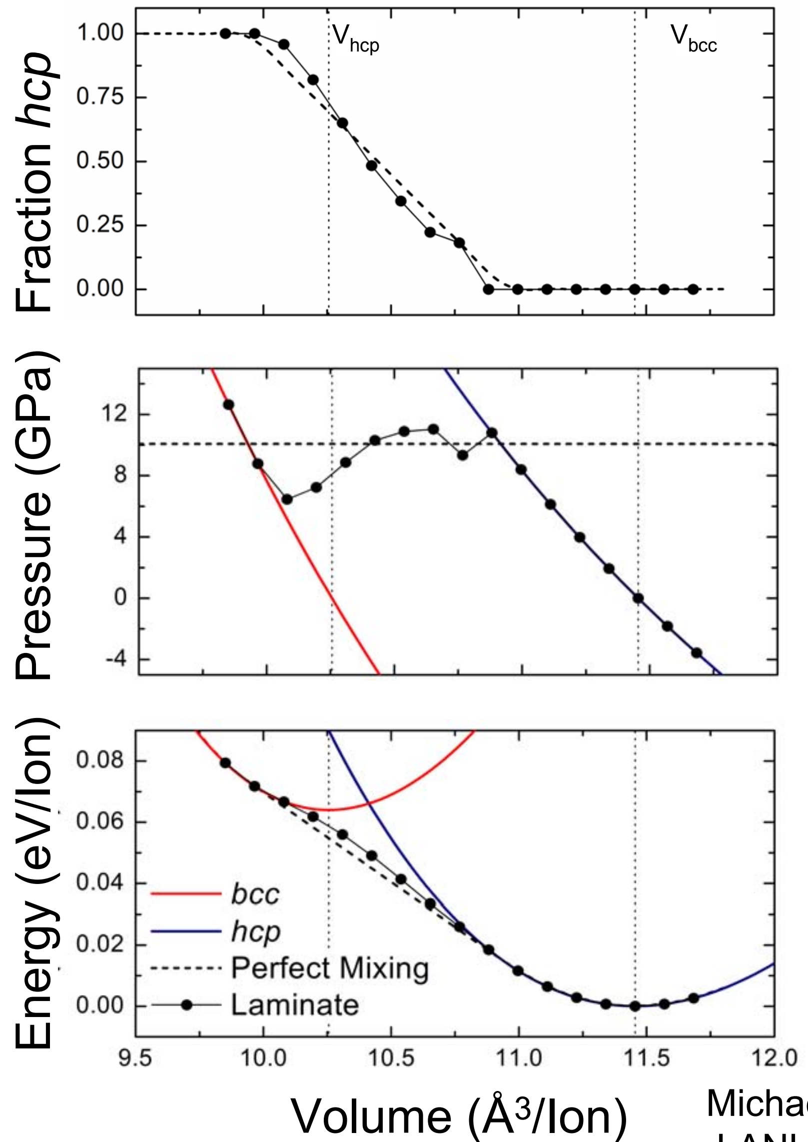




(K.J. Caspersen *et al. PRL* '04)

