Multiscale Modeling and Simulation of Solids

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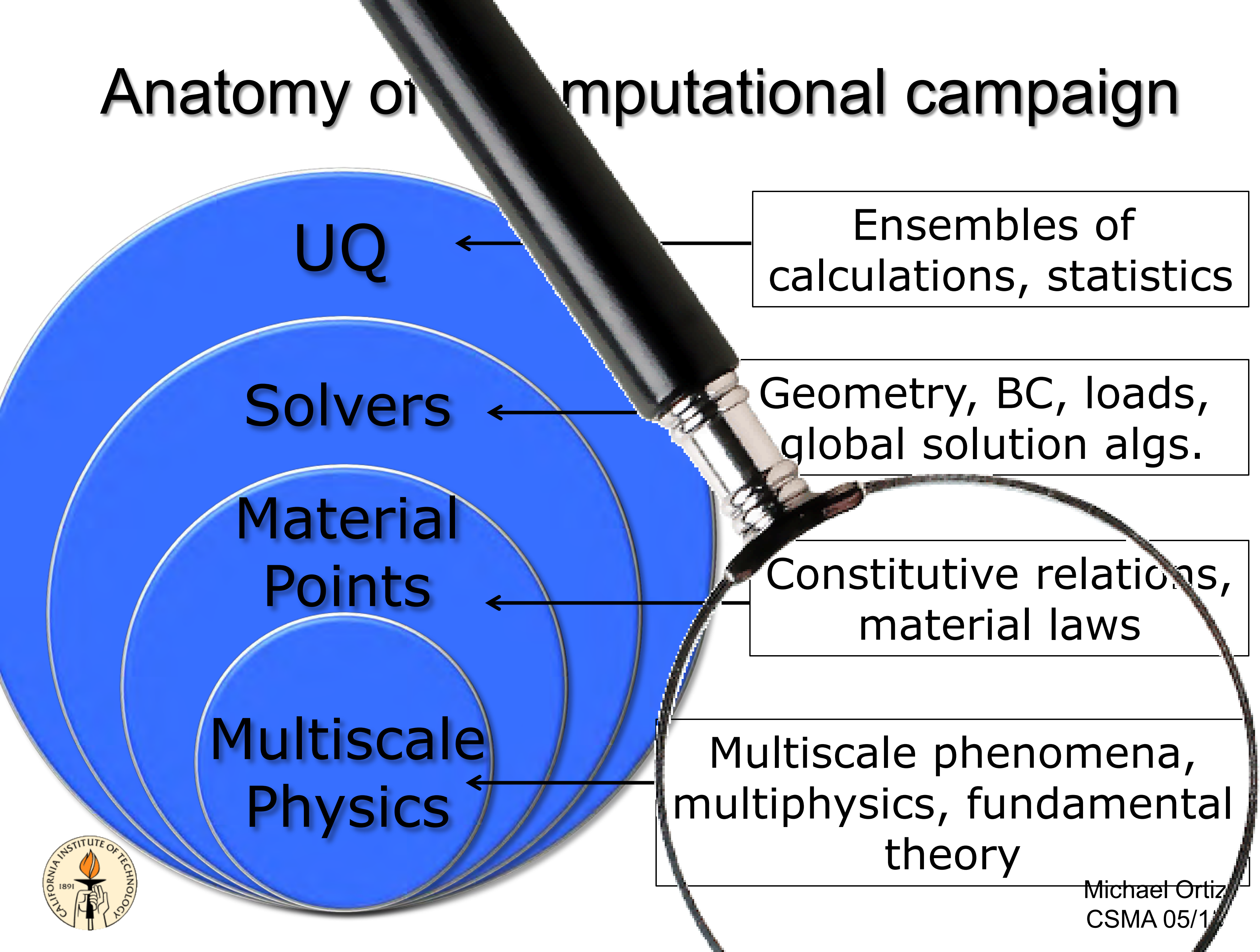
Anatomy o mputational campaign



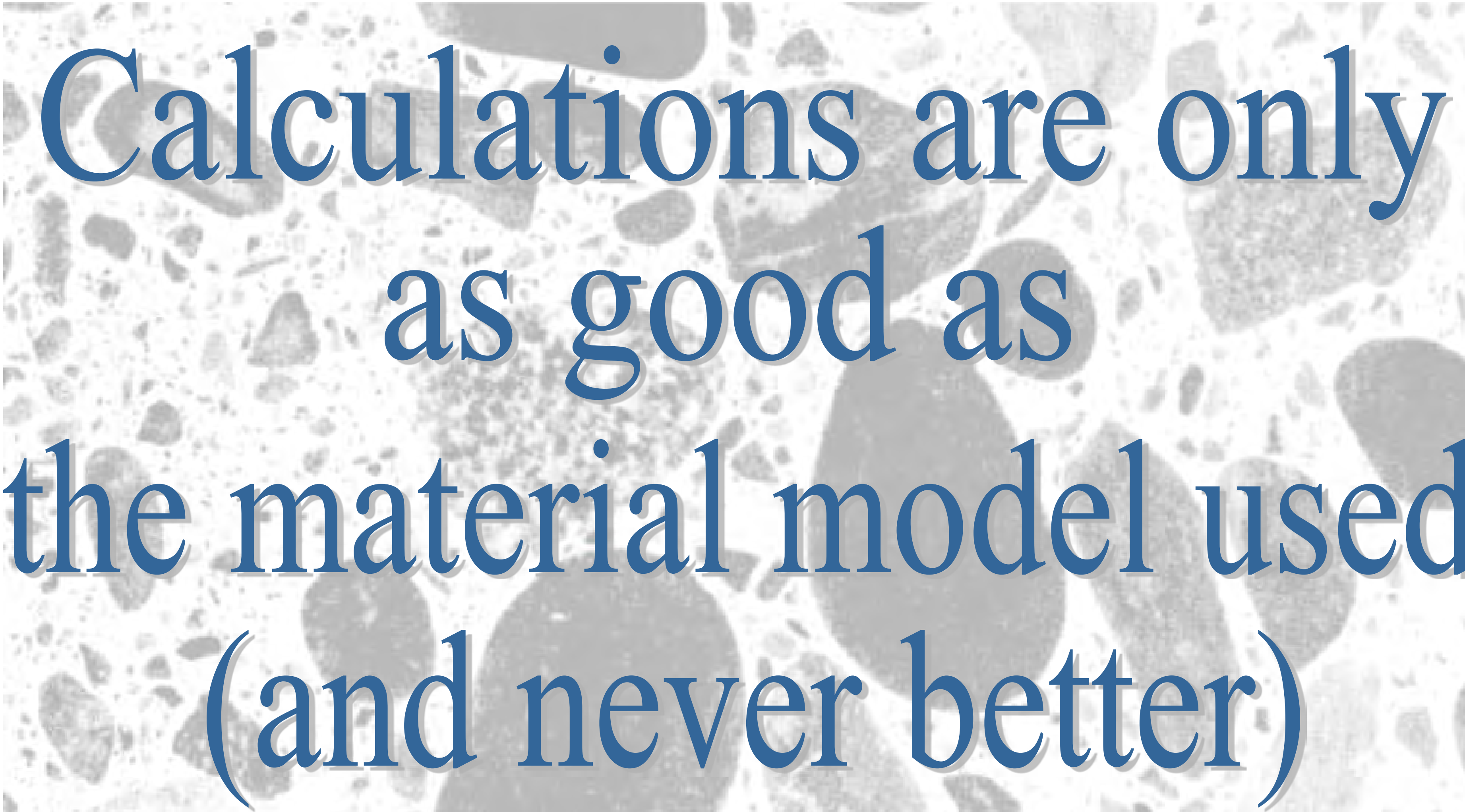
Ensembles of calculations, statistics

Geometry, BC, loads, global solution algs.

Constitutive relations, material laws

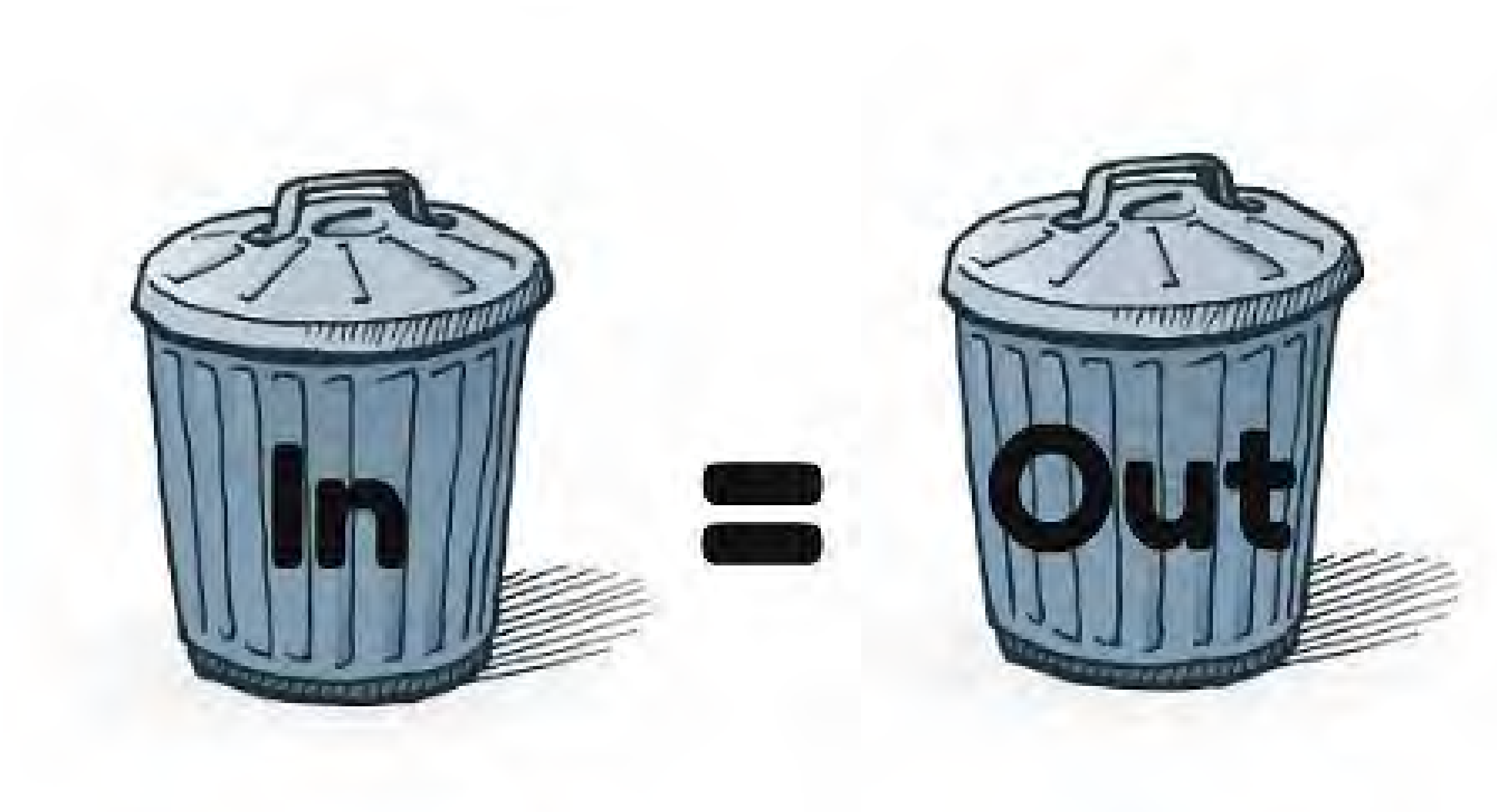
Multiscale phenomena, multiphysics, fundamental theory

Why material modeling? Reality check…



Calculations are only
as good as
the material model used
(and never better)

Why material modeling? Reality check…

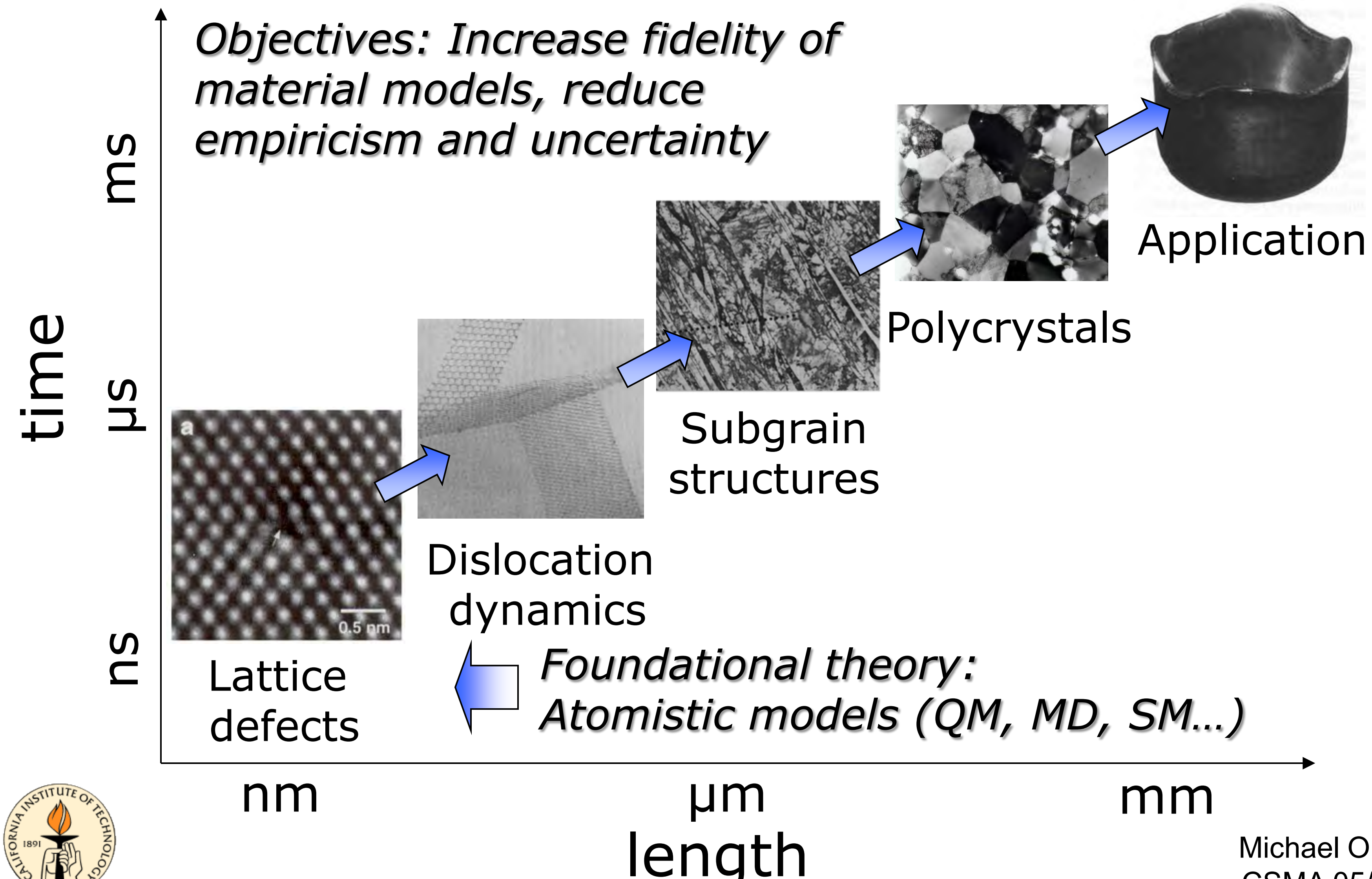


http://www.vivianpartnership.co.uk/garbage-in-garbage-out/

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



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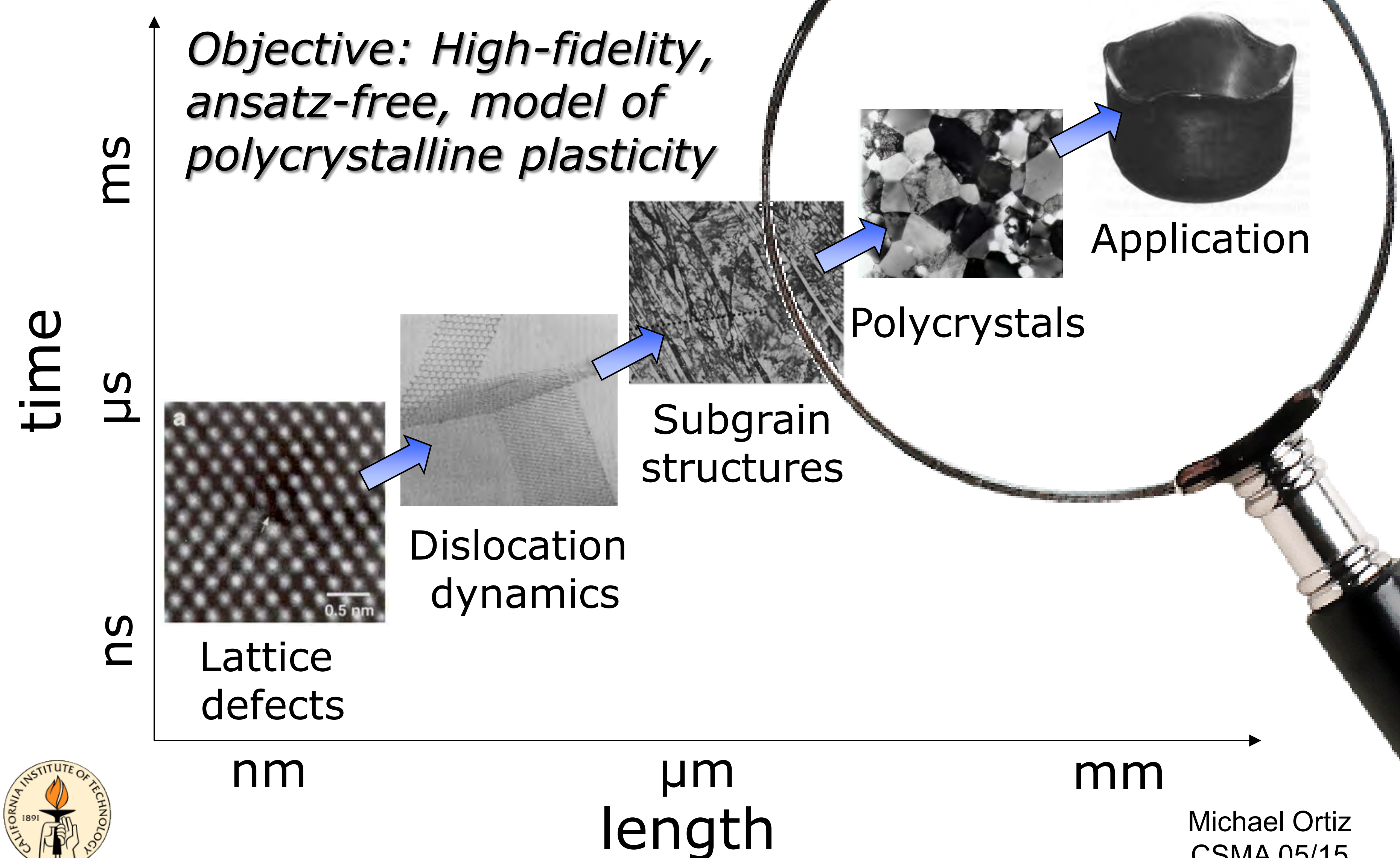
Multiscale modeling of materials

- 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? Where are we headed?

