Multiscale Analysis as a (Lossless) Approximation Scheme

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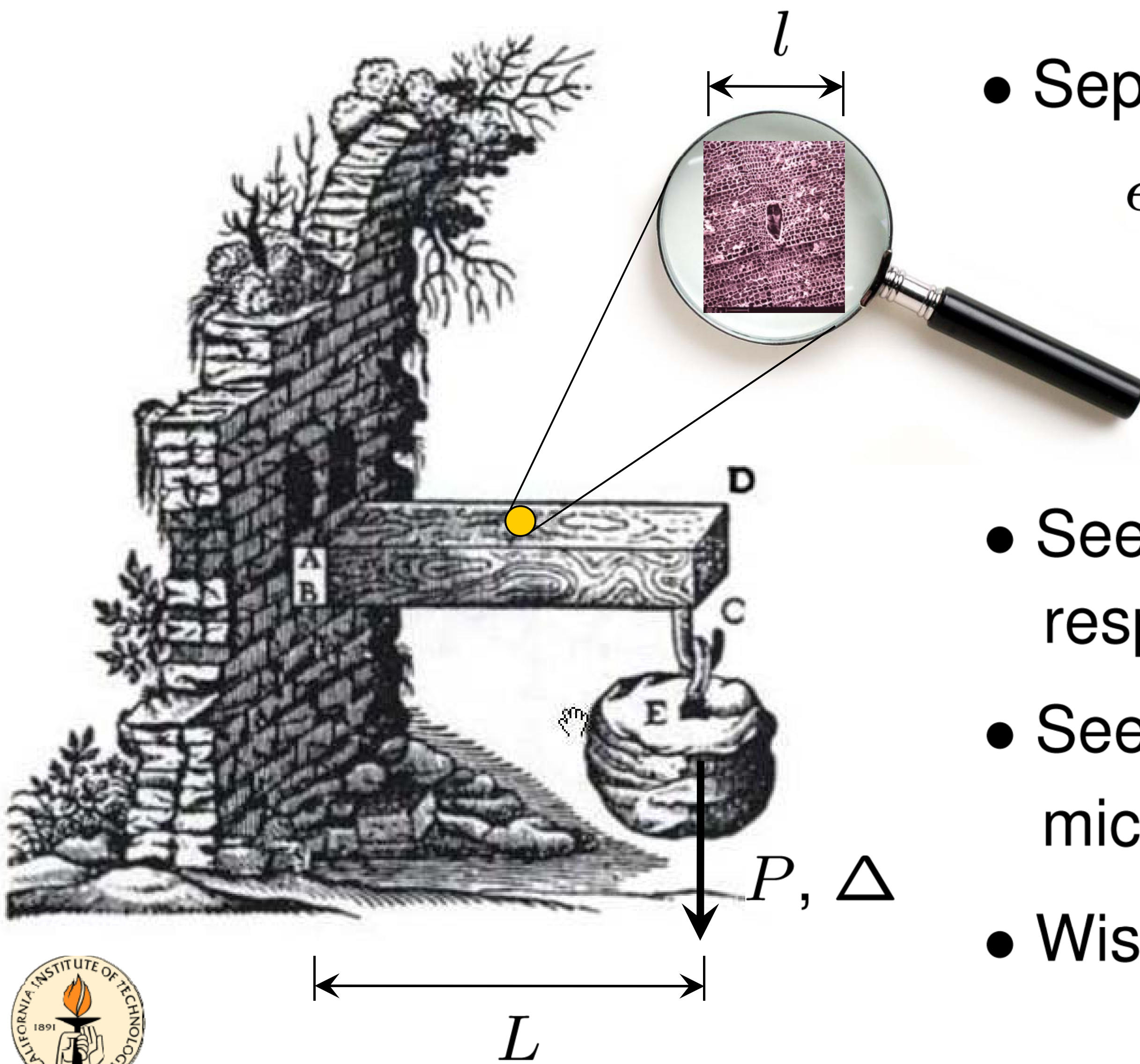
Outline

- Multiscale Analysis as an approximation scheme:
  - *What is (or is not) Multiscale Analysis?*
  - *When does it apply? To what avail?*
  - *How and to what does it converge?*
  - *What information is lost, if any?*
- The time-independent and time-dependent cases
- The rate-independent case, deformation theory
- Implementation and applications:
  - *Crystal plasticity*
  - *Initiation in energetic materials*

Separation of Scales - Homogeneization



- Separation of scales:

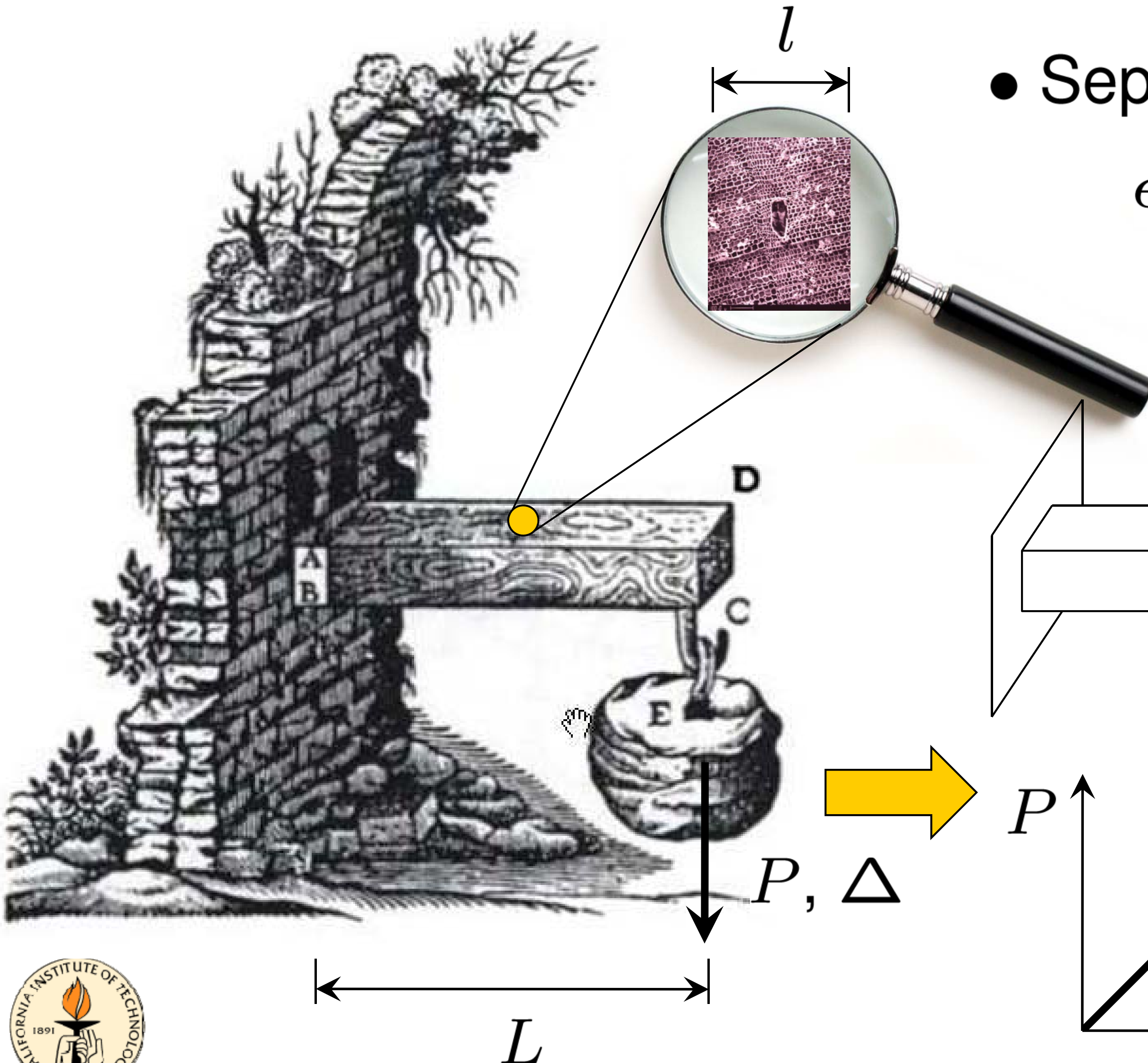
$$\epsilon = l/L \to 0$$

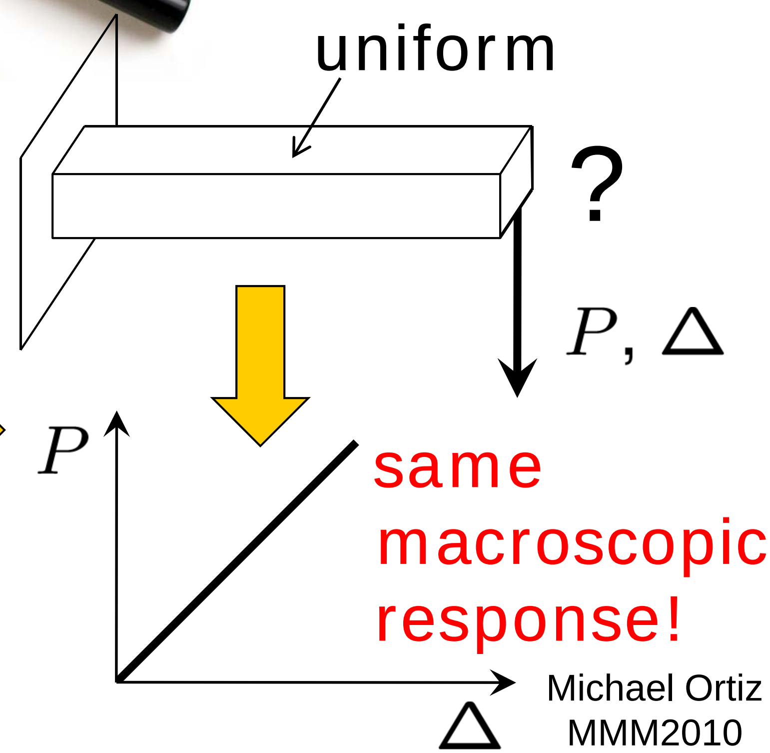
- Seek macroscopic response P-Δ
- Seek to eliminate microscopic scale
- Wish return option...