Phase transitions in Fe





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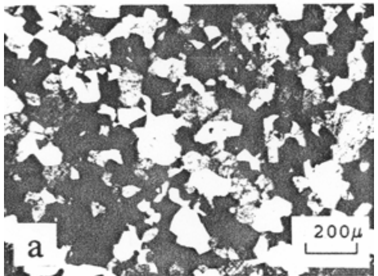
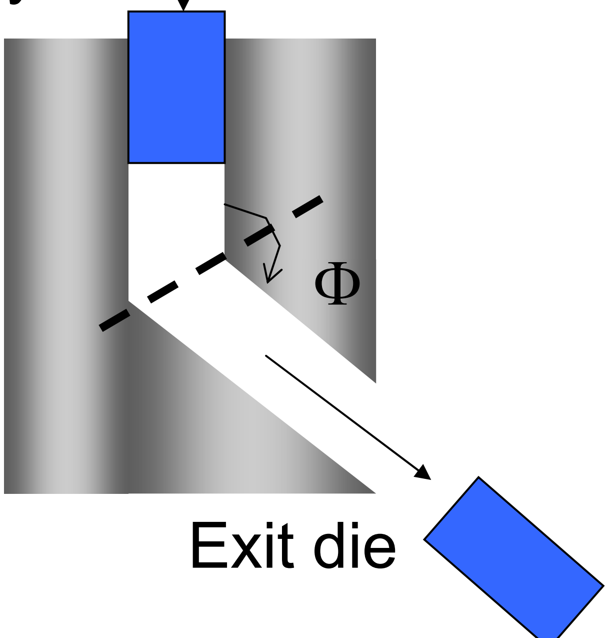
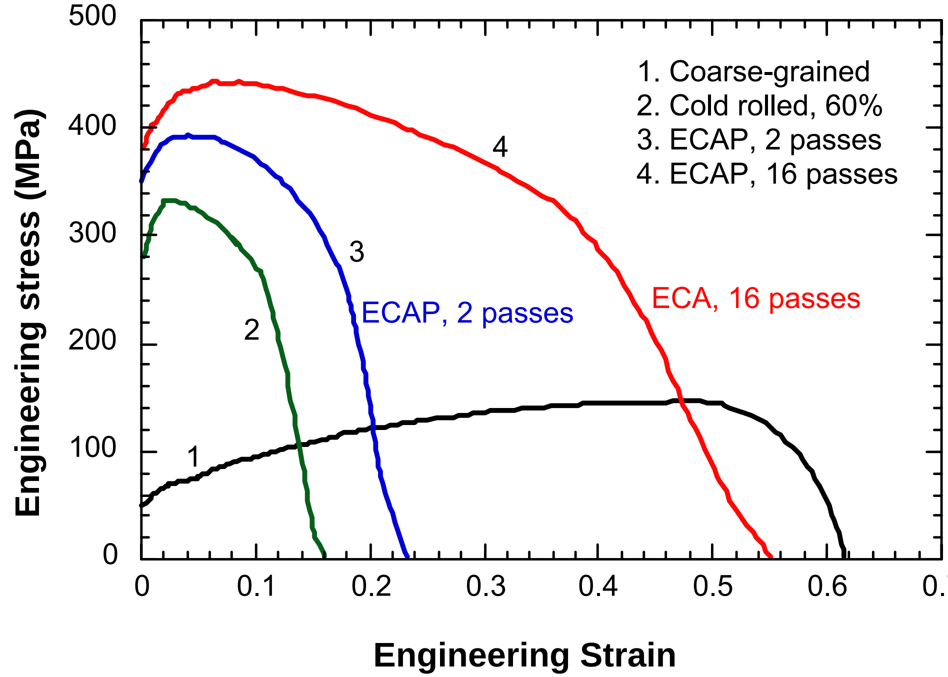
Equal Angular Channel Extrusion