Multiscale modeling of materials

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



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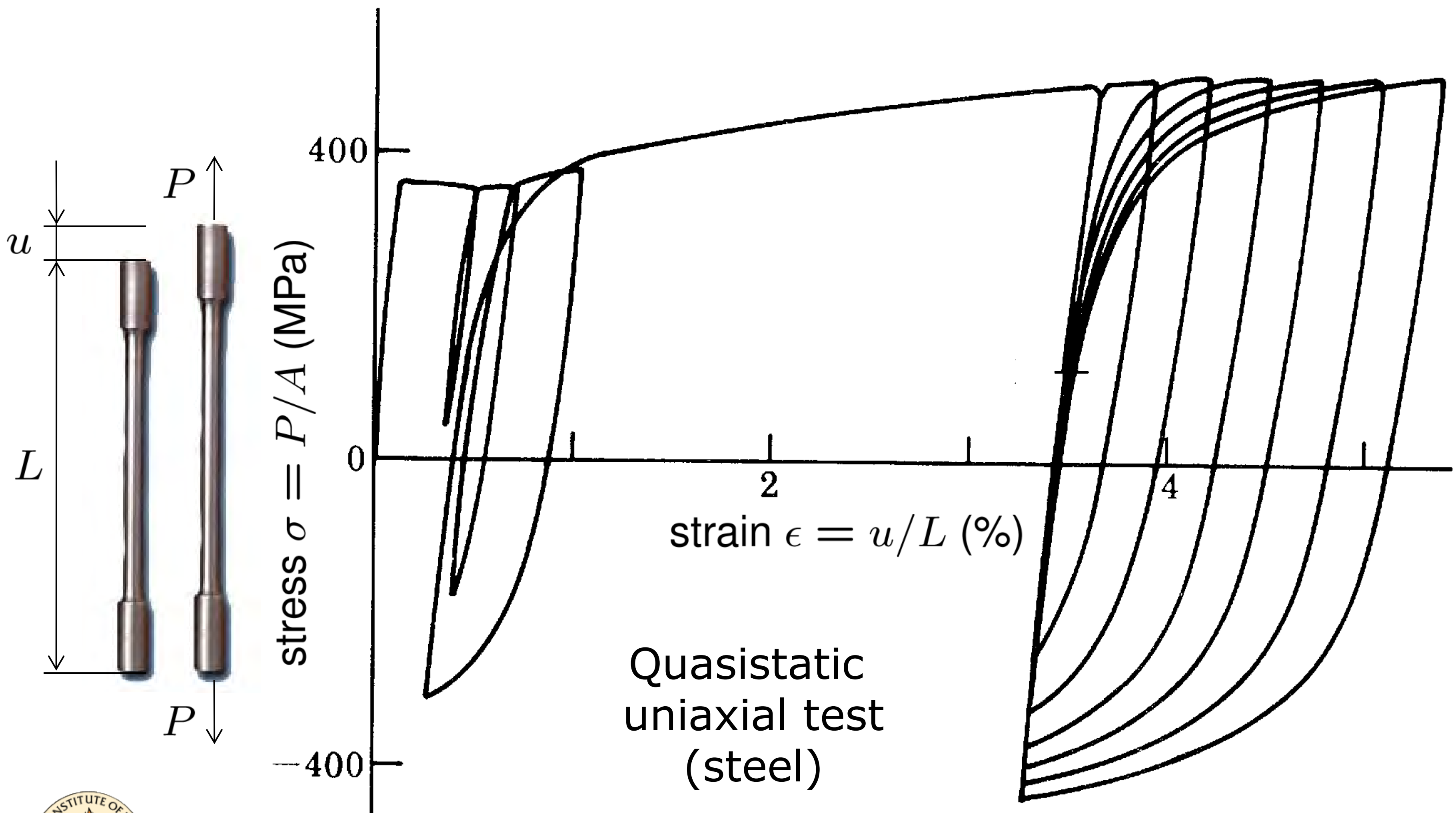
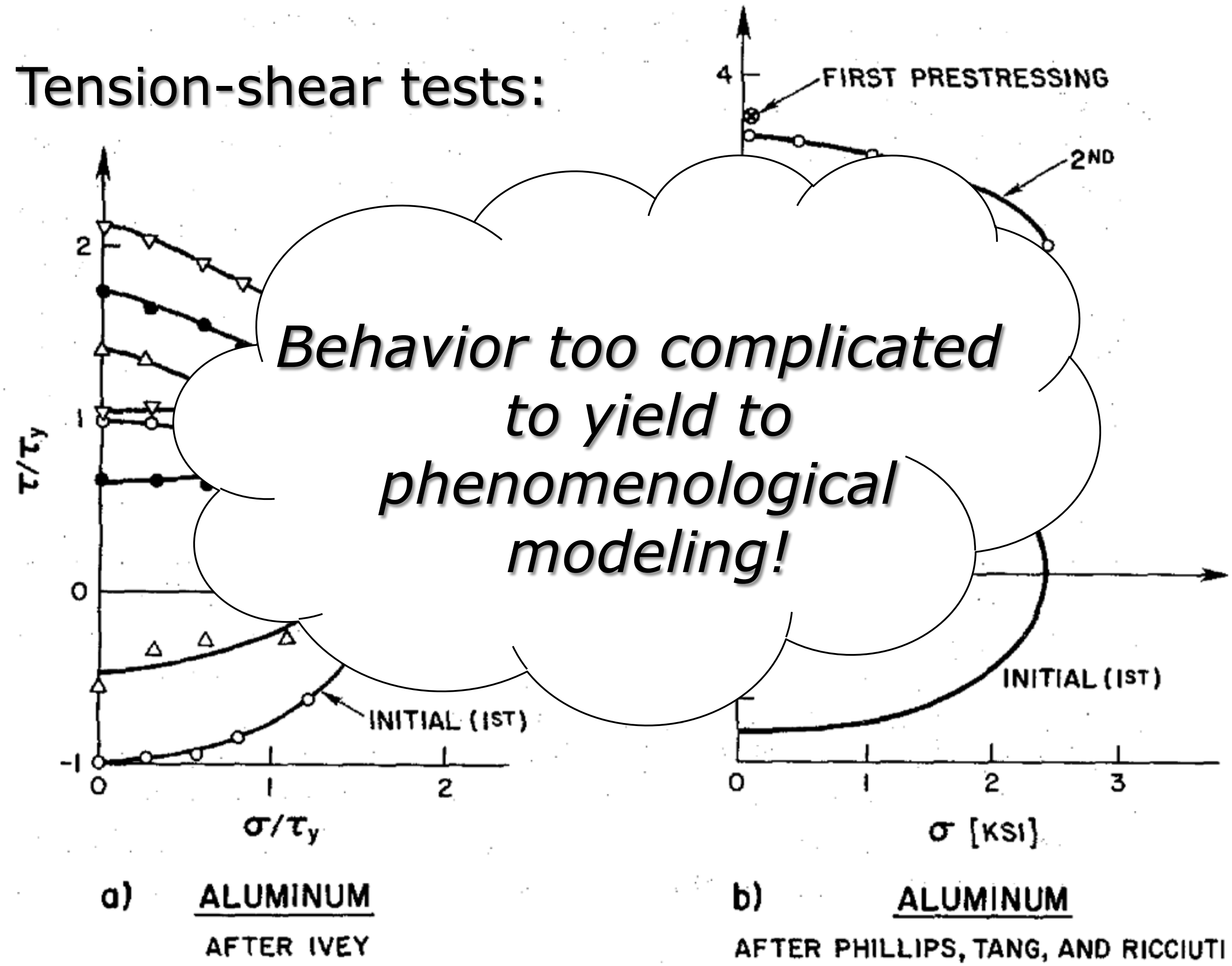
Quasistatic cyclic tension-compression



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

Multiaxial yielding and hardening

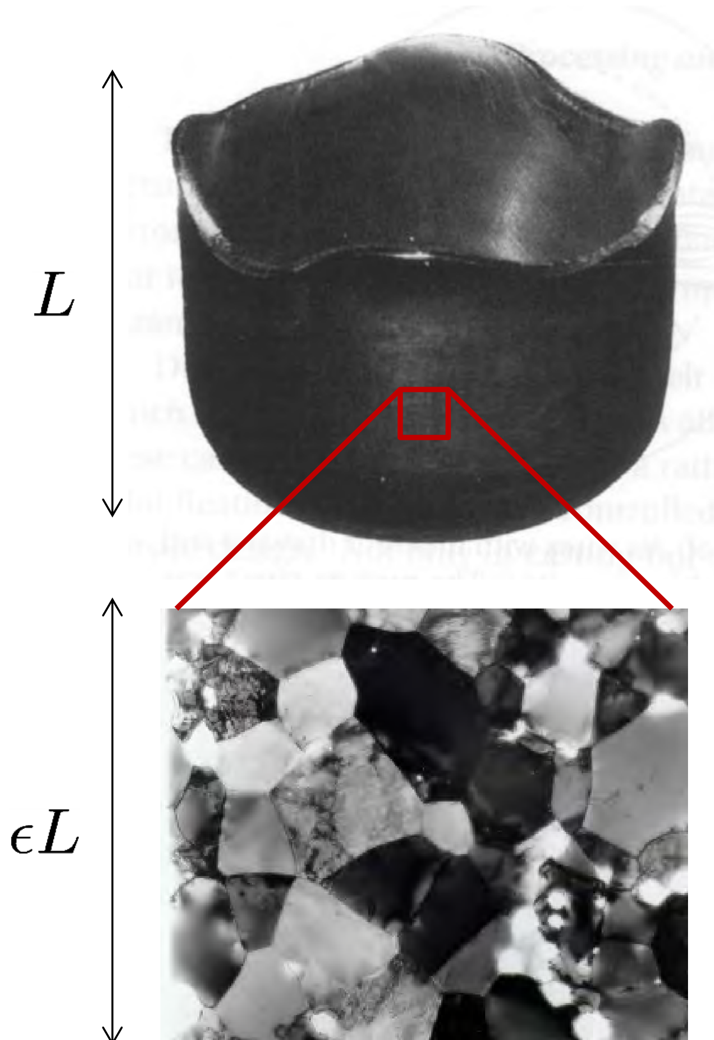
Tension-shear tests:



Behavior too complicated to yield to phenomenological modeling!

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

The big hammer: Homogenization

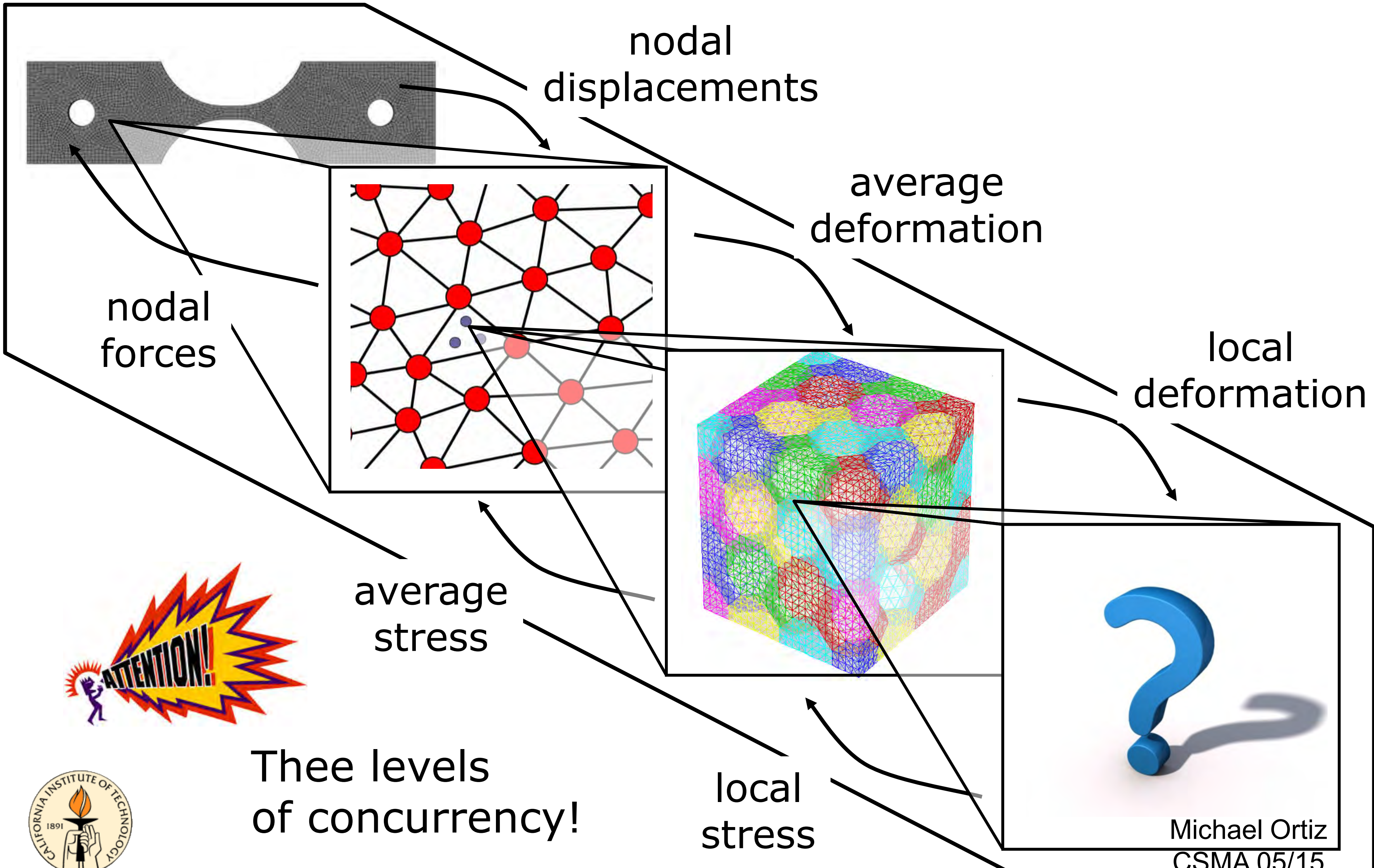


RVE

- 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 (C^3)



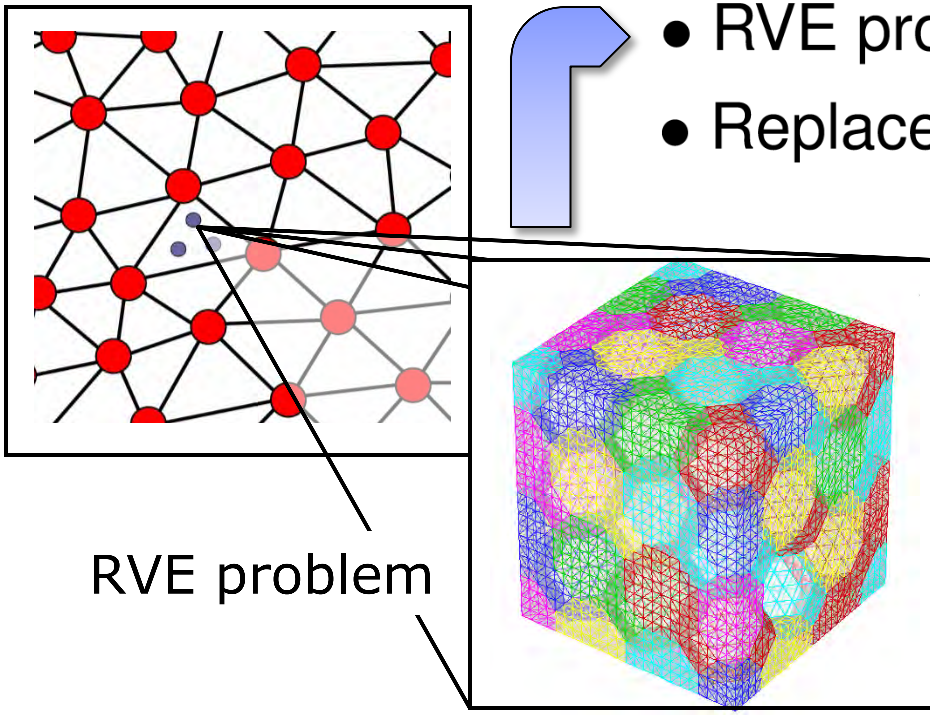
Thee levels of concurrency!

Polycrystals – Concurrent multiscale (C^3)

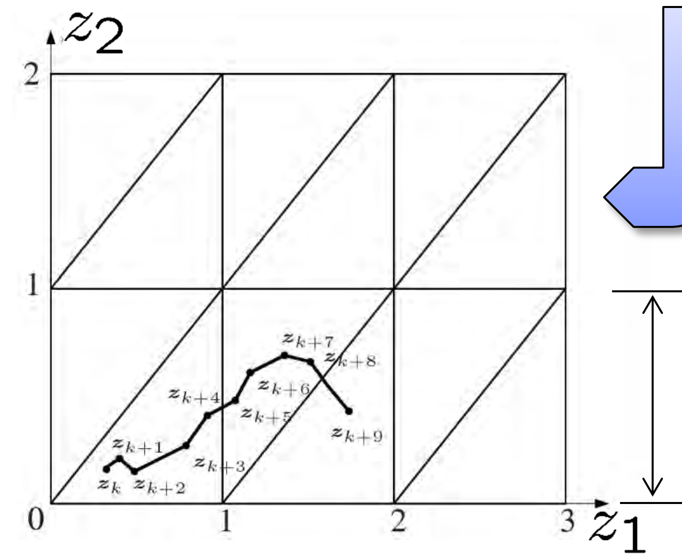
- Concurrent polycrystalline plasticity models (e.g., FE^2) implement homogenization theory
- They bypass the need to model polycrystalline plasticity analytically or phenomenologically
- Result in doubly convergent approximations as h (mesh size) and ε (RVE size) → 0[1]
- Essential difficulty: Too slow!
- 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.

Acceleration: Phase-space interpolation



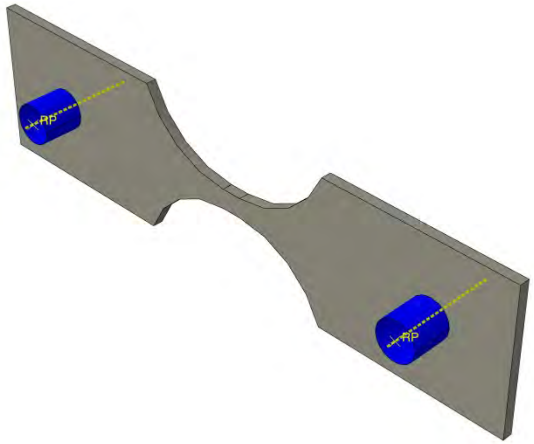
- RVE problem must supply $\boldsymbol{P}(\overbrace{\boldsymbol{F},\dot{\boldsymbol{F}},T}^{\boldsymbol{z}})$
- Replace by interpolant $\boldsymbol{P}_h(\boldsymbol{F},\dot{\boldsymbol{F}},T)$!



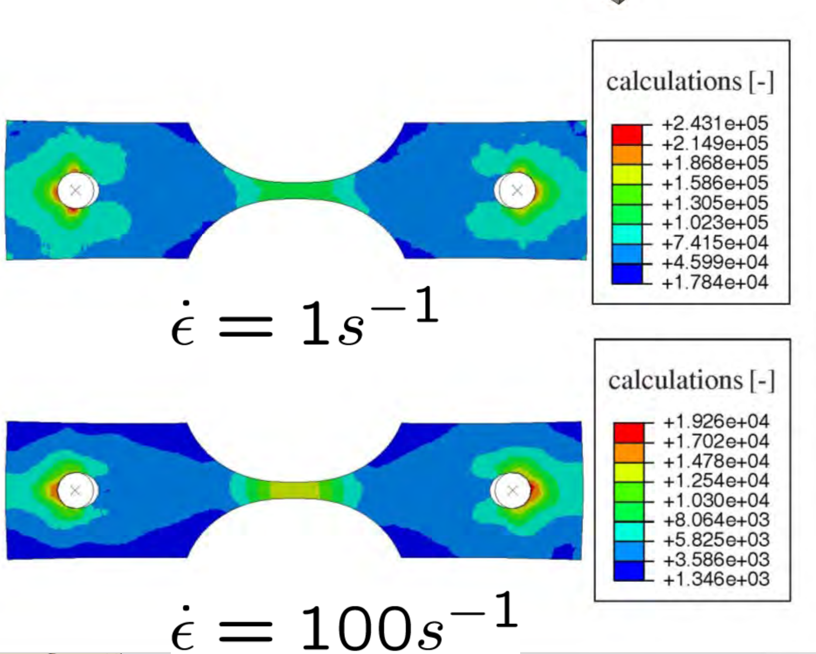
- Simplicial interpolation in high-dimensional spaces[1]
- One single RVE calculation per boundary crossing
- Speed-up = #steps/simplex @ constant accuracy

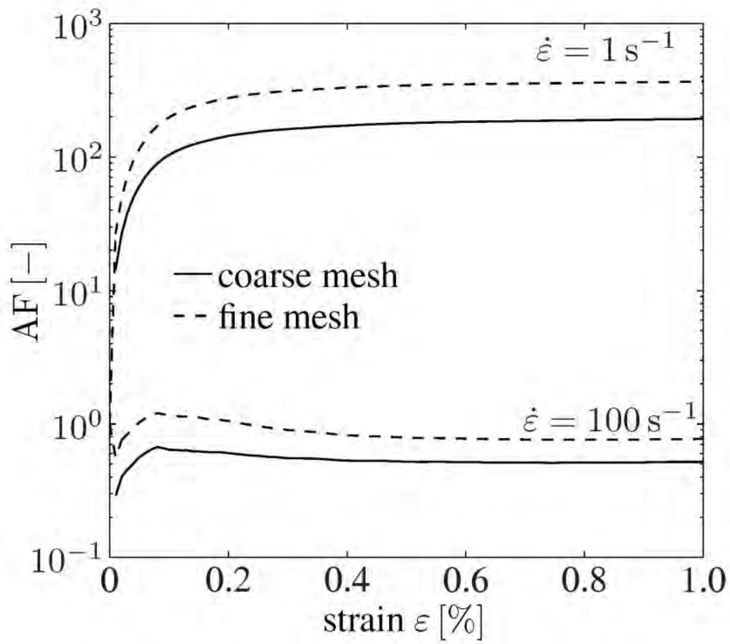
[1] Chien, M.J. and Kuh, E., *IEEE Transactions,* 1978; **25**(11):938–940.
Klusemann, B. and Ortiz, M., IJNME, 10.1002/nme.4887, 2015.

Acceleration: Phase-space interpolation



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





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

Multiscale modeling of materials

Objective: High-fidelity, ansatz-free, model of polycrysta...

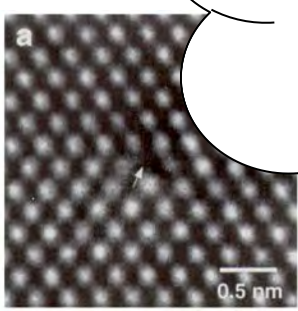
Acceleration may enable C^3 concurrent multiscale simulation of polycrystals (e.g., FE^2 +subgrain)

time

ms

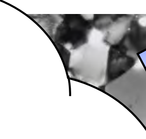
μs

ns



Lattice defects

dynamics



Application

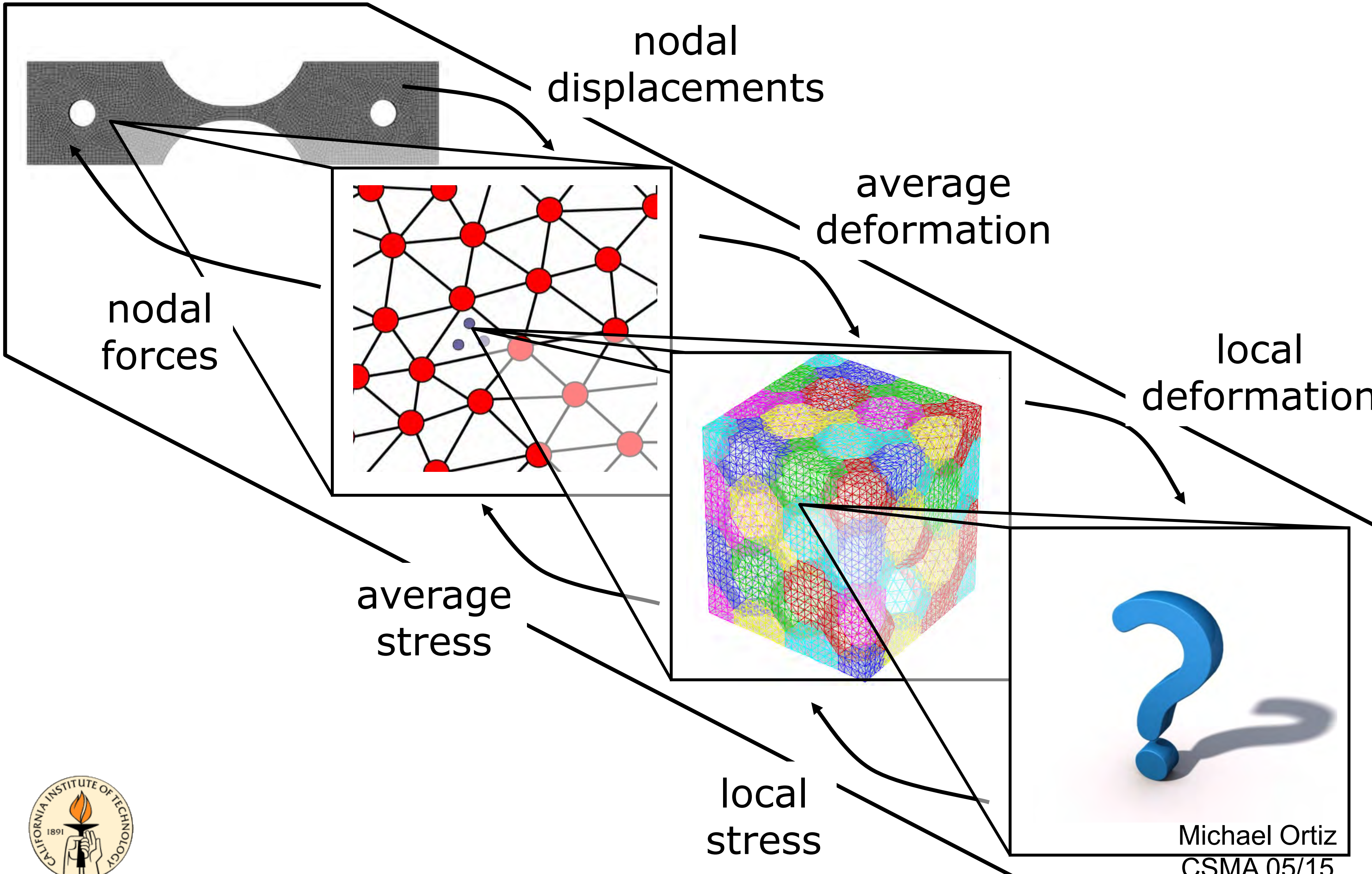
nm

μm

mm

length

Not done yet… Subgrain plasticity?



