Multiscale Modeling of Materials

M. Ortiz

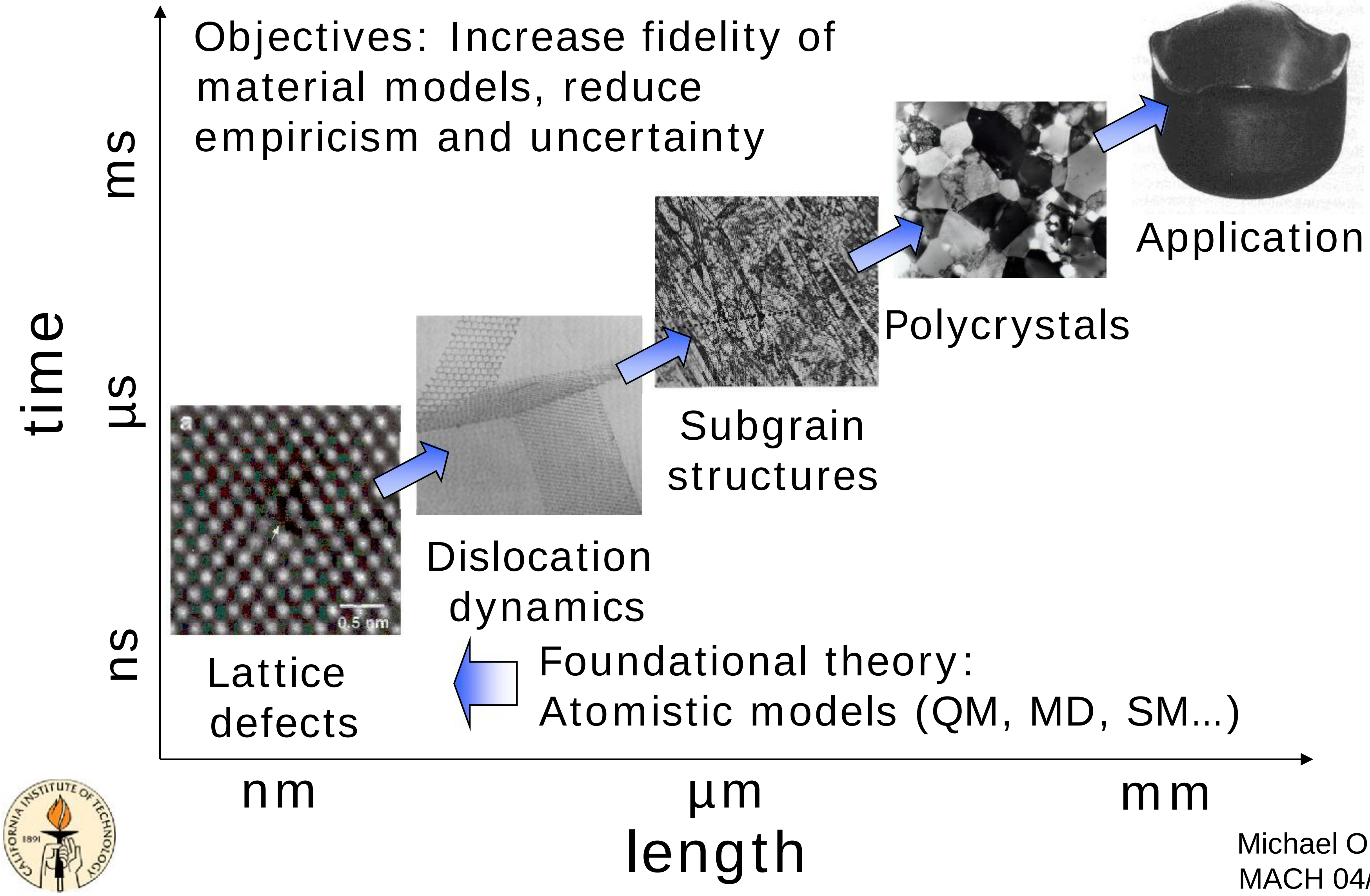
California Institute of Technology

MACH Conference,
Baltimore, April 8, 2015

Multiscale modeling of materials

- Multiscale modeling of materials provides a systematic means of generating high-fidelity, ansatz-free, models of materials
- Paradigm: Model the physics, not the data...
- But: Physics happens on multiple spatial and temporal scales...

Multiscale modeling – Strength of metals



Objectives: Increase fidelity of material models, reduce empiricism and uncertainty

Application

Polycrystals

Subgrain structures

Dislocation dynamics

Lattice defects

Foundational theory:
Atomistic models (QM, MD, SM...)

time

ms

μs

ns

nm

μm

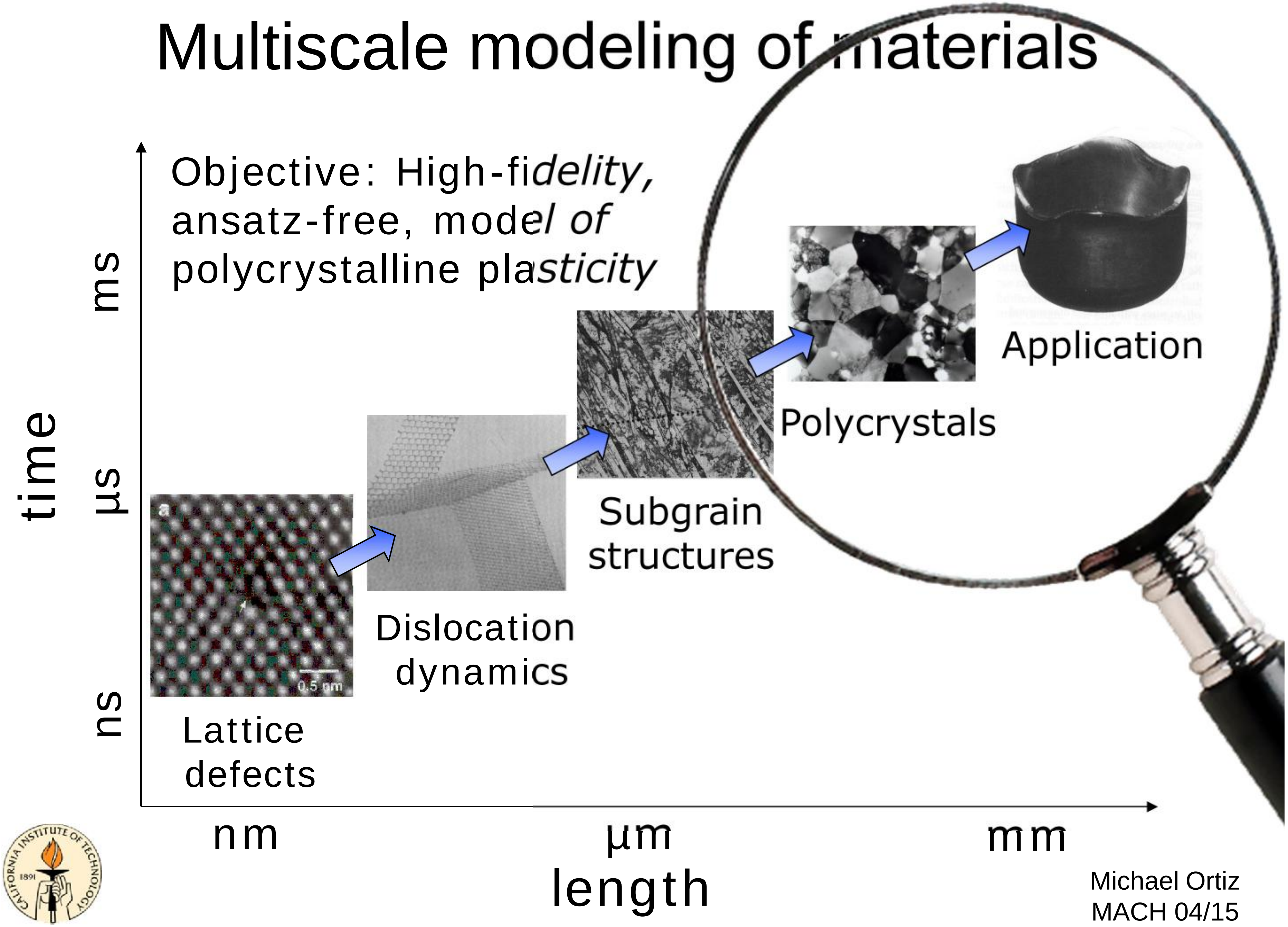
mm

length

Multiscale modeling of materials

- Multiscale modeling of materials provides a systematic means of generating high-fidelity, *ansatz*-free, models of materials
- Paradigm: Model the physics, not the data…
- But: Physics happens on multiple spatial and temporal scales…
- Require a multiplicity of approaches (analytical, computational, experimental), theories, tools, approximation and computational schemes...
- To date many challenges remain, but also some successes, recent advances...
- Where do we stand?

Multiscale modeling of materials



Objective: High-fidelity, ansatz-free, model of polycrystalline plasticity

Lattice defects

Dislocation dynamics

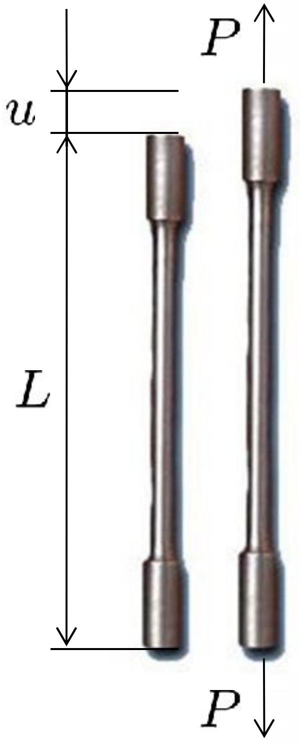
Subgrain structures

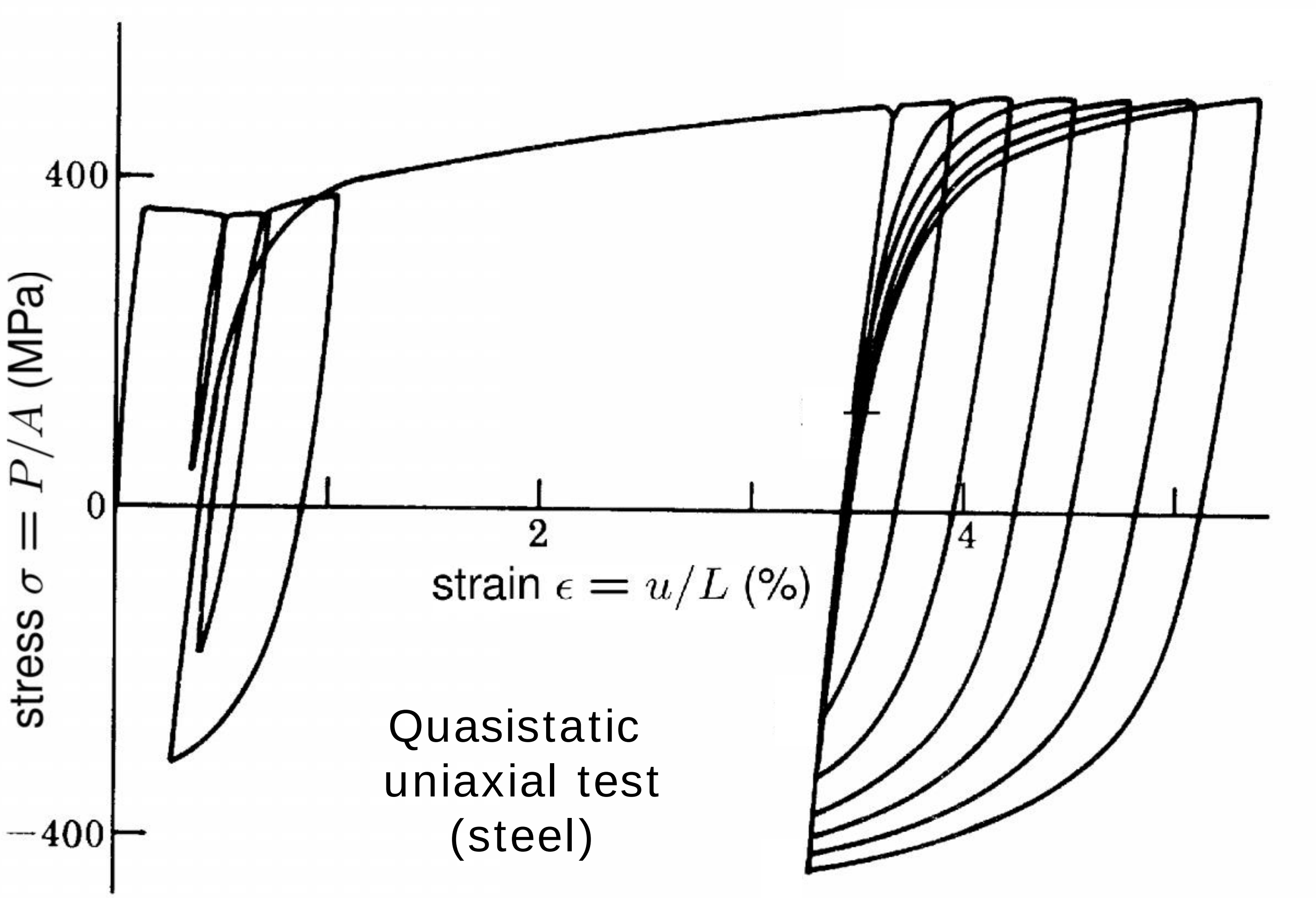
Polycrystals

Application

Michael Ortiz
MACH 04/15

Quasistatic cyclic tension-compression



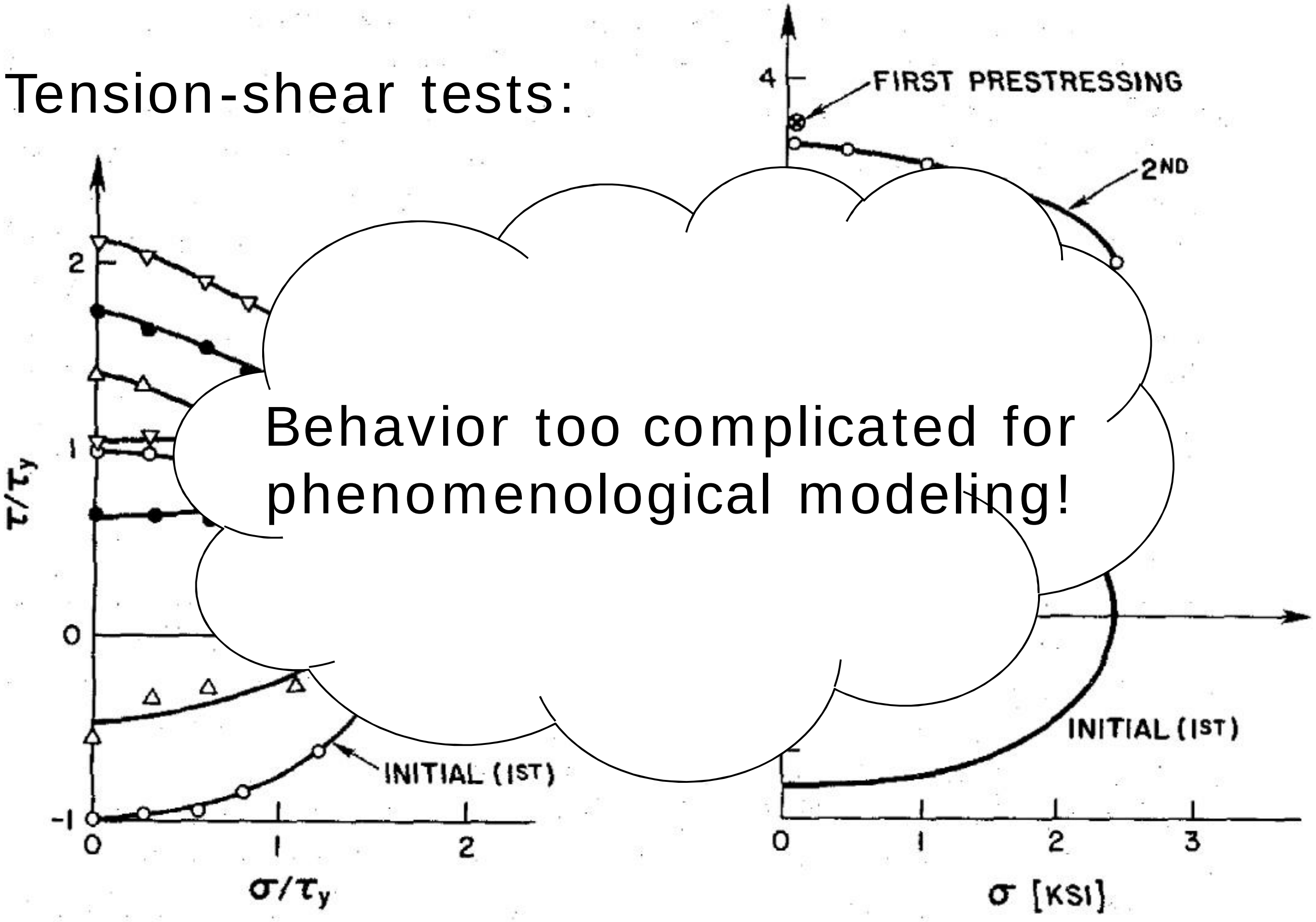


Quasistatic
uniaxial test
(steel)

M. Ortiz and E.P. Popov, *J. Eng. Mech. ASCE* **109** (4) 1042-1057 (1983)

Multiaxial yielding and hardening

Tension-shear tests:



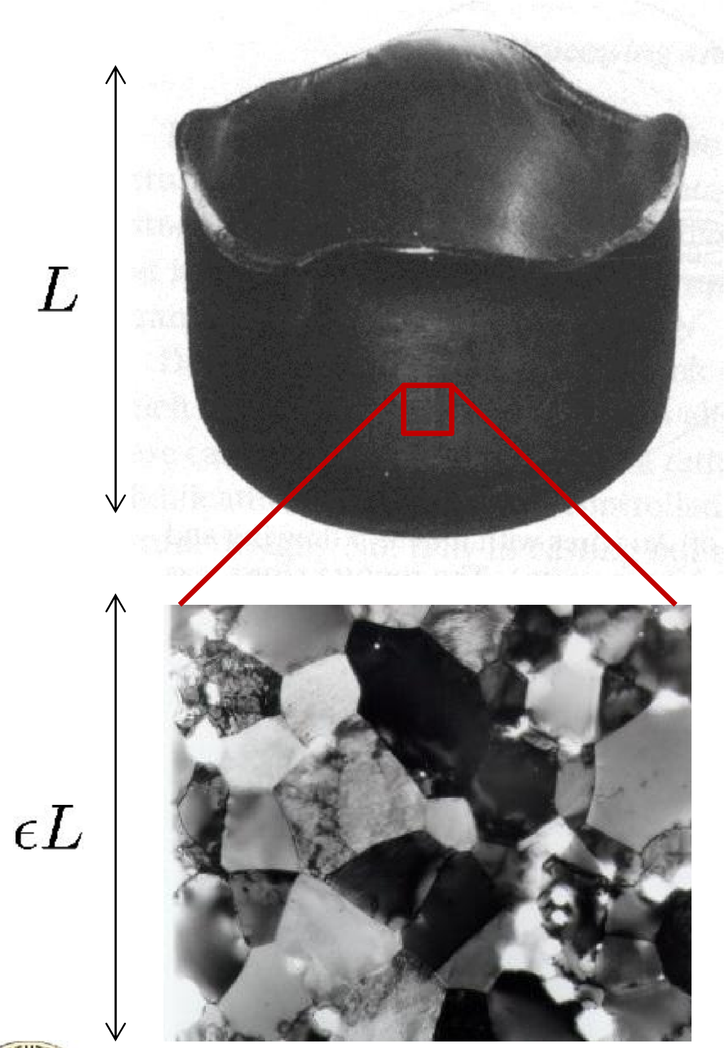
Behavior too complicated for phenomenological modeling!

a) **ALUMINUM**
AFTER IVEY

b) **ALUMINUM**
AFTER PHILLIPS, TANG, AND RICCIUTI

M. Ortiz and E.P. Popov, *J. Eng. Mech. ASCE* **109** (4) 1042-1057 (1983)

Polycrystals: Homogenization

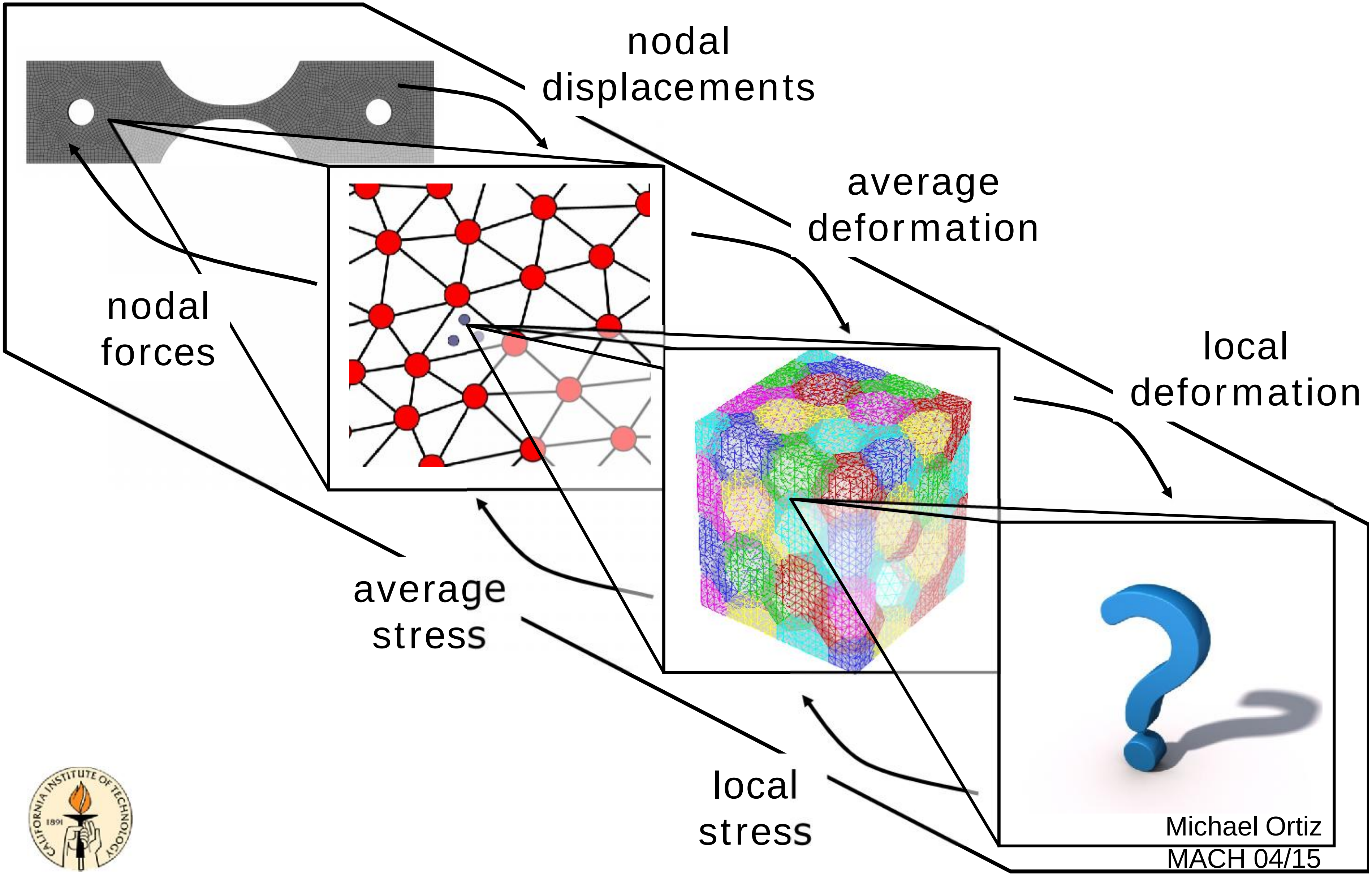


RVE

- Polycrystals:
  - Built-in microstructure (from casting, sintering…)
  - Assume strict separation of scales (ε ≪ 1)
- Known effective theory: Mathematical theory of homogenization
- Fundamental theorem[1]: Assume material is stable (no localization). Then, the effective behavior is that of an RVE subject to affine boundary conditions.
- But: Hard cell problem!

[1] G. dal Maso, *An Introduction to Γ-Convergence*, Birkhäuser (1993)

Polycrystals – Concurrent multiscale



Polycrystals – Concurrent multiscale

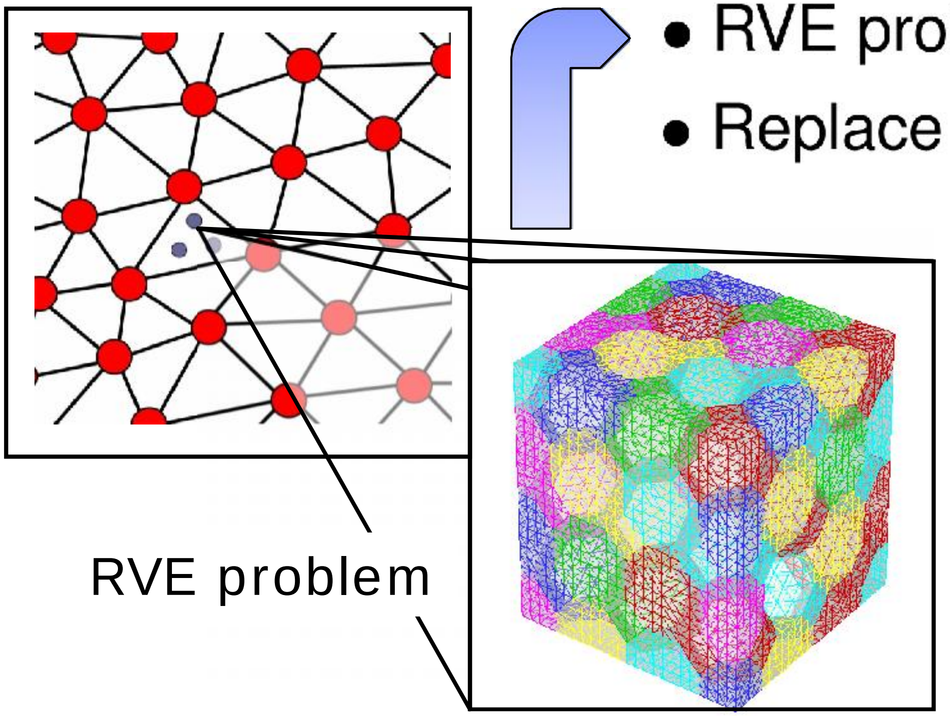
- Concurrent polycrystalline plasticity models (e.g., FE^2) implement homogenization theory
- They bypass the need to model pollycrystalline plasticity analytically or phenomenologically
- Result in doubly convergent approximations as h (mesh size) and ε (RVE size) → 0[1]
- Essential difficulty: Too slow!
- Path forward: Acceleration methods…
- Examples: Database methods (non-concurrent), adaptive tabulation (databasing on the fly), Kriging[2] (stochastic interpolation)…

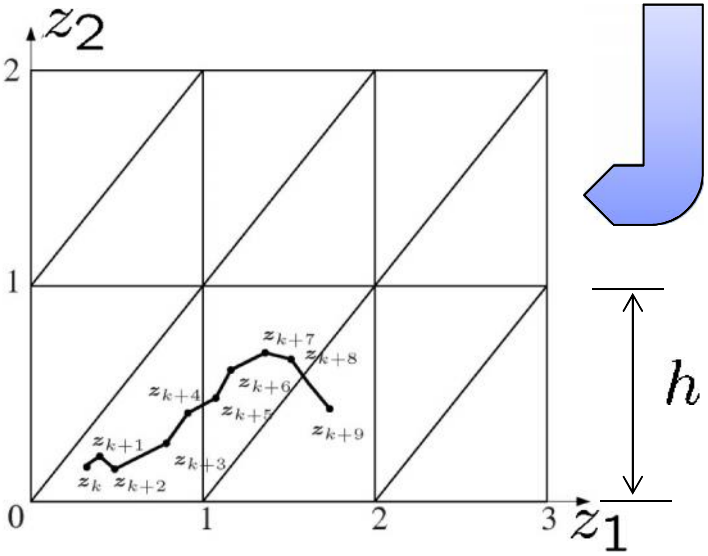
[1] Conti, S., Hauret, P. and Ortiz, M., *MSMSE*, 2007; ***6***:135-157.

[2] Barton, N.R., Knap, J., Arsenlis, A., Becker, R., Hornung, R.D. and Jefferson, D.R., *International Journal of Plasticity*. 2008; **24**(2):242-266.

Phase-space interpolation

- RVE problem must supply $\boldsymbol{P}(\overbrace{\boldsymbol{F}, \dot{\boldsymbol{F}}, T}^{\boldsymbol{z}})$
- Replace by interpolant $\boldsymbol{P}_h(\boldsymbol{F}, \dot{\boldsymbol{F}}, T)$!

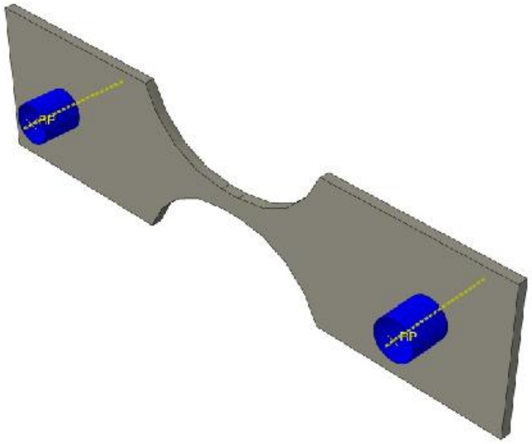

RVE problem



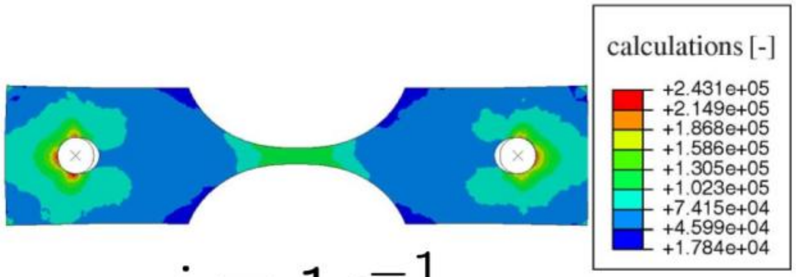
- Simplicial interpolation in high-dimensional spaces[1]
- One single RVE calculation per boundary crossing
- Speed-up = #steps/simplex @ constant accuracy

[1] Chien, M.J. and Kuh, E., *IEEE Transactions*, 1978; **25**(11):938–940.
Klusemann, B. and Ortiz, M., IJNME, 10.1002/nme.4887, 2015.

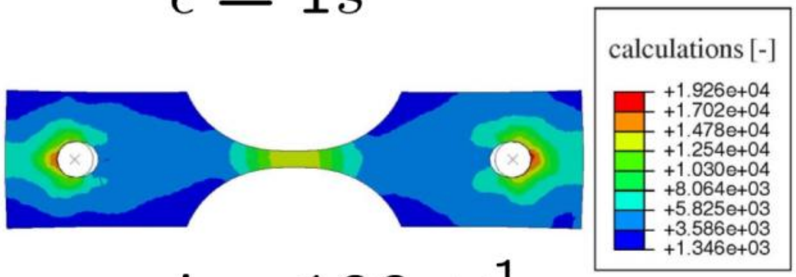
Phase-space interpolation



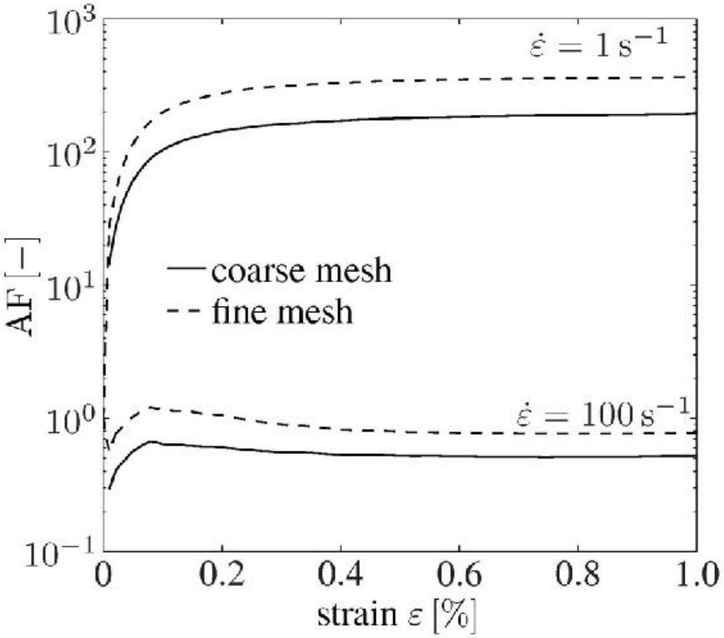
- Dynamic extension of tensile neo-Hookean specimen
- Explicit Newmark integration
- Hexahedral finite elements
- Quadratic interpol. of W(F)



$\dot{\epsilon} = 1s^{-1}$



$\dot{\epsilon} = 100s^{-1}$



Klusemann, B. and Ortiz, M., IJNME, 10.1002/nme.4887, 2015.

Multiscale modeling of materials

Objective: High-fidelity, ansatz-free, model of polycrystall

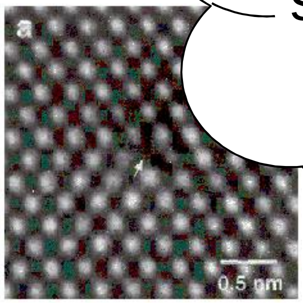
Acceleration may enable concurrent multiscale (FE^2) simulation of polycrystals