Separation of Scales - Homogeneization

- Separation of scales:

$$\epsilon = l/L \to 0$$

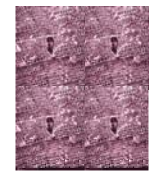




Gamma Convergence of functionals

- Equicoercive functionals $F_\epsilon : X \to [0, +\infty]$, e. g.:

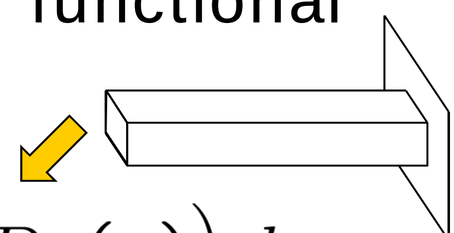
$$F_\epsilon(u) = \int_\Omega W\Big(\frac{x}{\epsilon}, Du(x)\Big)\, dx \to \text{inf!}$$

- Separation-of-scales limit: $\epsilon \to 0$: , ,  $\dots$

- $\Gamma - \lim\limits_{\epsilon \to 0} F_\epsilon = F_0$ (*wlsc*) iff, for all $f \in X^*$ (loadings),

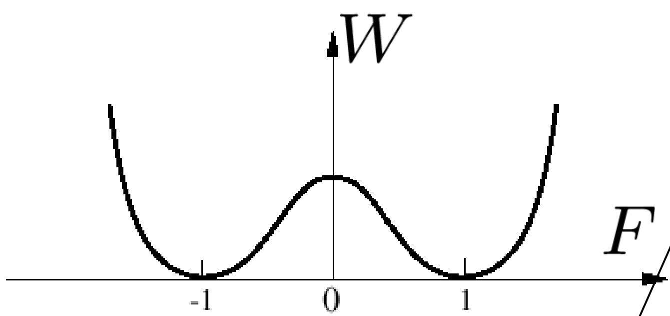
$$\underbrace{\inf_{u \in X} \Big(F_\epsilon(u) + \langle f, u \rangle\Big)}_{\text{minimum energies of sequence of functionals}} \longrightarrow \underbrace{\inf_{u \in X} \Big(F_0(u) + \langle f, u \rangle\Big)}_{\text{minimum energy of limiting functional}}$$

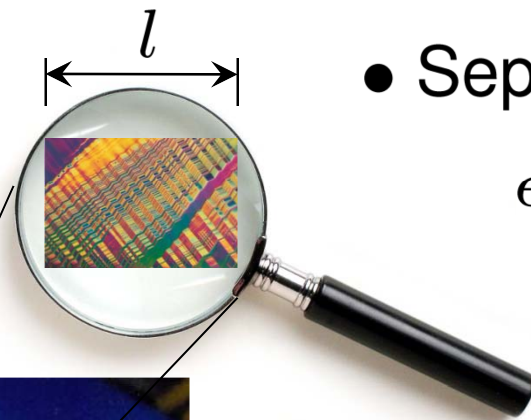
- Example: Homogeneization limit,



$$W_0(\xi) = \inf_{W^{1,1}_{\text{per}}(P)} \frac{1}{|P|} \int_P W\Big(x, \xi + Dv(x)\Big)\, dx$$

Separation of Scales - Relaxation

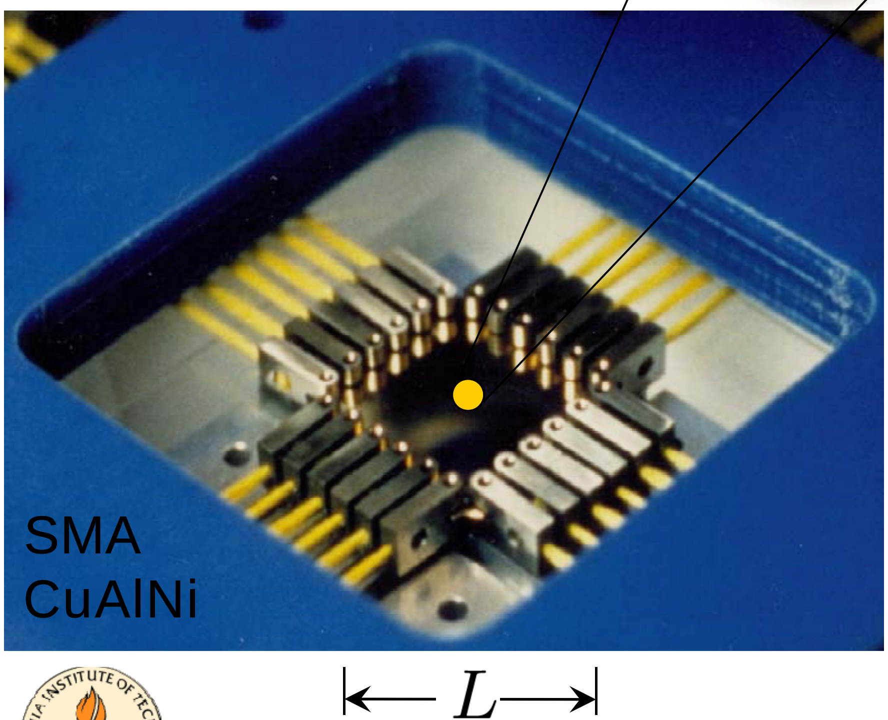


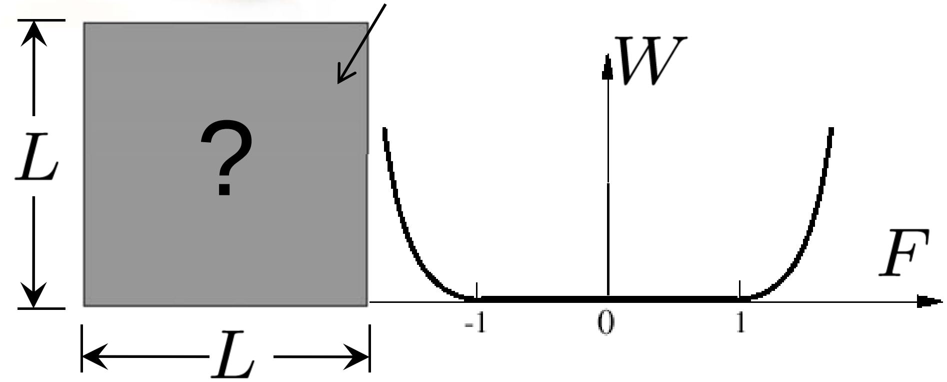


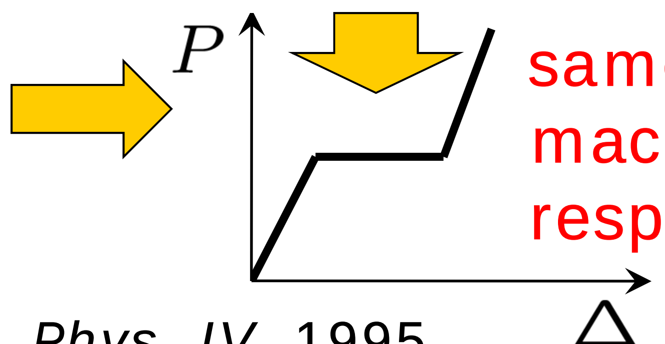
- Separation of scales:

$$\epsilon = l/L \to 0$$

no deformation microstructures!







same macroscopic response!

Chu, C. and James, R.D., *J. Phys. IV*, 1995

Separation of Scales - Relaxation

- Coercive functional $F : X \to [0, +\infty]$, e. g.:

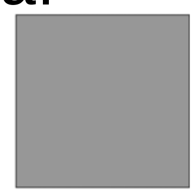
$$F(u) = \int_\Omega W\Big(Du(x)\Big)\,dx \to \text{inf!}$$

- F_0 is the *relaxation* of F iff:

  - F_0 stable w.r.t. affine deformations (*wlsc*),
  - For all applied loadings $f \in X^*$,

$$\underbrace{\inf_{u\in X}\Big(F(u) + \langle f, u\rangle\Big)}_{\text{minimum energy of original functional}} \longrightarrow \underbrace{\inf_{u\in X}\Big(F_0(u) + \langle f, u\rangle\Big)}_{\text{minimum energy of relaxed functional}}$$