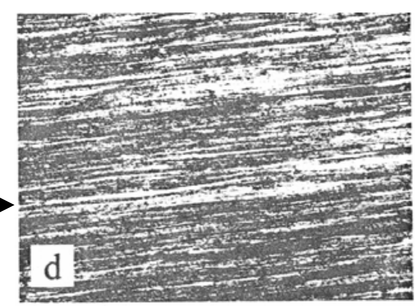


Entry die



Exit die





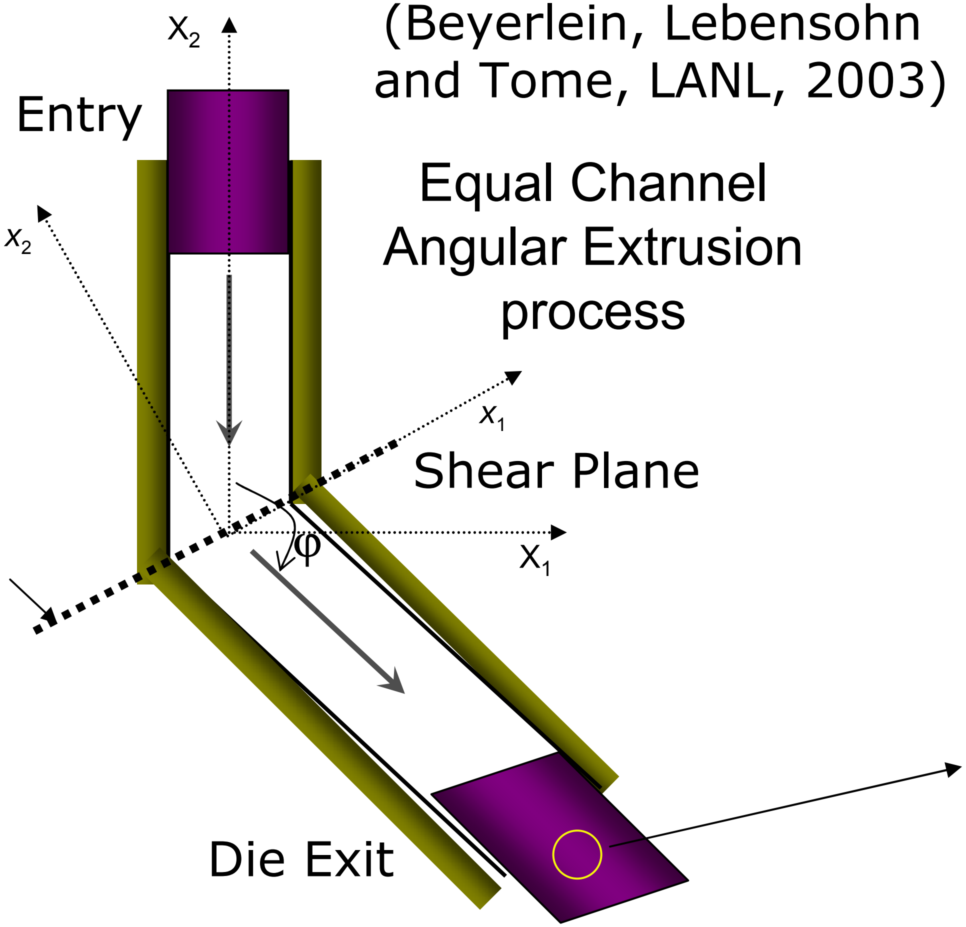
Nanoscale polycrystal

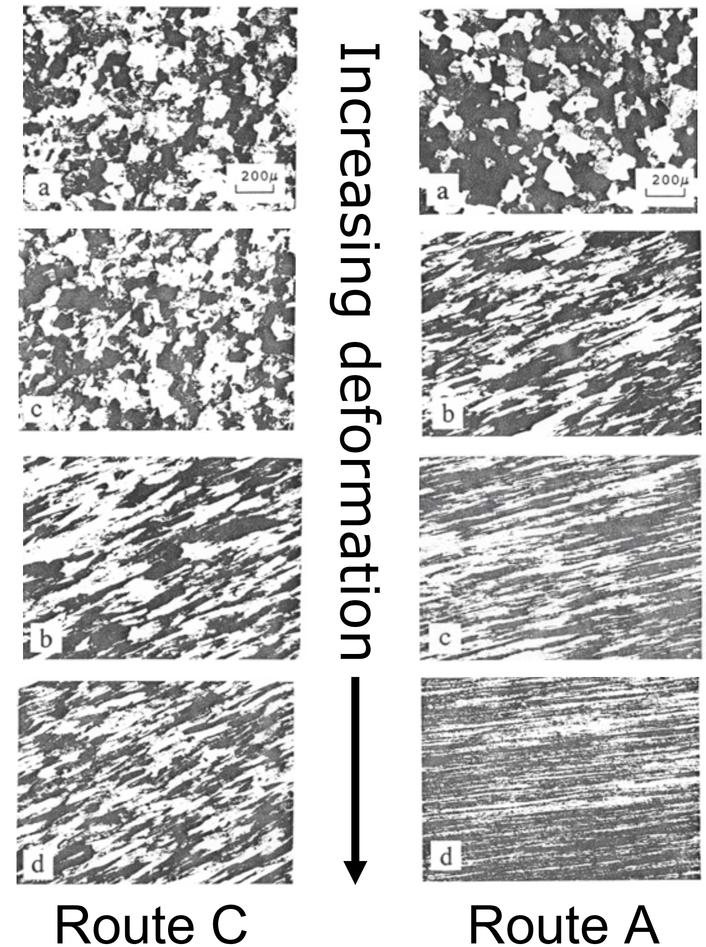
(Beyerlein, Lebensohn and Tome, LANL, 2003)

Equal Angular Channel Extrusion

(Beyerlein, Lebensohn and Tome, LANL, 2003)