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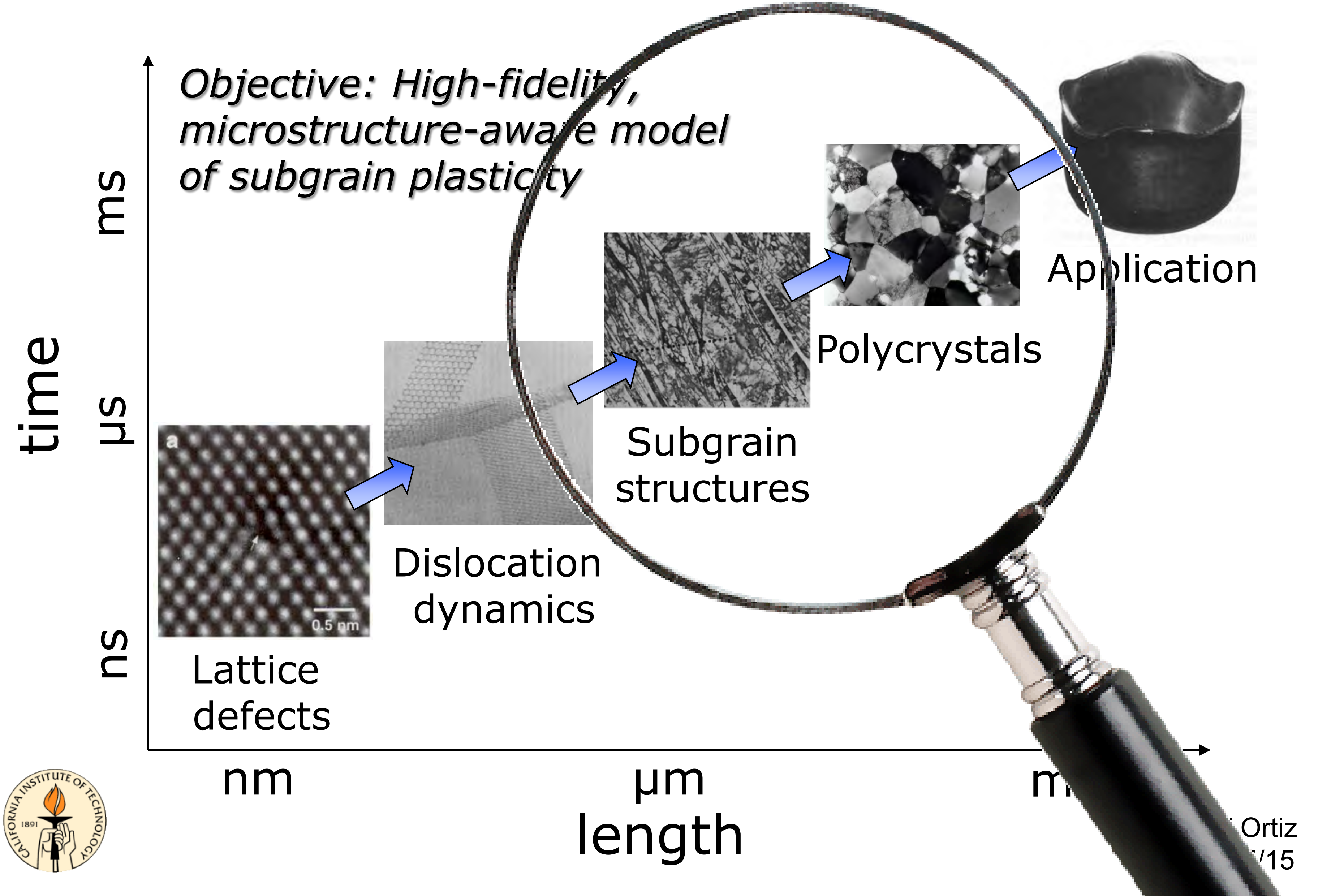
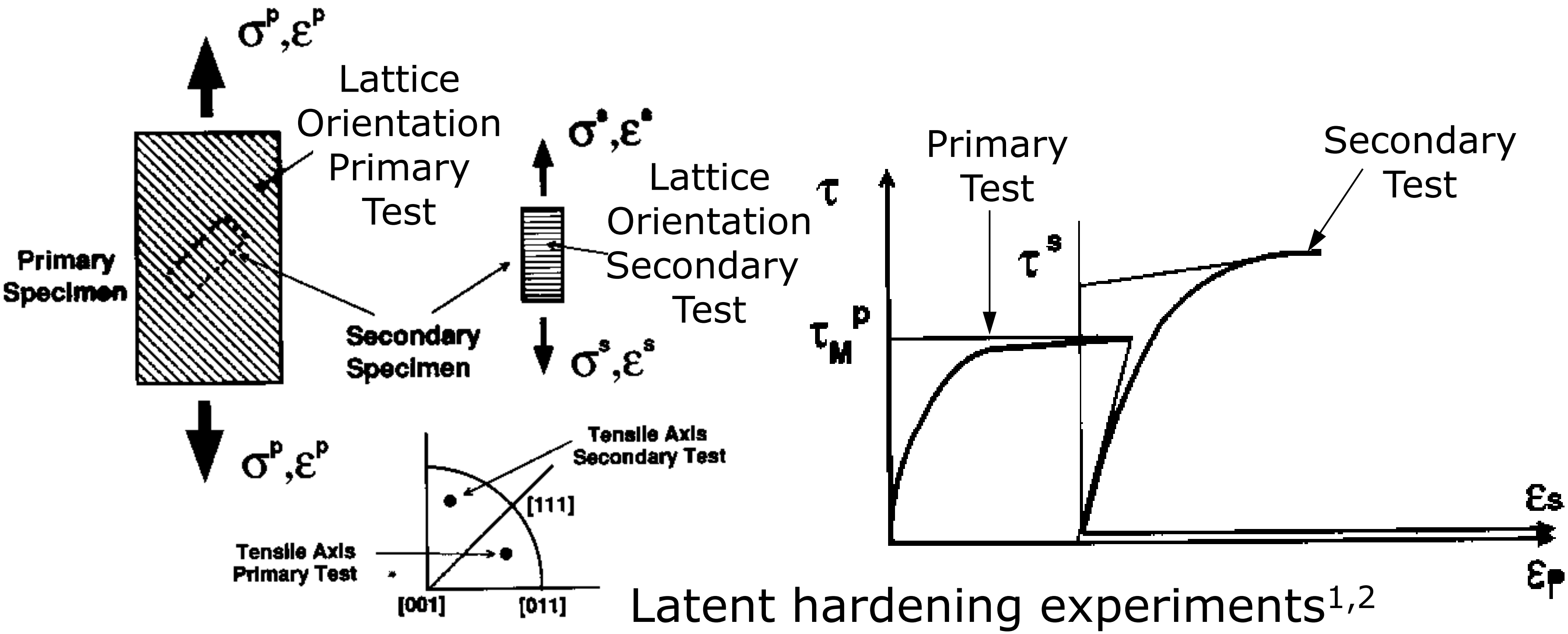
Multiscale modeling of materials



Strong latent hardening & microstructure



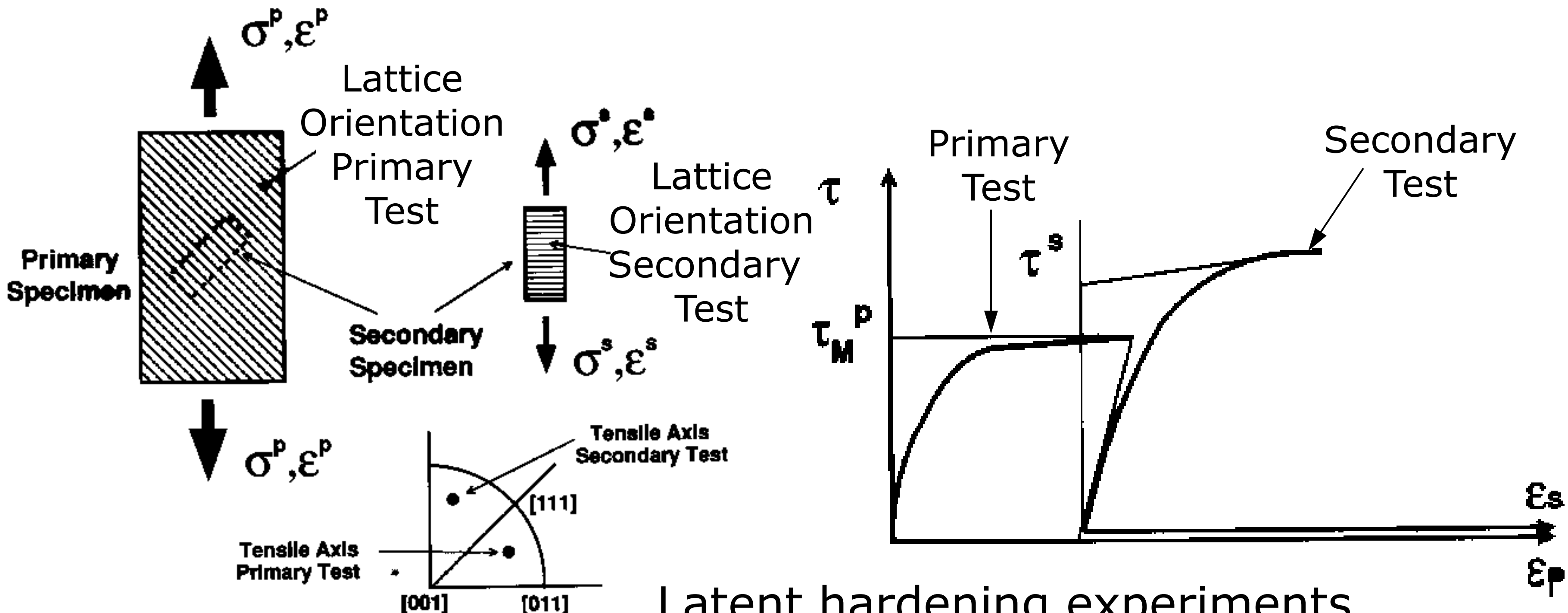
Latent hardening experiments[1,2]

- *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



Latent hardening experiments

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

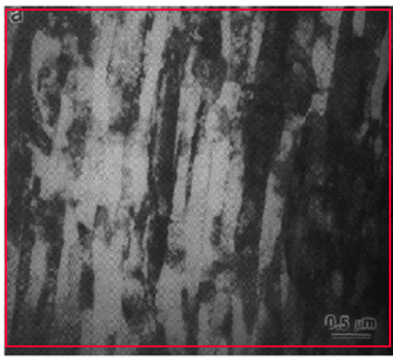
[1]Peirce, D., Asaro, R. and Needleman, A. *Acta Metall.*, **31** (1983) 1951.

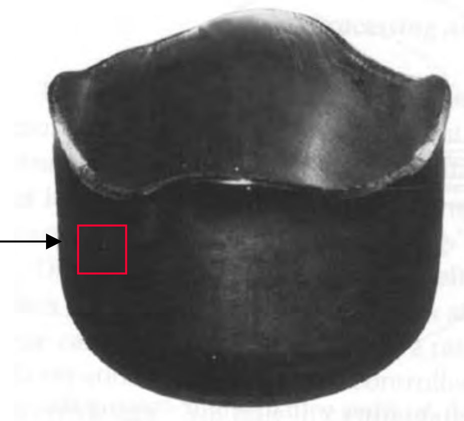
The big hammer: Relaxation

$$F(u) = \int_\Omega W(\nabla u)\, dx \to \text{inf!} \quad \Rightarrow \text{Too hard!}$$

$u =$

Ax





$$QW(A) = \inf \frac{1}{|E|} \int_E W(\nabla u)\, dx$$

Relaxation of the constitutive model (RVE calculation)

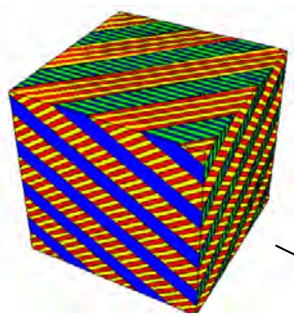
$$sc^- F(u) = \int_\Omega QW(\nabla u)\, dx \to \text{inf!}$$

Relaxed problem: no microstructure, same macro-response

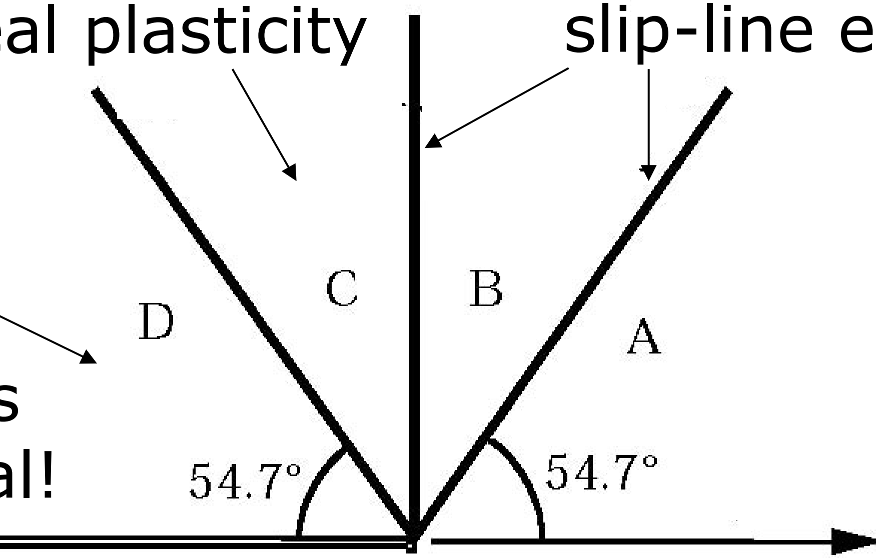
Strong latent hardening: Relaxation

- Exact relaxation is known analytically[1]:

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

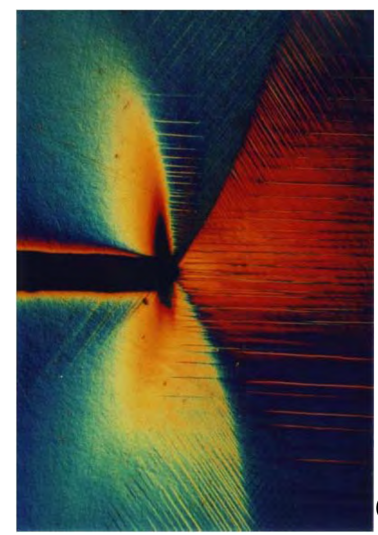


laminates
are optimal!



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

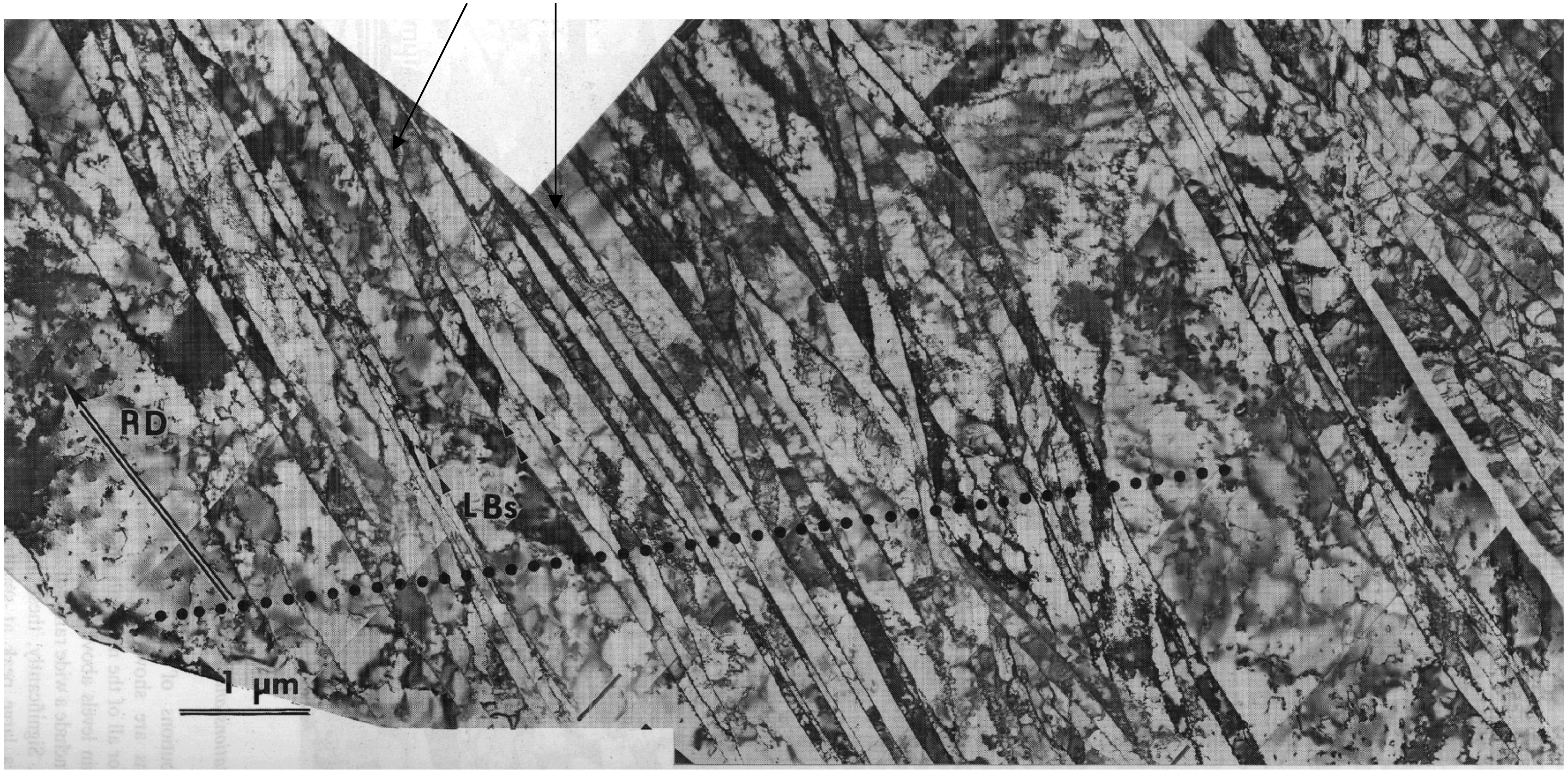
(Crone and Shield, *JMPS*, 2002)