- Example: Quasiconvex envelop

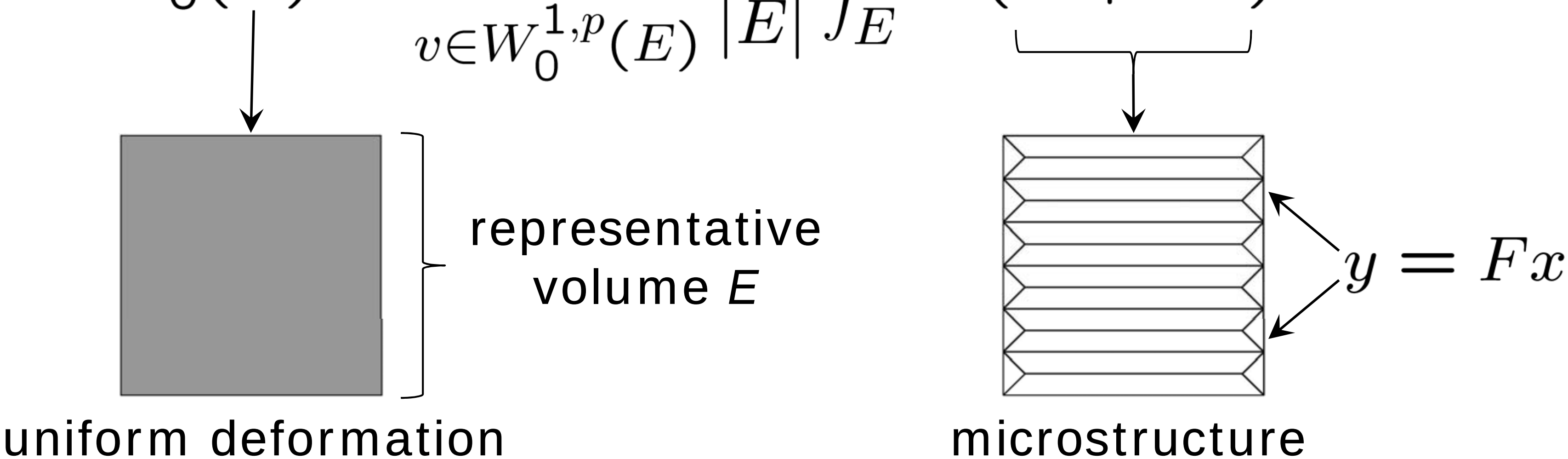


$$W_0(\xi) = \inf_{W_0^{1,p}(E)} \frac{1}{|E|}\int_E W\Big(\xi + Dv(x)\Big)\,dx$$

Separation of Scales - Relaxation

- Quasiconvex envelop:

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



- Microstructure construction, optimality (hard)
- List of problems whose relaxation is know explicitly is small but growing...

Relaxation as 'optimal' multiscale scheme

- The relaxed problem is well-posed, exhibits no microstructure, can be approximated by, e.g., finite elements
- The relaxed and unrelaxed problems deliver the same macroscopic response (e.g., force-displacement curve: *convergence*!)
- All microstructures are pre-accounted for by the relaxed problem (no physics lost)
- Microstructures can be reconstructed from the solution of the relaxed problem (no loss of information: *return* option!)
- Relaxation is an 'optimal' multiscale method!

Time-dependent microstructure

Copper single crystal
(Mughrabi, Phil. Mag. **23**, 869, 1971)

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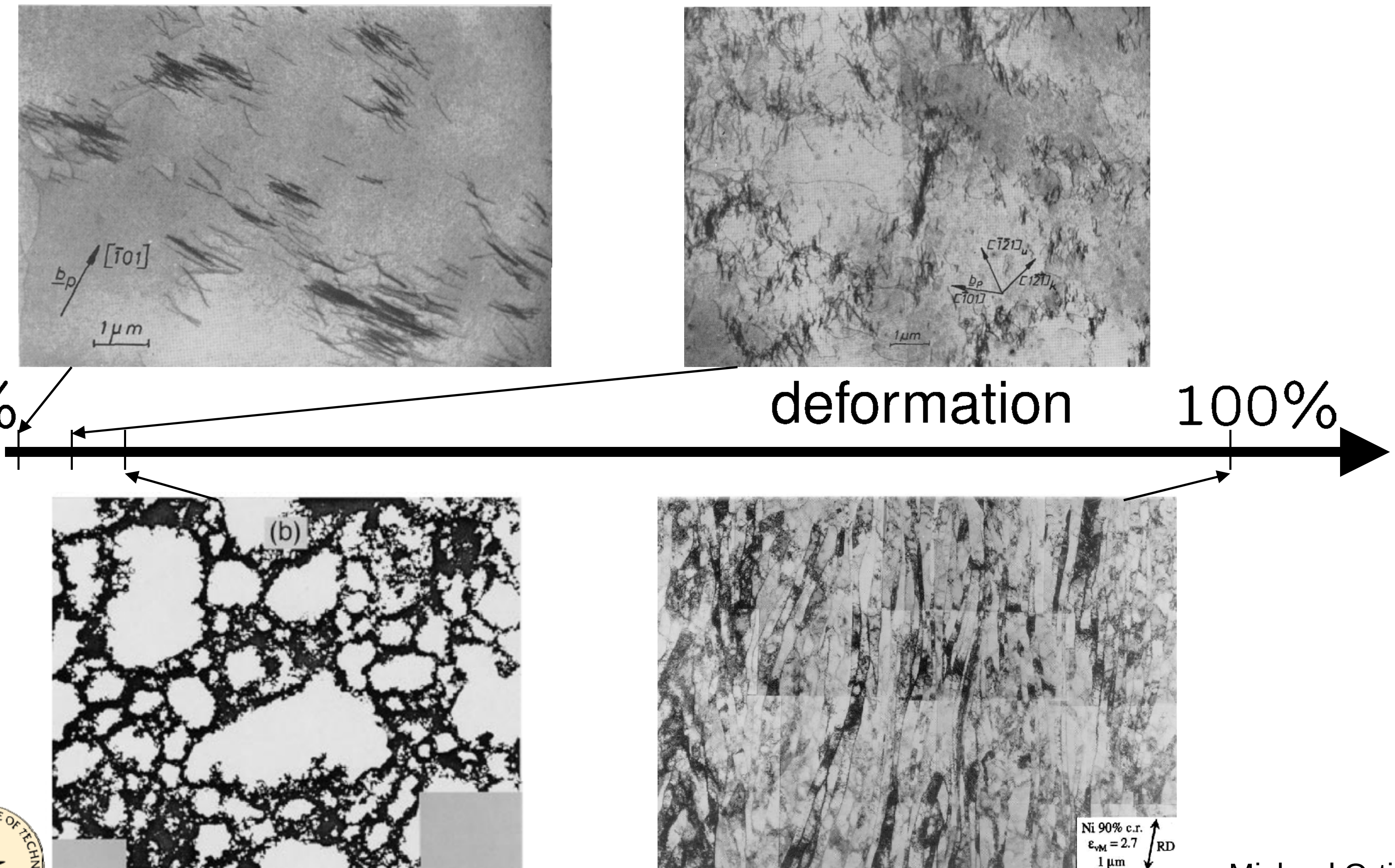

Copper single crystal
(Mughrabi, Phil. Mag. **23**, 869, 1971)

90% cold-rolled Ni (Hansen, Huang and Hughes, Mat. Sci. Engin. A **317**, 3, 2001)

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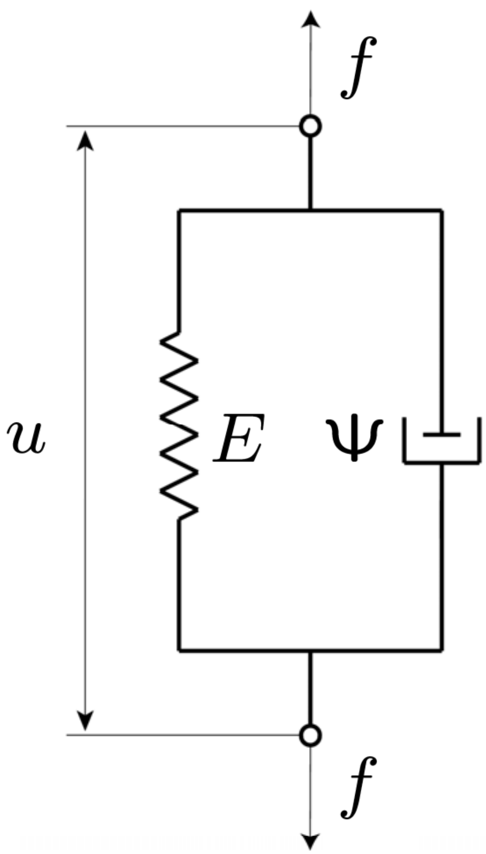
Time-dependent problems

- Time-dependent problems: $\partial\Psi(u,\dot{u}) + DE(t,u) = 0$



- Energy-dissipation functional: $F_\epsilon(u) = \int_0^T \mathrm{e}^{-t/\epsilon}[\frac{1}{\epsilon}E(t,u) + \Psi(u,\dot{u})]\,dt \to \inf!$
- Rate-independence + monotonic loading:

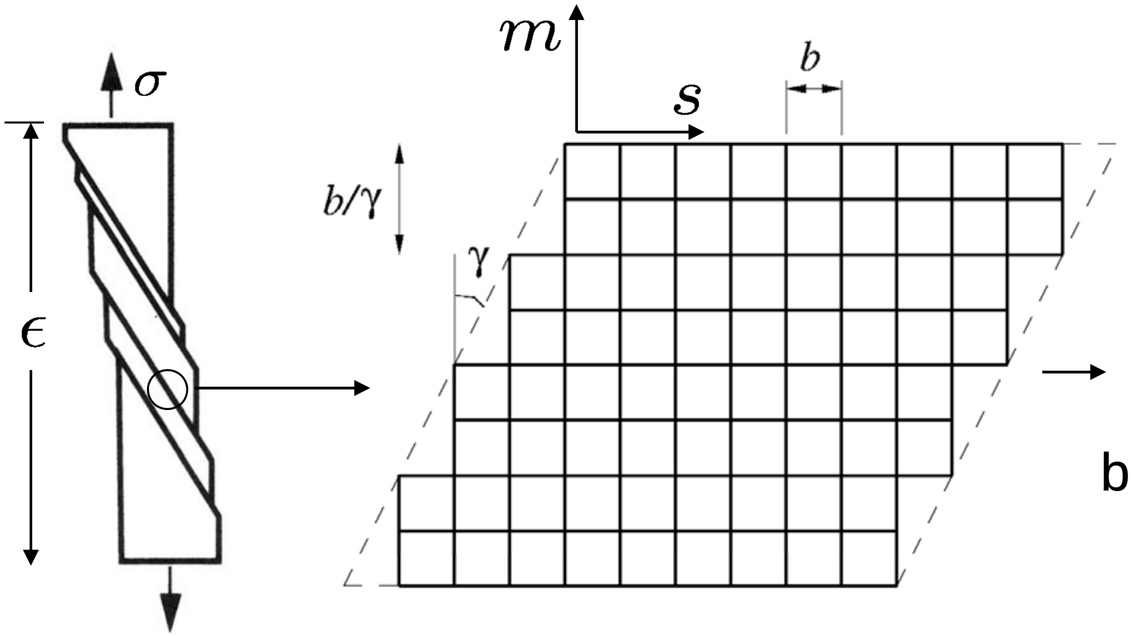
$$\Psi(u(t),\dot{u}(t)) = \frac{d}{dt}P(u(t))$$