time

ms

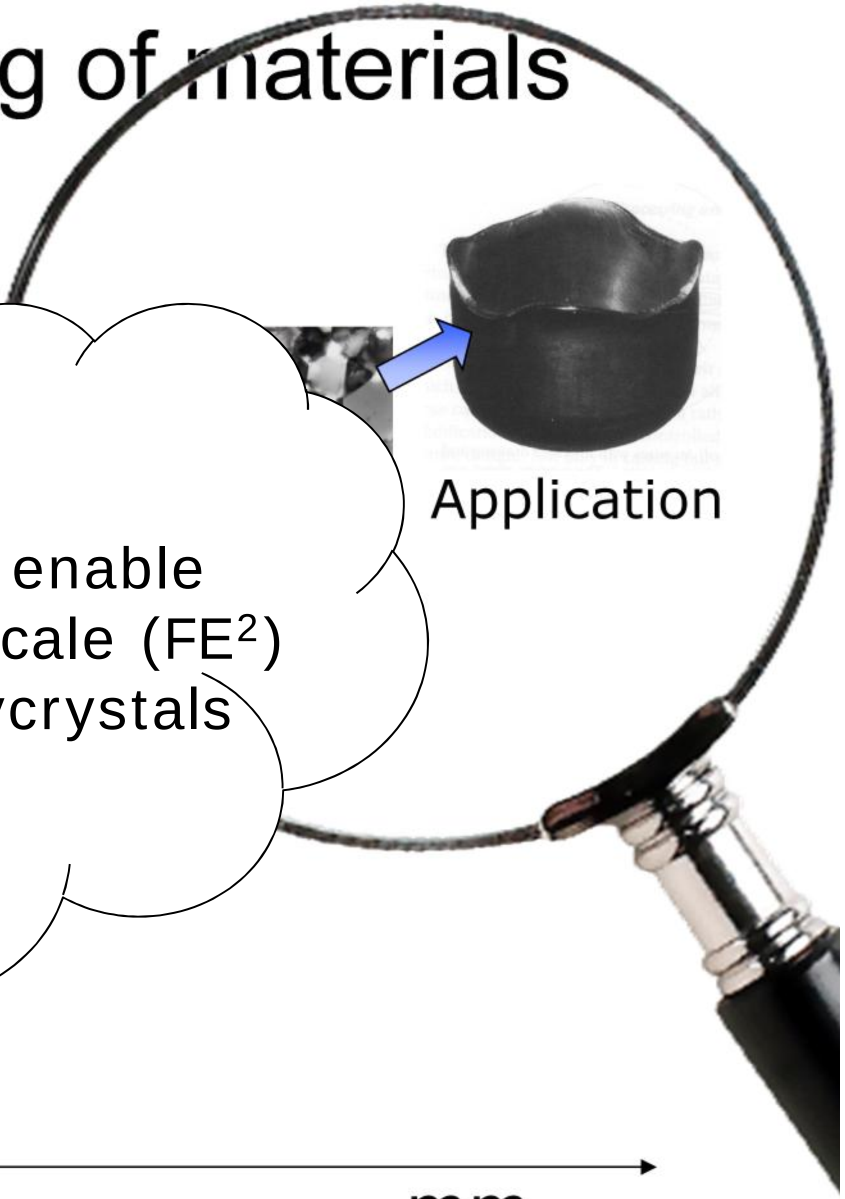
μs

ns



Lattice defects

dynamics



Application

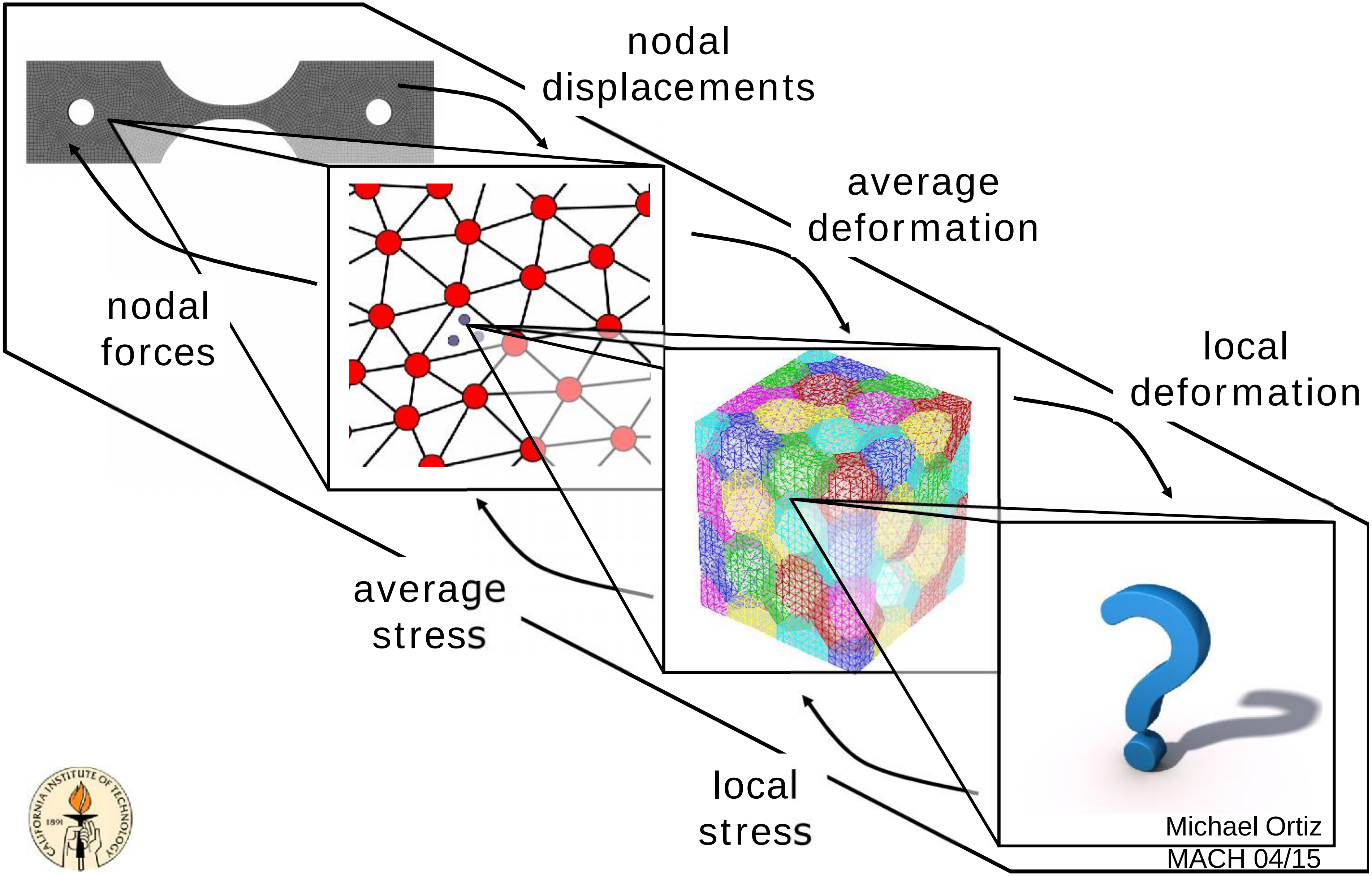
nm

μm

mm

length

Not done yet… Subgrain plasticity?



nodal displacements

average deformation

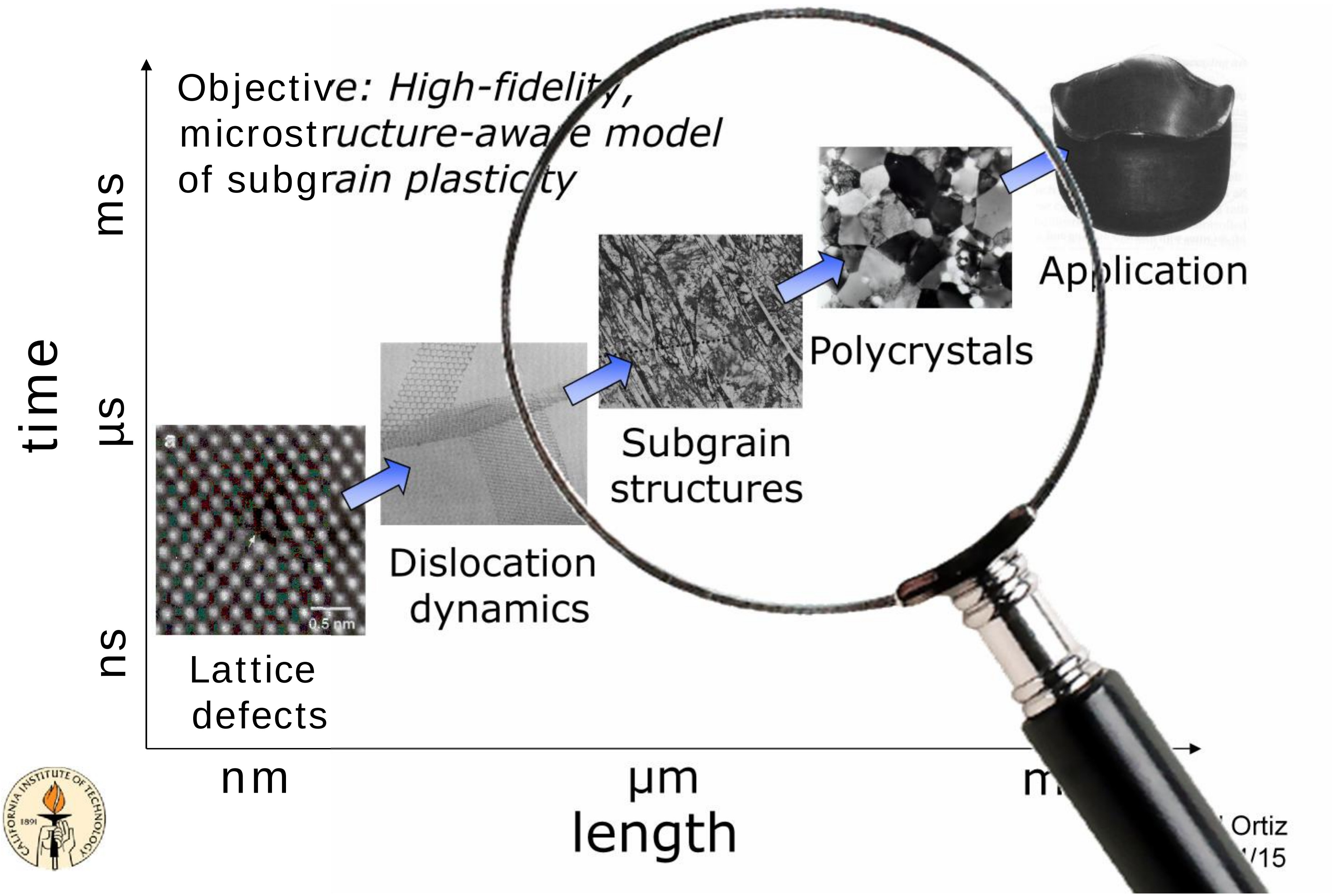
local deformation

nodal forces

average stress

local stress

Multiscale modeling of materials



Objective: *High-fidelity, microstructure-aware model of subgrain plasticity*

Lattice defects

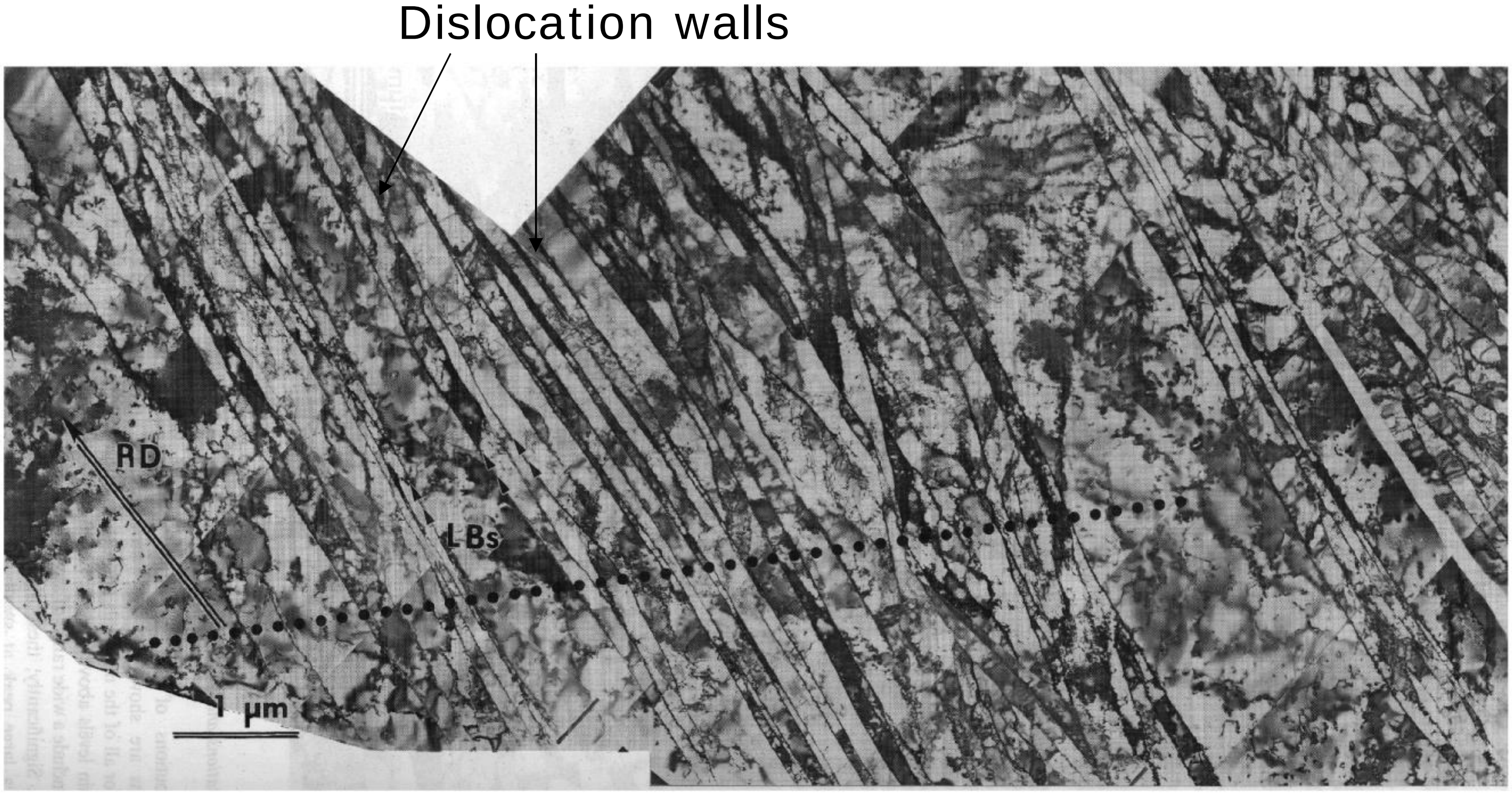
Dislocation dynamics

Subgrain structures

Polycrystals

Application

Subgrain dislocation structures - Static

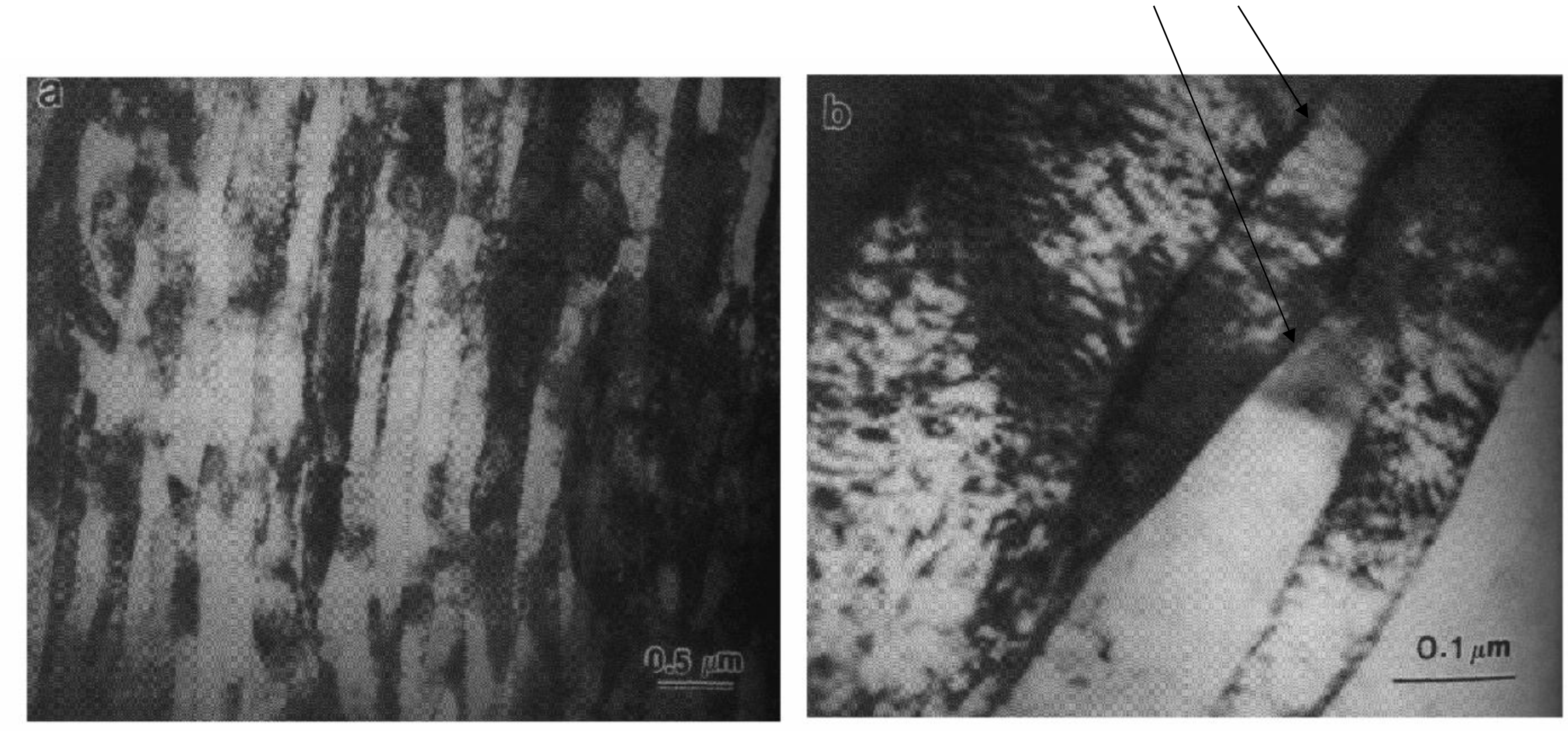

Dislocation walls

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

Michael Ortiz
MACH 04/15

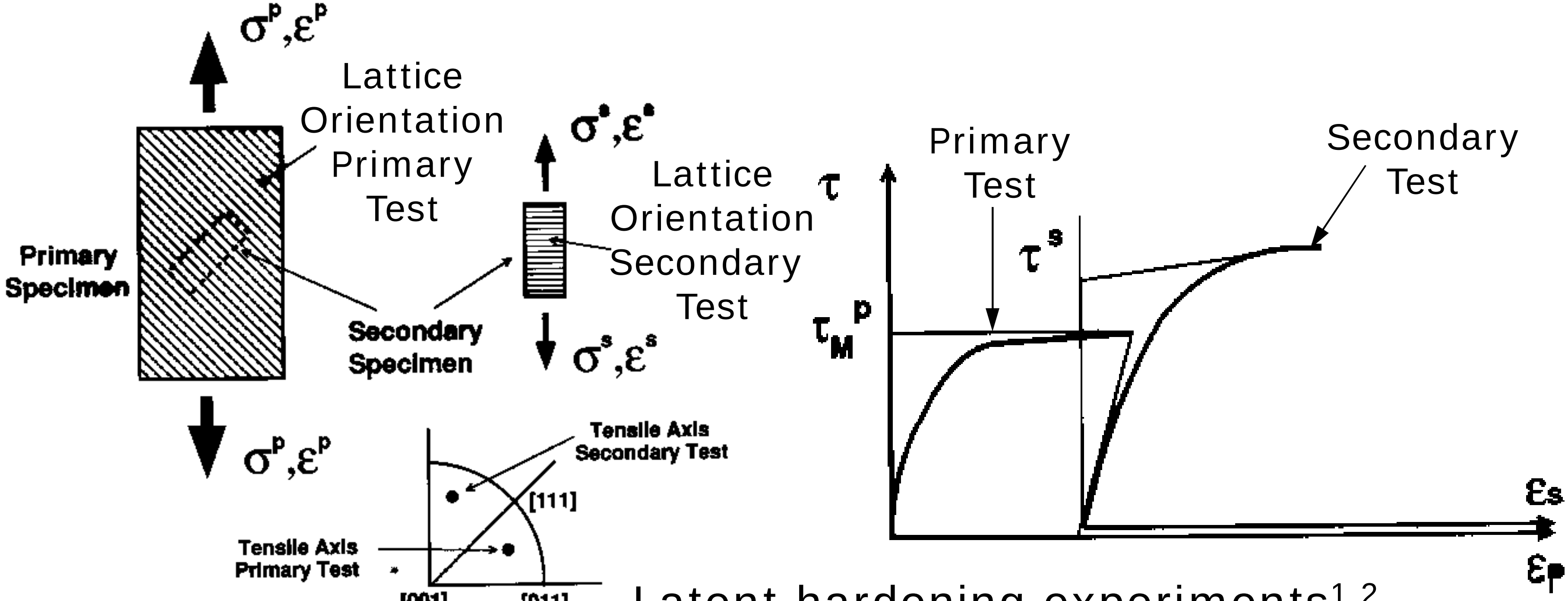
Subgrain dislocation structures - Shock

Dislocation walls



Shocked Ta (Meyers et al., 1995)