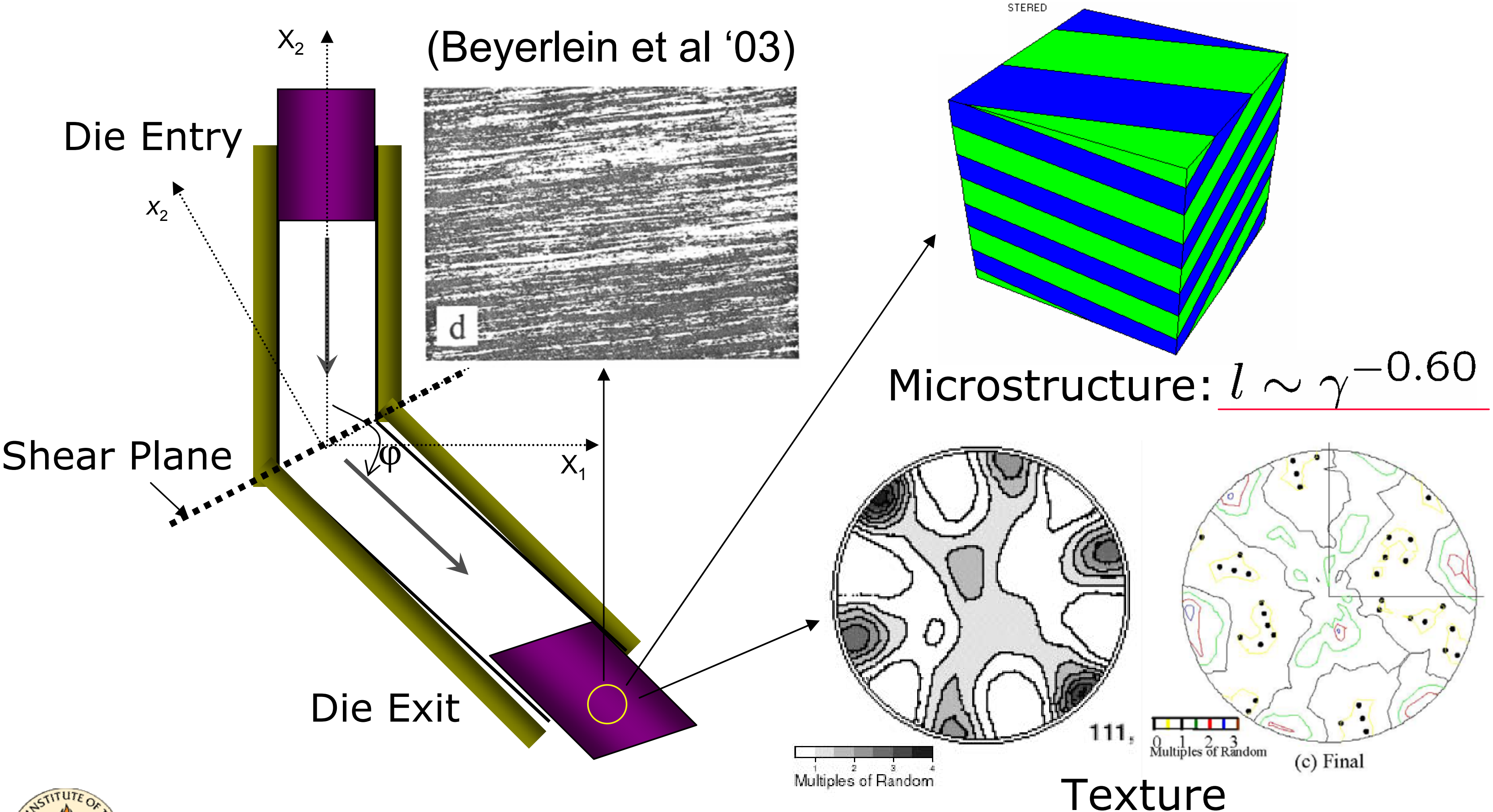
Equal Channel Angular Extrusion process





Evolution of dislocation structures in Cu specimen. Lamellar width: $l \sim \gamma^{-0.65}$

Equal Angular Channel Extrusion

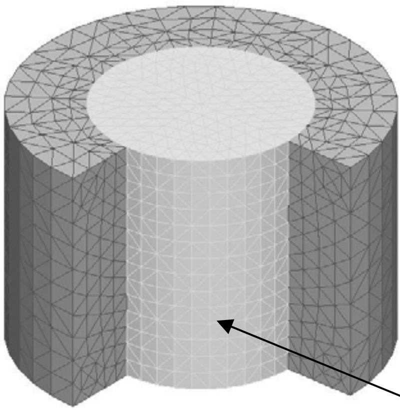


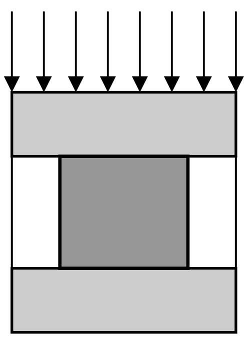
(Sivakumar and Ortiz ´03)