- Deformation theory: $F_\epsilon(u) = \int_0^T \mathrm{e}^{-t/\epsilon}[E(t,u) + P(u)]\,\frac{dt}{\epsilon} \to \inf!$

$$u(t) \in \operatorname{argmin}\Big(E(t,\cdot) + P(\cdot)\Big)$$

Mielke, A. & MO, *ESAIM:COCV,* 2008

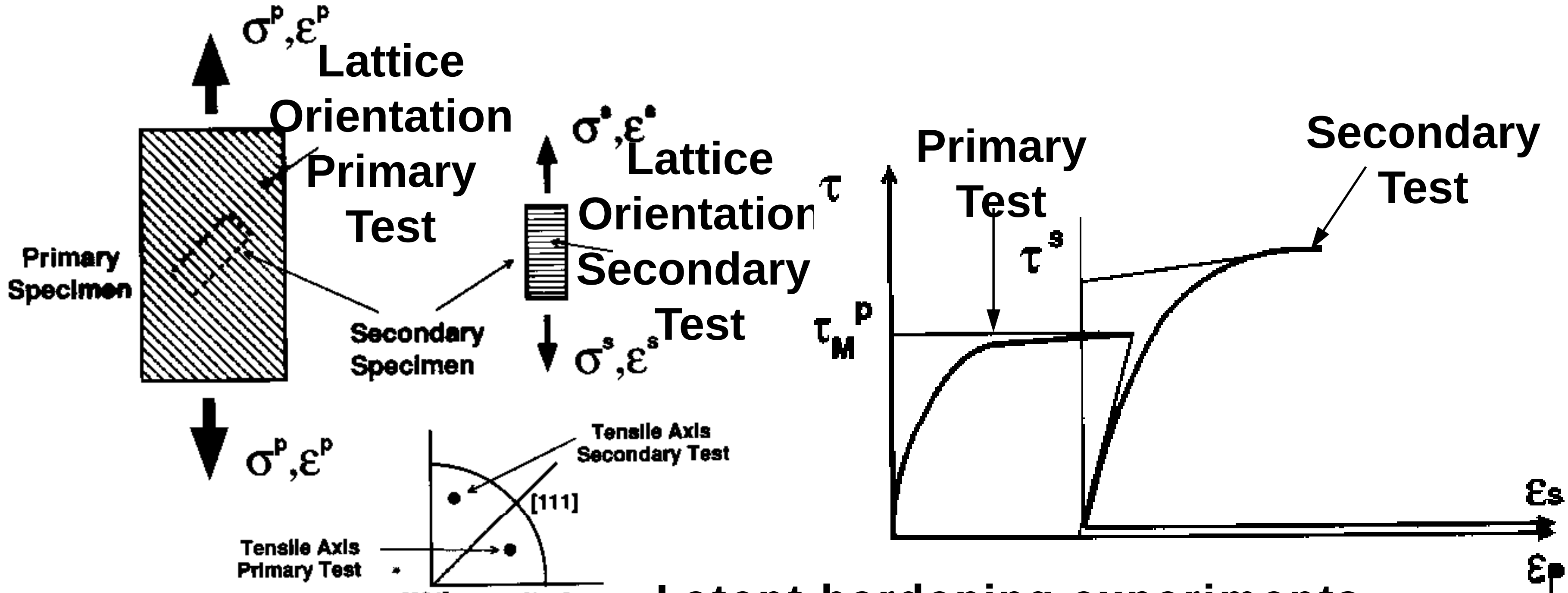
Application to crystal plasticity



Irreversible accommodation of shear deformation by crystallographic slip

- Elastic energy: $E(u, \gamma) = \int_\Omega W^e(\nabla u - \sum \gamma s \otimes m)\, dx$
- Plastic work: $P(\gamma) = \int_\Omega W^p(\gamma)\, dx \longleftarrow$ non-convex!
- Monotonicity: $\gamma(t_2) > \gamma(t_1)$, if $t_2 > t_1$

Strong latent hardening



Latent hardening experiments

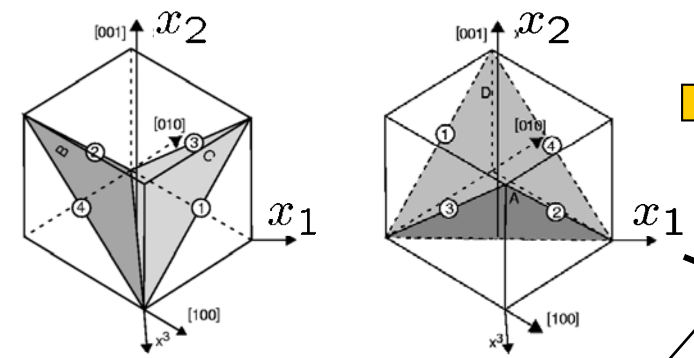
UF Kocks, *Acta Metallurgica*, **8** (1960) 345

UF Kocks, *Trans. Metall. Soc. AIME*, **230** (1964) 1160

- Strong latent hardening: Crystals much 'prefer' to activate a single slip system at each material point, though the active system may vary from point to point

Non-convexity - Strong latent hardening

- Linear hardening: $W^p = \tau_0 \sum_\alpha \gamma^\alpha + \sum_\alpha \sum_\beta h_{\alpha\beta} \gamma^\alpha \gamma^\beta$
- Example: FCC crystal deforming on $(1\bar{1}0)$-plane

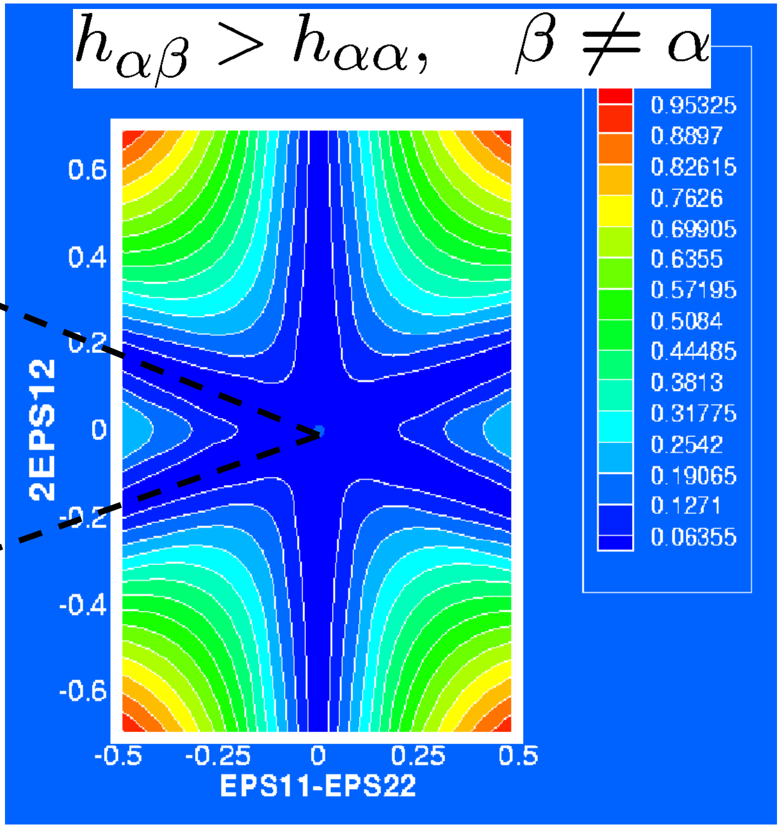


$$\beta^p \in \gamma s \otimes m + so(3)$$

(Single slip)