Strong latent hardening & microstructure



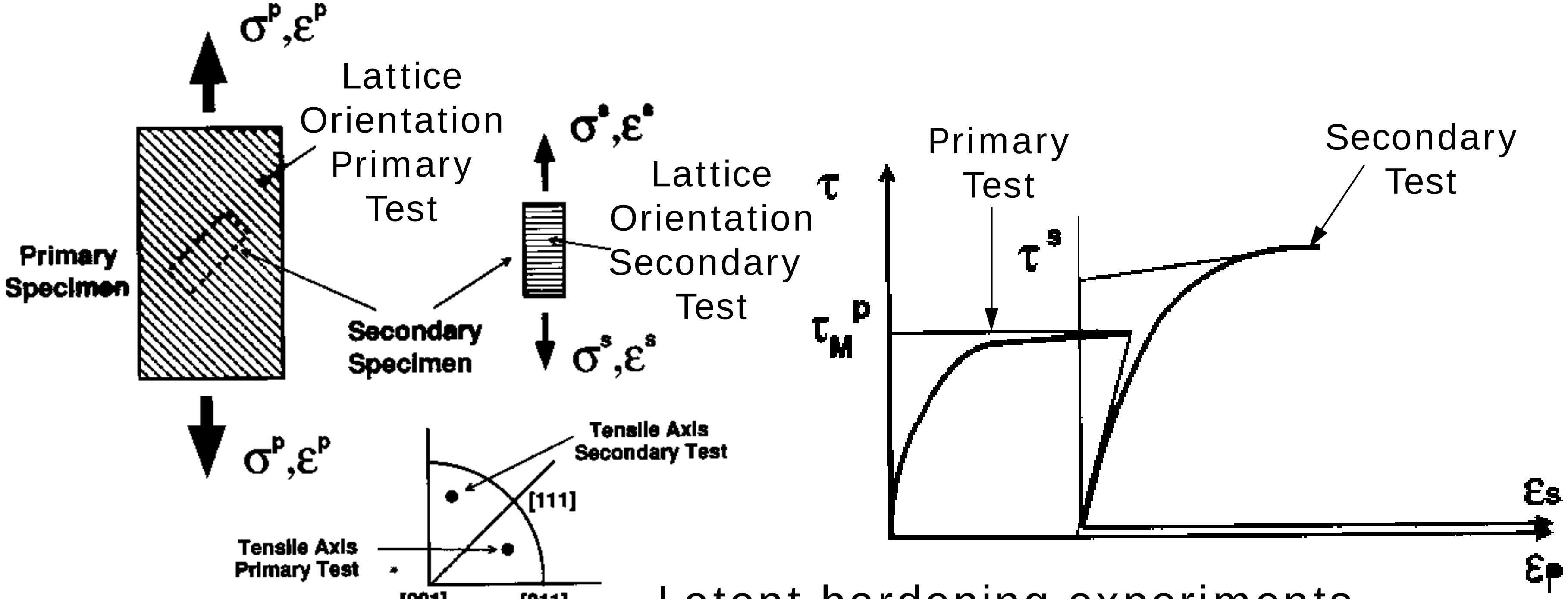
Latent hardening experiments[1,2]

- Strong latent hardening: Activity on one slip system hardens other systems much more than it hardens the system itself (owing to dislocation multiplication and forest hardening...)

[1] Kocks, U.F., *Acta Metallurgica*, **8** (1960) 345

[2] Kocks, U.F., *Trans. Metall. Soc. AIME*, **230** (1964) 1160

Strong latent hardening & microstructure



Lattice Orientation Primary Test

Lattice Orientation Secondary Test

Primary Test

Secondary Test

Latent hardening experiments

- Classical model[1]: $\dot{\tau}_\alpha = \sum_{\beta=1}^{N} \left[qh + (1-q)h\delta_{\alpha\beta} \right] \left| \dot{\gamma}_\beta \right|$
- Strong latent hardening: $q > 1$ → Nonconvexity!

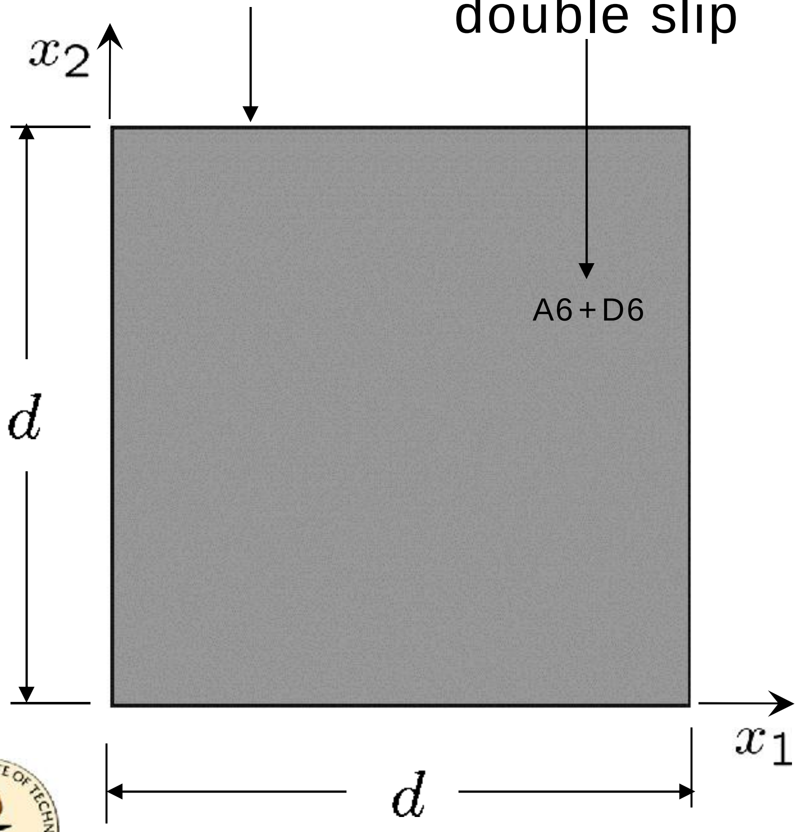
---

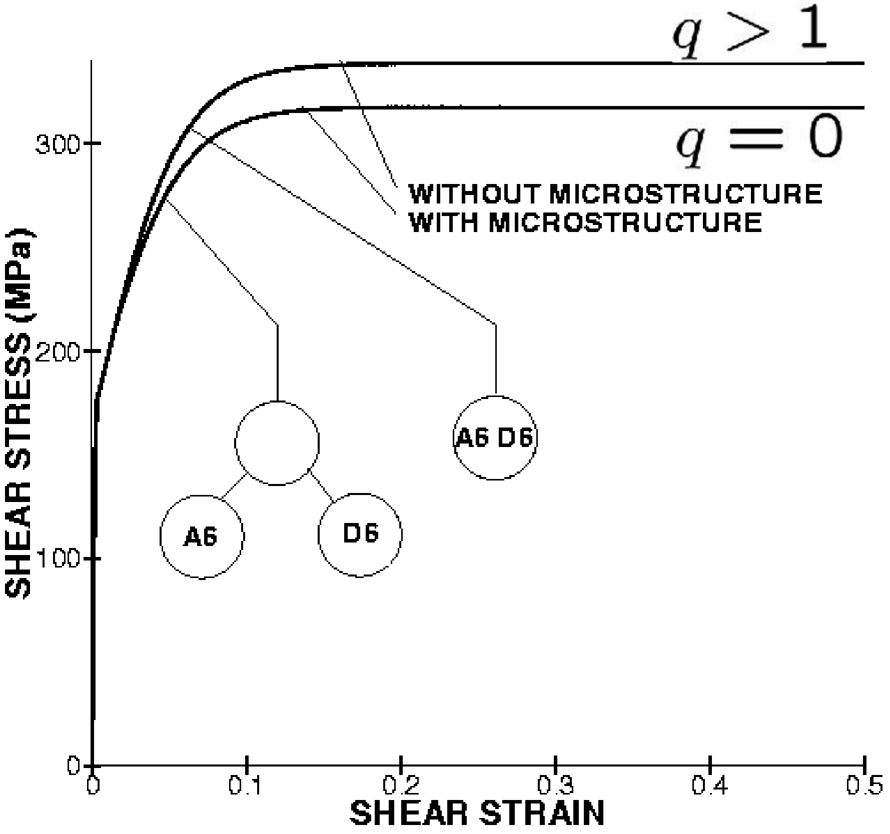
[1] Peirce, D., Asaro, R. and Needleman, A. *Acta Metall.*, **31** (1983) 1951.

Strong latent hardening & microstructure

affine boundary conditions $u_1 = \gamma x_2$

uniform double slip

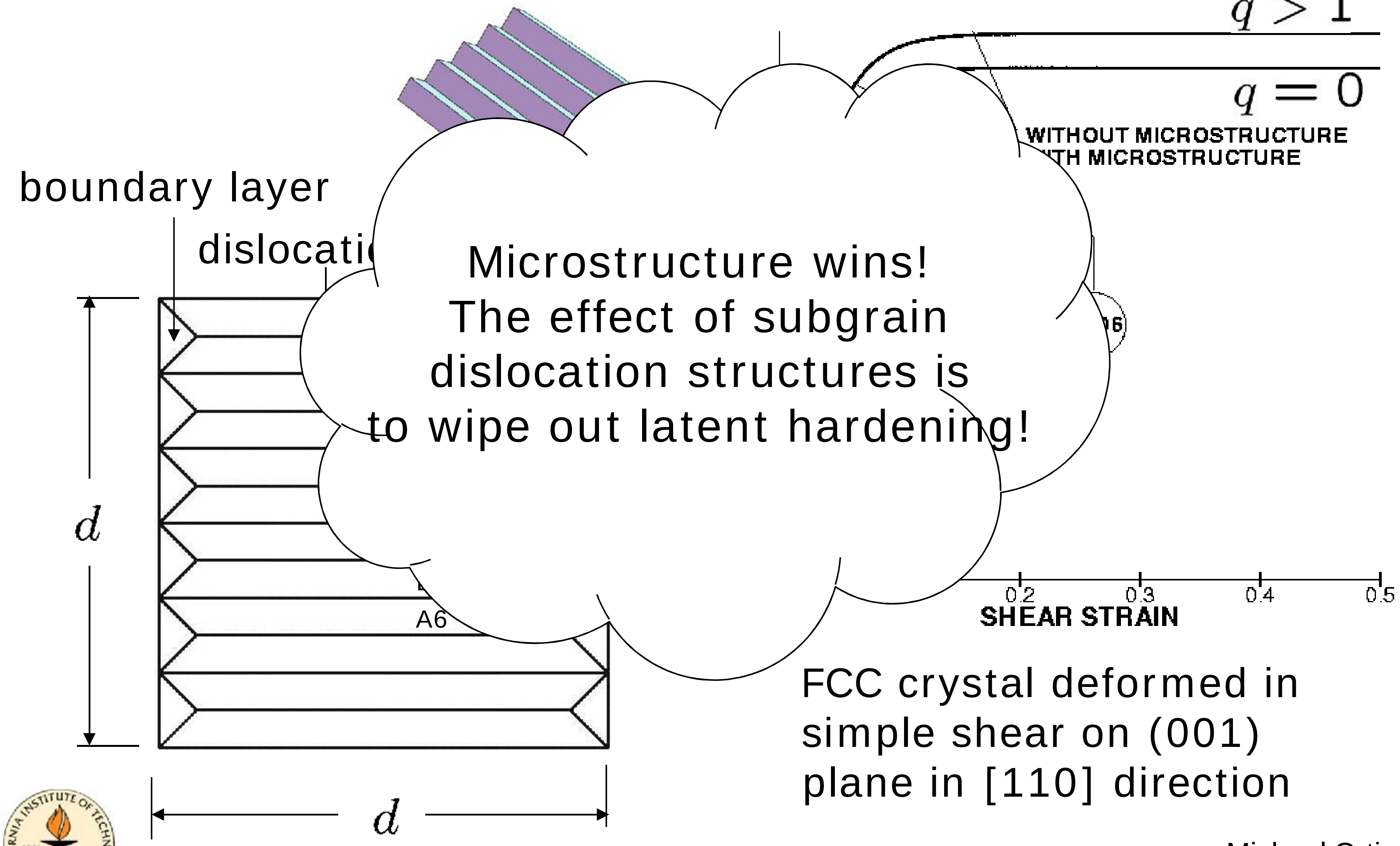




FCC crystal deformed in simple shear on (001) plane in [110] direction

M Ortiz, EA Repetto and L Stainier *JMPS*,**48**(10) 2000, p. 2077.

Strong latent hardening & microstructure

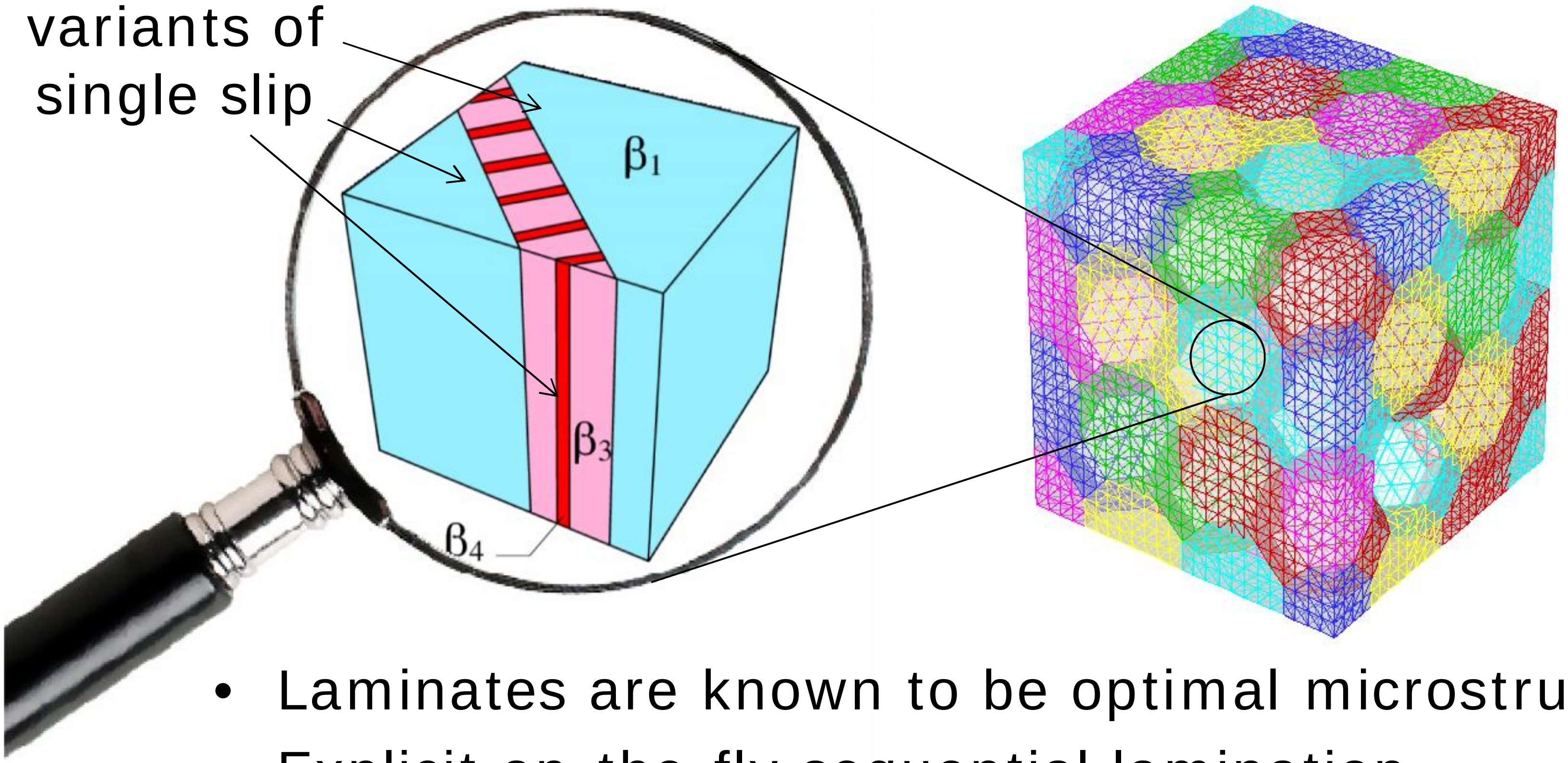


Microstructure wins!
The effect of subgrain
dislocation structures is
to wipe out latent hardening!

FCC crystal deformed in
simple shear on (001)
plane in [110] direction

M Ortiz, EA Repetto and L Stainier *JMPS*,**48**(10) 2000, p. 2077.

Optimal subgrain structures – Laminates



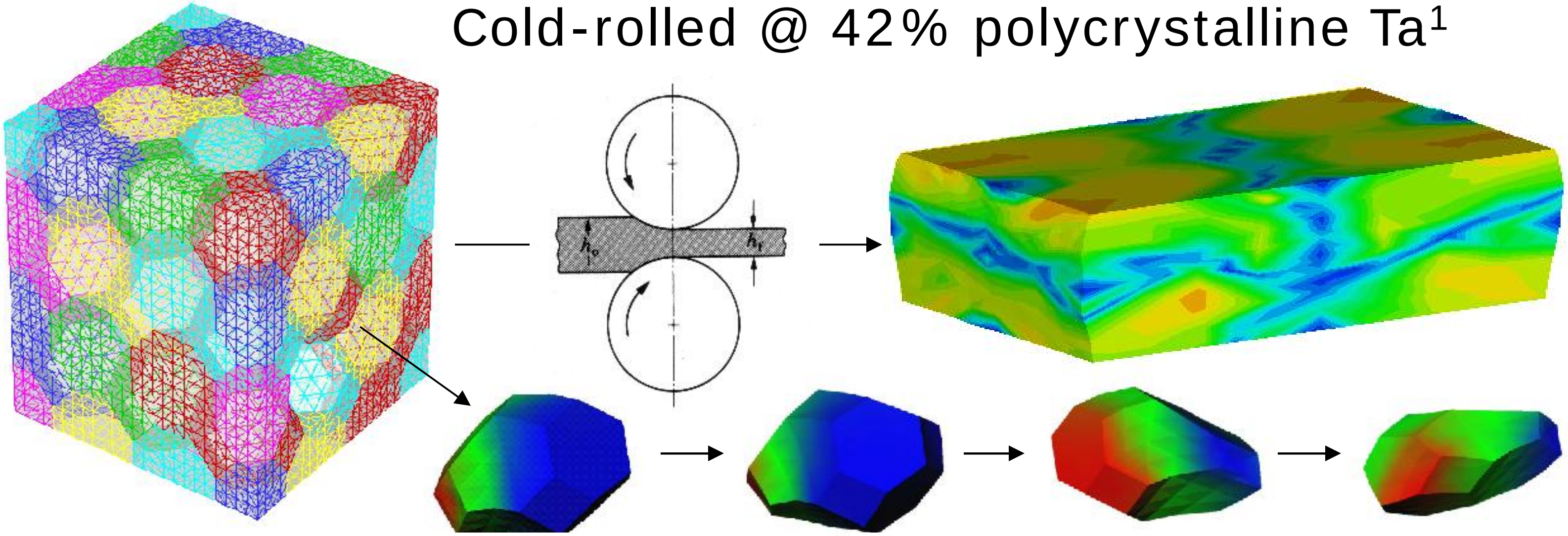
- Laminates are known to be optimal microstructures[1]
- Explicit on-the-fly sequential lamination construction delivers effective response[1,2]
- Caveat emptor: All other bases are sub-optimal! (e.g., Fourier, spectral, p-enrichment...)