[1]S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

Subgrain dislocation structures - Static

Dislocation walls



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

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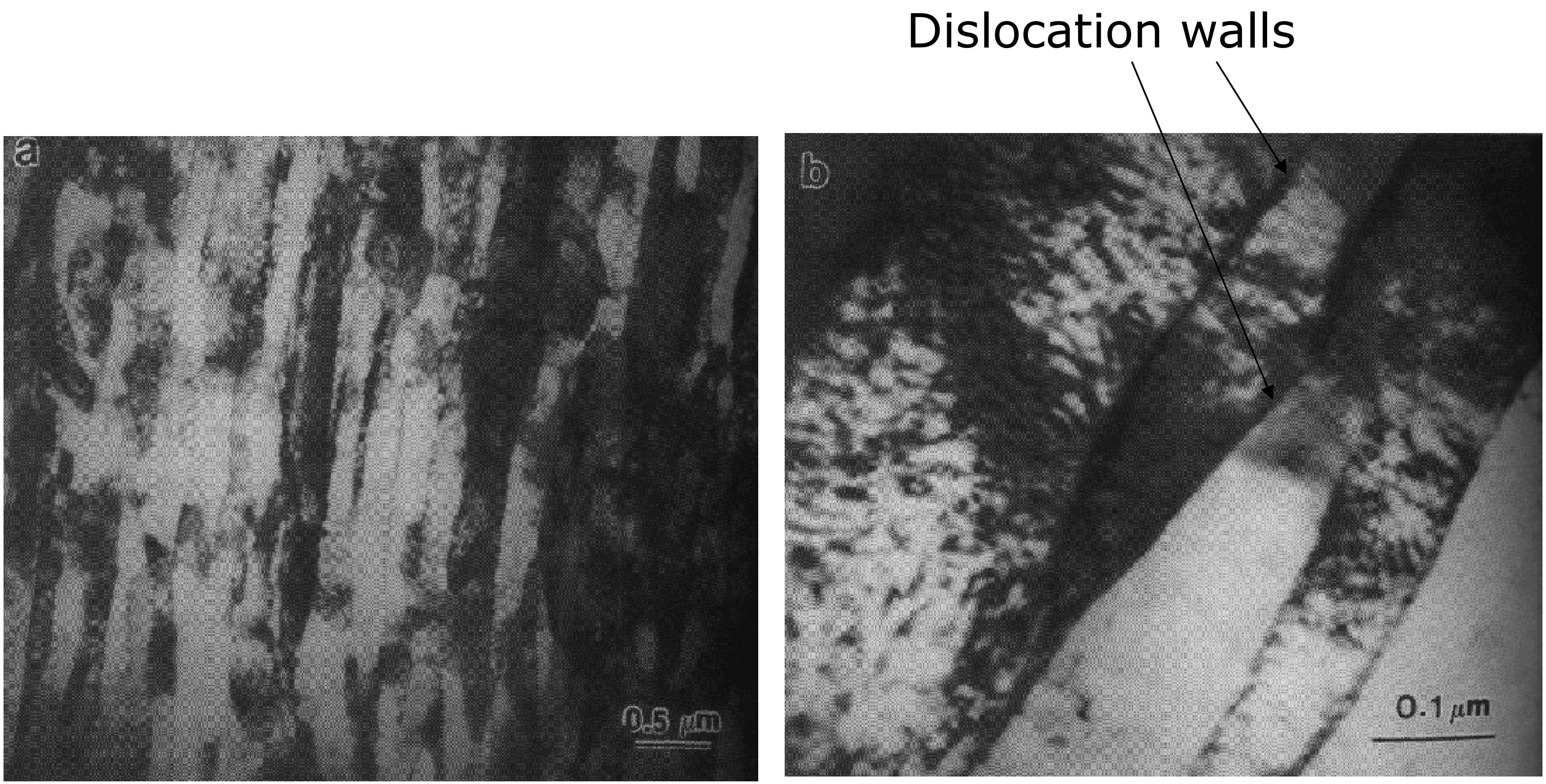
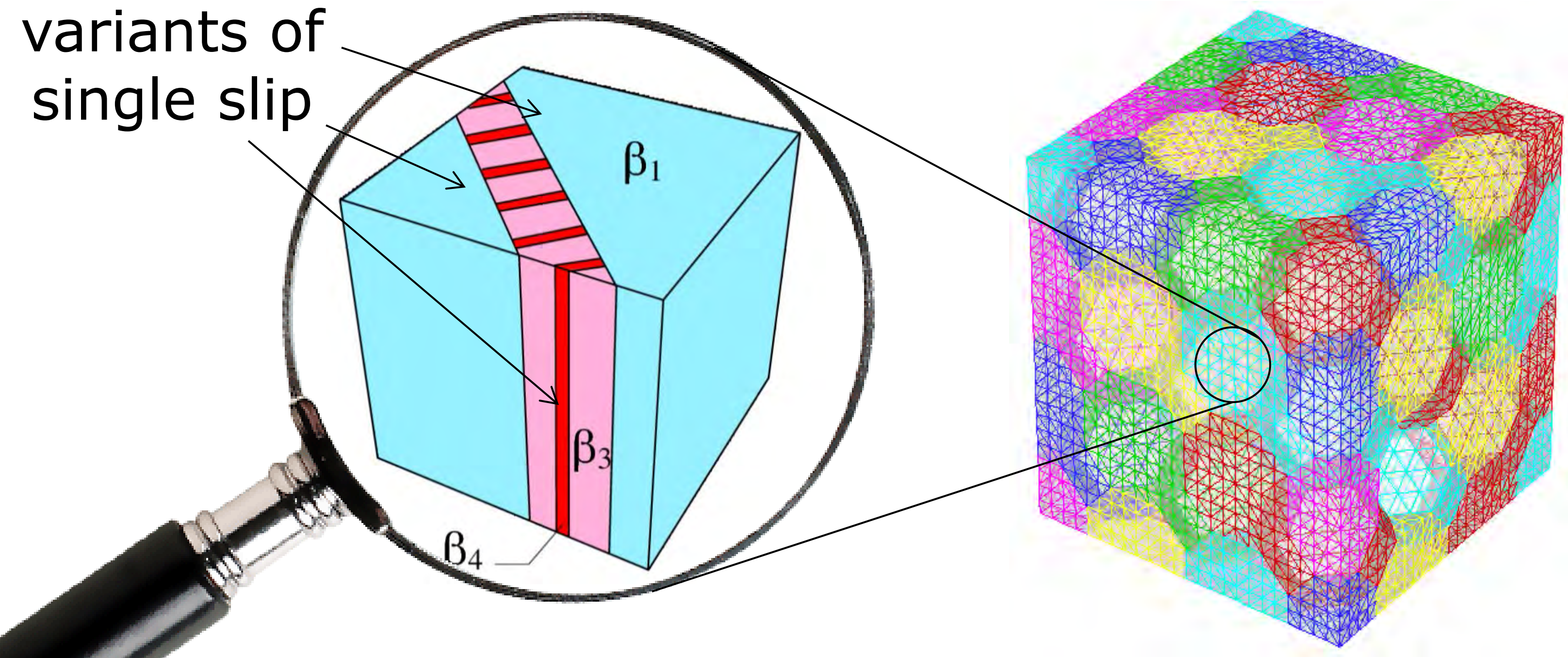
Subgrain dislocation structures - Shock



Shocked Ta (Meyers et al., 1995)

Optimal subgrain structures – Laminates

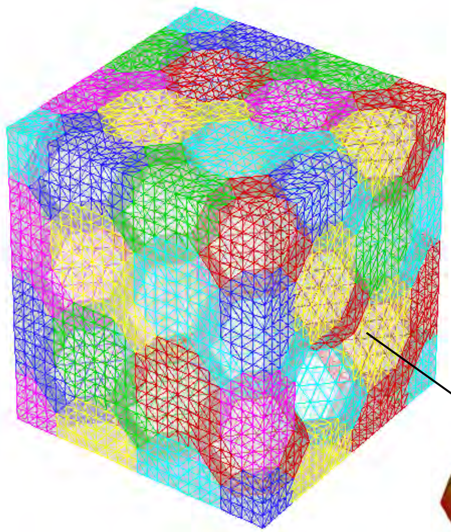


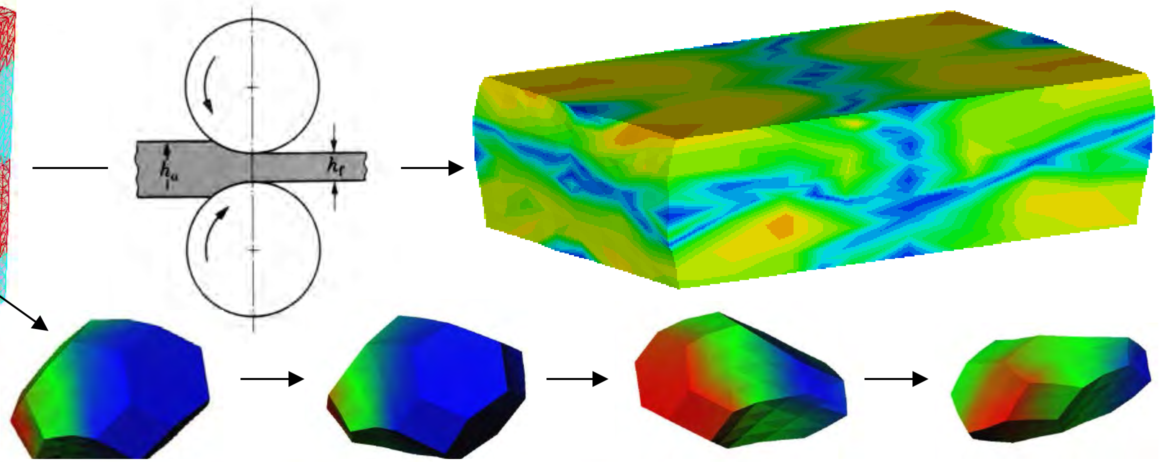
- *Laminates* are known to be optimal microstructures[1]
- Explicit *on-the-fly sequential lamination* construction delivers effective response[1,2]
- *Caveat emptor:* All other bases are sub-optimal! (e.g., Fourier, spectral, p-enrichment…)

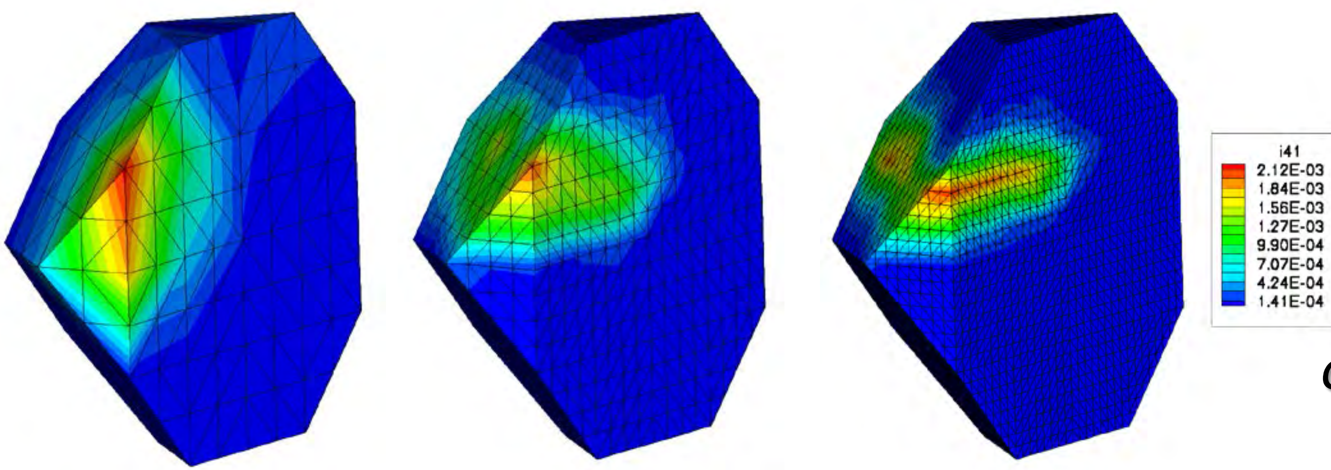
[1]Conti, S. and Ortiz, M., *ARMA*, 176: 103-147, 2005.
[2]Hansen, B., Bronkhorst, C.A., Ortiz, M., MSMSE, 18: 055001, 2010.

Suboptimal subgrain structures

Cold-rolled @ 42% polycrystalline Ta[1]





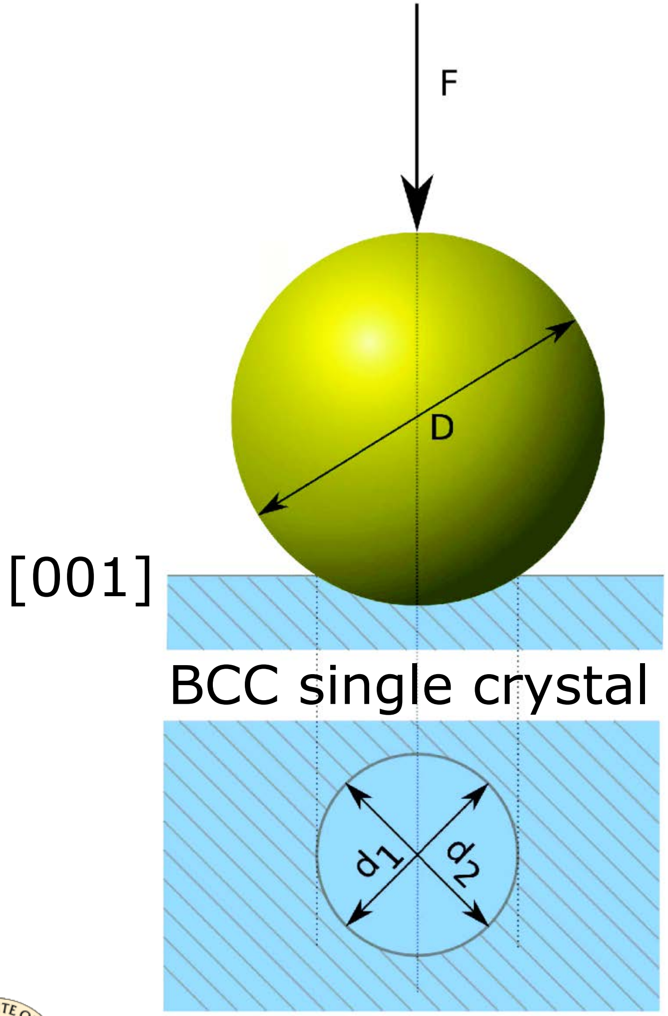


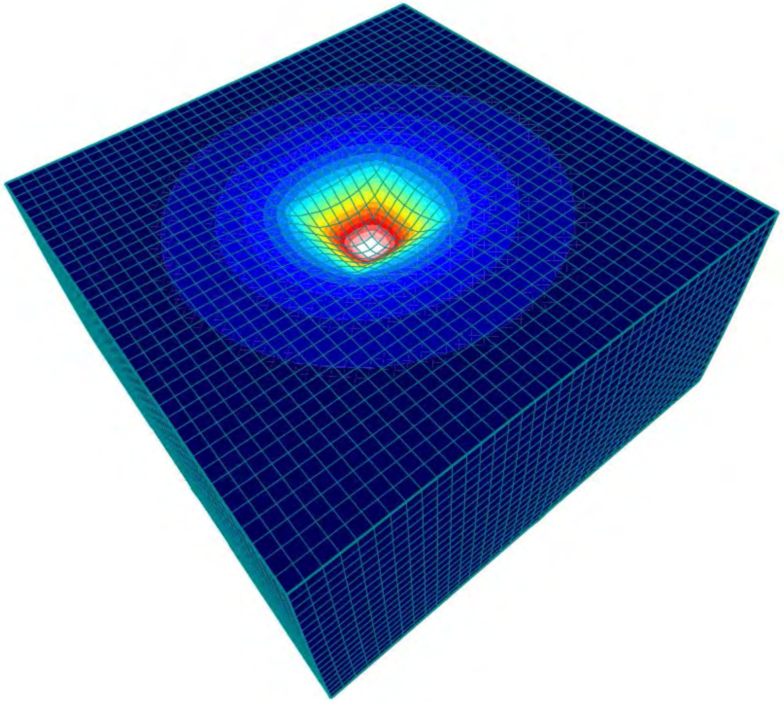
Slow or no convergence!

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

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

Optimal *vs.* suboptimal microstructures



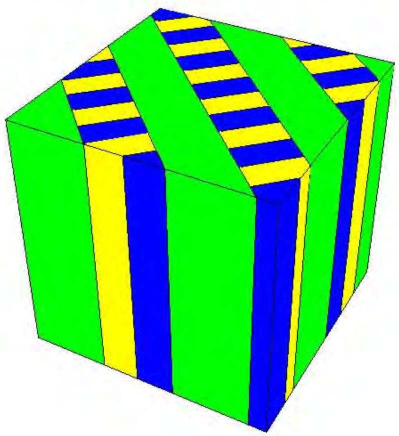


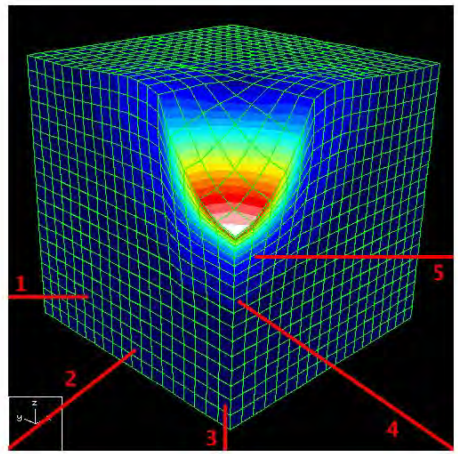
Indentation of [001] surface
of BCC single crystal
32,000 nodes
27,436 hexahedral elements

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

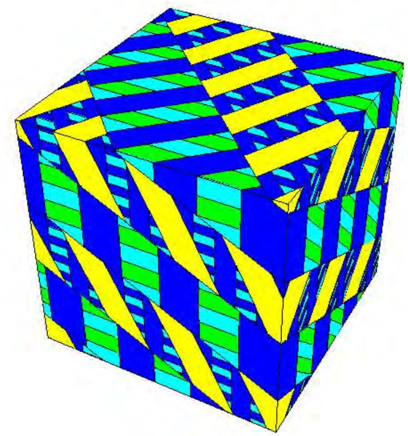
Optimal *vs*. suboptimal microstructures

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

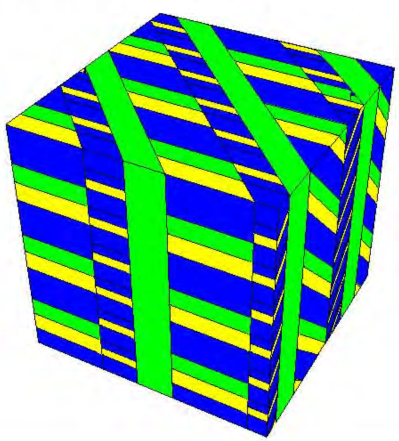




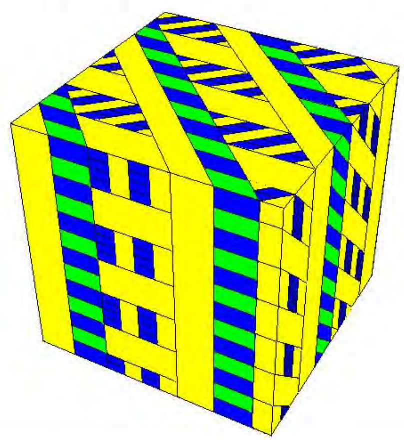
rank 4/14, $|\gamma|_\infty$ = 0.43



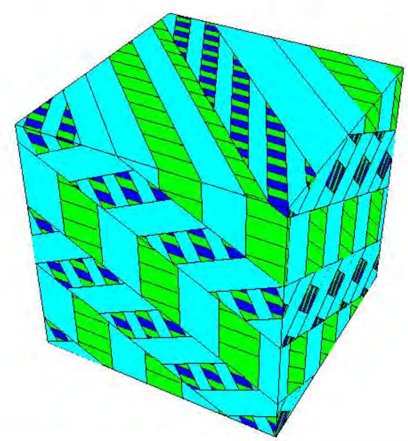
rank 4/12, $|\gamma|_\infty$ = 0.02



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



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



Conti, S., Hauret, P. and Ortiz, M.,
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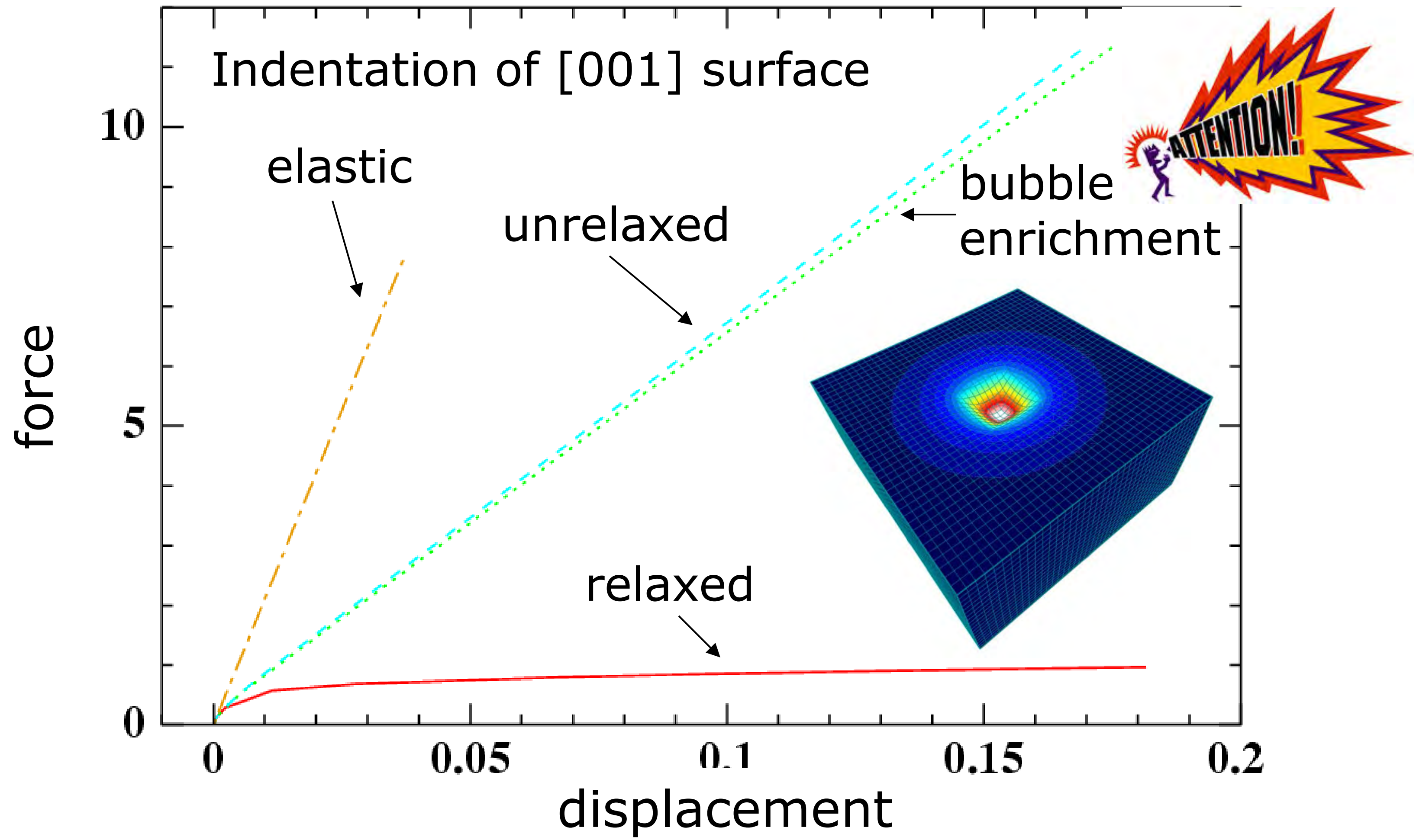
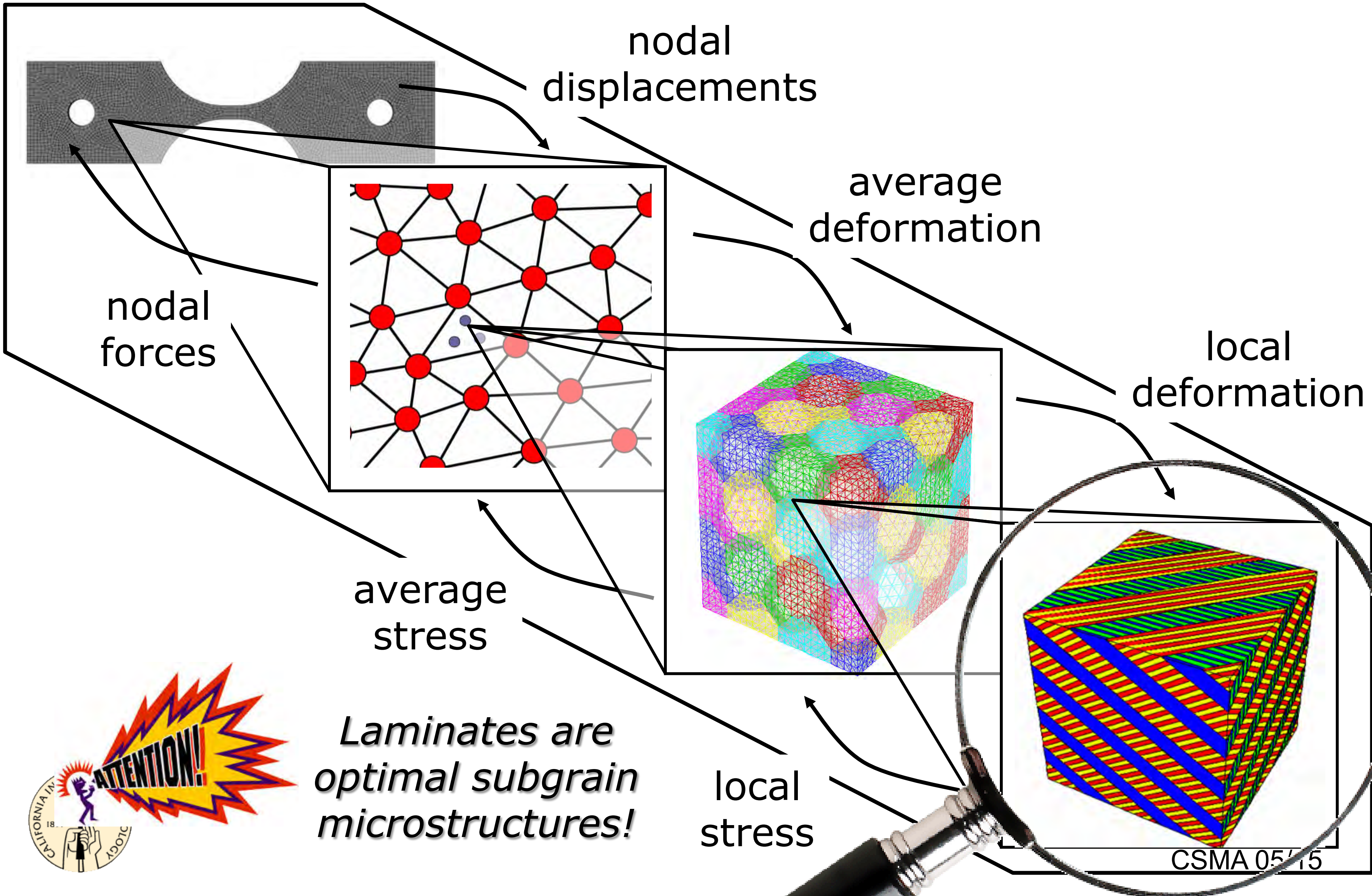
Optimal *vs.* suboptimal microstructures