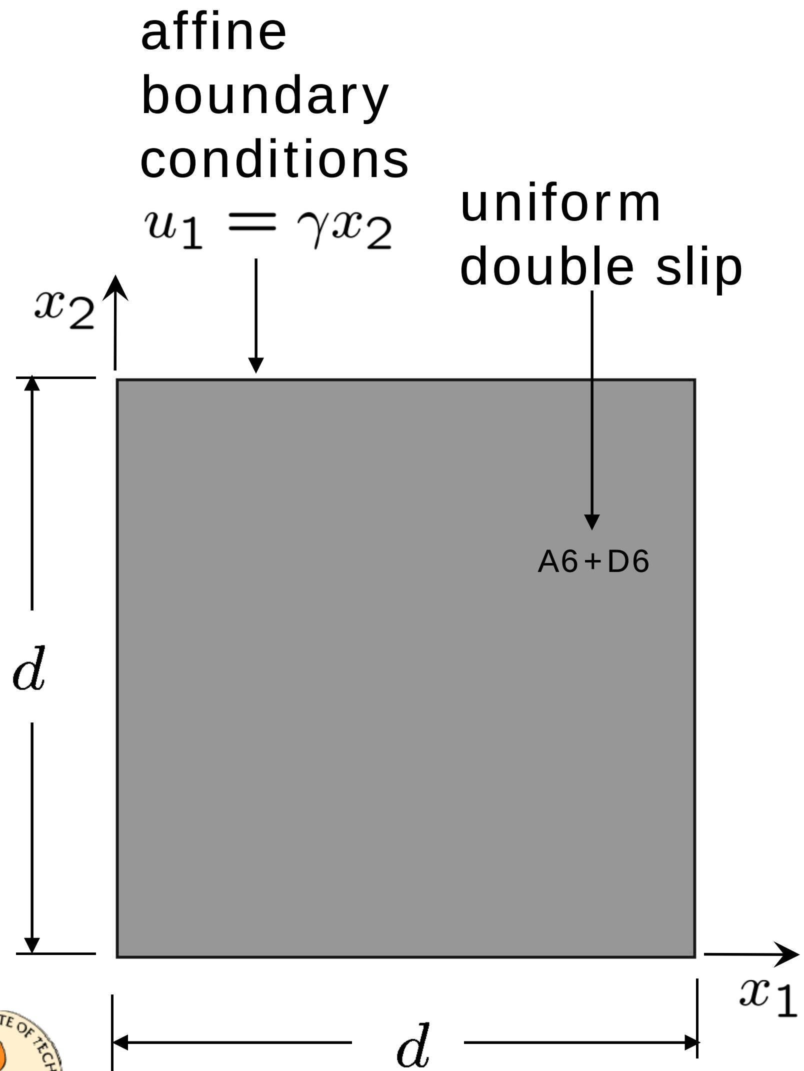
- $W(\nabla u)$ non-convex!

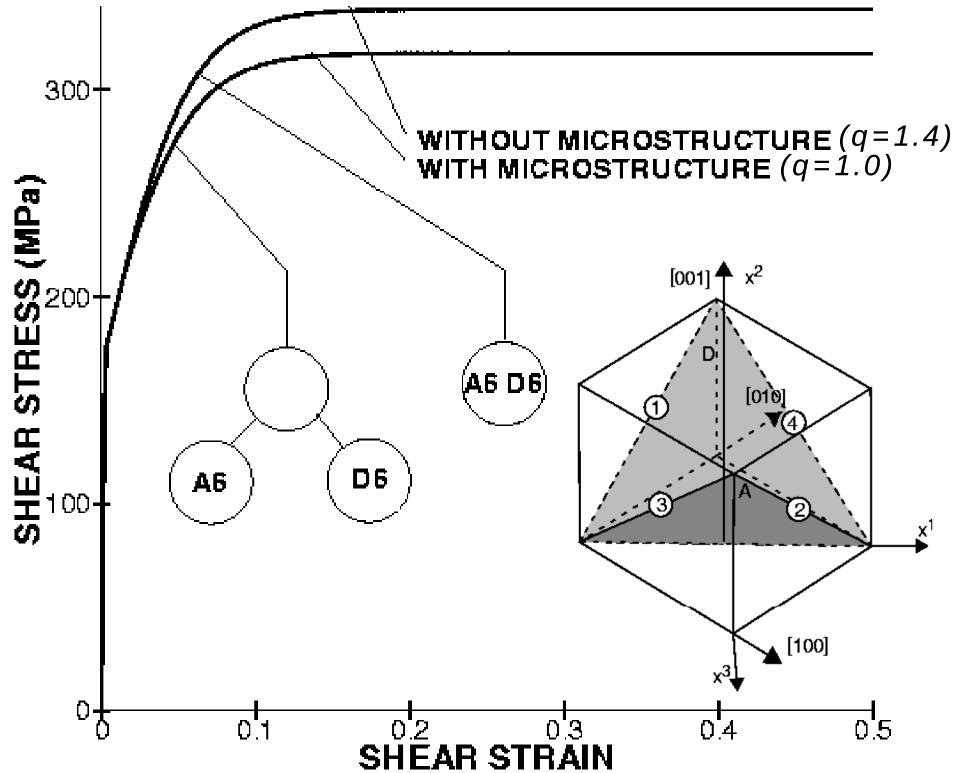
(Ortiz and Repetto, *JMPS*, **47**(2) 1999, p. 397)