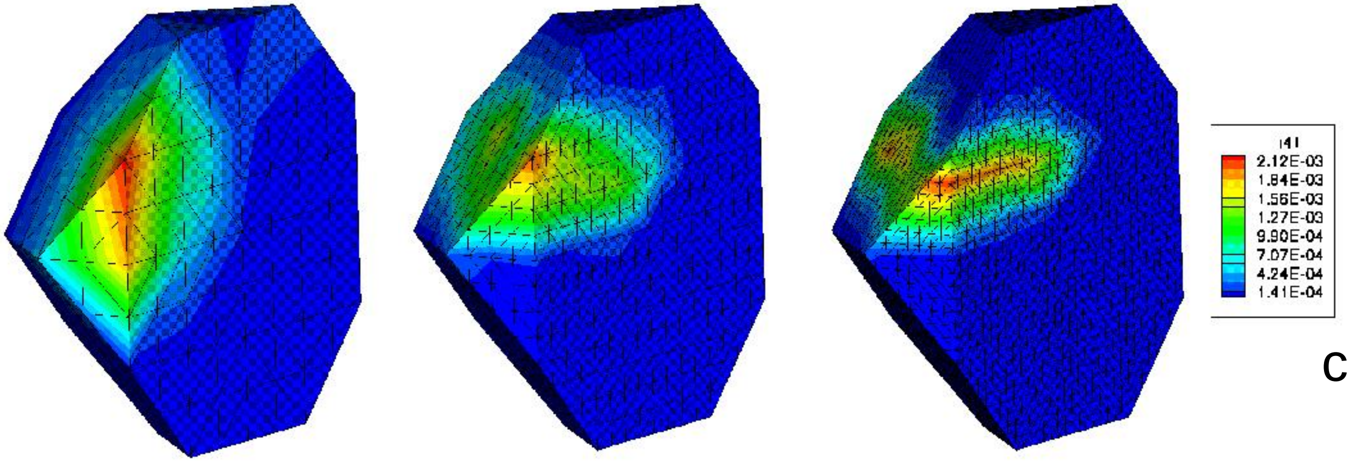
[1] Conti, S. and Ortiz, M., *ARMA*, 176: 103-147, 2005.

[2] Hansen, B., Bronkhorst, C.A., Ortiz, M., MSMSE, 18: 055001, 2010.

Suboptimal subgrain structures

Cold-rolled @ 42% polycrystalline Ta[1]



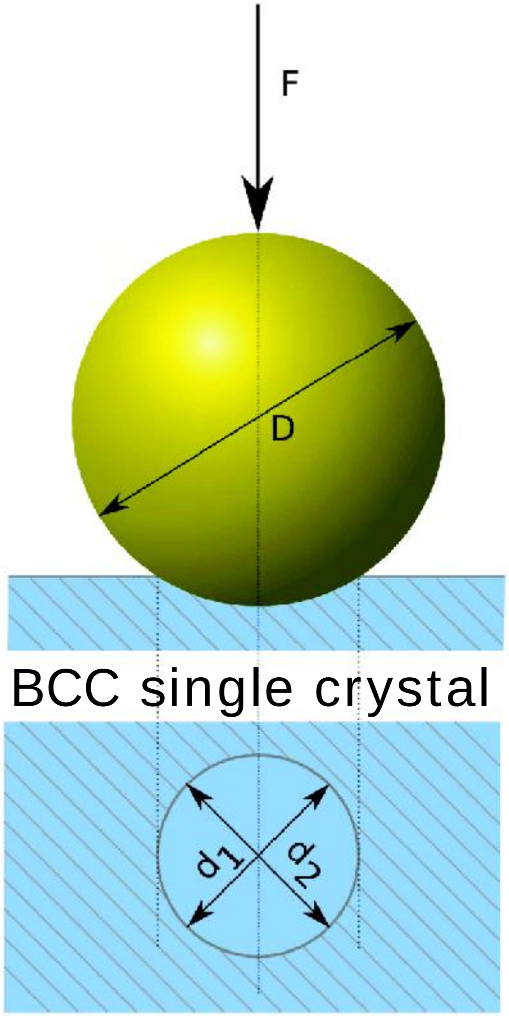


192 elmts 1,536 elmts. 12,288 elmts.

Slow or no convergence!

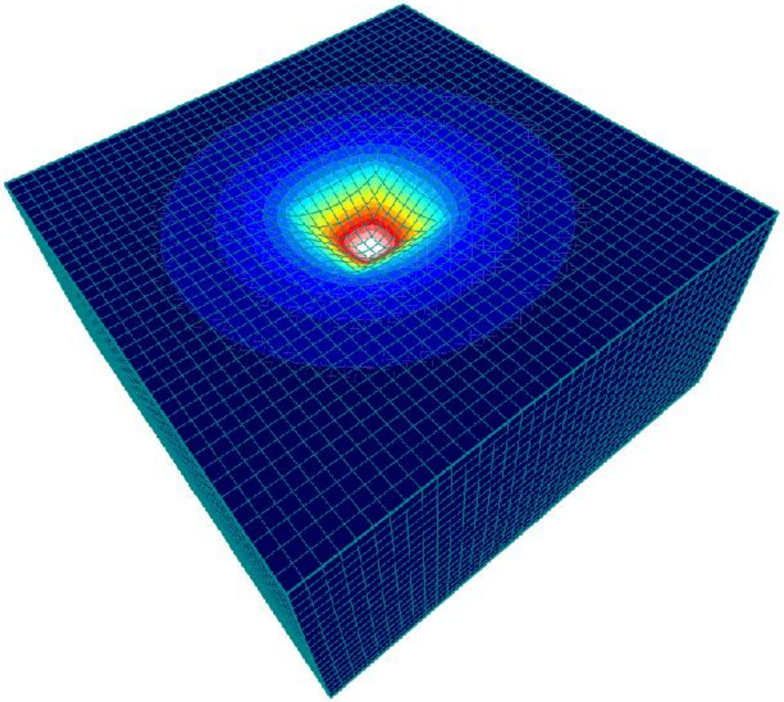
Zhao, Z., Radovitzky, R. and Cuitino A. (2004) Acta Mater., 52(20) 5791.

Optimal *vs.* suboptimal microstructures



[001]

BCC single crystal

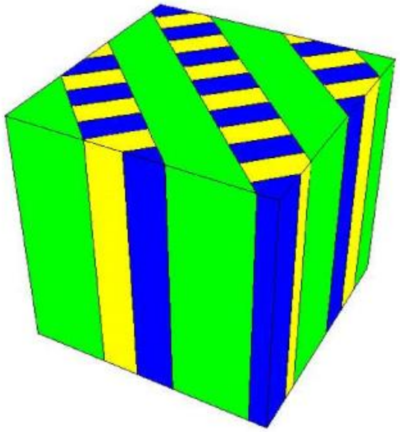


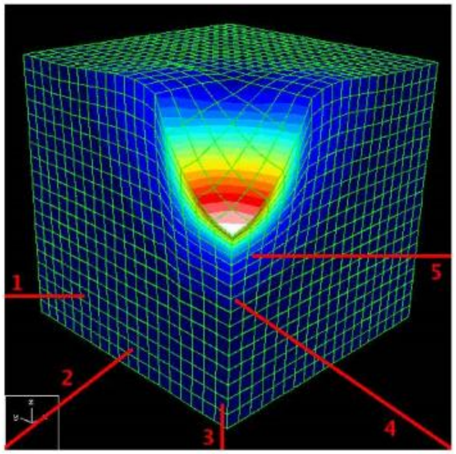
Indentation of [001] surface
of BCC single crystal
32,000 nodes
27,436 hexahedral elements

Conti, S., Hauret, P. and Ortiz, M.,
SIAM Multiscale Model. Simul., 6: 135-157, 2007

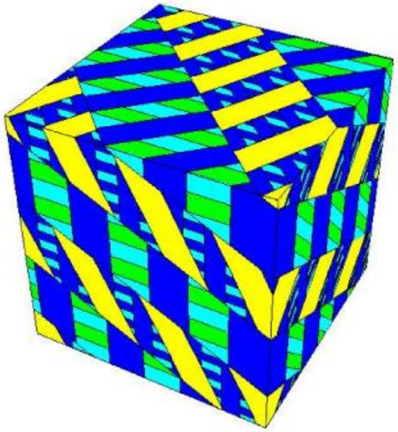
Optimal *vs*. suboptimal microstructures

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

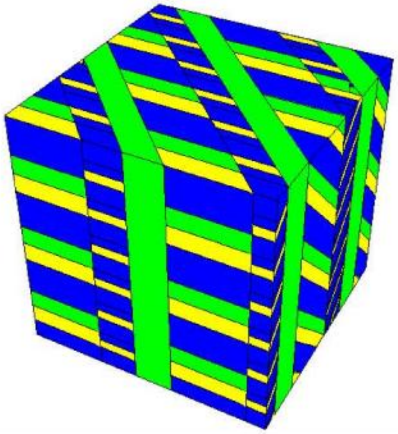




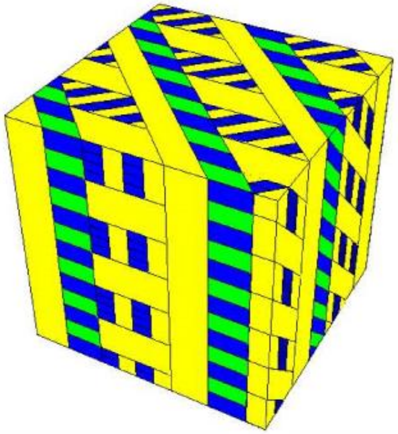
rank 4/14, $|\gamma|_\infty$ = 0.43



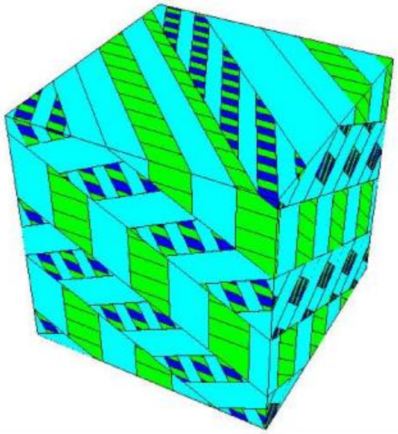
rank 4/12, $|\gamma|_\infty$ = 0.02



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

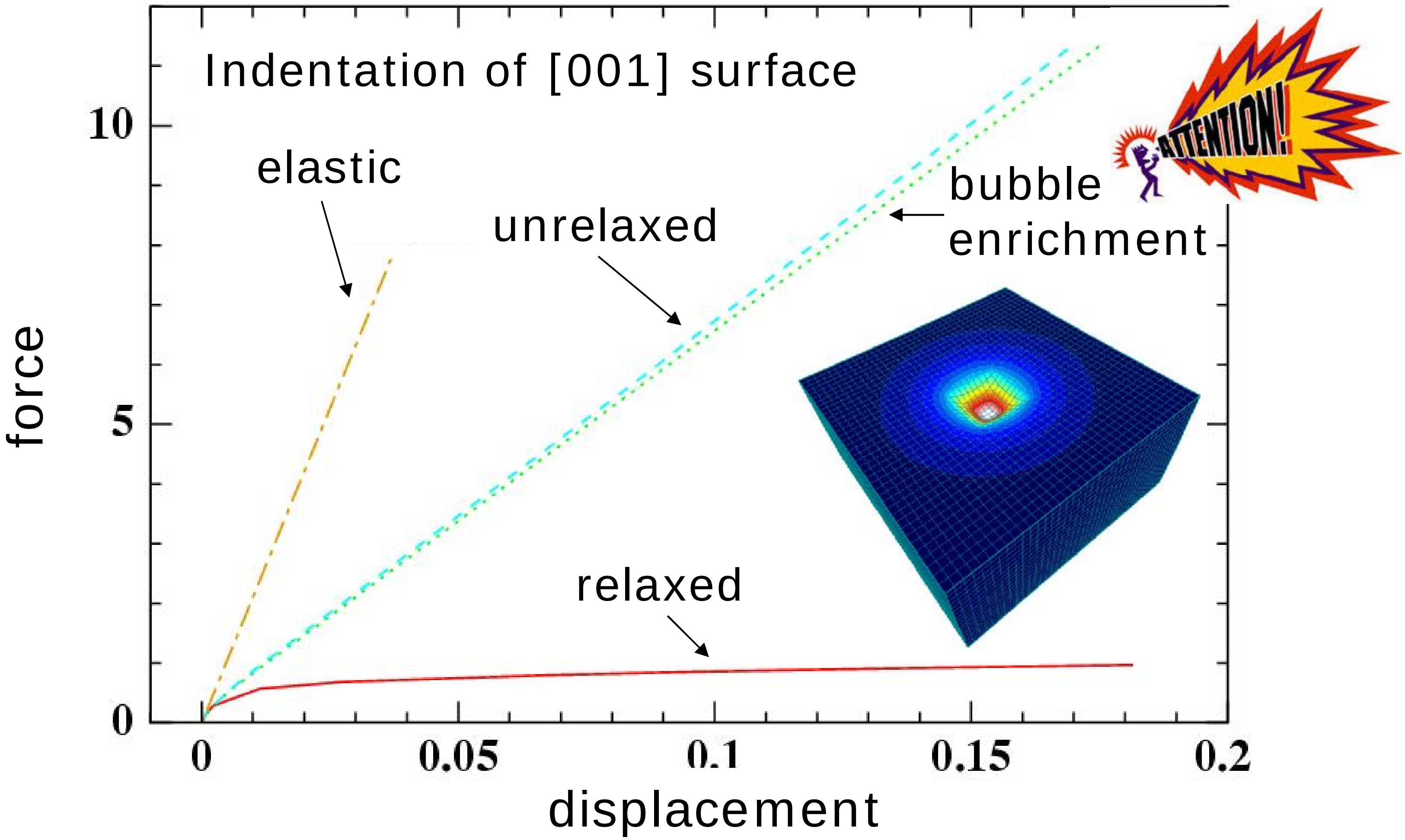


rank 4/16, $|\gamma|_\infty$ = 0.21



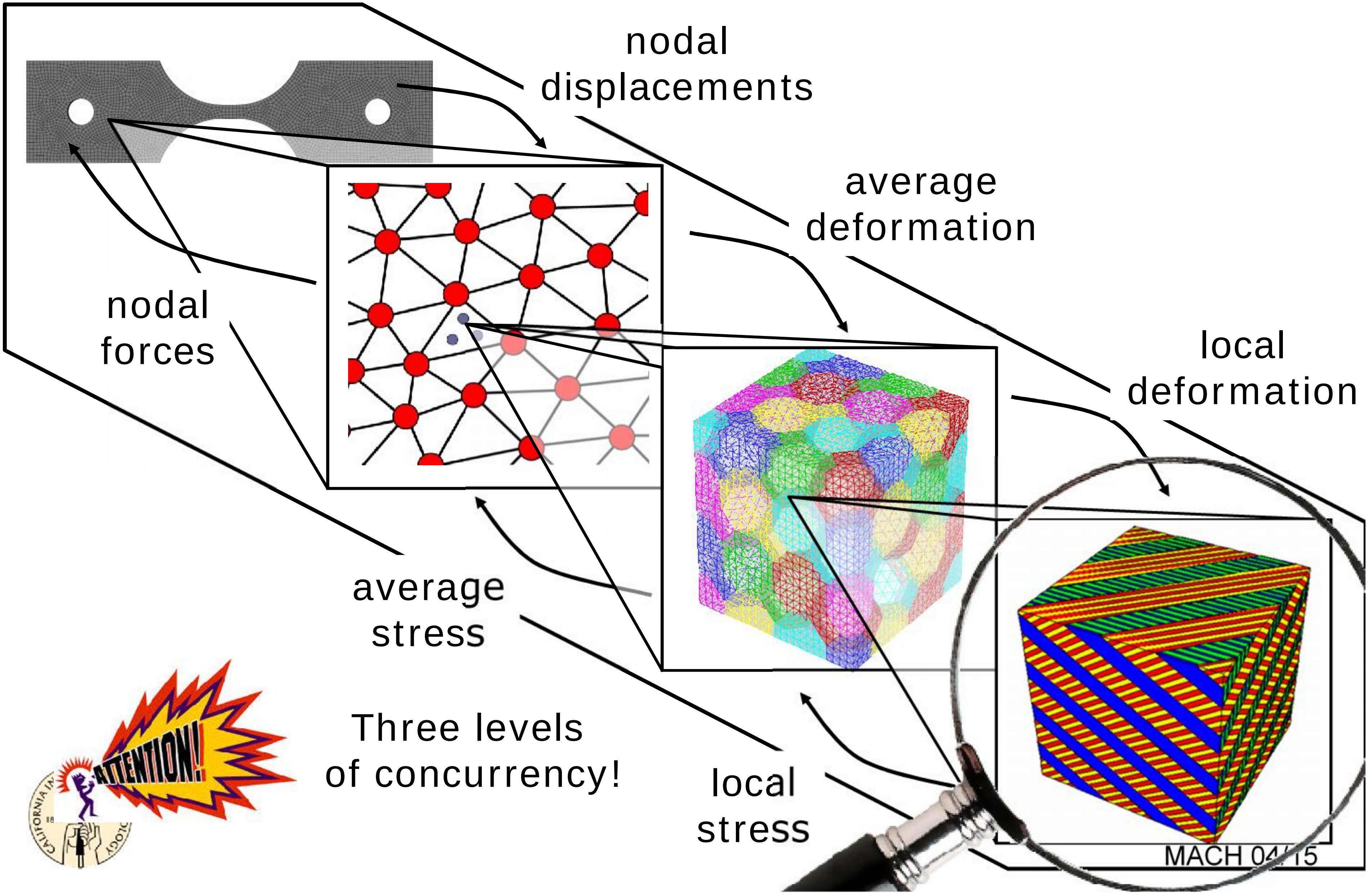
Conti, S., Hauret, P. and Ortiz, M.,
SIAM Multiscale Model. Simul., 6: 135-157, 2007