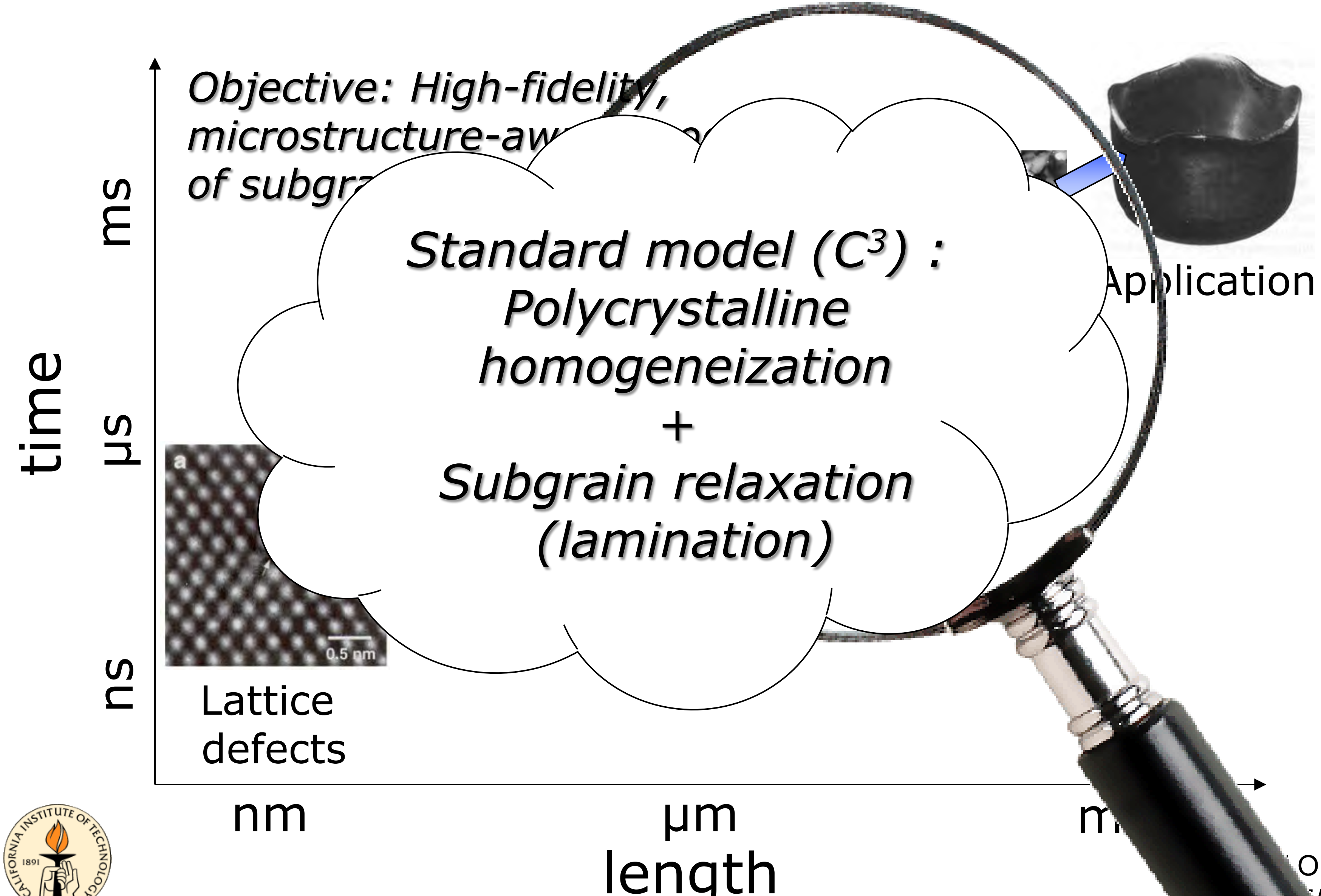
Conti, S., Hauret, P. and Ortiz, M.,
SIAM Multiscale Model. Simul., 6: 135-157, 2007

Polycrystals – Concurrent multiscale (C^3)



Laminates are optimal subgrain microstructures!

Multiscale modeling of materials

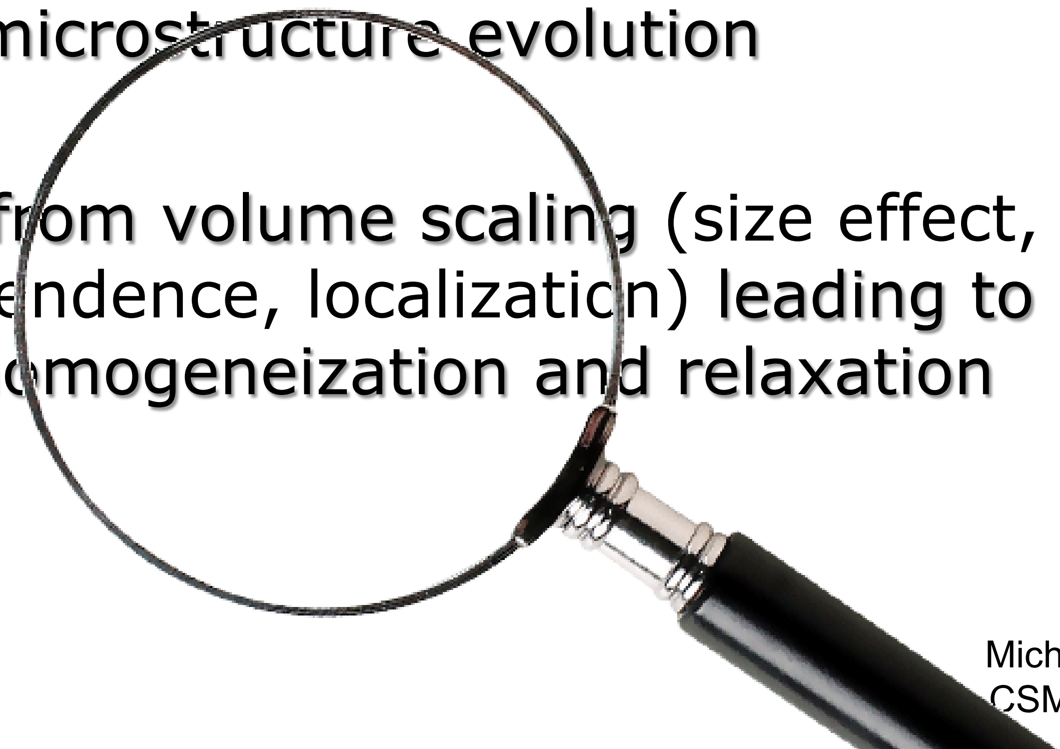


Standard model: Pitfalls

'Standard model' may fail due to:

Non-proportional loading (unloading, cycling loading, change of loading path direction) leading to microstructure evolution

Departures from volume scaling (size effect, domain dependence, localization) leading to failure of homogeneization and relaxation



Non-local microplasticity

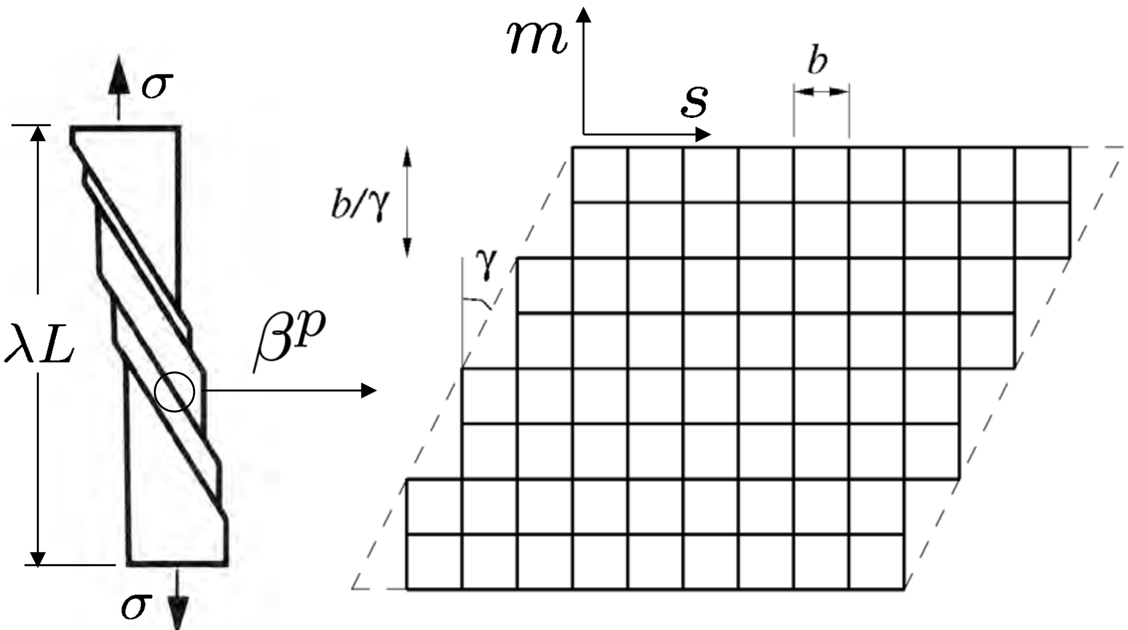
Scaling laws such as Hall-Petch suggest the existence of an intrinsic material length scale

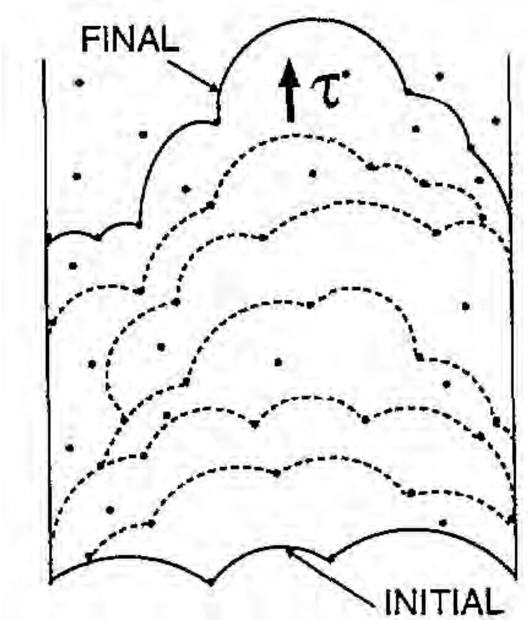
Modeling assumption: Account for dislocation self-energy using a line-tension approximation

The resulting deformation-theoretical energy is non-local (specifically, depends on $\nabla\gamma$)

Intrinsic length-scale: Burgers vector

Crystal plasticity – Linearized kinematics





- Kinematics: $\epsilon^p(\gamma) = \dfrac{1}{|\Omega|}\displaystyle\int_{J_u} [\![u]\!] \odot m \, d\mathcal{H}^2 \equiv \sum \gamma s \odot m$

- Energy: $E(u,\gamma) = \displaystyle\int_\Omega [\, W^e(\nabla u - \epsilon^p(\gamma)) + T\,|\nabla\gamma \times m| \,]\, dx$

- Dissipation: $\psi(\dot\gamma) = \begin{cases} \tau_c|\dot\gamma|, & \text{single slip,} \\ +\infty, & \text{otherwise.} \end{cases}$

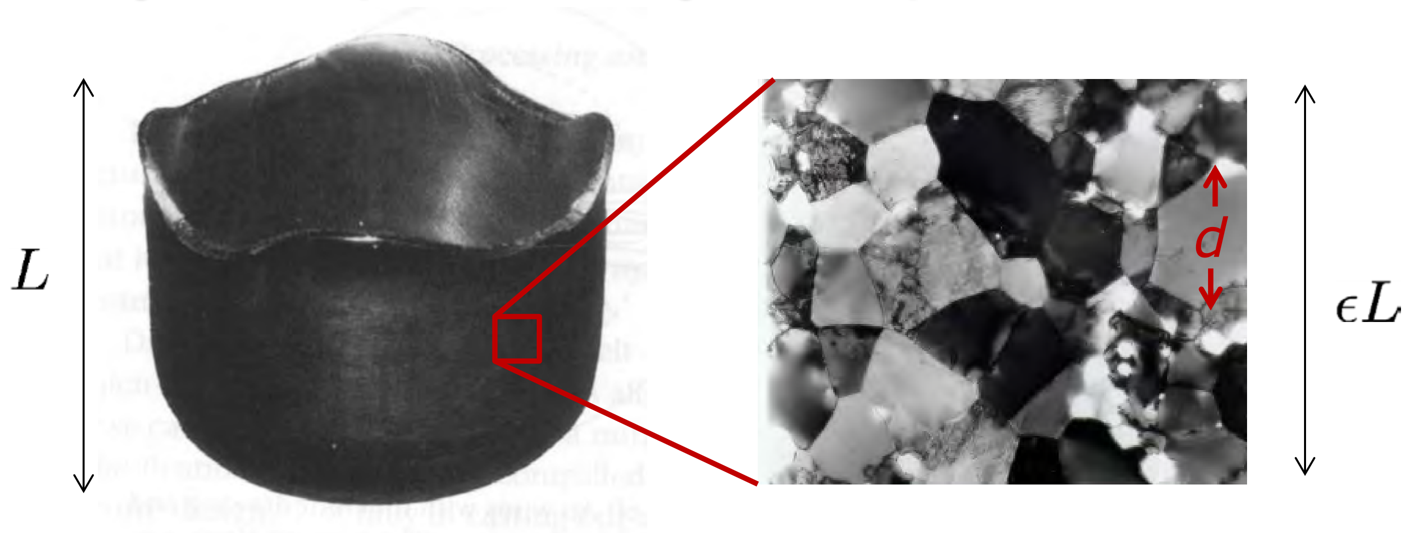
The big hammer: Optimal scaling

- Suppose: Energy $= E(u, \epsilon_1, \dots, \epsilon_N)$
- Optimal (matching) upper and lower bounds:

$$C_L \epsilon_1^{\alpha_1} \dots \epsilon_N^{\alpha_N} \leq \inf E(\cdot, \epsilon_1, \dots, \epsilon_N) \leq C_U \epsilon_1^{\alpha_1} \dots \epsilon_N^{\alpha_N}$$

- The exponents $\alpha_1, \dots, \alpha_N$ are *sharp*, *universal*
- The constants C_L and C_U are often lax, imprecise...
- Upper bound by construction, *ansatz*-free lower bound
- Originally applied to branched microstructures in martensite (Kohn-Müller 92, 94; Conti 00)
- Applications to micromagnetics (Choksi-Kohn-Otto 99), thin films (Belgacem *et al* 00)...

Crystal plasticity – Optimal scaling



Theorem [Conti & MO, ARMA, 2005] *There are constants c and c' such that*

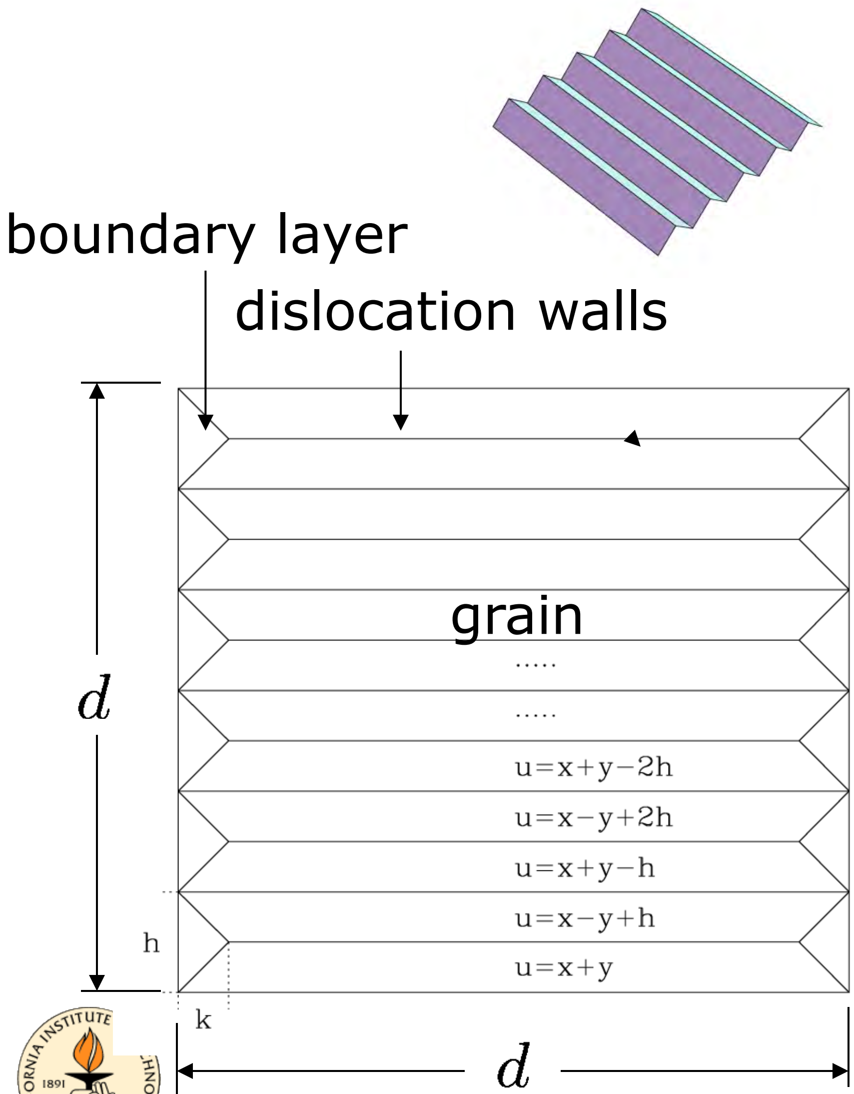
$$cE_0(T,\gamma,\tau_0,\mu,d) \leq \inf E \leq c' E_0(T,\gamma,\tau_0,\mu,d)$$

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

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

S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

Optimal scaling – Laminate construction



- Energy:

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

- Yield stress:

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

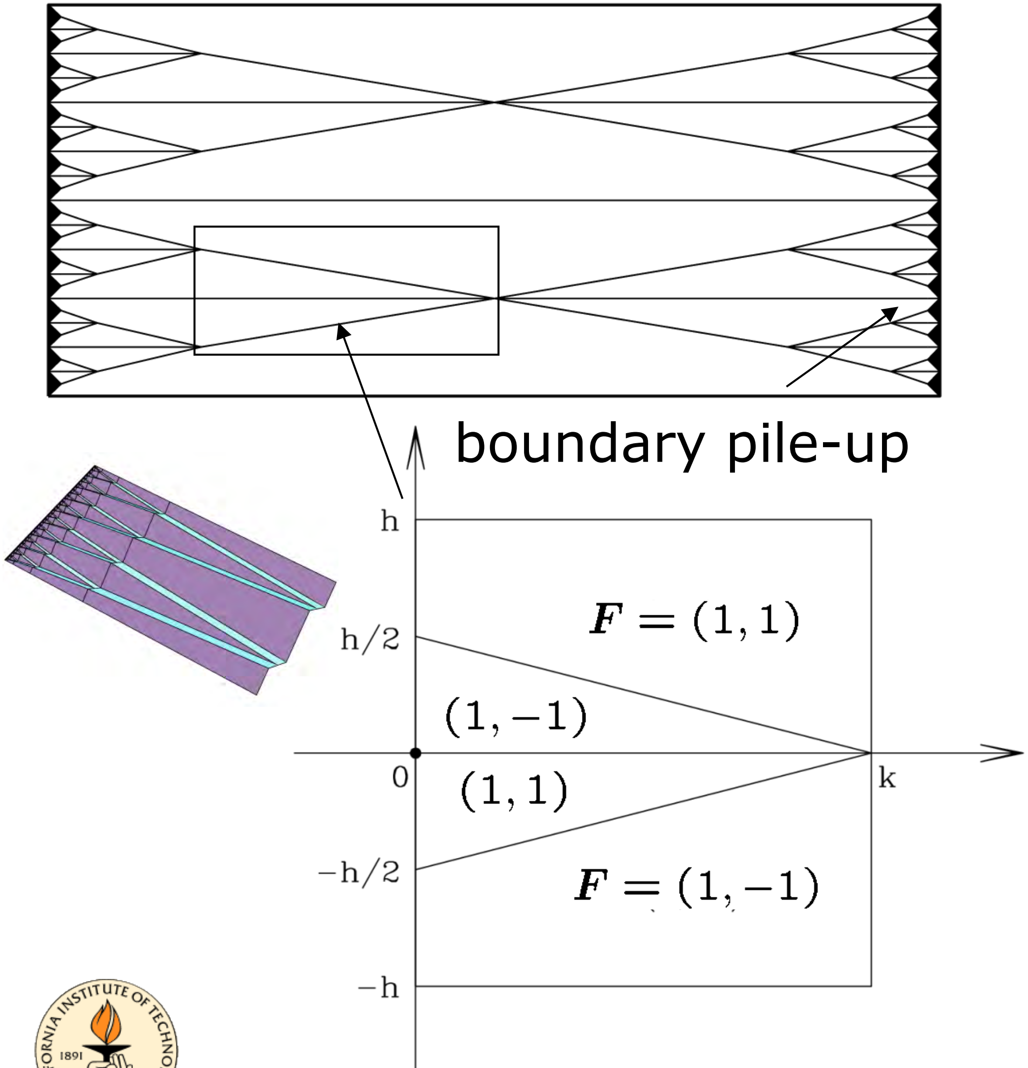
parabolic hardening + Hall-Petch scaling