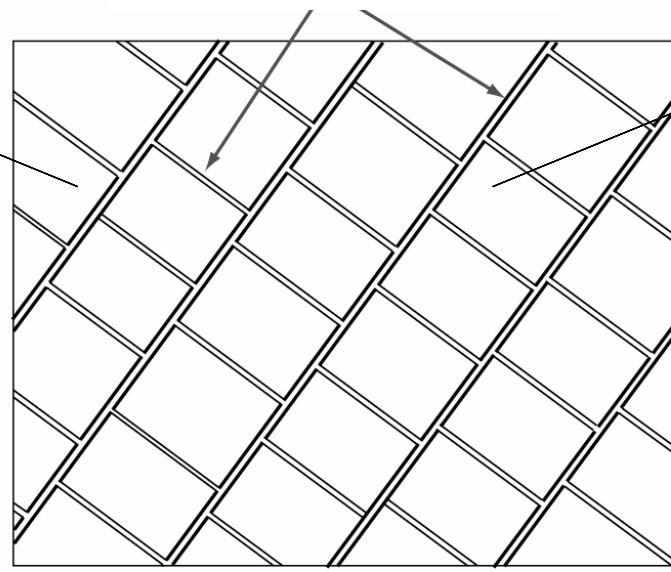
Distributed brittle damage

Sintered aluminum nitride (AlN)
Confined with a brass sleeve

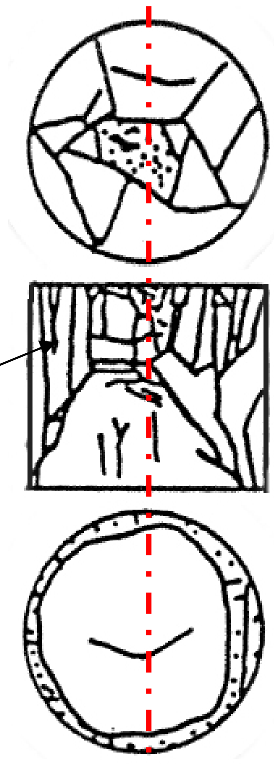
(Chen and Ravichandran ’96)







Sequential faulting construction
(Pandolfi, Conti and Ortiz ’05)



Damage distribution

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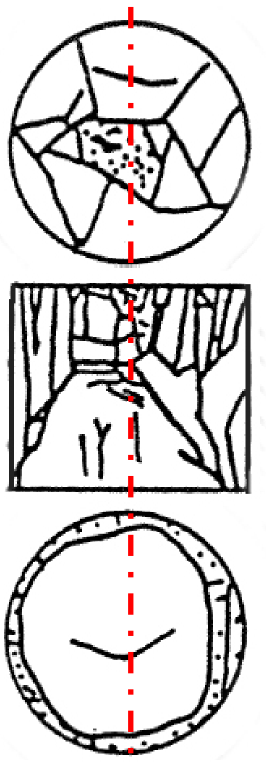
Distributed brittle damage

Experiments (Chen and Ravichandran ’96)

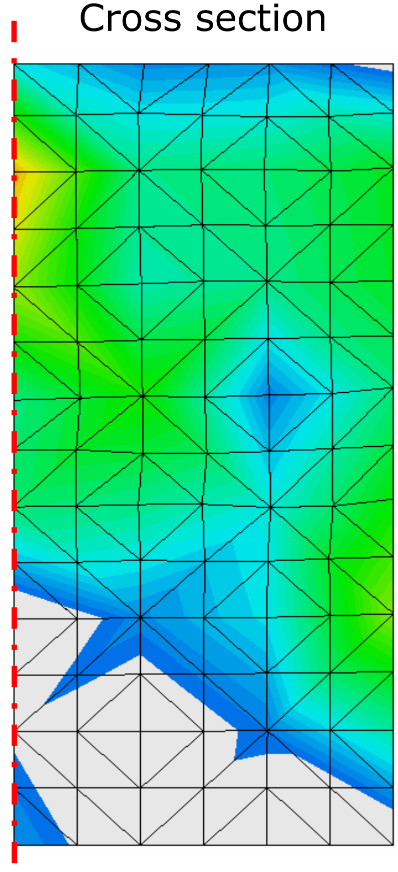
Top view

Cross Section

Bottom view

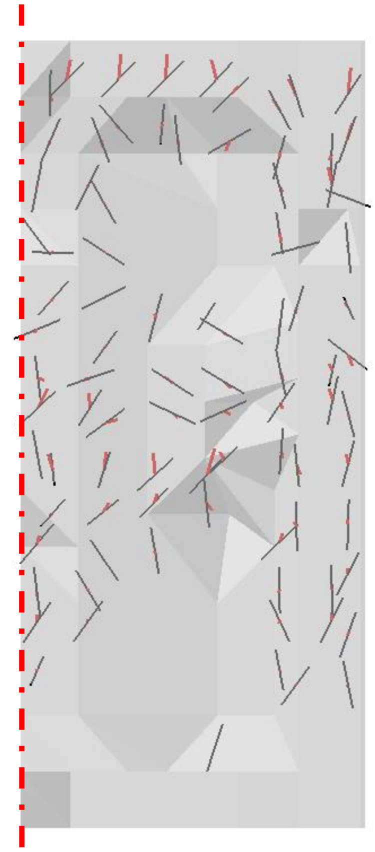


Damage contour levels Cross section

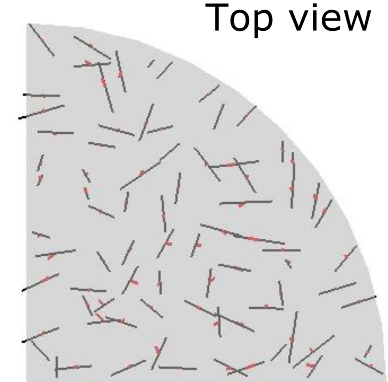


Fault planes (black) and opening (red)