Optimal *vs.* suboptimal microstructures



Conti, S., Hauret, P. and Ortiz, M.,
SIAM Multiscale Model. Simul., 6: 135-157, 2007

Polycrystals – Concurrent multiscale (C^3)



nodal displacements

average deformation

local deformation

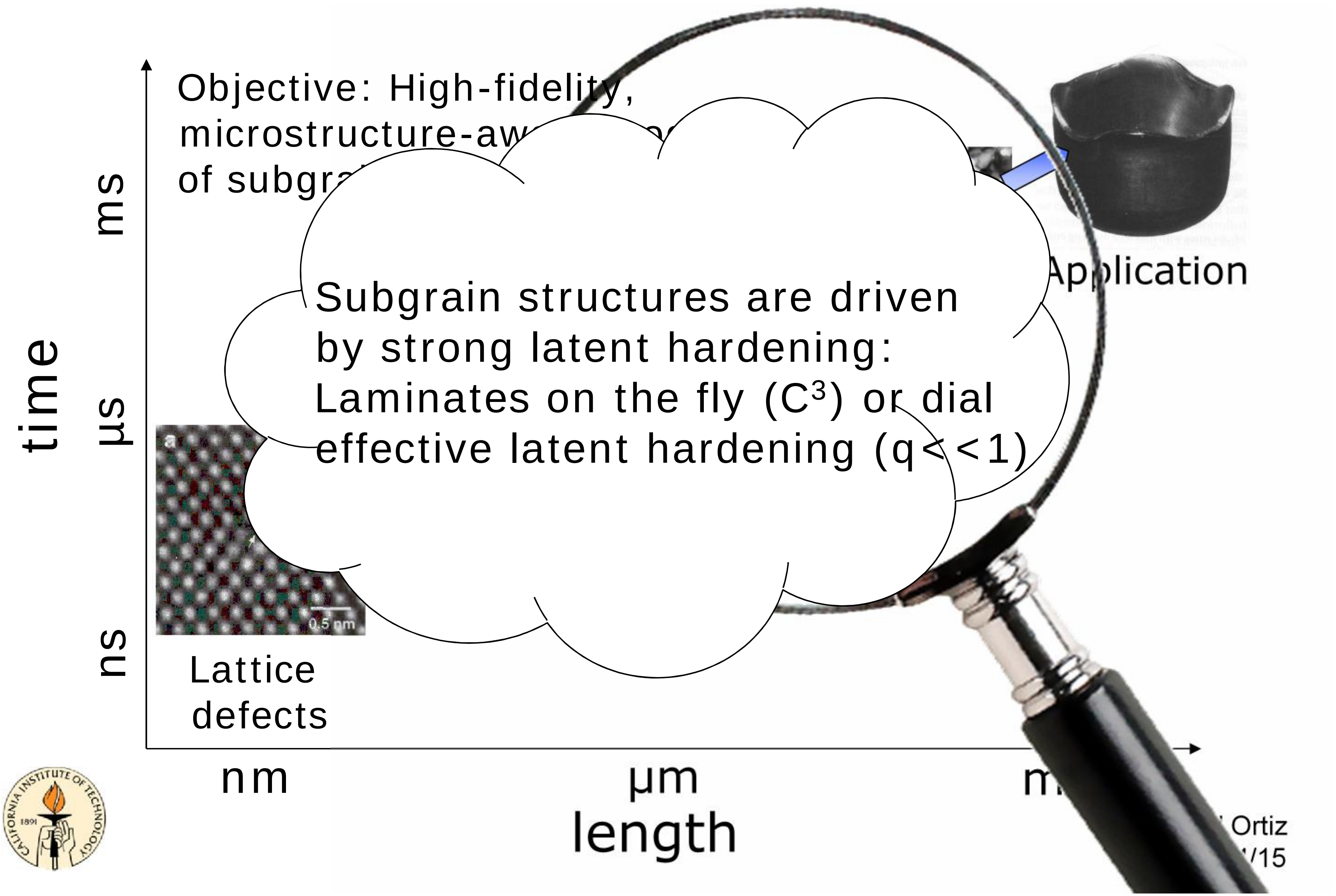
nodal forces

average stress

local stress

Three levels of concurrency!

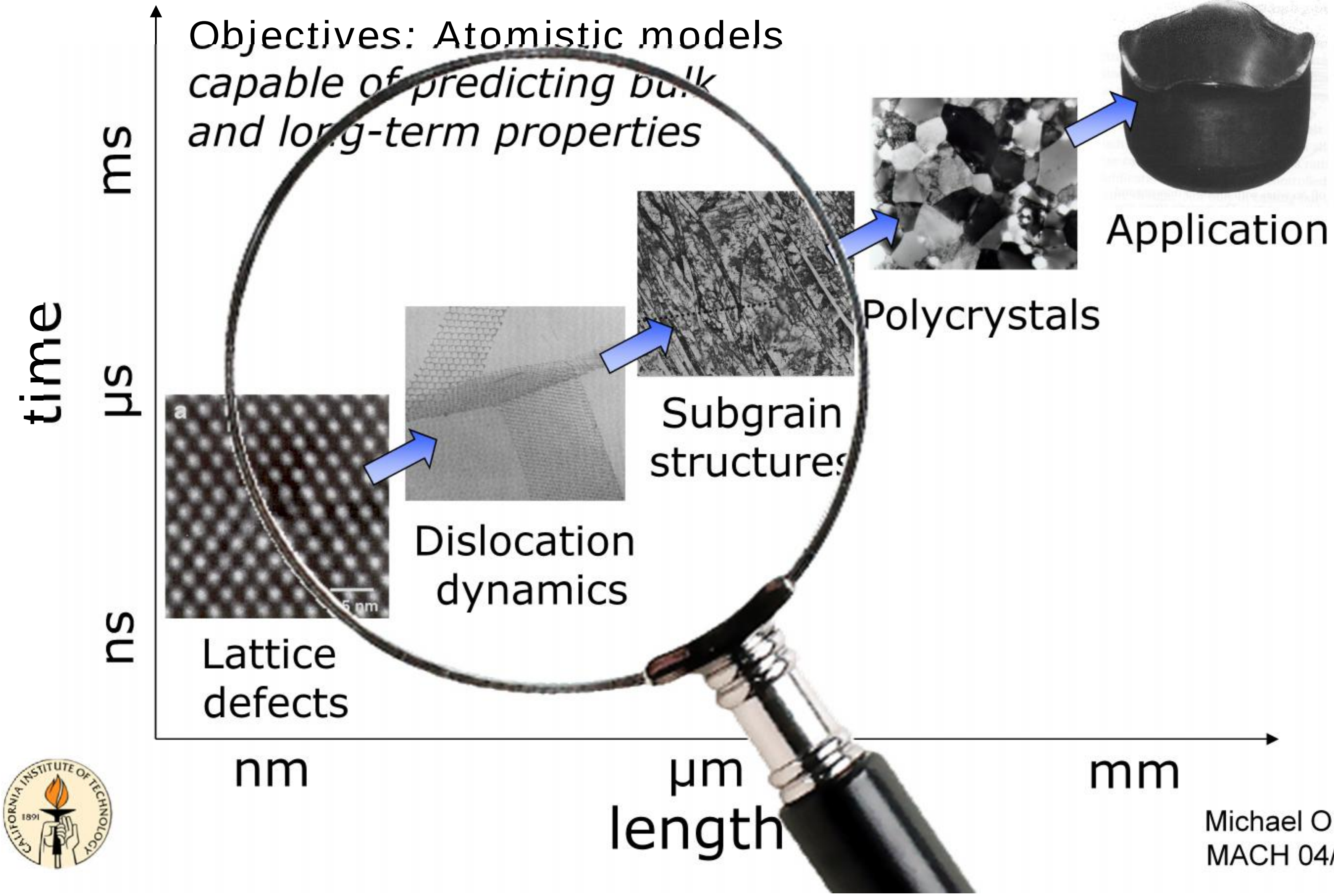
Multiscale modeling of materials



Objective: High-fidelity,
microstructure-aw
of subgr

Subgrain structures are driven by strong latent hardening: Laminates on the fly (C^3) or dial effective latent hardening ($q<<1$)

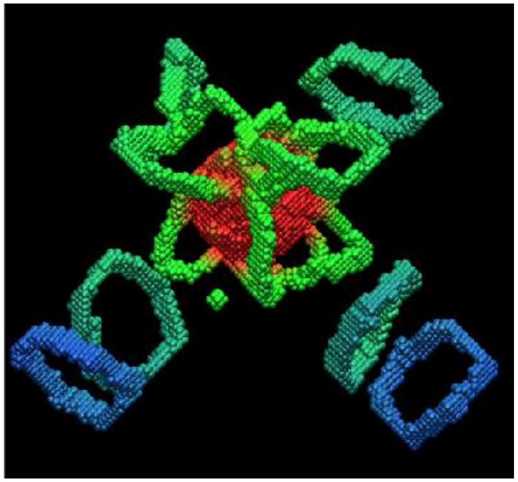
Multiscale modeling of materials



Objectives: Atomistic models *capable of predicting bulk and long-term properties*

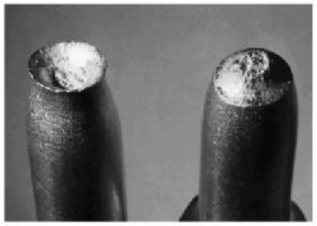
The essential difficulty…

10^{10} s^{-1}, 100 nm

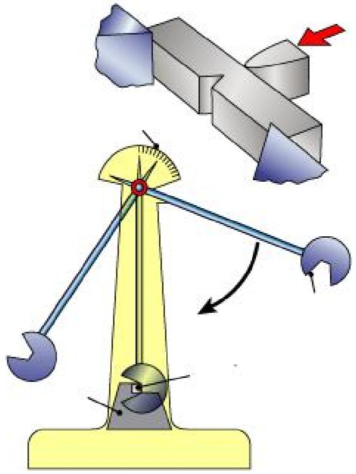


MD simulation of nanovoids growth in Ta[1]

10^{3} s^{-1}, 1 cm



Cup-cone ductile fracture



Charpy test

- Many mechanical properties are rate-controlled by lattice defects
- MD can access strain rates ~ 10^8-10^{12} s^{-1}, nano-samples
- Engineering applications involve lower strain rates, larger sizes
- Materials testing:
  - Servo-hydraulic: 1 s^{-1}
  - Hopkinson bar: 10^4 s^{-1}
  - Plate impact: 10^7 s^{-1} a
- MD outside realm of typical engineering application and materials testing…

[1] Tang, Y., Bringa, E.M., Remington, B.A., and Meyers, M.A., *Acta Materialia*, **59**:1354, 2011

Paradigm shift: Deterministic-to-Statistical

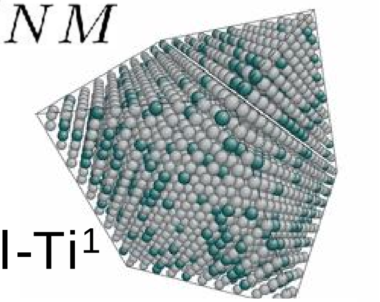
- Treat atomic-level fluctuations statistically (away from equilibrium) through maximum-entropy principle
- Approximate grand-canonical free entropy using variational meanfield theory
- Append Onsager-like empirical atomic-level kinetic laws (heat and mass transport)
- Treat (smooth) mesodynamics by implicit integration (large time steps >> MD!)
- Quasicontinuum spatial coarse-graining

[1] Y. Kulkarni, J. Knap & MO, *J. Mech. Phys. Solids*, **56** (2008) 1417.

[2] G. Venturini, K. Wang, I. Romero, M.P. Ariza & MO, *J. Mech. Phys. Solids*, **73** (2014) 242-268.

Max-Ent Non-Equilibrium SM

- Grand-canonical ensemble, N atoms, M species:
  - State: $(\{\boldsymbol{q}\},\{\boldsymbol{p}\},\{\boldsymbol{n}\}) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N} \times \mathcal{O}_{NM}$
  - Atomic positions: $\{\boldsymbol{q}\} = \{\boldsymbol{q}_1, \dots, \boldsymbol{q}_N\}$
  - Atomic momenta: $\{\boldsymbol{p}\} = \{\boldsymbol{p}_1, \dots, \boldsymbol{p}_N\}$
  - Occupancy: $n_{ik} = \begin{cases} 1, & \text{site } i \text{ occupied by species } k, \\ 0, & \text{otherwise.} \end{cases}$



Al-Ti[1]

- Ensemble average of observable: $\langle A \rangle =$

$$\sum_{\{\boldsymbol{n}\}\in\mathcal{O}_{NM}} \int A(\{\boldsymbol{q}\},\{\boldsymbol{p}\},\{\boldsymbol{n}\})\ \underset{\substack{\uparrow \\ \text{grand-canonical pdf}}}{\rho}(\{\boldsymbol{q}\},\{\boldsymbol{p}\},\{\boldsymbol{n}\})\, dq\, dp$$

J. von Pezold, A. Dick, M. Friak and J. Negebauer, Phys. Rev. B, 81 (2010) 094203.

Max-Ent Non-Equilibrium SM

- Assume $H = \sum_{i=1}^{N} h_i$, (e. g., EAM, TB...)
- Principle of max-ent[1]: $\mathcal{S}[p] = -k_B \langle \log \rho \rangle \to$ max!

subject to:
$$\left.\begin{array}{l} \langle \boldsymbol{q}_i \rangle = \bar{\boldsymbol{q}}_i, \ \langle \boldsymbol{p}_i \rangle = \bar{\boldsymbol{p}}_i, \\ \langle h_i \rangle = e_i, \ \langle n_{ik} \rangle = x_{ik} \end{array}\right\} \text{local constraints!}$$

- Lagrangian: reciprocal temperatures chemical potentials

$$\mathcal{L}[p, \{\beta\}, \{\gamma\}] = \mathcal{S}[p] - k_B \{\overset{\downarrow}{\beta}\}^T \{\langle h \rangle\} - k_B \{\overset{\downarrow}{\boldsymbol{\gamma}}\}^T \{\langle \boldsymbol{n} \rangle\}$$

- Gran-canonical pdf: $\underline{\rho = \frac{1}{\Xi} \mathrm{e}^{-\{\beta\}^T \{h\} - \{\gamma\}^T \{\boldsymbol{n}\}},}$

on affine subspace $\Big\{ \langle \{\boldsymbol{q}\} \rangle = \{\bar{\boldsymbol{q}}\}, \langle \{\boldsymbol{p}\} \rangle = \{\bar{\boldsymbol{p}}\} \Big\}$

[1] E.T. Jaynes, *Physical Review Series* II, **106**(4) (1957) 620–630; **108**(2) (1957) 171–190.

Non-Equilibrium Statistical Mechanics

- From max-ent principle, free entropy:

$$\Phi = k_B \log \int \mathrm{e}^{-\{\beta\}^T \{h(q,p)\}}\, dq\, dp$$

reciprocal atomic temperatures

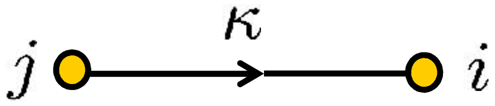
local atomic Hamiltonians

- Mesoscopic dynamics:

$$\frac{d\bar{\boldsymbol{q}}_i}{dt} = \frac{\partial \bar{H}}{\partial \bar{\boldsymbol{p}}_i}, \qquad \frac{d\bar{\boldsymbol{p}}_i}{dt} = -\frac{\partial \bar{H}}{\partial \bar{\boldsymbol{q}}_i}, \qquad \bar{H} = \sum_{i=1}^{N} \frac{1}{k_B} \frac{\partial \Phi}{\partial \beta_i}$$

- Temperature field evolution, discrete heat equation:

$$\underbrace{\frac{d}{dt}\frac{1}{k_B}\frac{\partial \Phi}{\partial \beta_i}}_{\text{internal energy of atom i}} = \sum_{j \neq i} \underbrace{\partial \psi(\beta_i - \beta_j)}_{\text{heat flux into atom i}}$$



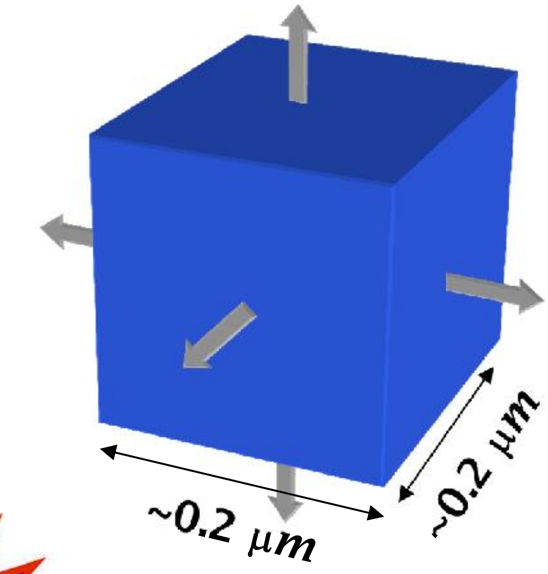
Non-Equilibrium Statistical Mechanics

	Molecular dynamics	N.E. Stat. Mech.
Configuration space	Phase space (q,p)	•Temperature field •Atomic-fraction field
Governing equations	ΣF=ma	•Diffusive transport •Mesodynamics
Spatial resolution	Atomic lattice	•Temperature grads. •Concentration grads.
Temporal resolution	•Thermal vibrations •Transition states	•Mesoscopic dynamics •Diffusional transients
Time-scale bridging	Non-equilibrium statistical mechanics	
Spatial-scale bridging	Quasicontinuum method	

- Paradigm shift: From Newtonian dynamics to diffusional transport (heat and mass)
- Time step limited by diffusional time scale!