- Lamellar width:

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

S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

Optimal scaling – Branching construction



- Energy:

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

- Yield stress:

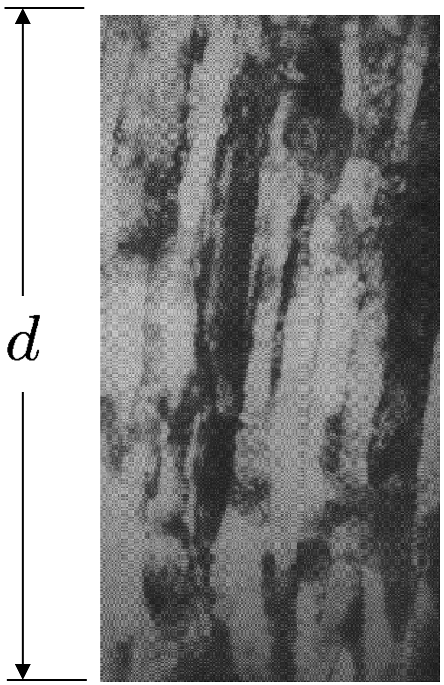
$$\tau \sim \tau_0 + \left(\frac{T}{bd} \right)^{2/3} (G\gamma)^{1/3}$$

- Microstructure size:

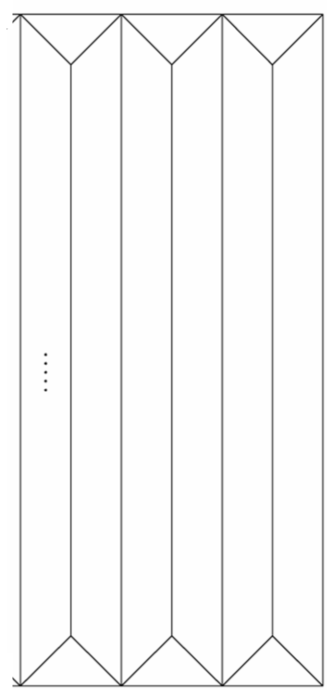
$$l \sim \left(\frac{Td^2}{G\gamma b} \right)^{1/3}$$

S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

Optimal scaling – Microstructures

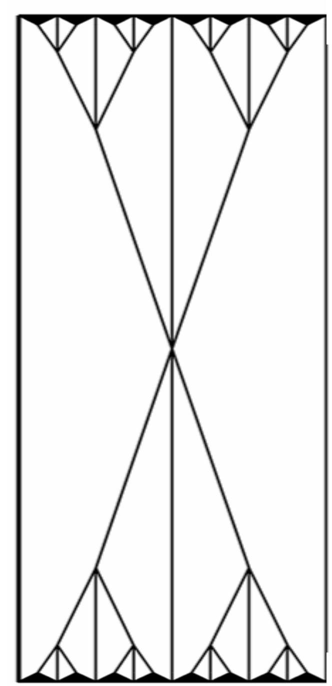


Shocked Ta
(Meyers et al ´95)



Laminate

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



Branching

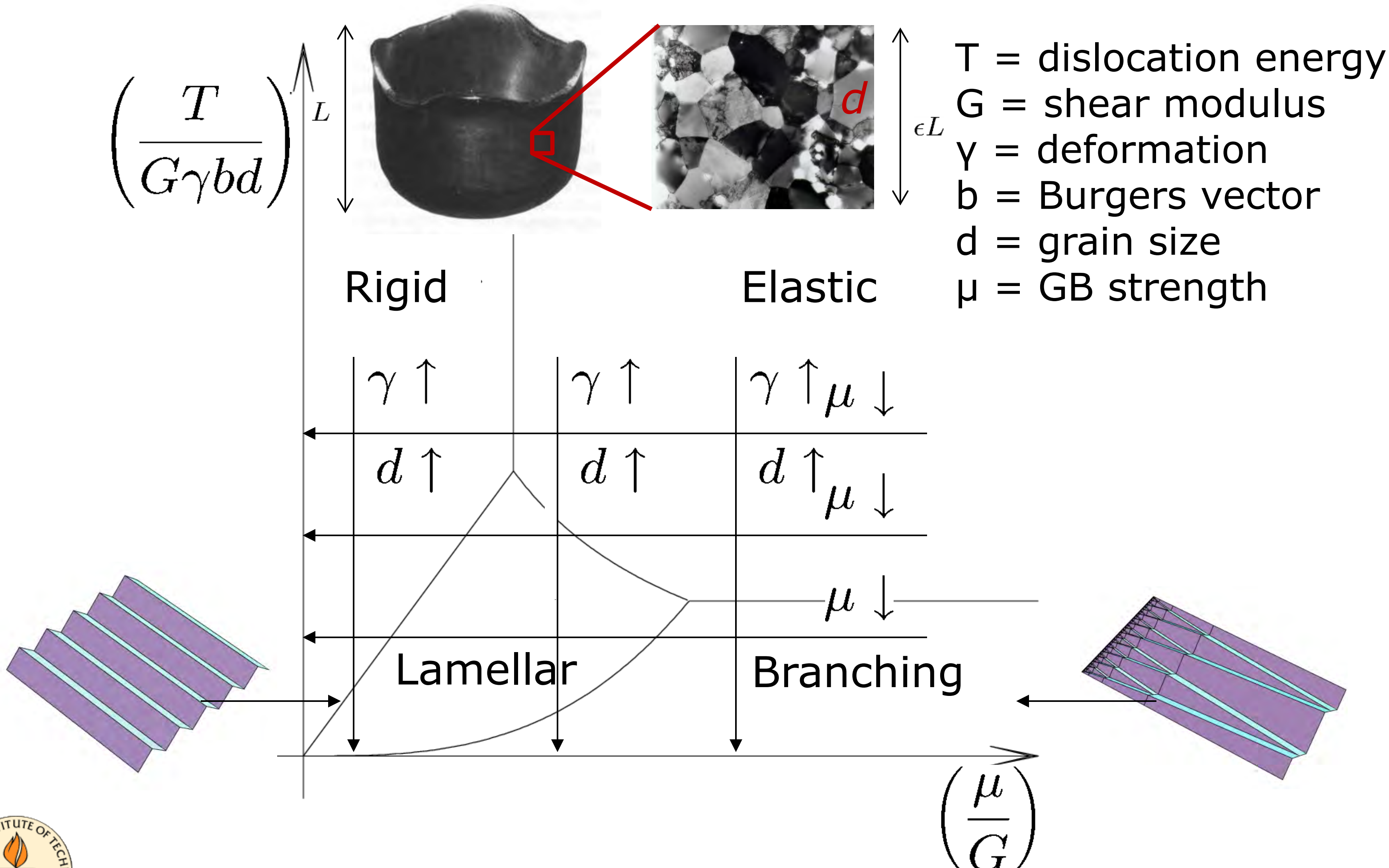
$\tau \sim d^{-2/3}$

LiF impact
(Meir and Clifton ´86)

Dislocation structures corresponding to the lamination and branching constructions

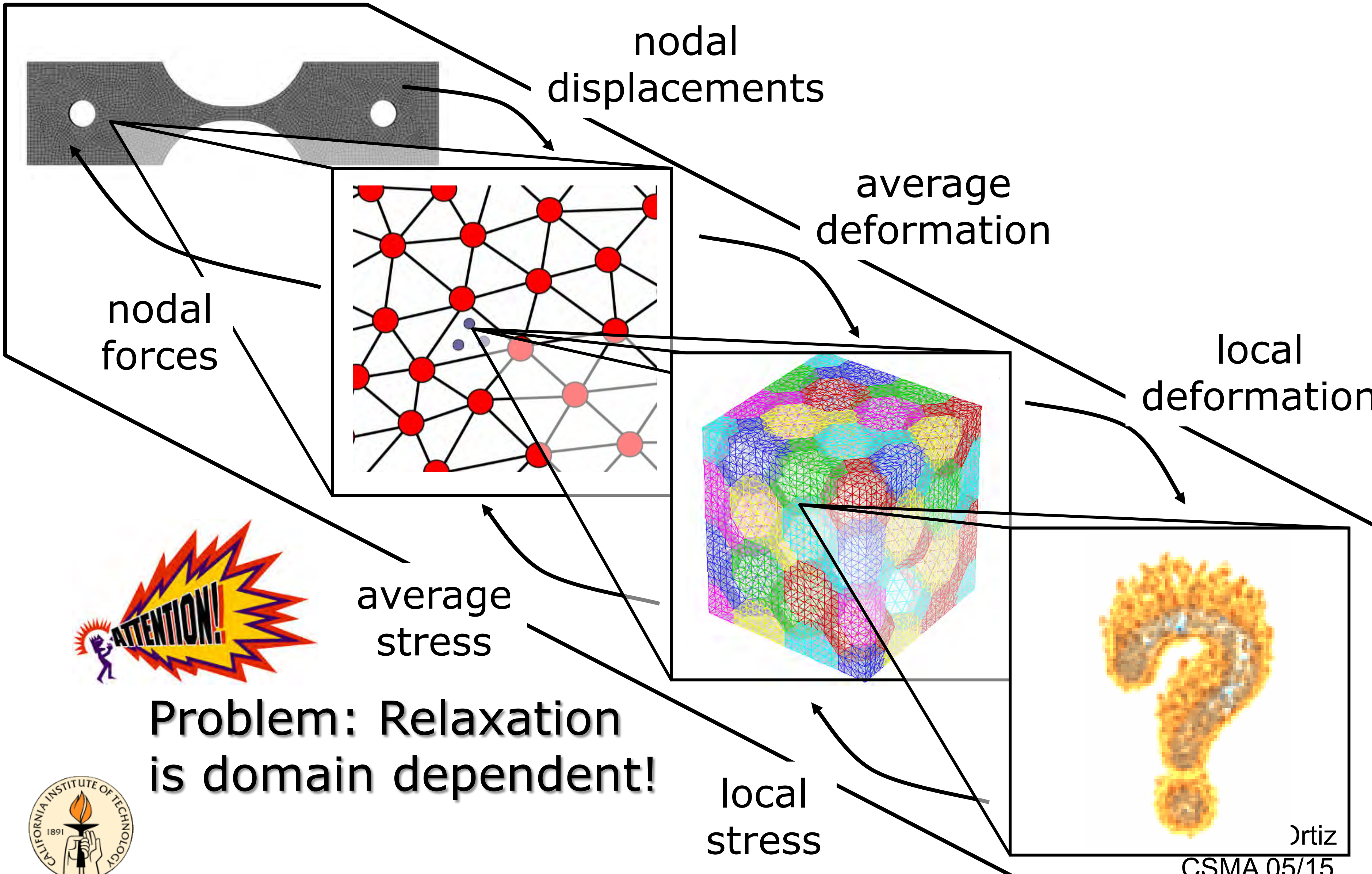
S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

Optimal scaling – Phase diagram



S. Conti and M. Ortiz, *ARMA*, **176** (2005), pp. 103–147

Polycrystals – Concurrent multiscale (C^3)

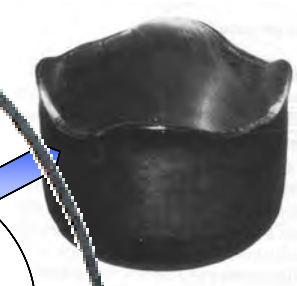


Problem: Relaxation is domain dependent!

Multiscale modeling of materials

Objective: High-fidelity,
microstructure-aw
of subgra

Open problem:
Size and shape-dependent
effective models of
subgrain microstructure



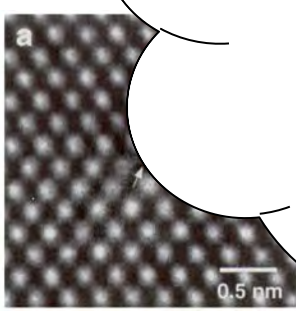
Application

time

ms

μs

ns



Lattice
defects

nm

μm

m

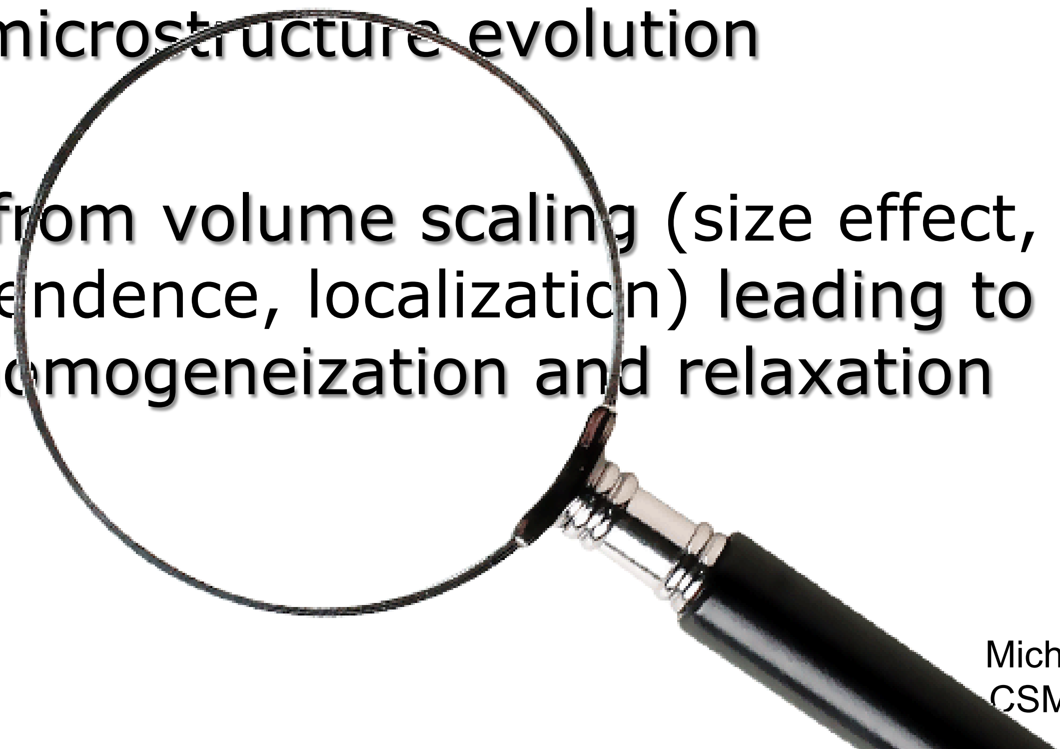
length

Standard model: Pitfalls

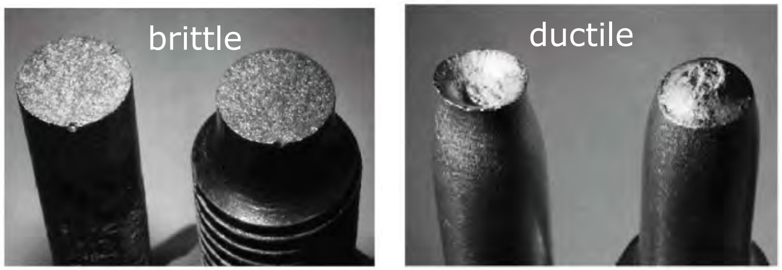
'Standard model' mail fail due to:

Non-proportional loading (unloading, cycling loading, change of loading path direction) leading to microstructure evolution

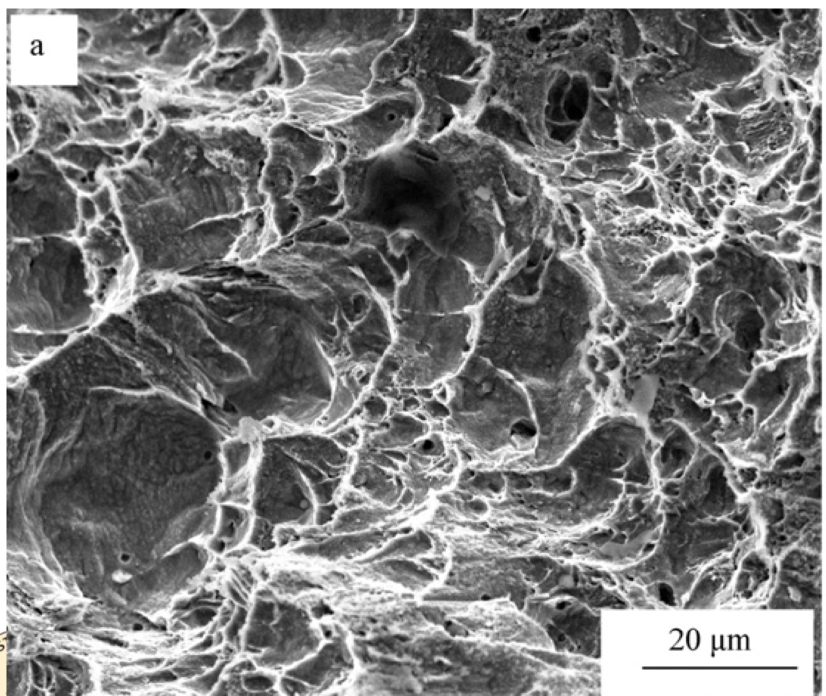
Departures from volume scaling (size effect, domain dependence, localization) leading to failure of homogeneization and relaxation



Localization – Fracture scaling



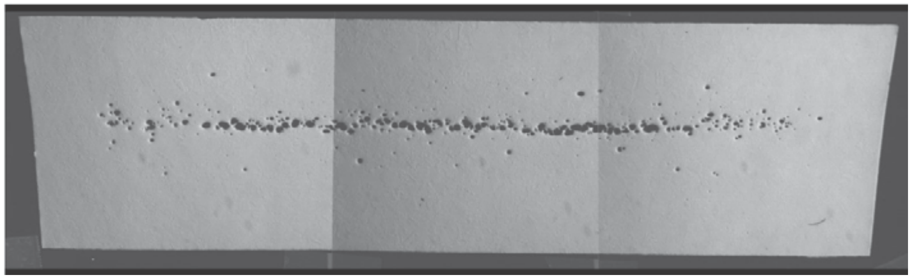
(Courtesy NSW HSC online)



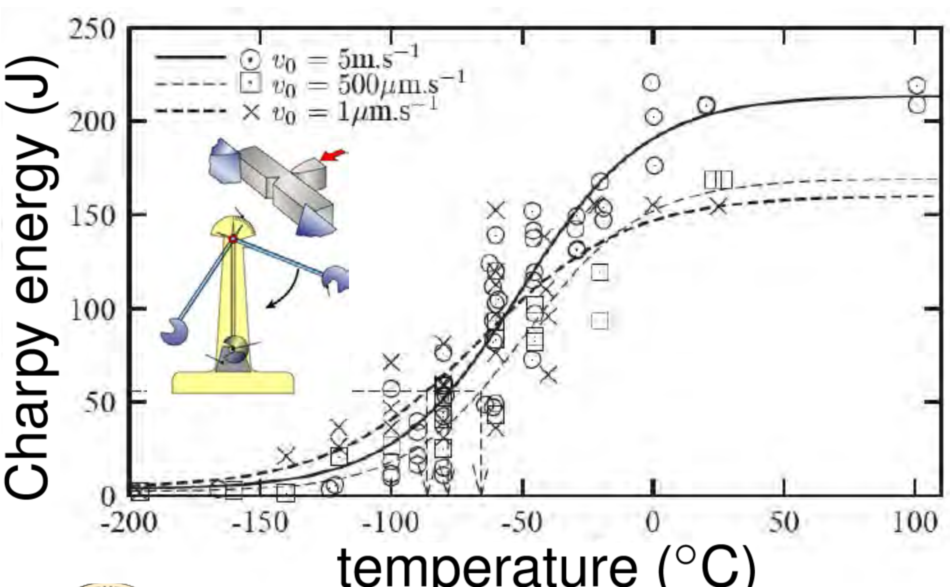
- Ductile fracture in metals occurs by *void nucleation, growth and coalescence*
- Fractography of ductile-fracture surfaces exhibits profuse *dimpling*, vestige of microvoids
- Ductile fracture entails large amounts of *plastic deformation* (*vs*. surface energy) and dissipation.