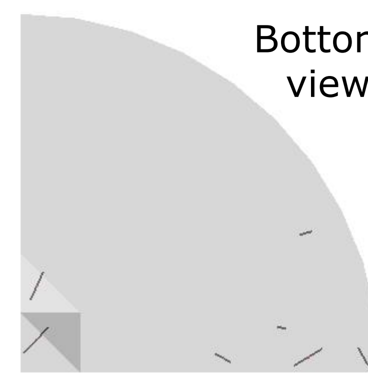
Cross section



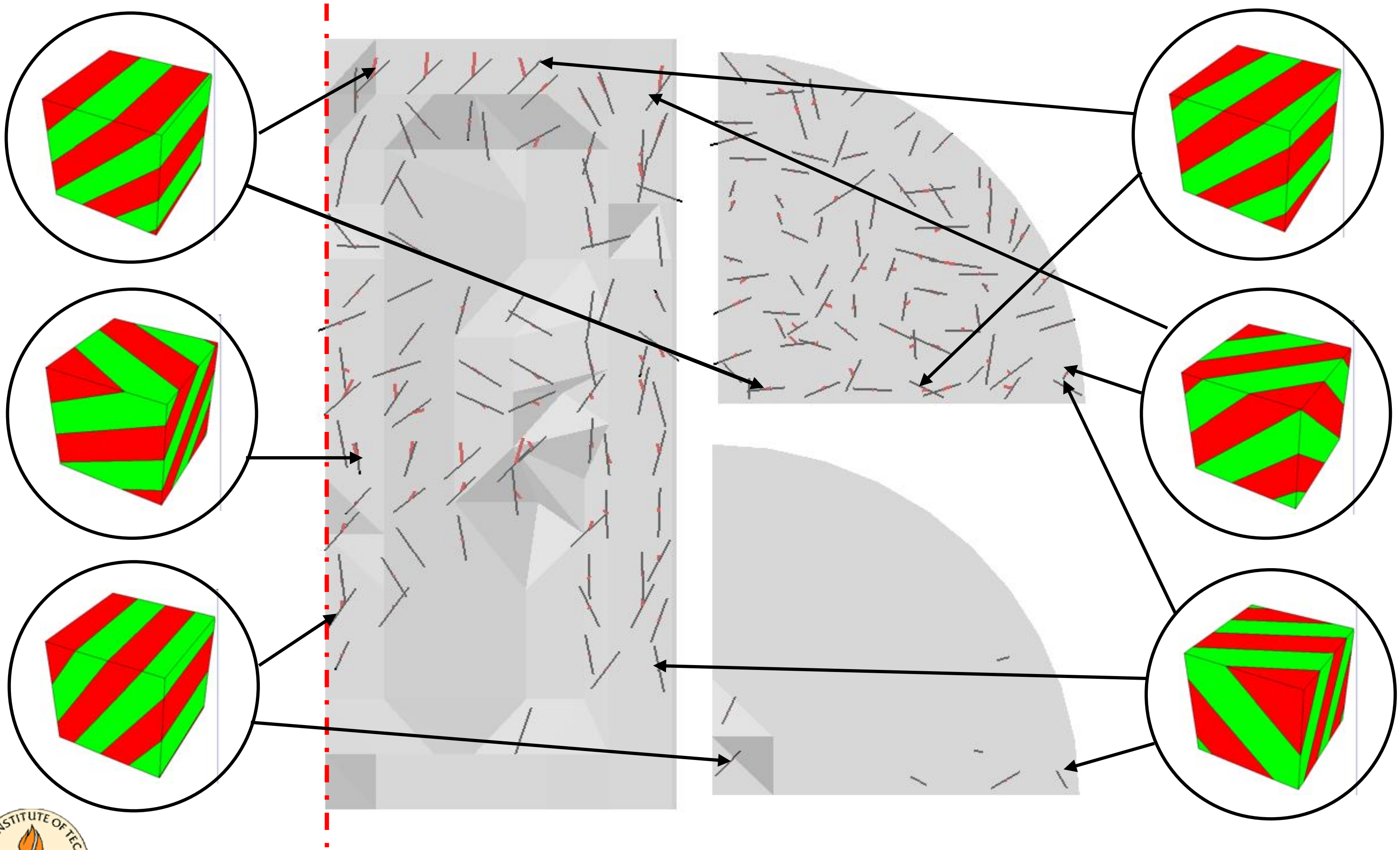
Top view



Bottom view



Distributed brittle damage



Normals (black) and opening displacement (red)