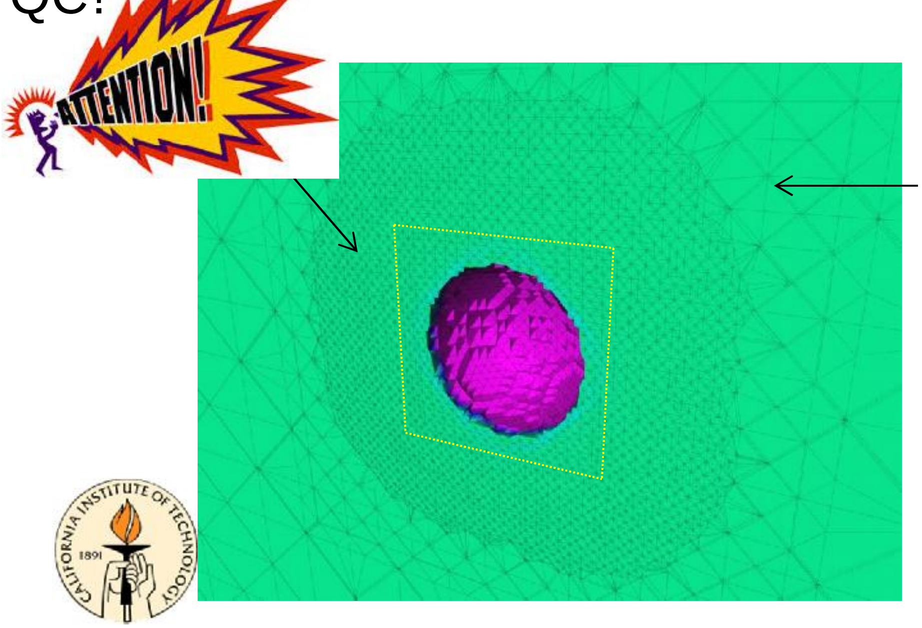
Y. Kulkarni et al., J. Mech. Phys. Solids, 56:1417-1449, 2008

Application: Nanovoid cavitation in Cu[1]



- Parameters:
  - T_0 (initial) = 300K
  - Full Size = $72a_0$
  - Atomistic Zone = $14a_0$
  - Diameter = $12a_0$
  - Strain Rate = 10^5-10^{12} s^{-1}
- Loading: Triaxial, uniaxial
- Potential: EAM-Mishin[2]

QC!



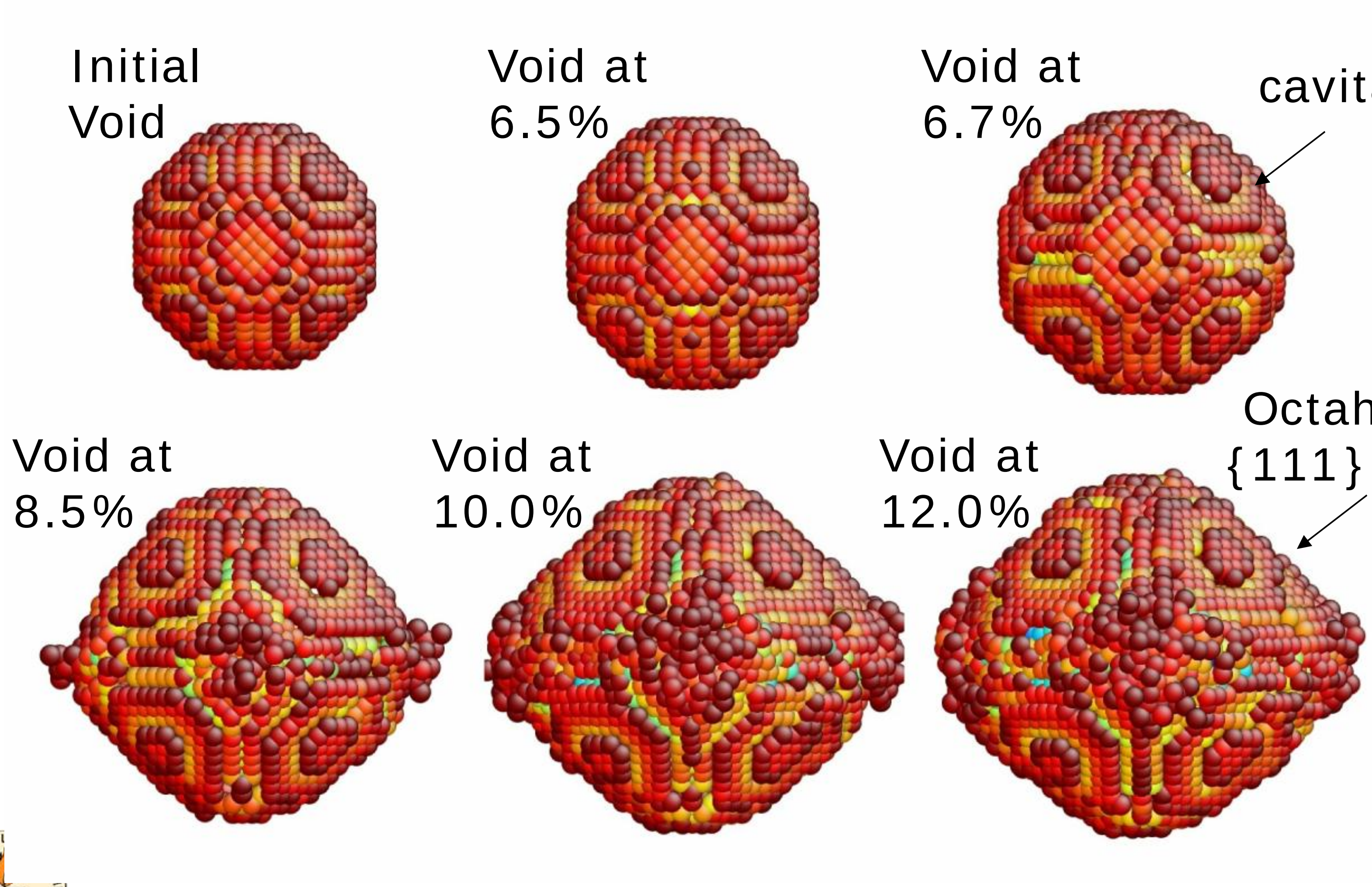
Initial quasicontinuum mesh with full atomistic resolution near void

[1] M. Ponga, M. Ortiz and P. Ariza, *Mechanics of Materials* (submitted)

[2] Y. Mishin, M. Mehl, D. Papaconstantopoulos, A. Voter, A. and J. Kress, *Phys. Rev. B*, **63** (2001) 224106.

Application: Nanovoid cavitation in Cu

Uniaxial loading



Initial Void

Void at 6.5%

Void at 6.7%

cavitation

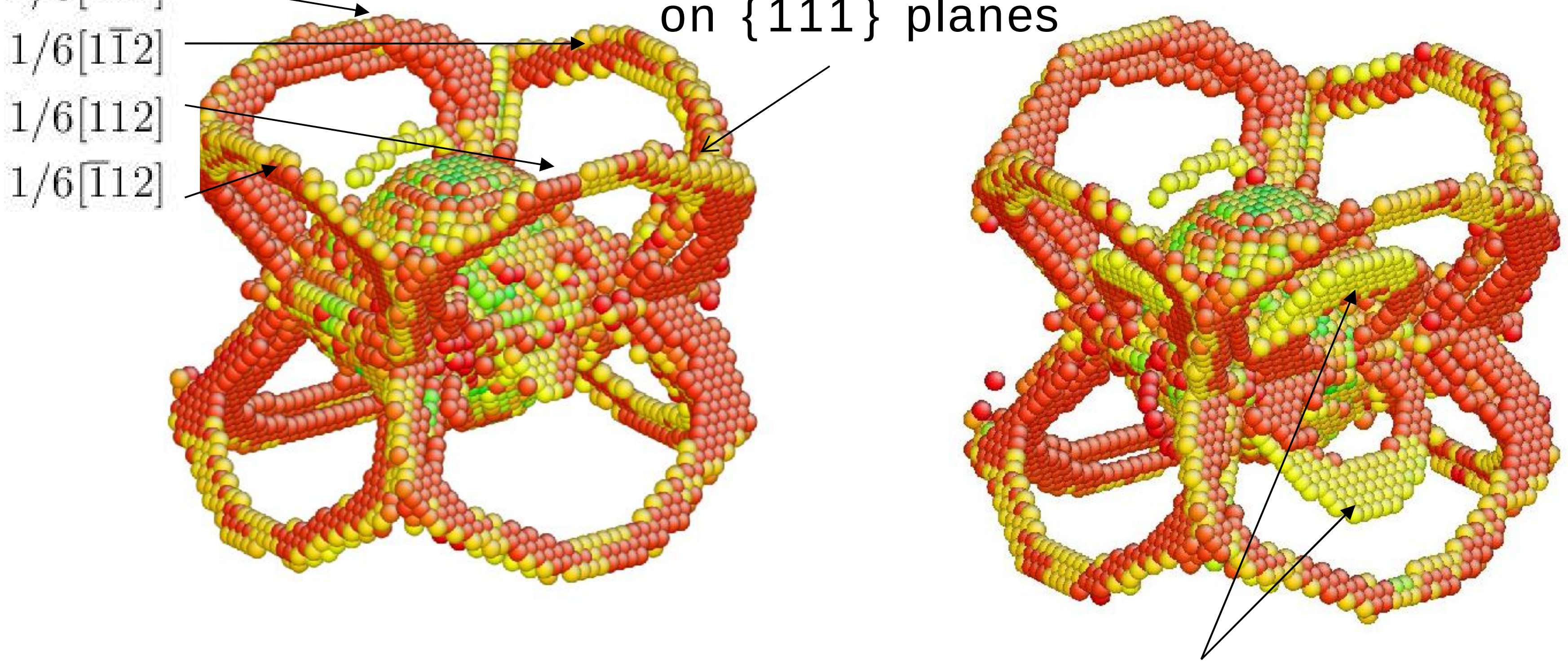
Void at 8.5%

Void at 10.0%

Void at 12.0%

Octahedron {111} planes

Application: Nanovoid cavitation in Cu



$1/6[\bar{1}\bar{1}2]$

$1/6[1\bar{1}2]$

$1/6[112]$

$1/6[\bar{1}12]$

Leading Shockley partial dislocations on {111} planes

Uniaxial loading,
$\varepsilon = 6.6\%$

Trailing Shockley partial dislocations on {111} planes

Application: Nanovoid cavitation in Cu

Shear to Prismatic loop reactions:

On <110> directions

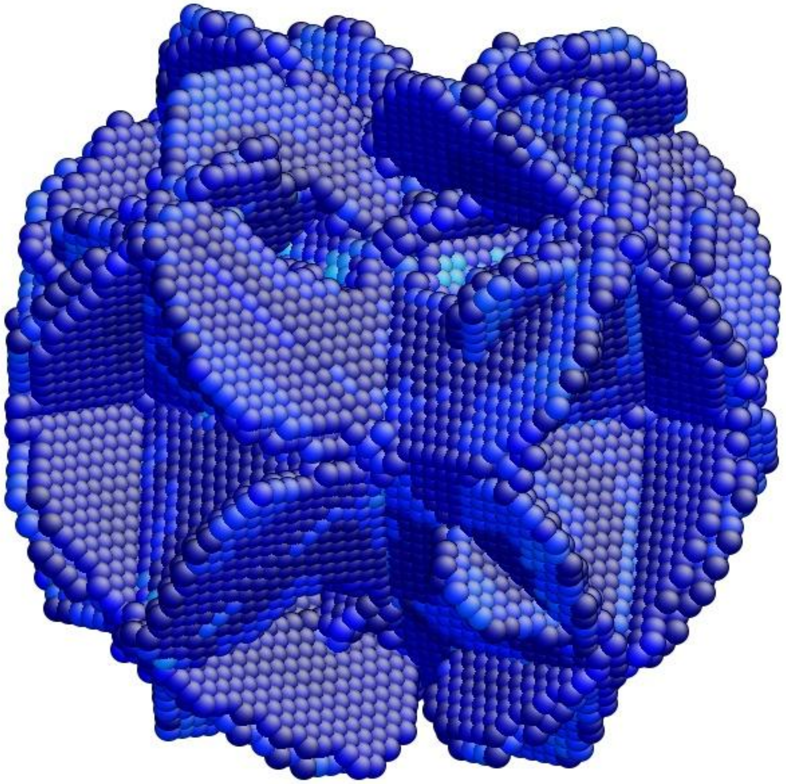
$$1/6[\bar{2}11] + 1/6[\bar{2}1\bar{1}] + 1/6[\bar{1}21] + 1/6[\bar{1}2\bar{1}] \rightarrow [\bar{1}10]$$
$$1/6[\bar{2}\bar{1}\bar{1}] + 1/6[\bar{2}\bar{1}1] + 1/6[\bar{1}\bar{2}\bar{1}] + 1/6[\bar{1}\bar{2}1] \rightarrow [\bar{1}\bar{1}0]$$
$$1/6[1\bar{2}1] + 1/6[1\bar{2}\bar{1}] + 1/6[2\bar{1}1] + 1/6[2\bar{1}\bar{1}] \rightarrow [1\bar{1}0]$$
$$1/6[211] + 1/6[12\bar{1}] + 1/6[21\bar{1}] + 1/6[121] \rightarrow [110]$$

On <110> directions

$$1/6[\bar{2}\bar{1}\bar{1}] + 1/6[\bar{1}\bar{1}\bar{2}] + 1/6[\bar{2}1\bar{1}] + 1/6[\bar{1}1\bar{2}] \rightarrow [\bar{1}0\bar{1}]$$
$$1/6[1\bar{1}\bar{2}] + 1/6[2\bar{1}\bar{1}] + 1/6[21\bar{1}] + 1/6[11\bar{2}] \rightarrow [10\bar{1}]$$
$$1/6[2\bar{1}1] + 1/6[211] + 1/6[1\bar{1}2] + 1/6[112] \rightarrow [101]$$
$$1/6[1\bar{1}2] + 1/6[\bar{2}11] + 1/6[\bar{2}\bar{1}1] + 1/6[\bar{1}\bar{1}2] \rightarrow [\bar{1}01]$$

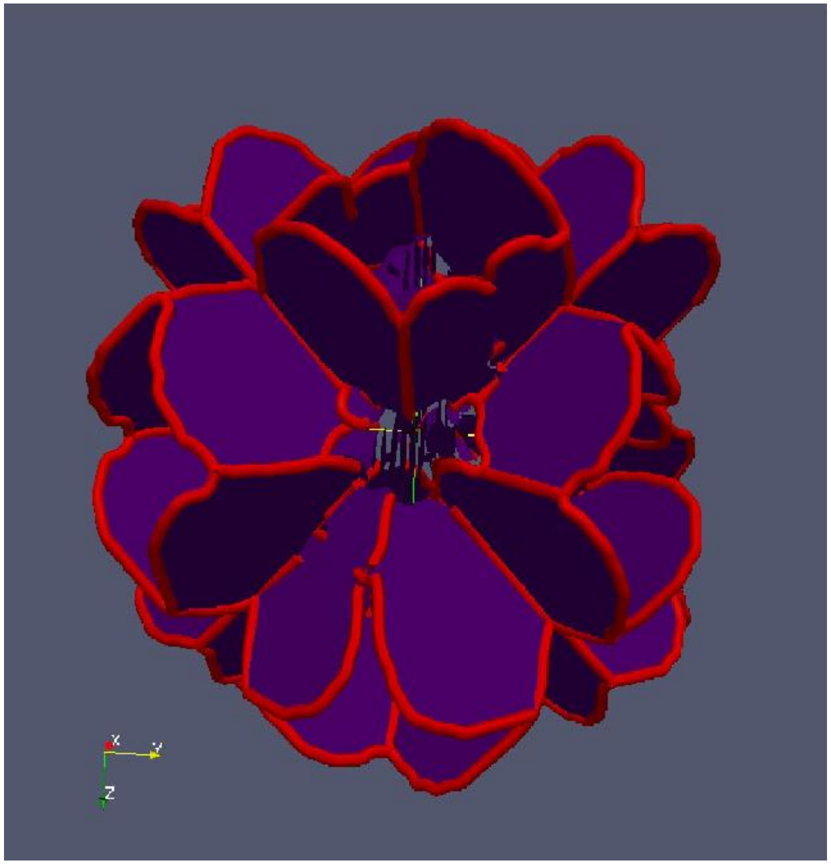
On <110> directions

$$1/6[\bar{1}21] + 1/6[\bar{1}12] + 1/6[\bar{1}21] + 1/6[112] \rightarrow [011]$$
$$1/6[1\bar{2}\bar{1}] + 1/6[\bar{1}\bar{2}\bar{1}] + 1/6[1\bar{1}\bar{2}] + 1/6[\bar{1}\bar{1}\bar{2}] \rightarrow [0\bar{1}\bar{1}]$$
$$1/6[\bar{1}\bar{2}1] + 1/6[1\bar{2}1] + 1/6[\bar{1}\bar{1}2] + 1/6[1\bar{1}2] \rightarrow [0\bar{1}1]$$
$$1/6[1\bar{2}1] + 1/6[11\bar{2}] + 1/6[\bar{1}1\bar{2}] + 1/6[12\bar{1}] \rightarrow [01\bar{1}]$$