Fracture surface in SA333 steel, room temp., $d\varepsilon/dt=3\times10^{-3}s^{-1}$
(S.V. Kamata, M. Srinivasa and P.R. Rao, Mater. Sci. Engr. A, ***528*** *(2011) 4141–4146)*

Localization – Fracture scaling



Void sheet in copper disk[1]

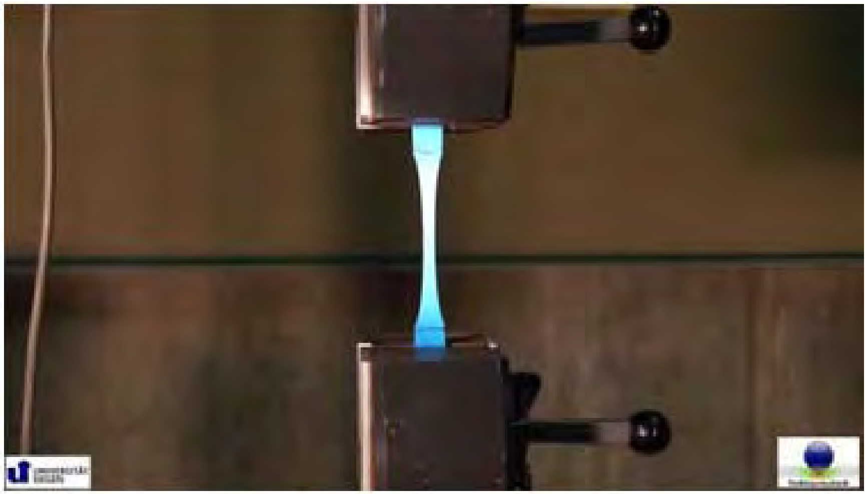


Charpy energy of A508 steel[2]

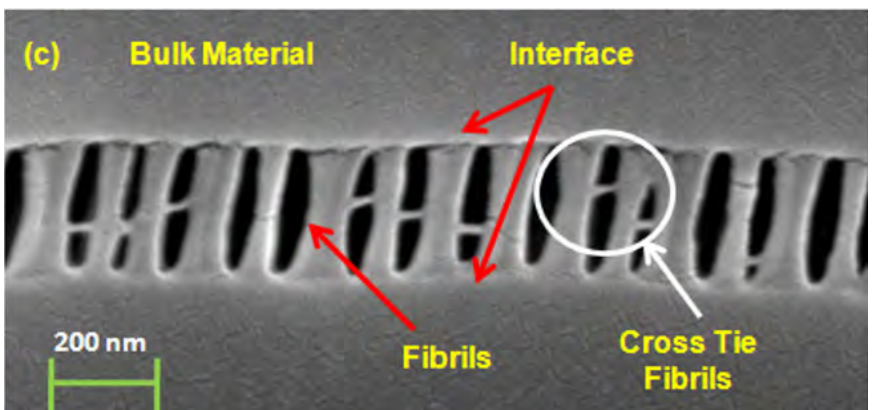
- Fracture energy scales with crack area: $E \sim L^2$
- A number of ASTM engineering standards are in place to characterize ductile fracture properties (J-testing, Charpy test)
- In general, the specific fracture energy for ductile fracture is greatly in excess of that required for brittle fracture…

[1]Heller, A., Science & Technology, LLNL, pp. 13-20, July/August, 2002
[2]Tanguy *et al.*, *Eng. Frac. Mechanics*, 2005

Fracture of polymers



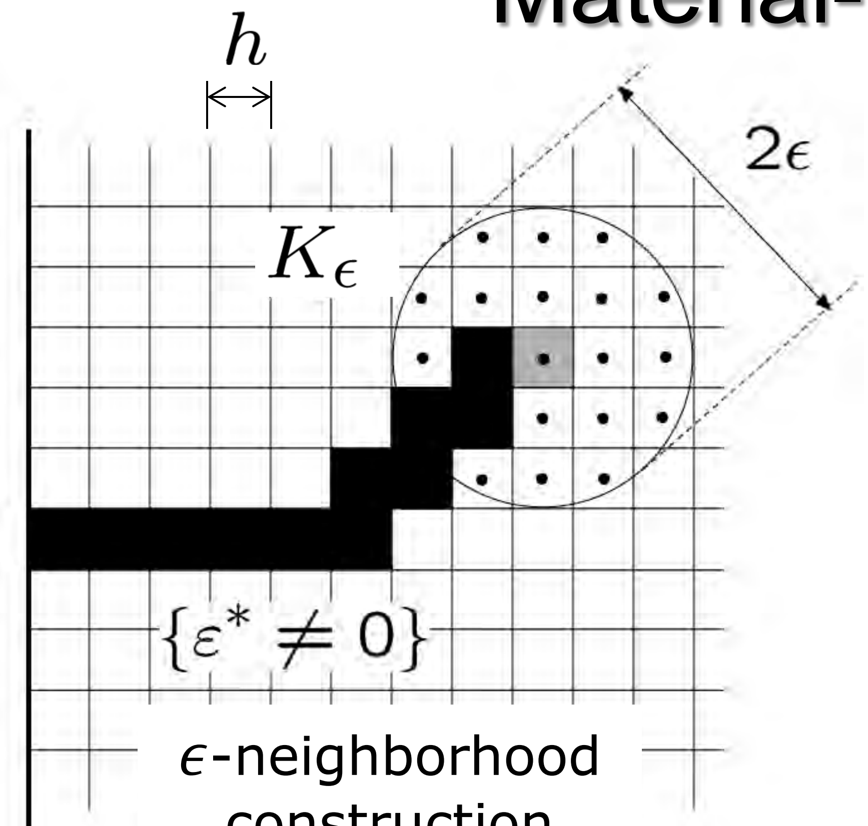
T. Reppel, T. Dally, T. and K. Weinberg, Technische Mechanik, 33 (2012) 19-33.



Crazing in 800 nm polystyrene thin film (C. K. Desai *et al*., 2011)

- Polymers undergo entropic elasticity and damage due to chain stretching and failure
- Polymers fracture by means of the crazing mechanism consisting of fibril nucleation, stretching and failure
- The free energy density of polymers saturates in tension once the majority of chains are failed: p=0!
- Crazing mechanism is incompatible with strain-gradient elasticity…

Numerical implementation
Material-point erosion



ϵ-neighborhood construction

- ϵ-neighborhood construction: Choose $h \ll \epsilon \ll L$
- Erode material point if

$$\frac{h^2}{|K_\epsilon|}\int_{K_\epsilon} W(\nabla u)\, dx \geq J_c$$

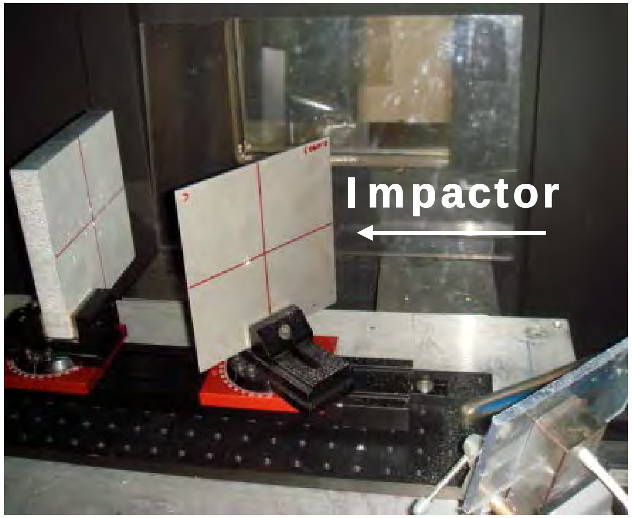
- For linear elasticity, proof of Γ-convergence to Griffith fracture

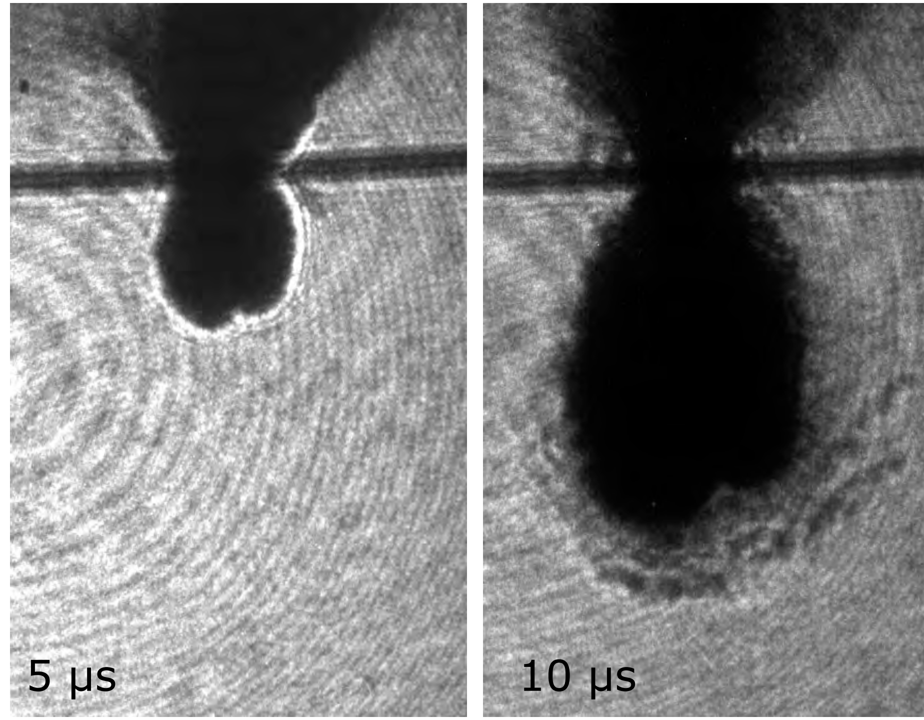
Theorem[1]: Suppose $\epsilon = \epsilon(h)$ and $h/\epsilon(h) \to 0$ as $h \to 0$. Then, $\Gamma - \lim_{h\to 0} E_{h,\epsilon(h)} =$ Griffith energy

[1]Schmidt, B., *et al.*, *SIAM Multi. Model.*, **7** (2009) 1237.

Michael Ortiz
CSMA 05/15

Application to hypervelocity impact

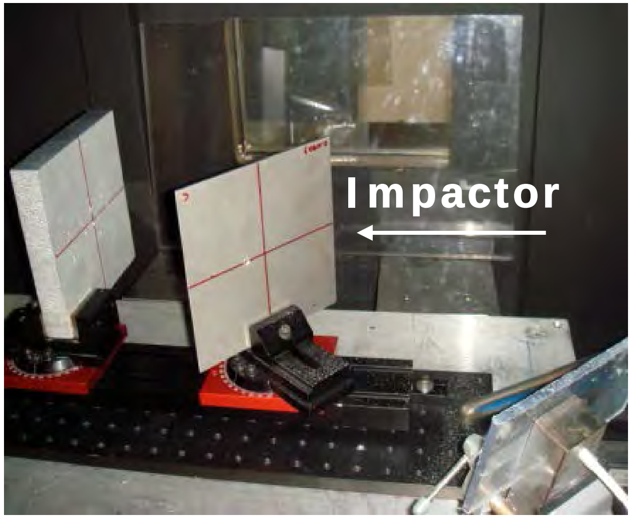


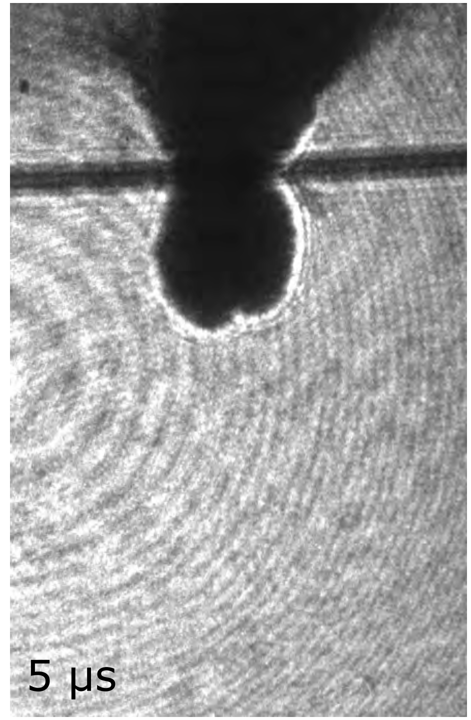


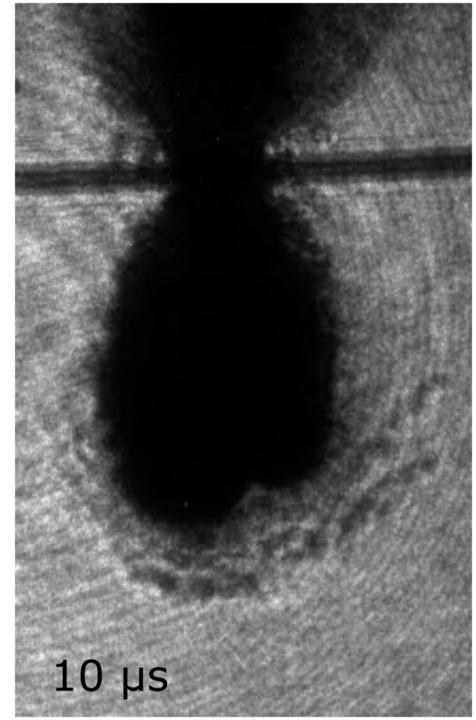
Hypervelocity impact (5.7 Km/s) of 0.96 mm thick aluminum plates by 5.5 mg nylon 6/6 cylinders (Caltech)

Pandolfi, A. & Ortiz, M. , *IJNME,* **92** *(*2012) 694.
Pandolfi, A., Li, B. & Ortiz, M. , *Int. J. Fract.,* **184** *(*2013) 3.
Li, B., Stalzer, M. & Ortiz, M., *IJNME,* **100** (2014) 40.

Application to hypervelocity impact







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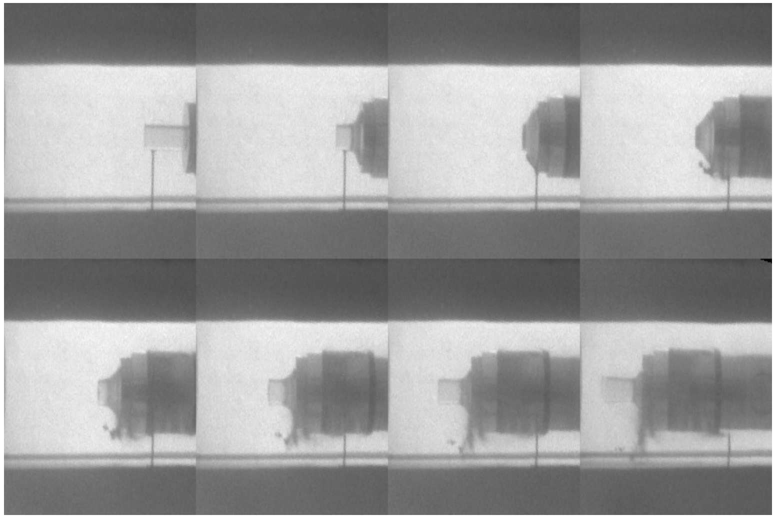
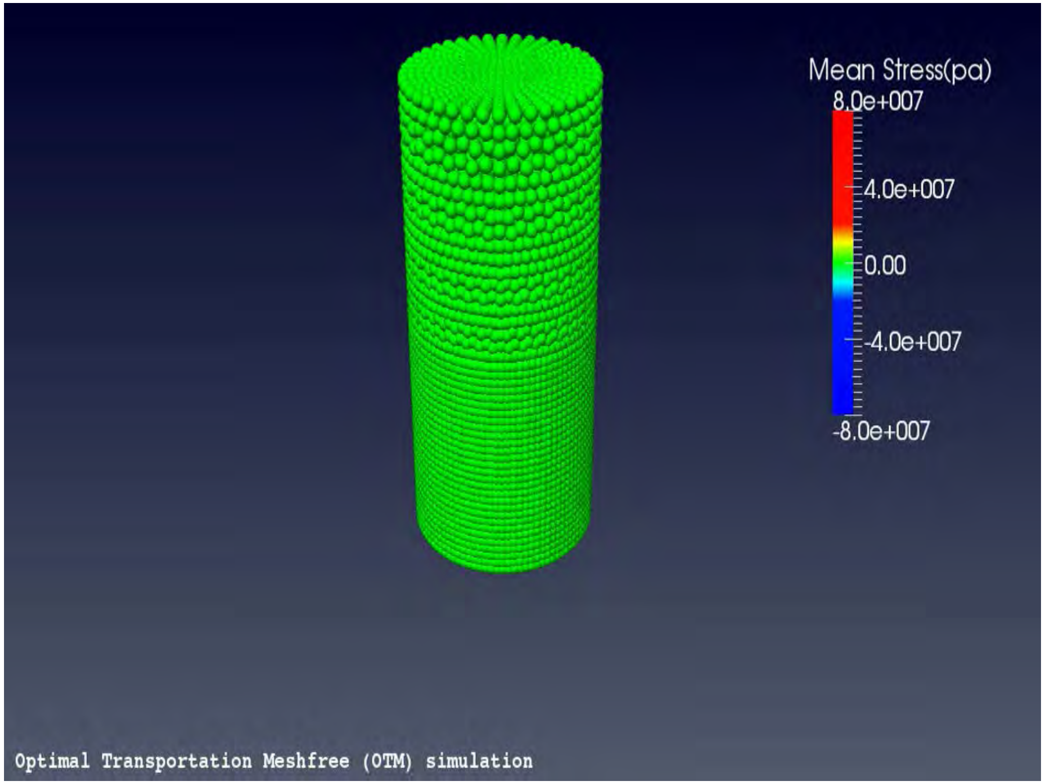
Li, B., Stalzer, M. & Ortiz, M., *IJNME,* **100** (2014) 40.

Taylor-anvil tests on polyurea



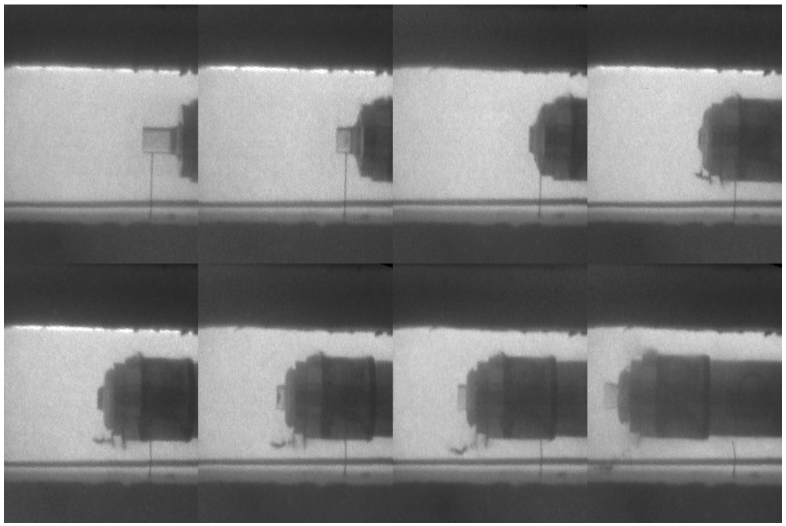
Shot #854:
R0 = 6.3075 mm,
L0 = 27.6897 mm,
v = 332 m/s



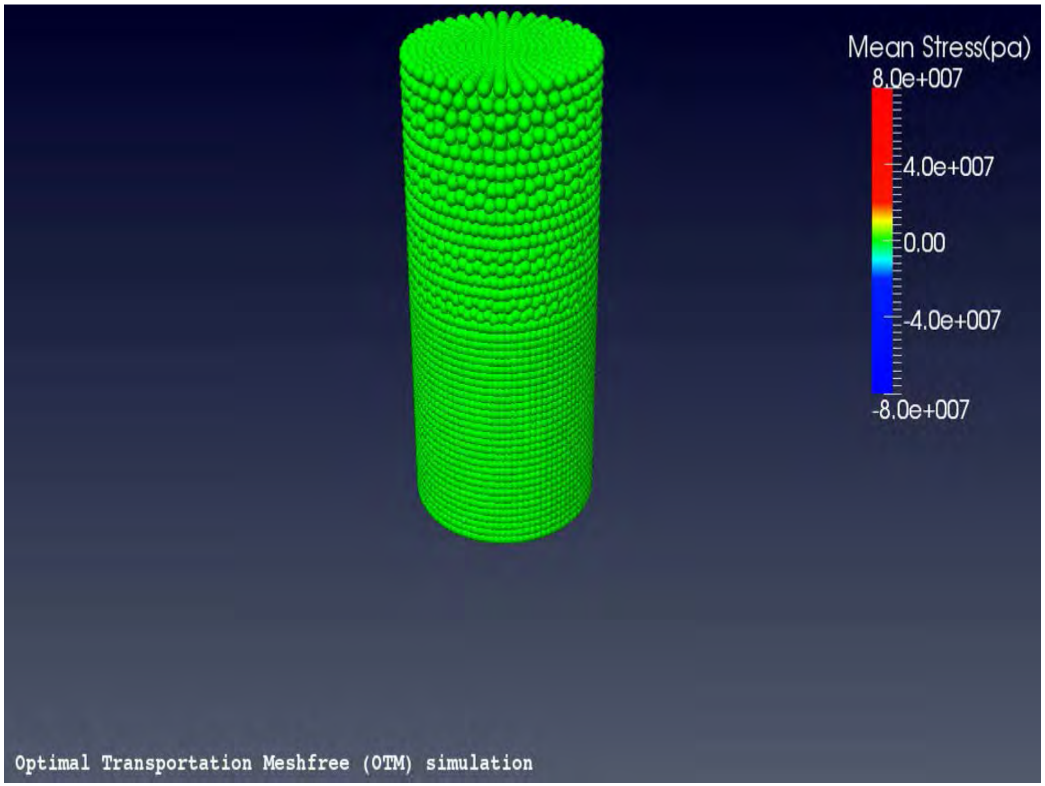
Experiments conducted by W. Mock, Jr. and J. Drotar,
at the Naval Surface Warfare Center (Dahlgren Division)
Research Gas Gun Facility, Dahlgren, VA 22448-5100, USA

S. Heyden *el al.*, *JMPS*, **74** (2015) 175.

Experiments and simulations



Shot #861:
R0 = 6.3039 mm,
L0 = 27.1698 mm,
v = 424 m/s



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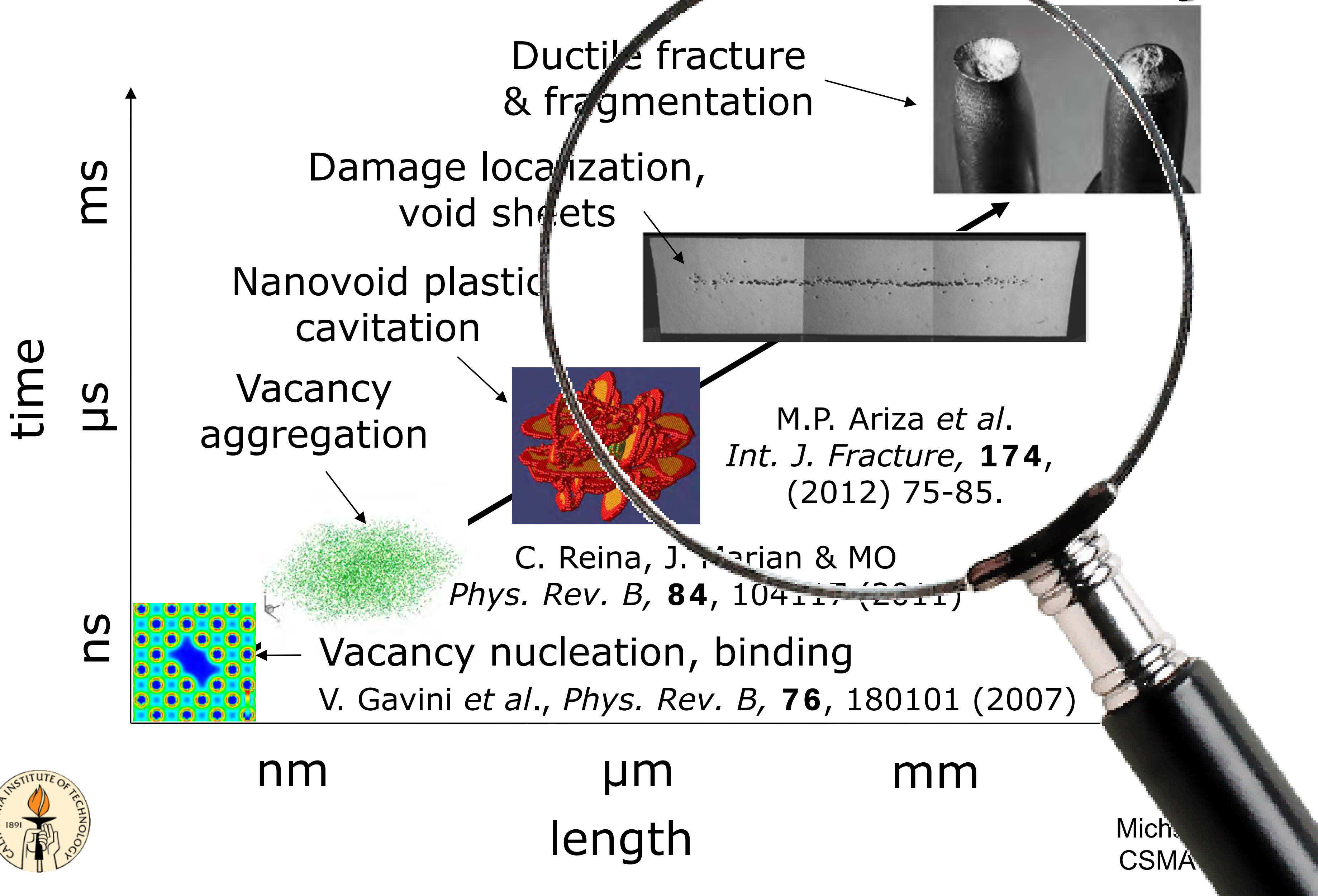
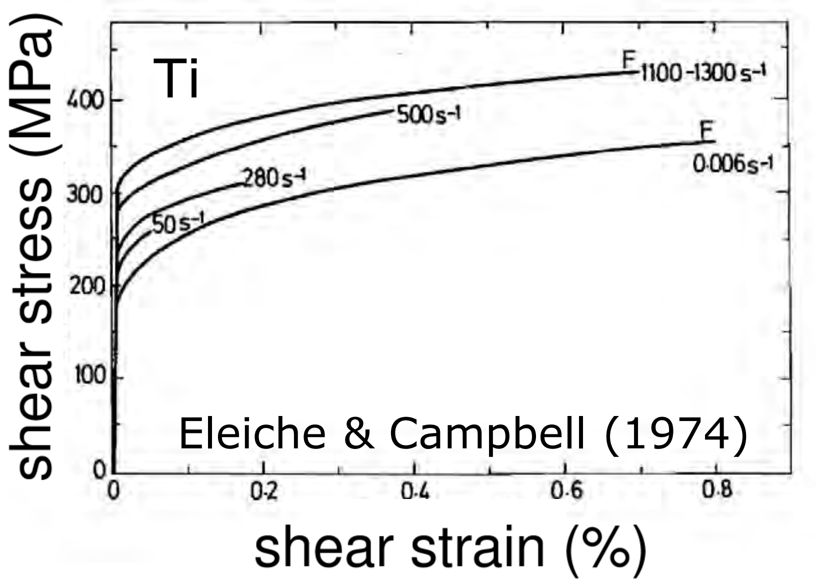
S. Heyden *el al.*, *JMPS*, **74** (2015) 175.