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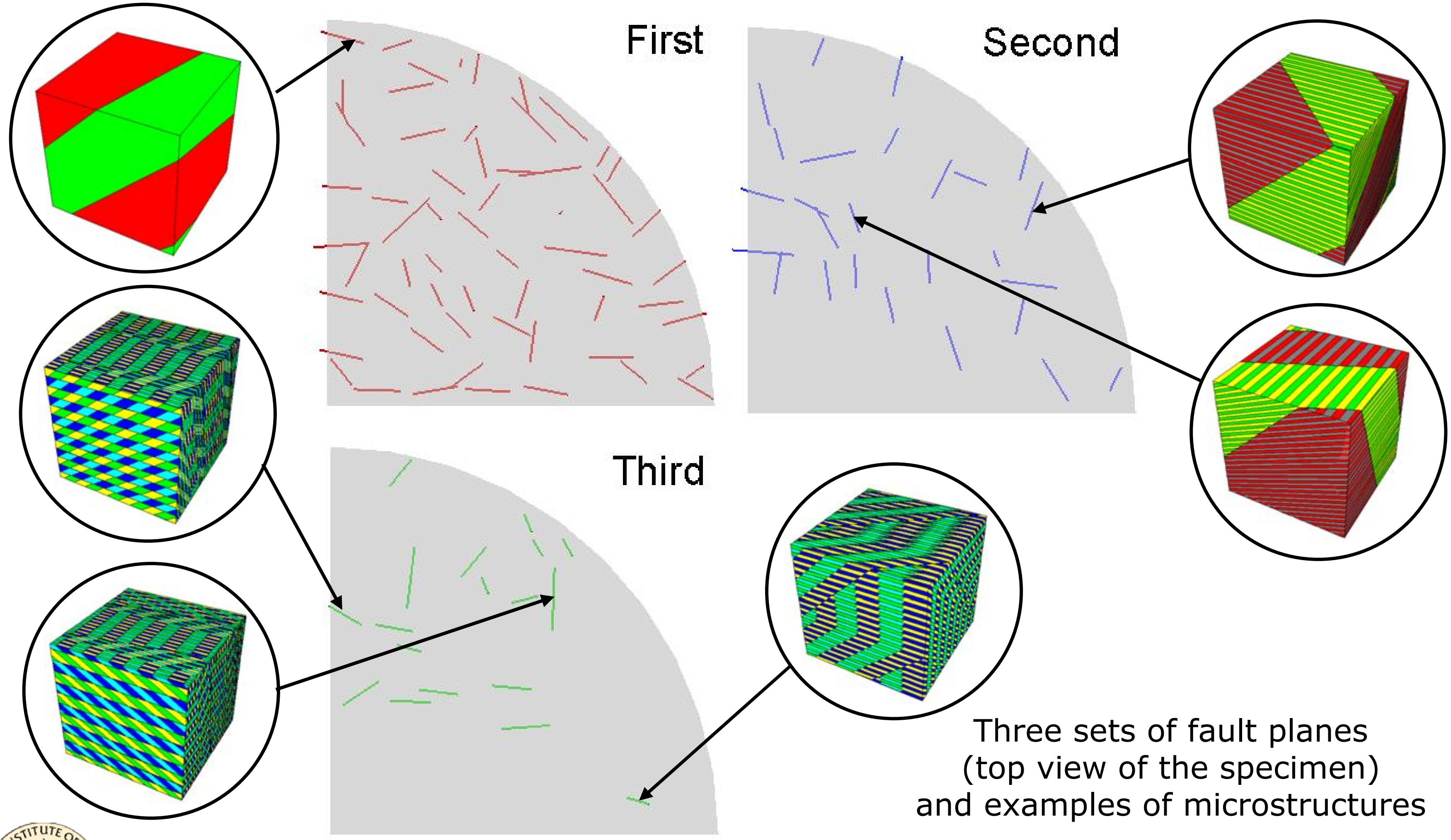
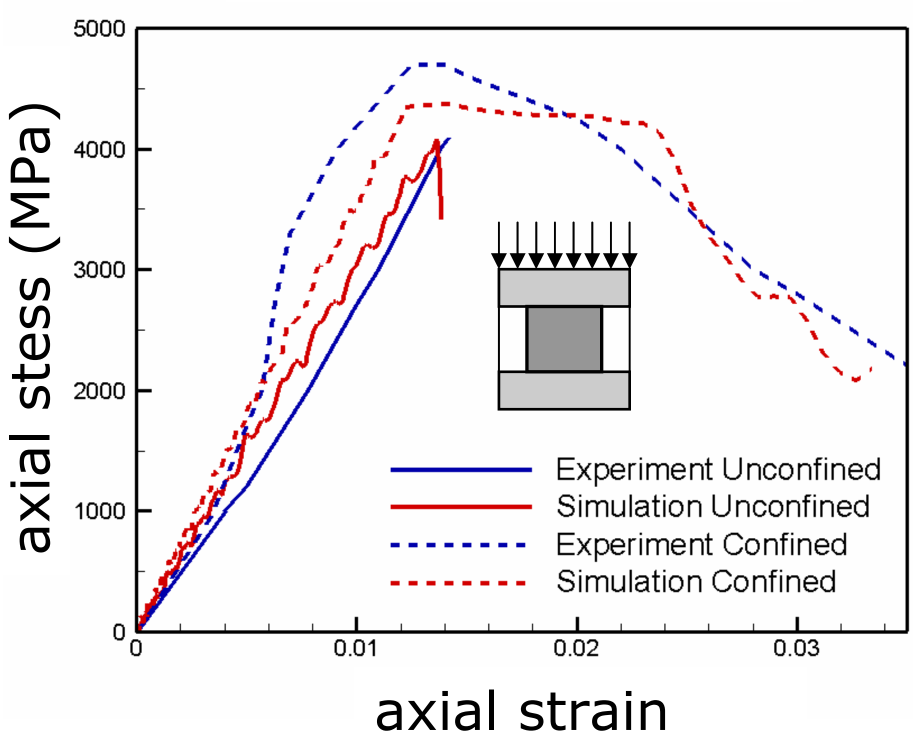
Distributed brittle damage