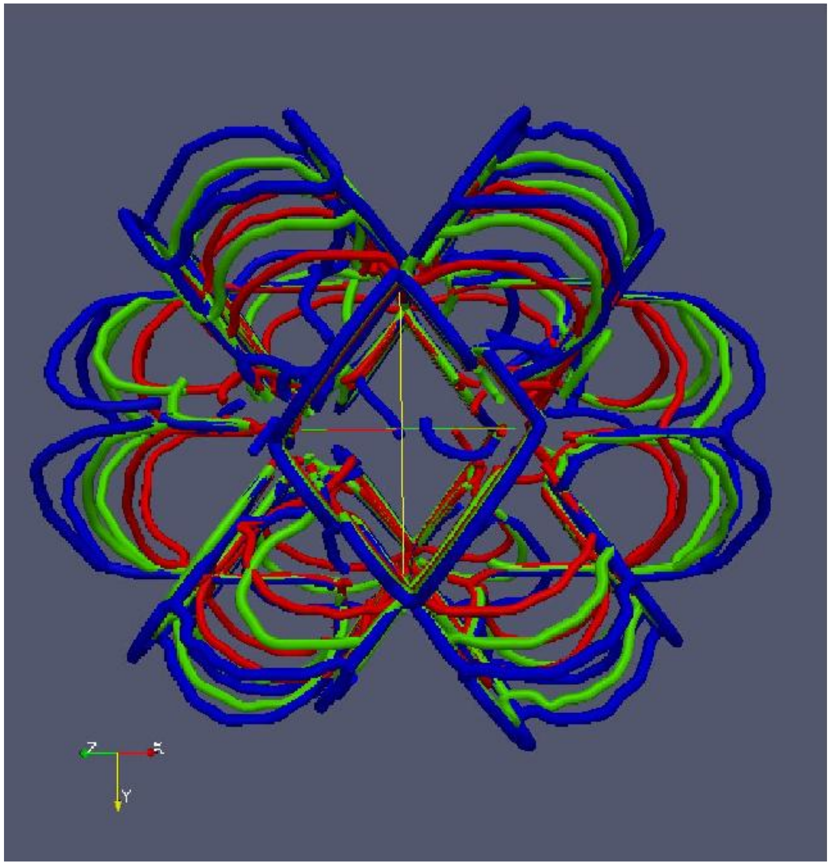


Triaxial loading

Application: Nanovoid cavitation in Cu



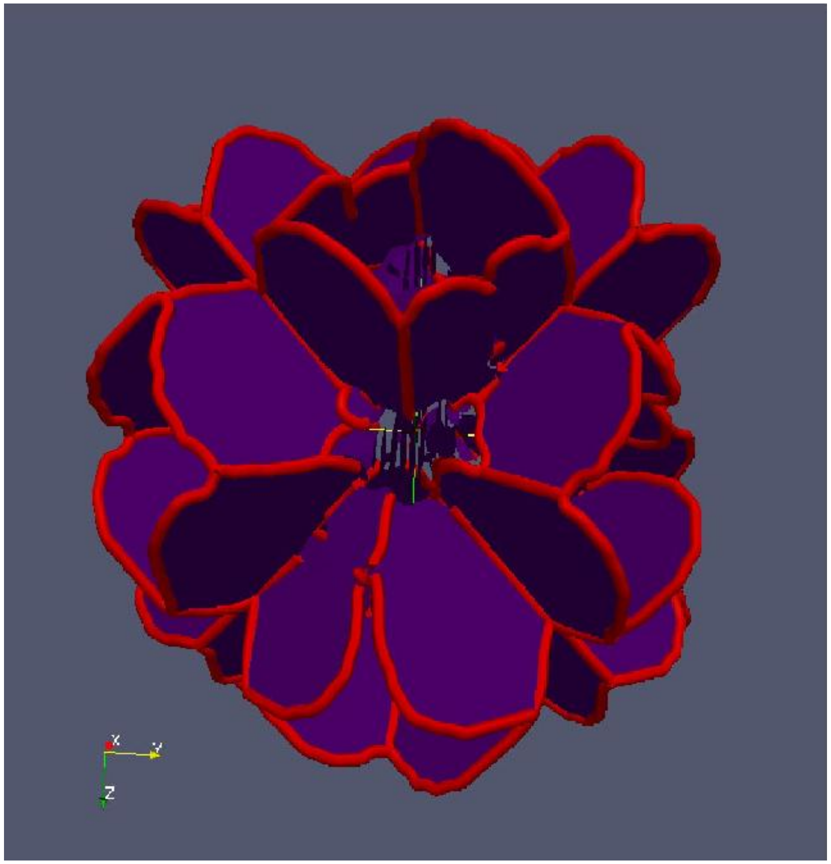
Prismatic loop structure, triaxial loading



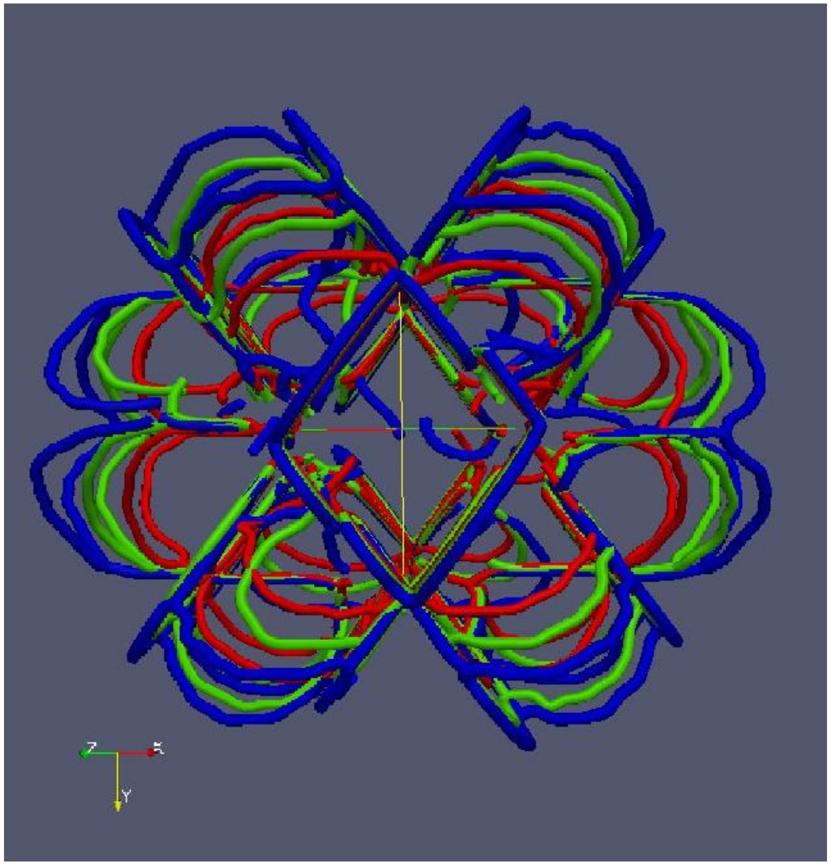
Prismatic loop evolution ($\varepsilon = 5, 6, 7\%$)

(Images obtained with DXA and Paraview)

Application: Nanovoid cavitation in Cu



Prismatic loop structure,
triaxial loading

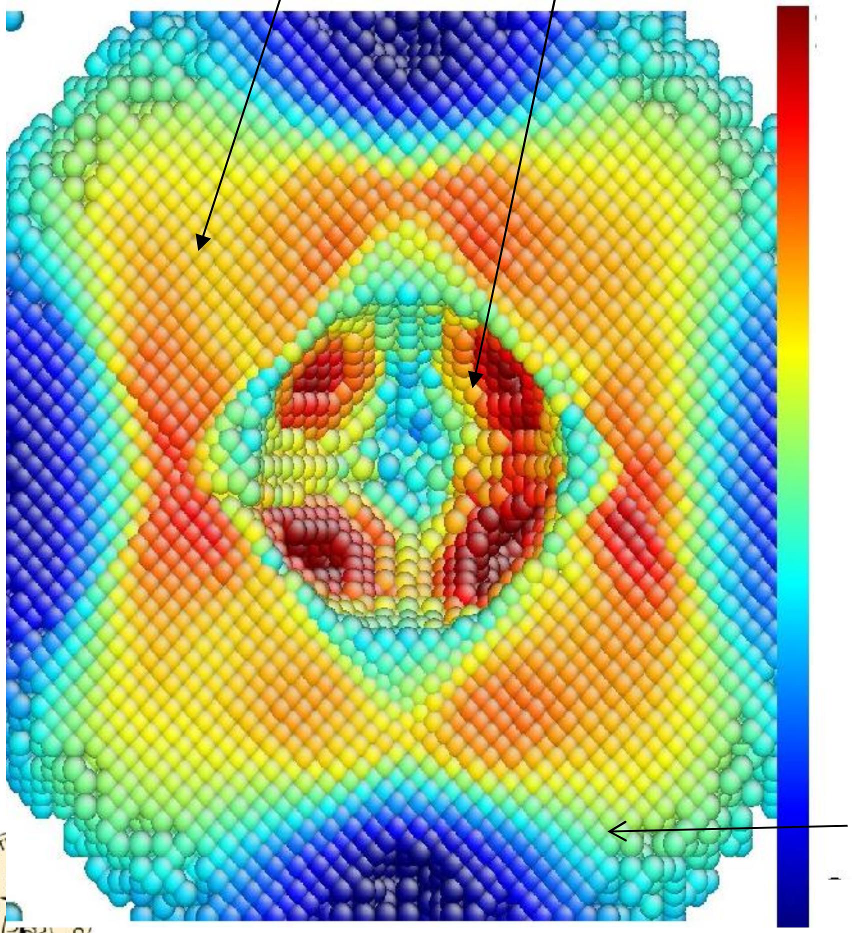


Prismatic loop evolution
(ε = 5, 6, 7%)

(Images obtained with DXA and Paraview)

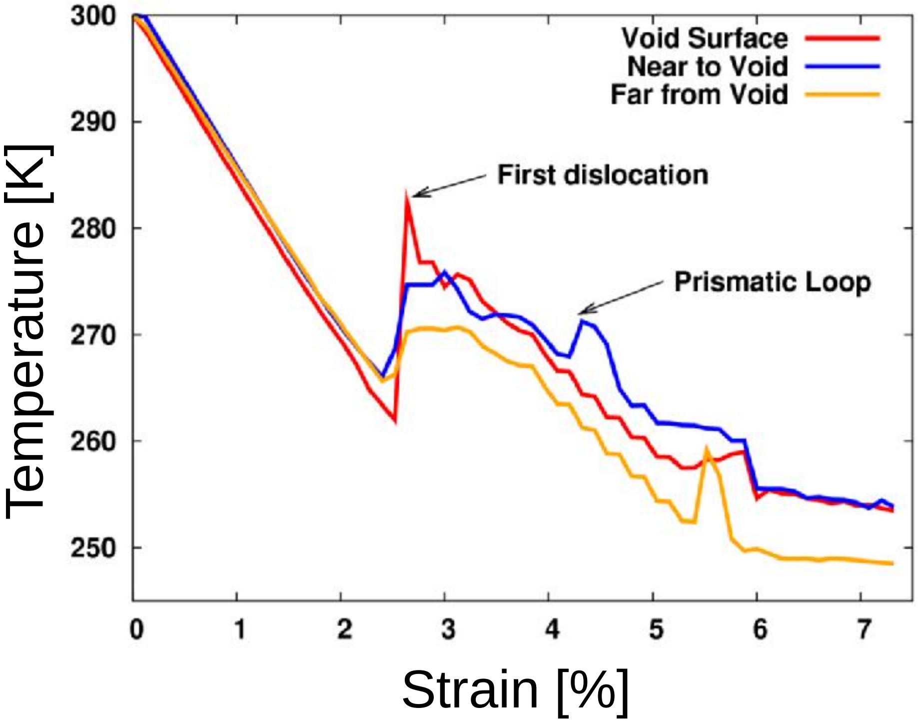
Application: Nanovoid cavitation in Cu

Temperature increase on {111} planes due to dislocation activity



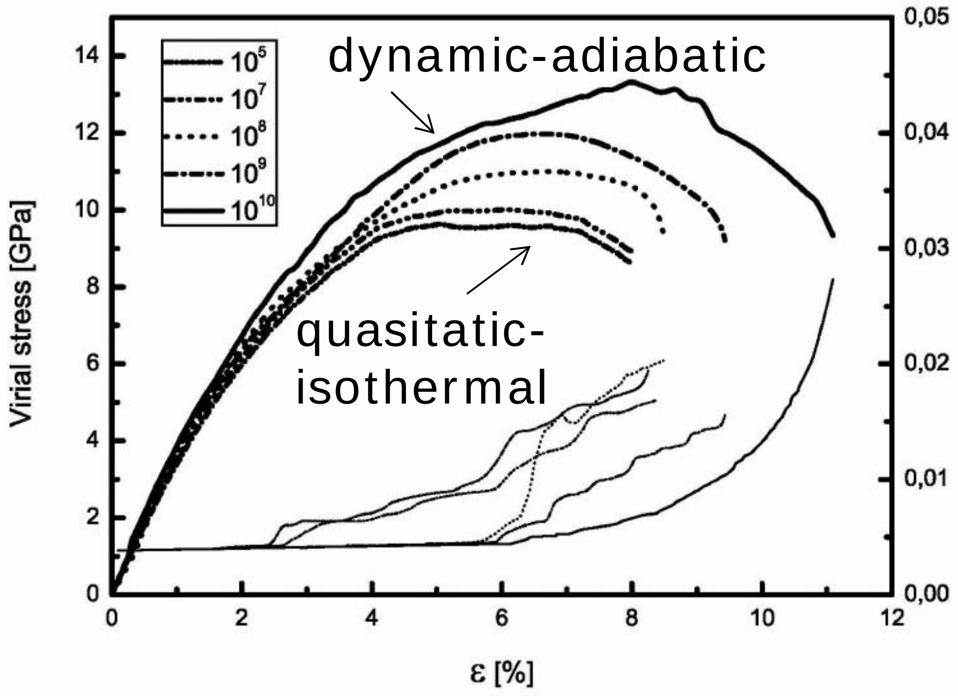
Temperature field @ ε=2.7%

Temperature evolution



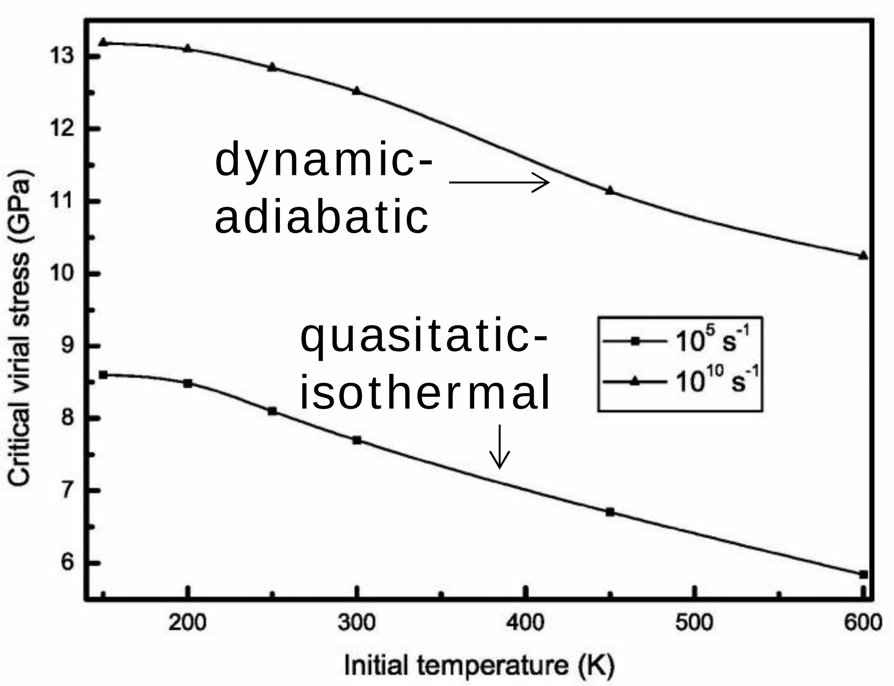
Michael Ortiz
MACH 04/15

Application: Nanovoid cavitation in Cu



dynamic-adiabatic

quasitatic-isothermal



dynamic-adiabatic

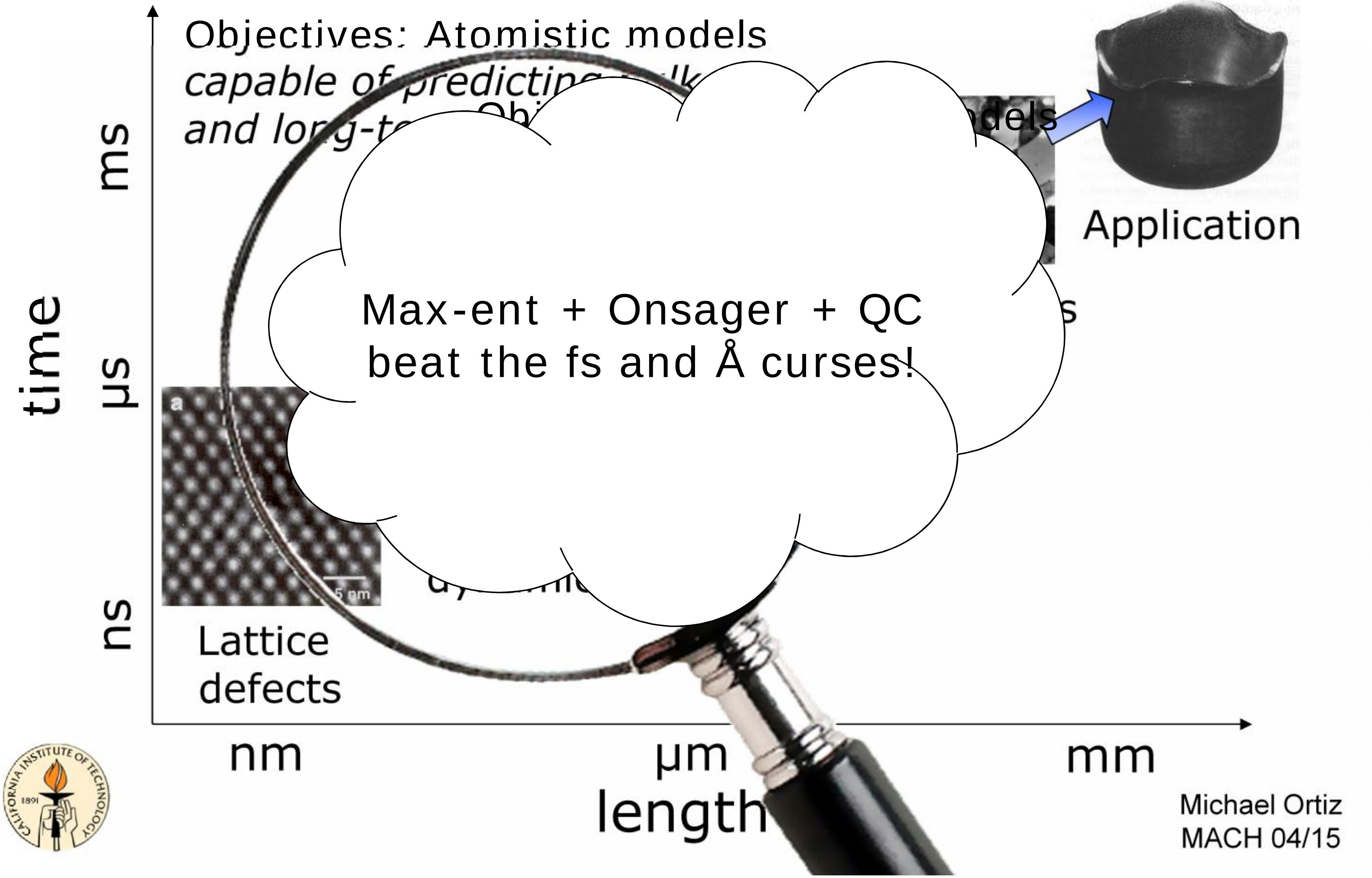
quasitatic-isothermal

- Transition between quasistatic-isothermal to dynamic-adiabatic behavior at 10^7-10^8 s^{-1}

  (not accessible to molecular dynamics!) ←

- Quasistatic regime: Time scale set by heat conduction
- Dynamic regime: Time scale set by microinertia

Multiscale modeling of materials



Objectives: Atomistic models capable of predicting bulk... and long-te...

Max-ent + Onsager + QC beat the fs and Å curses!

Concluding remarks

- Multiscale modeling of materials is still very much a work in progress…
- There are major gaps in theory, analysis, scientific computing that need to be plugged…
  - Nonlinear analysis of evolving microstructures
  - Beyond strict separation of scales: Scaling, size effect
- Most current schemes are computational
- Analysis and experiment have a much more important role to play (we compute too much!)

THANK YOU!