$W(\nabla u)$

Strong latent hardening & microstructure

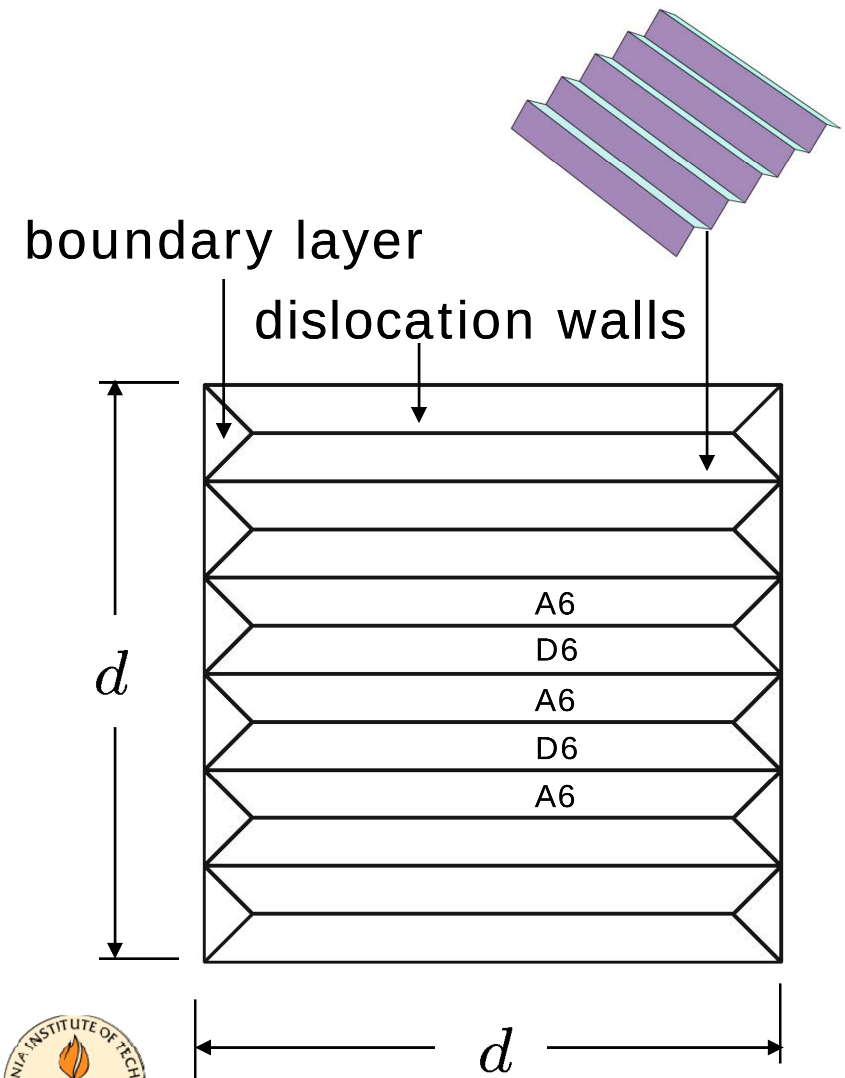


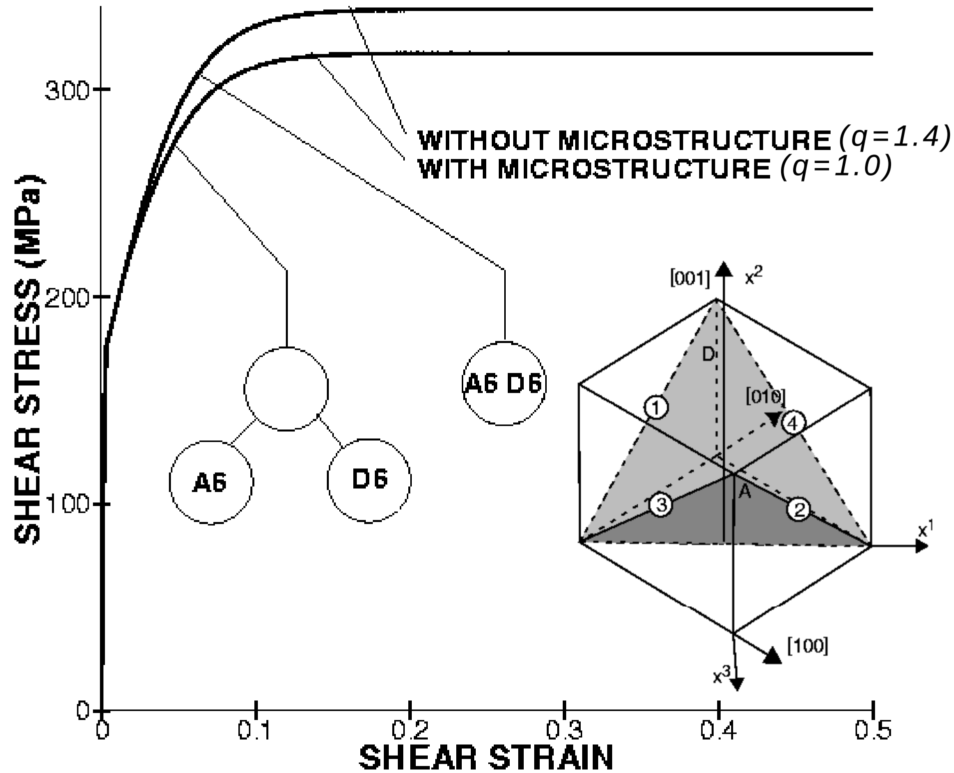


FCC crystal deformed in simple shear on (001) plane in [110] direction

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

Strong latent hardening & microstructure





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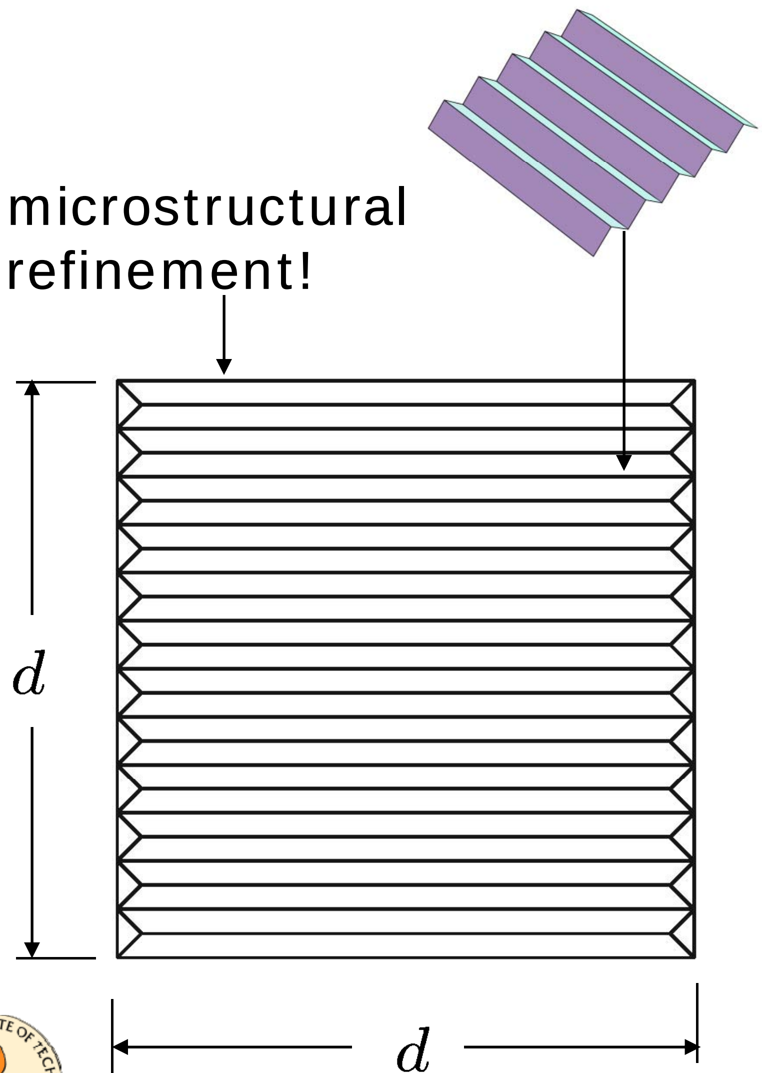

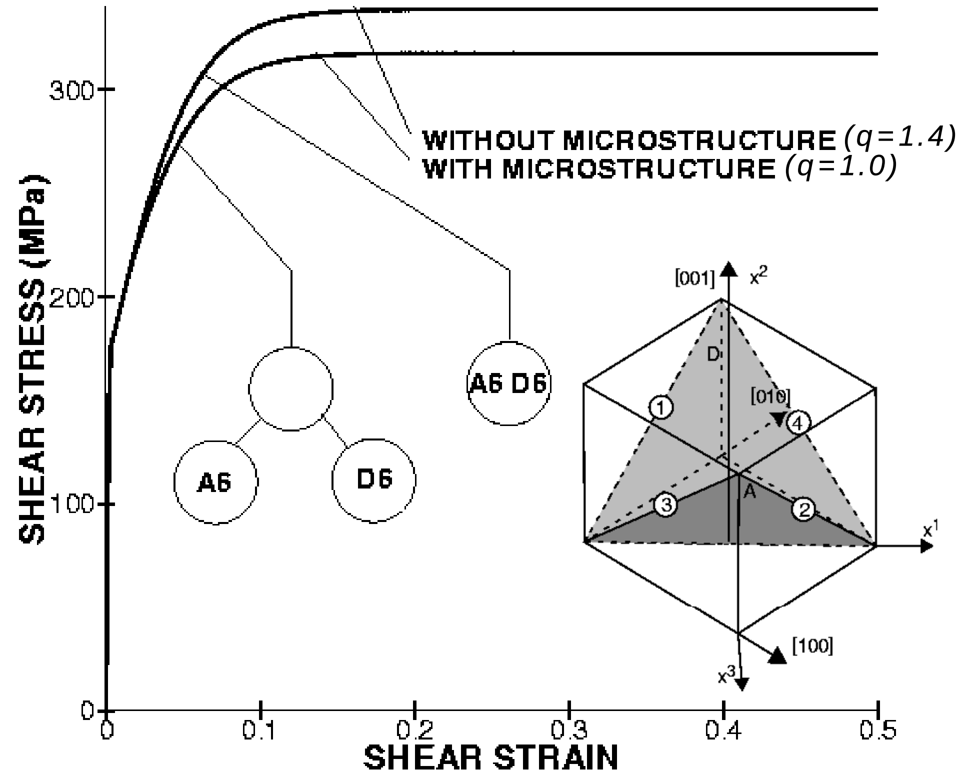

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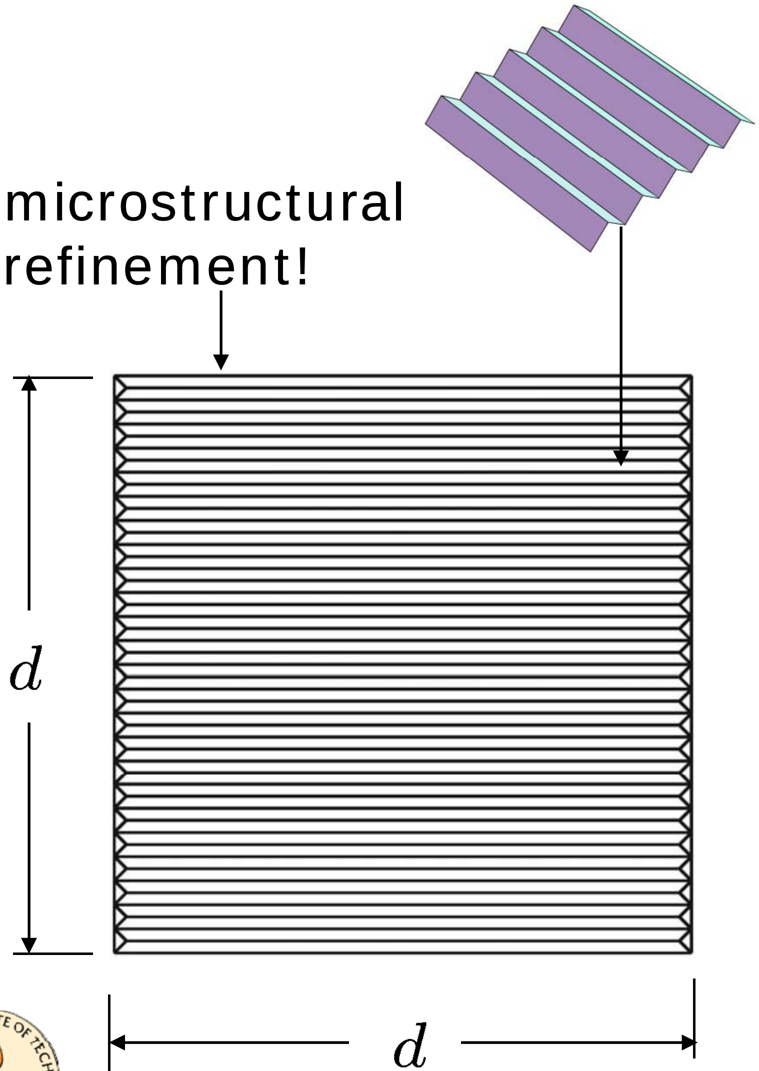