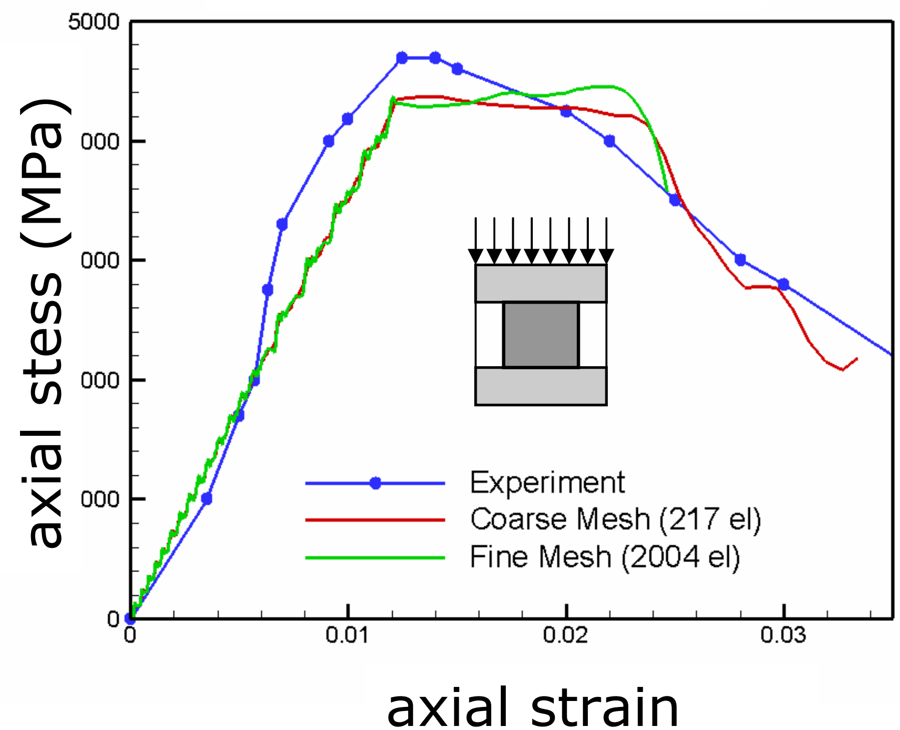
Three sets of fault planes
(top view of the specimen)
and examples of microstructures

Distributed brittle damage

Comparison with experiment



Mesh size analysis



Validation and verification of sequential faulting construction

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Relaxation – Outlook

- Relaxation is an example of a top-down multiscale method that relies on:
  - *Strict separation of scales*
  - *Well-posed macroscopic problem*
  - *Sub-grid evaluation of microstructure*
- Relaxation is an example of a *concurrent multiscale computing*: it resolves macroscopic and microscopic lengthscales concurrently during same calculation
- Challenges:
  - *Nonlocal effects (eg, interfacial energy), size effects*
  - *Kinetics (eg, interfacial motion, pinning)*
  - *Relaxation beyond sequential lamination*

Conclusion

- "…we are shifting our emphasis from developing parallel-architecture machines and codes to improved weapons science and increased physics understanding…" (***Randy Christensen***).
- "Better physics and computational mathematics is much more important than better 'computer science' " (***Doug Post***).
- "Prediction Challenge—Developing **predictive** codes with complex scientific models" (***Doug Post***).
- "The credibility of our simulation capabilities is central to the credibility of the certification of the nuclear stockpile. That credibility is established through V&V analyses." (***Cynthia Nitta***).

Conclusion

- “In anticipation of ASC Purple in 2005, we are shifting our emphasis from developing parallel-architecture machines and codes to improved weapons science and increased physics understanding of nuclear weapons.” (***Randy Christensen***).
- “The computers come, and after a few years, they go, But the codes and code teams endure.” (***Mike McCoy***).
- “The credibility of our simulation capabilities is central to the credibility of the certification of the nuclear stockpile. That credibility is established through V&V analyses.” (***Cynthia Nitta***).