Ductile fracture – Multiscale hierarchy



Naïve model: Local plasticity

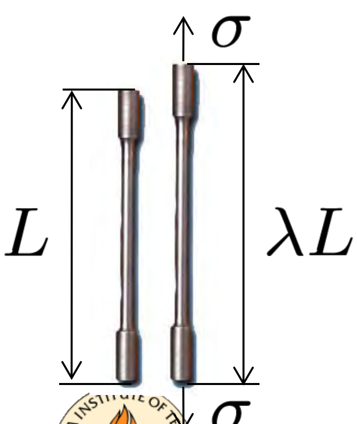


- Deformation theory: Minimize

$$E(y) = \int_\Omega W\Big(Dy(x)\Big)\,dx$$

- Growth of $W(F)$?
- Asume power-law hardening:

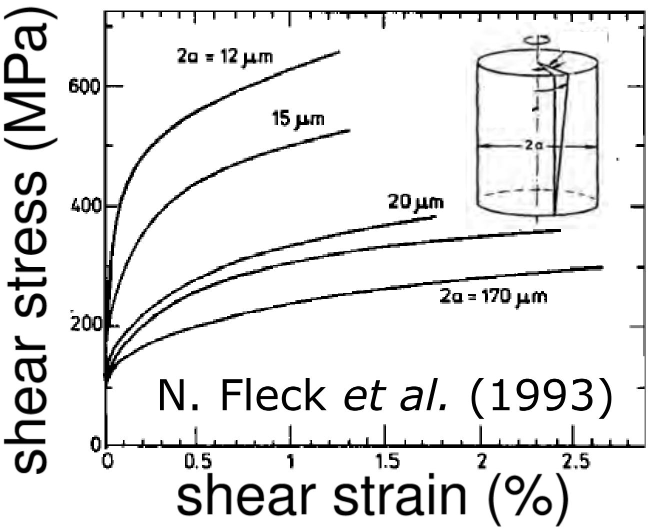
$$\sigma \sim K\epsilon^n = K(\lambda - 1)^n$$

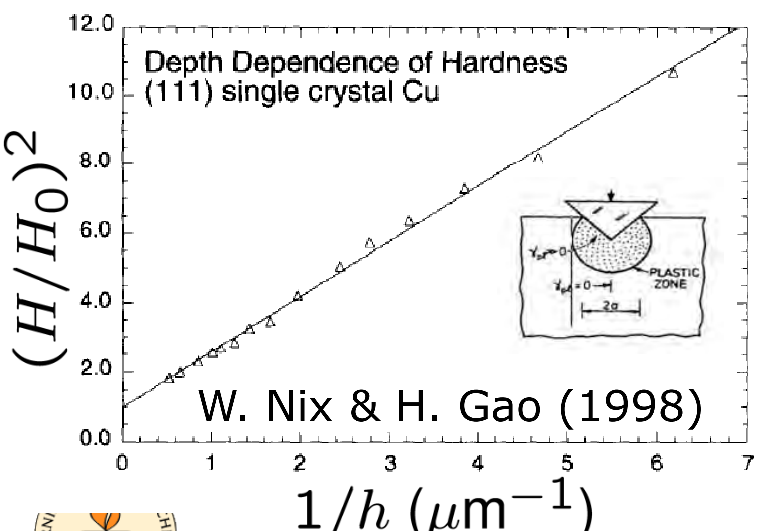


- Nominal stress: $\partial_\lambda W = \sigma/\lambda = K(\lambda - 1)^n/\lambda$
- For large λ: $\partial_\lambda W \sim K\lambda^{n-1} \Rightarrow W \sim K\lambda^n$
- In general: $W(F) \sim |F|^p,\ p = n \in (0,1)$

$\Rightarrow$ Sublinear growth!

Strain-gradient plasticity





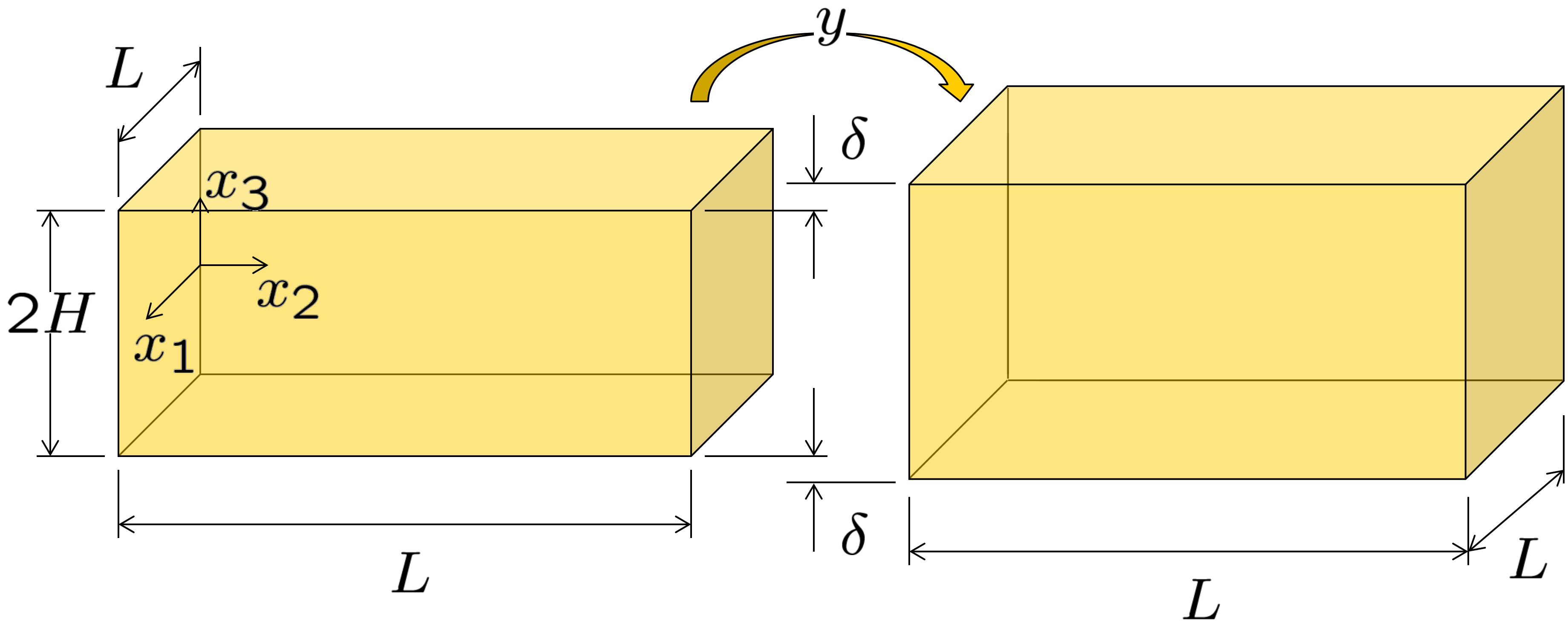
- The yield stress of metals is observed to increase in the presence of strain gradients
- Deformation theory of strain-gradient plasticity:

$$E(y) = \int_\Omega W\Big(Dy(x), D^2 y(x)\Big)\, dx$$

$y : \Omega \to \mathbb{R}^n$, volume preserving

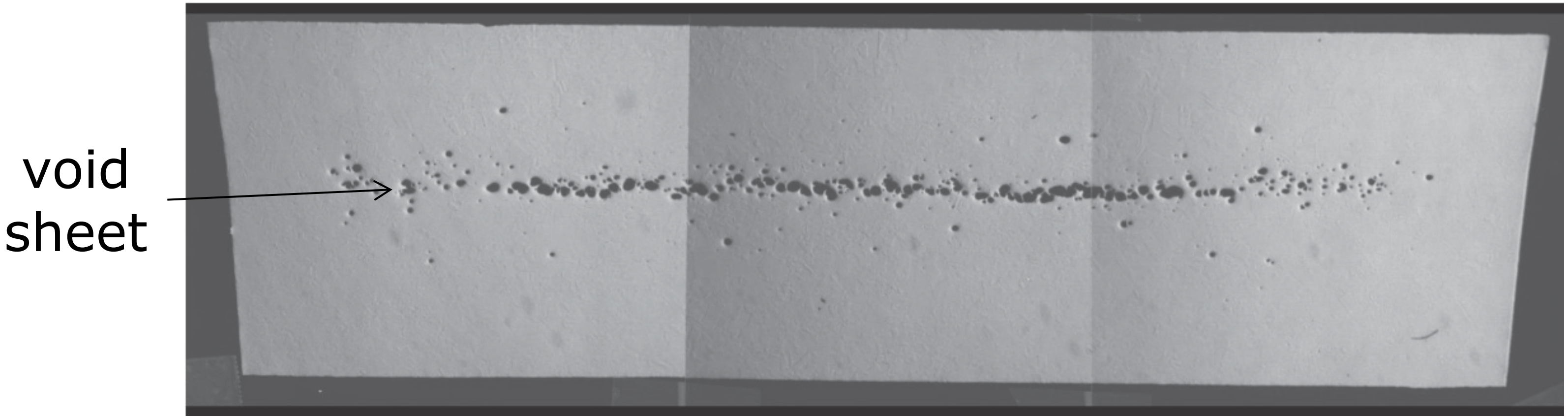
- Strain-gradient effects may be expected to oppose localization
- Question: Can fracture scaling be understood as the result of strain-gradient plasticity?

The big hammer: Optimal scaling

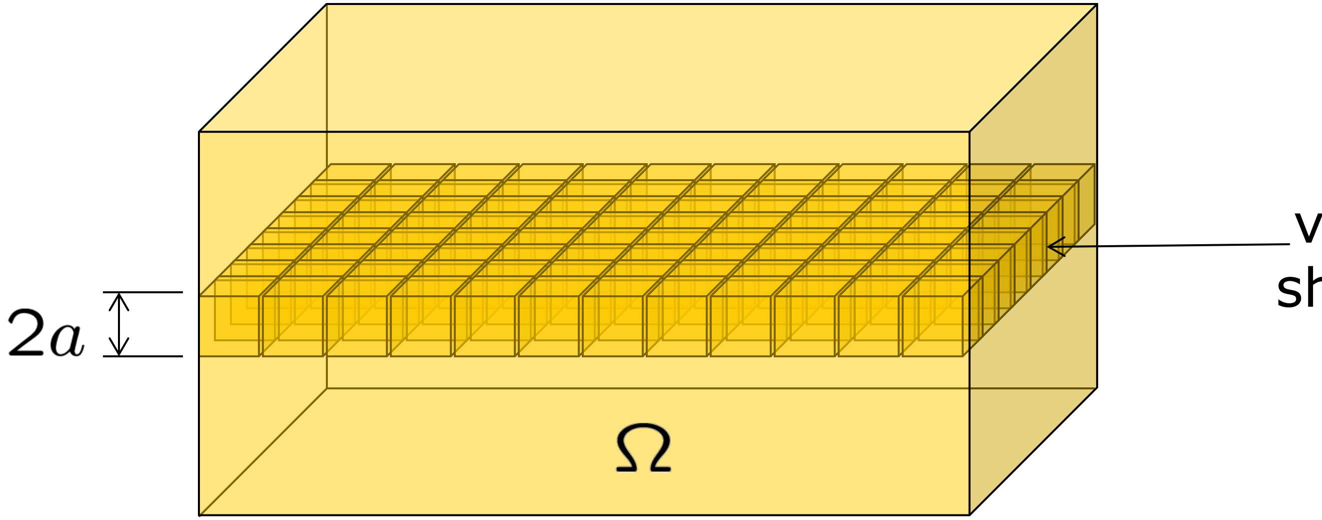


- Approach: Optimal scaling
- Slab: $\Omega = [0, L]^2 \times [-H, H]$, periodic
- Uniaxial extension: $y_3(x_1, x_2, \pm H) = x_3 \pm \delta$

Optimal scaling – Upper bound



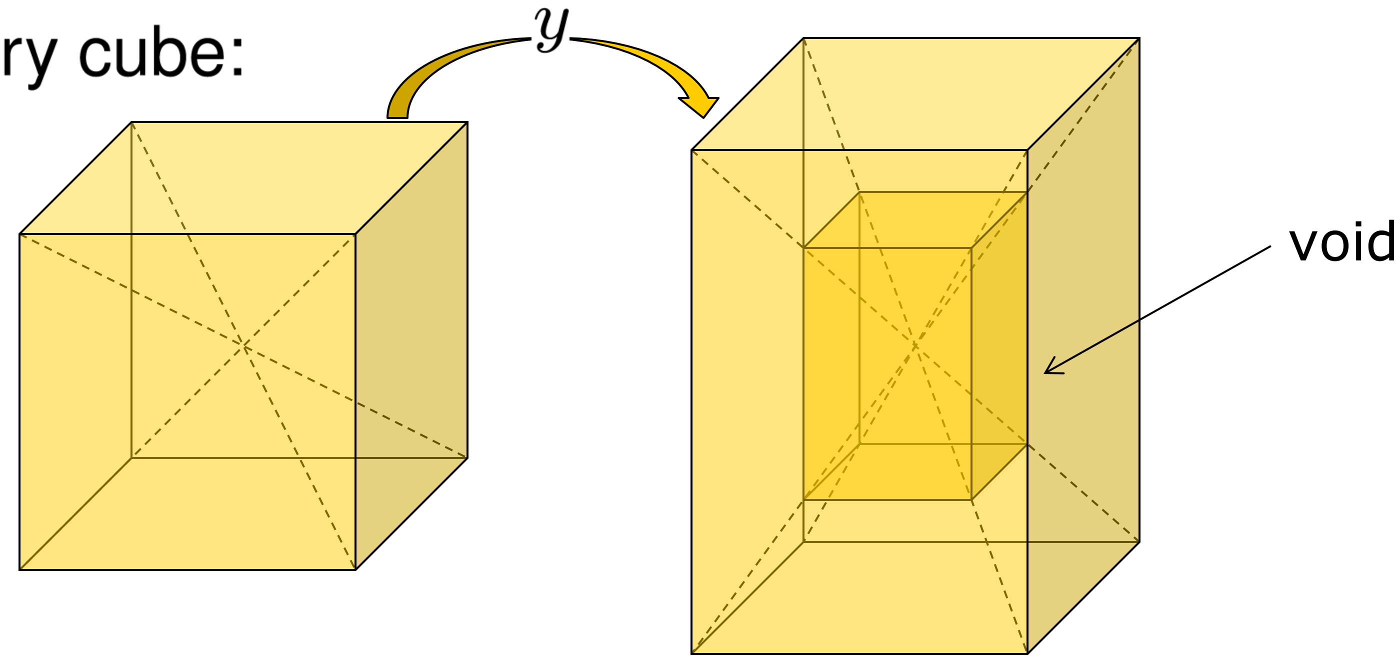
Heller, A., Science & Technology Review Magazine, LLNL, pp. 13-20, July/August, 2002



L. Fokoua, S. Conti and M. Ortiz, *ARMA*, **212** (2014) pp. 331-357.

Optimal scaling – Upper bound

- In every cube:

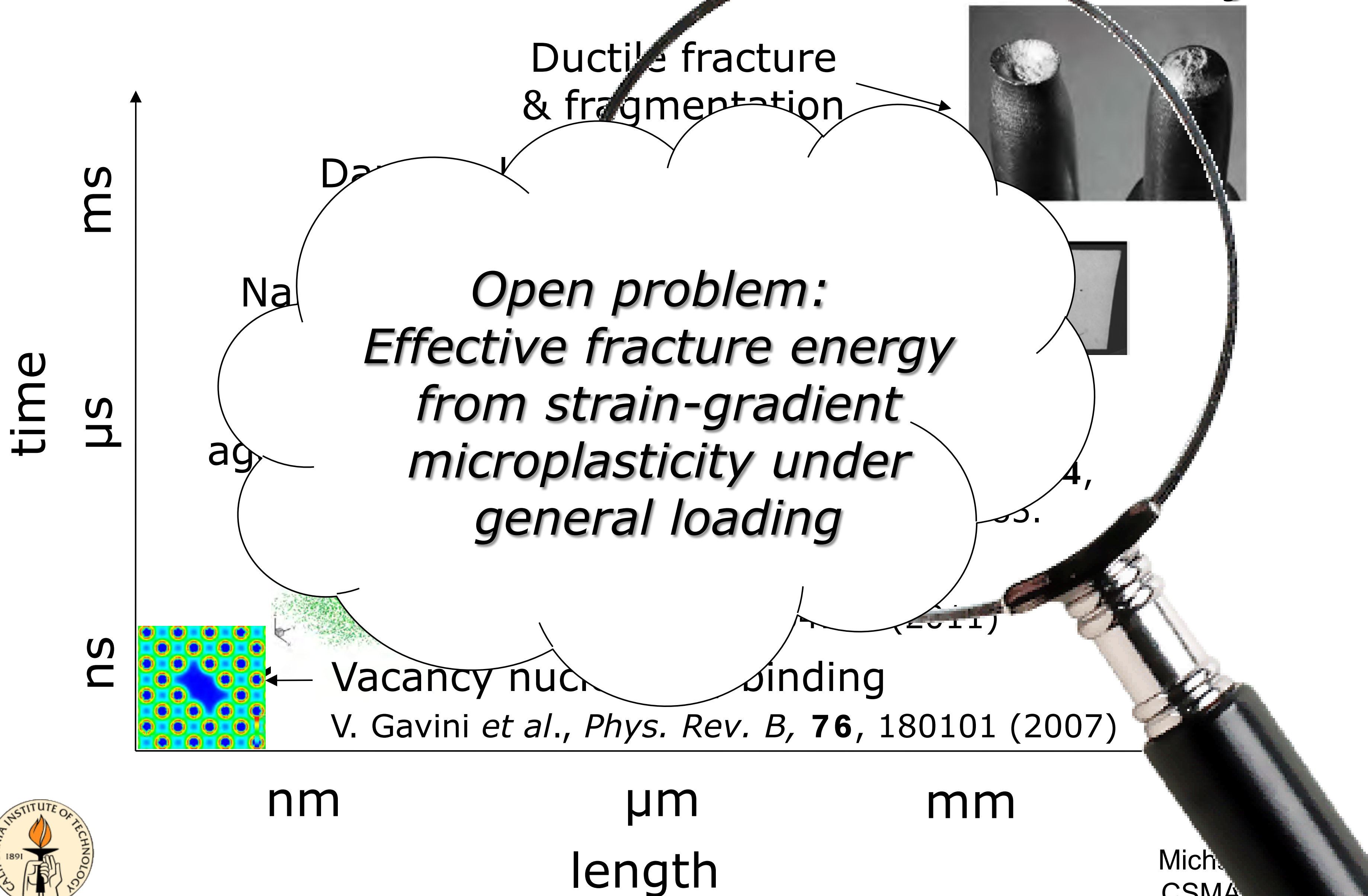


- Calculate, estimate: $E \leq CL^2 \left(a^{1-p} \delta^p + \ell \delta / a \right)$
- Optimize: $a = (\ell \delta^{1-p})^{1/(2-p)} \Rightarrow E \leq C_U L^2 \ell^{\frac{1-p}{2-p}} \delta^{\frac{1}{2-p}}$

void growth! fracture!

L. Fokoua, S. Conti and M. Ortiz, *ARMA*, **212** (2014) pp. 331-357.

Ductile fracture – Multiscale hierarchy



Concluding remarks

The well-understood setting:

Rate-independent, proportional loading and local behavior (deformation theory of plasticity + relaxation)

Still open:

Rate-dependent, non-proportional loading and non-local or localized behavior

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!