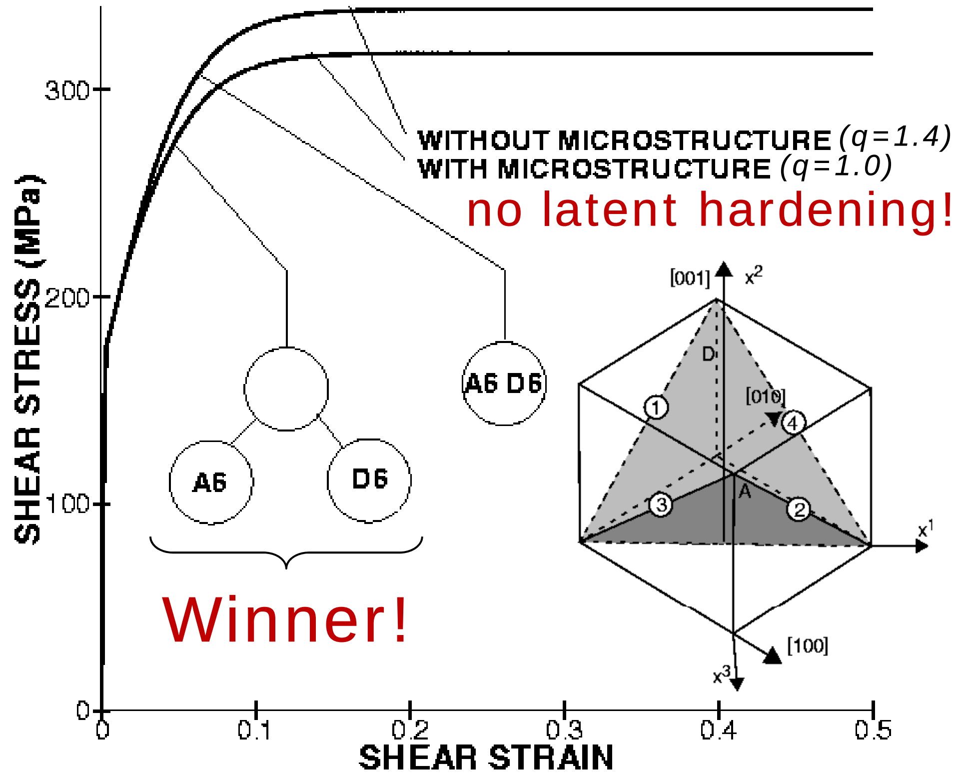

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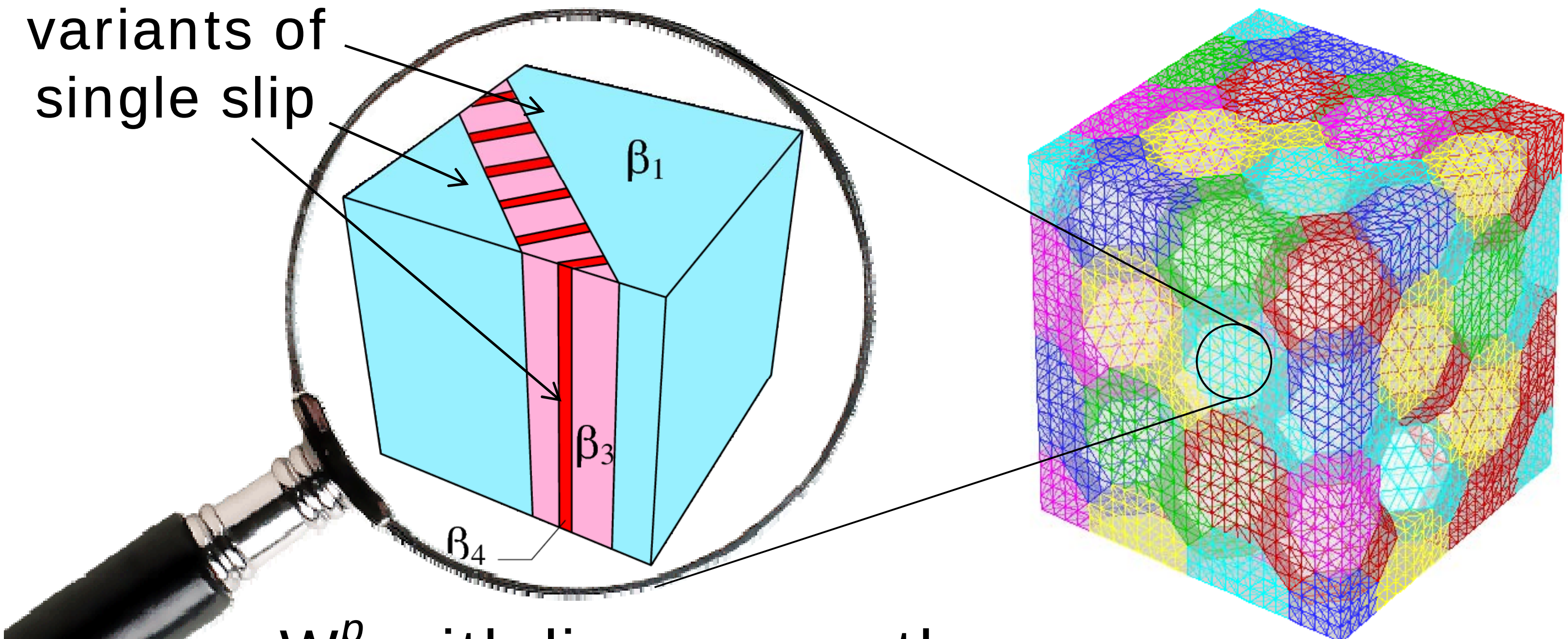
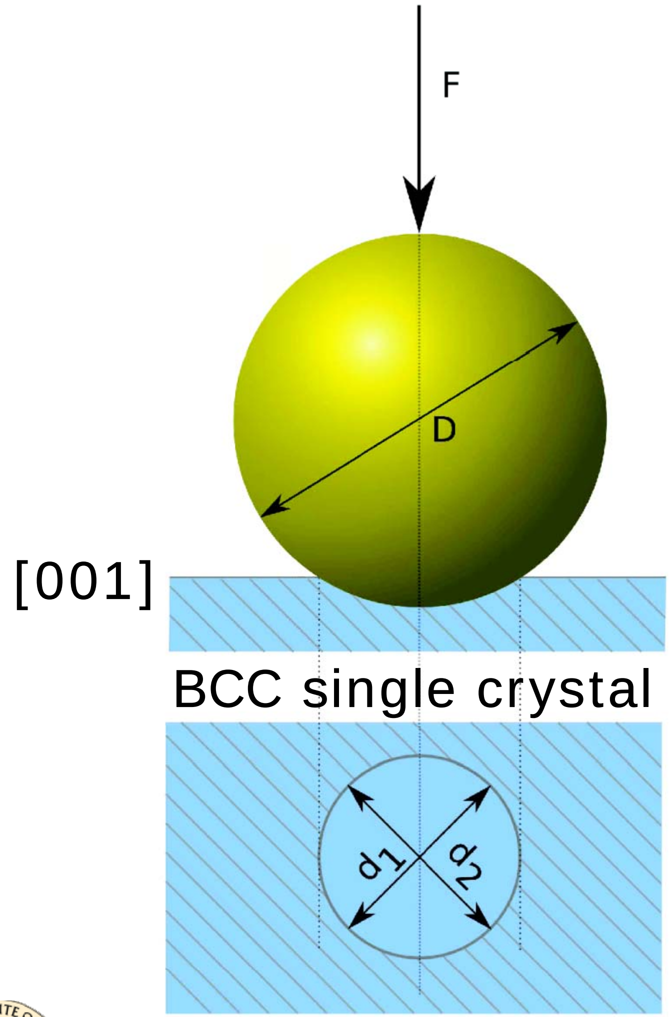
Crystal plasticity – Relaxation

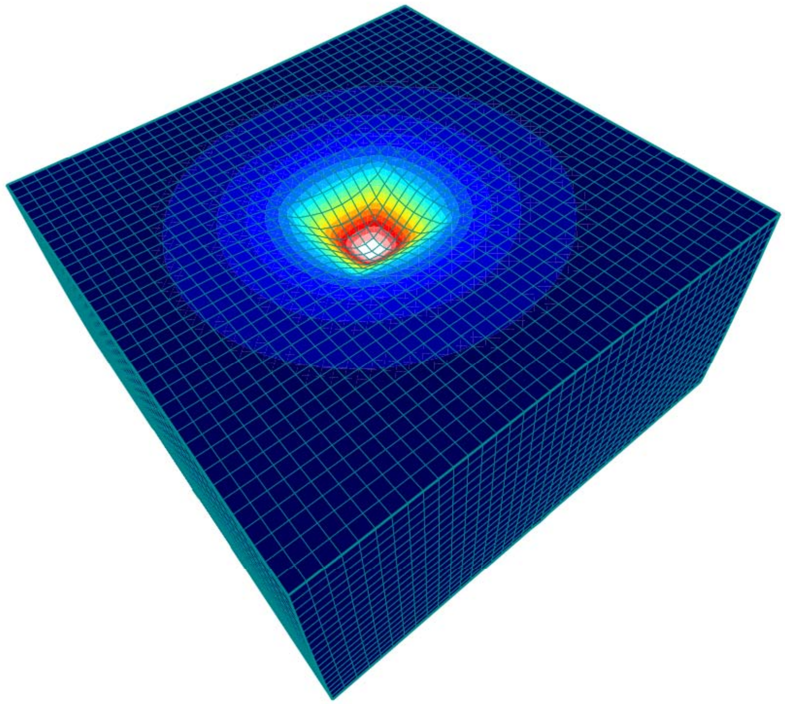


- W^p with linear growth
- Explicit lamination-type construction delivers:
  - *Quasi-convex envelop W_0 in close form: ideal plasticity + no latent hardening*
  - *Optimal microstructures as post-processing step*
- Some variants take the form of slip lines...

Conti, S. & MO, *ARMA,* 2005

Example – Single-crystal indentation



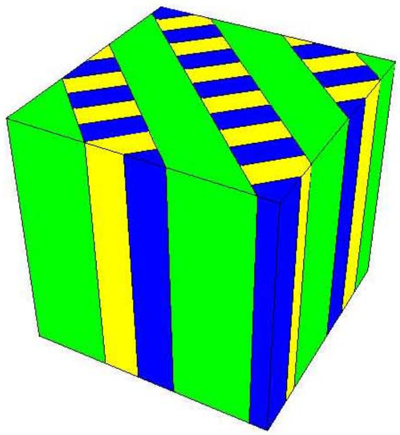


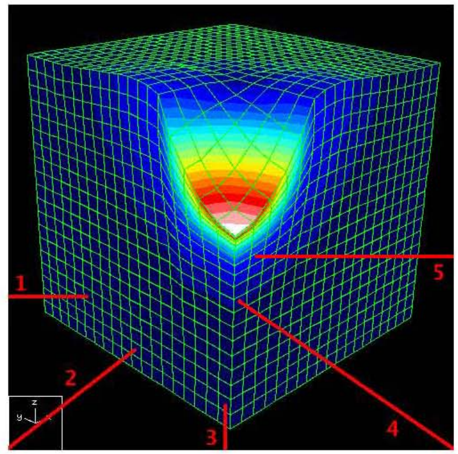
Indentation of [001] surface
of BCC single crystal
32,000 nodes
27,436 hexahedral elements

Conti, S., Hauret, P. and MO,
SIAM Multiscale Model. Simul., 2005

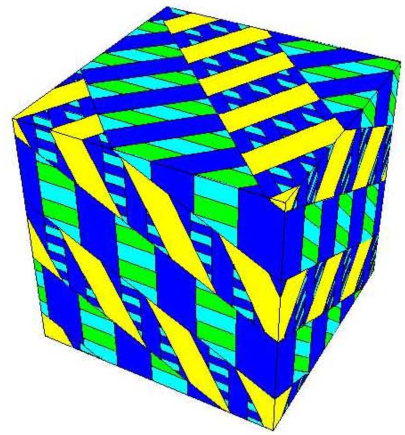
Example – Single-crystal indentation

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

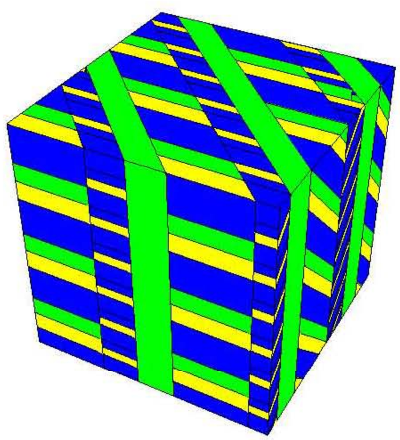




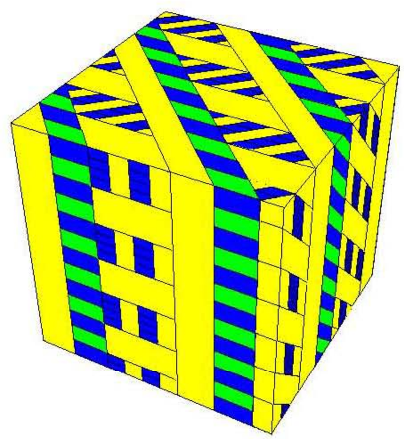
rank 4/14, $|\gamma|_\infty = 0.43$



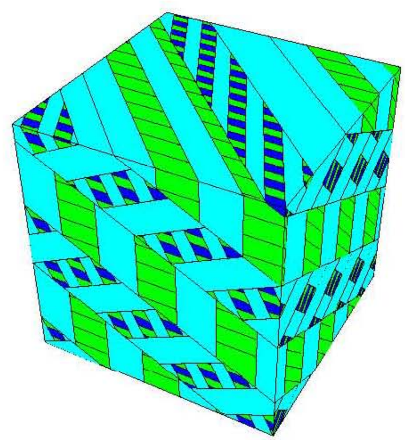
rank 4/12, $|\gamma|_\infty = 0.02$



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



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



Conti, S., Hauret, P. and MO,
SIAM Multiscale Model. Simul., 2005

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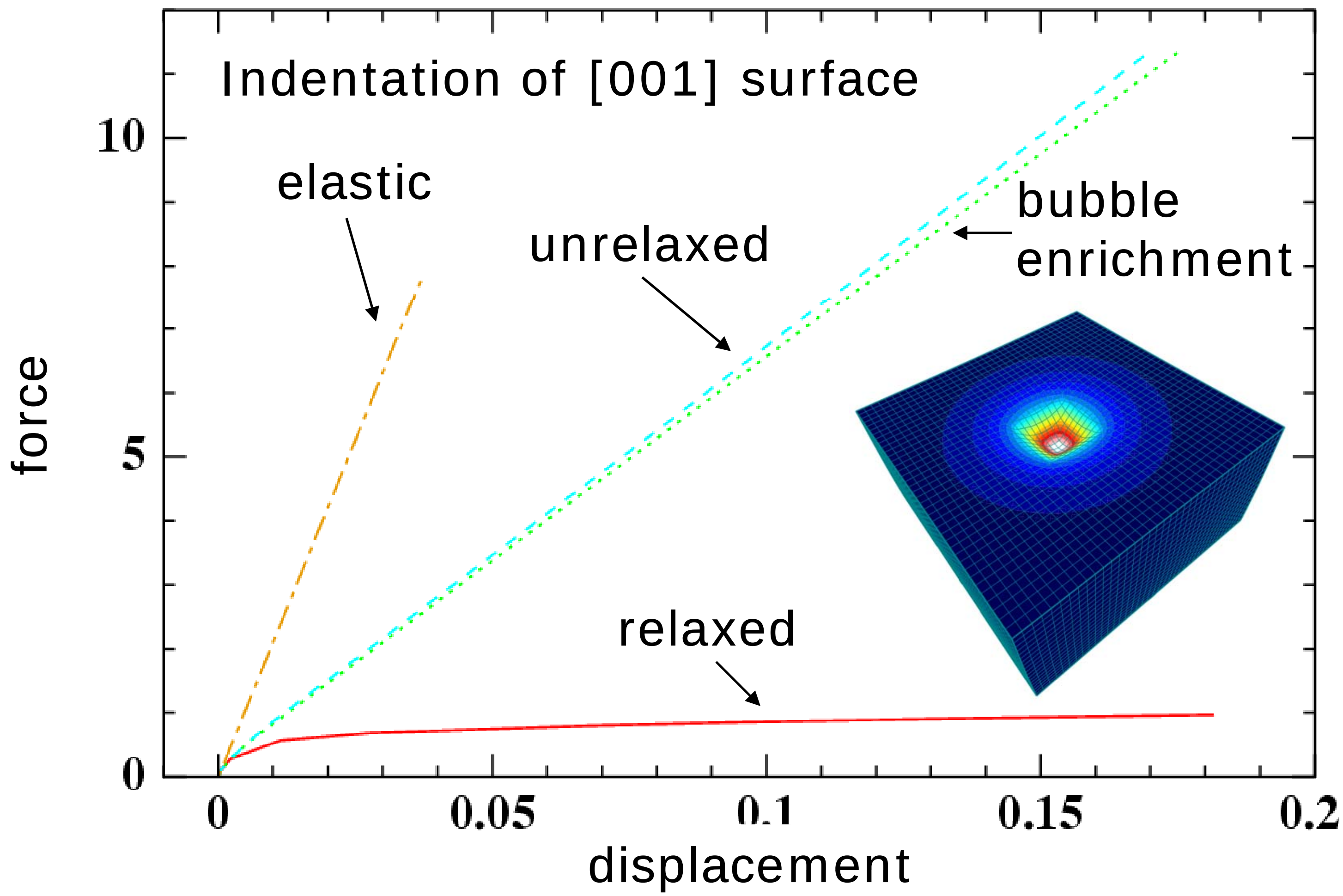


Conti, S., Hauret, P. and MO,
SIAM Multiscale Model. Simul., 2005

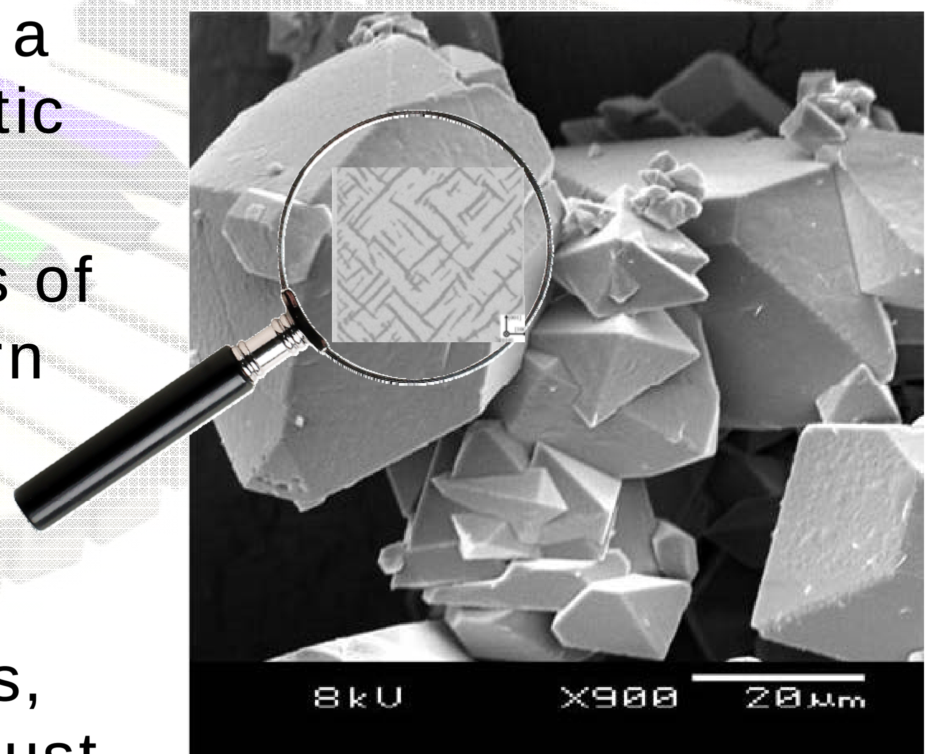
Application to High Explosives (HE)

- Detonation sensitivity: Ease with which an explosive can be detonated
- What factors determine detonation sensitivity?
- In high explosives localized ***hot spots*** cause detonation initiation

Detonation of high-explosive (RDX, PETN, HMX)

High-Explosives - Initiation

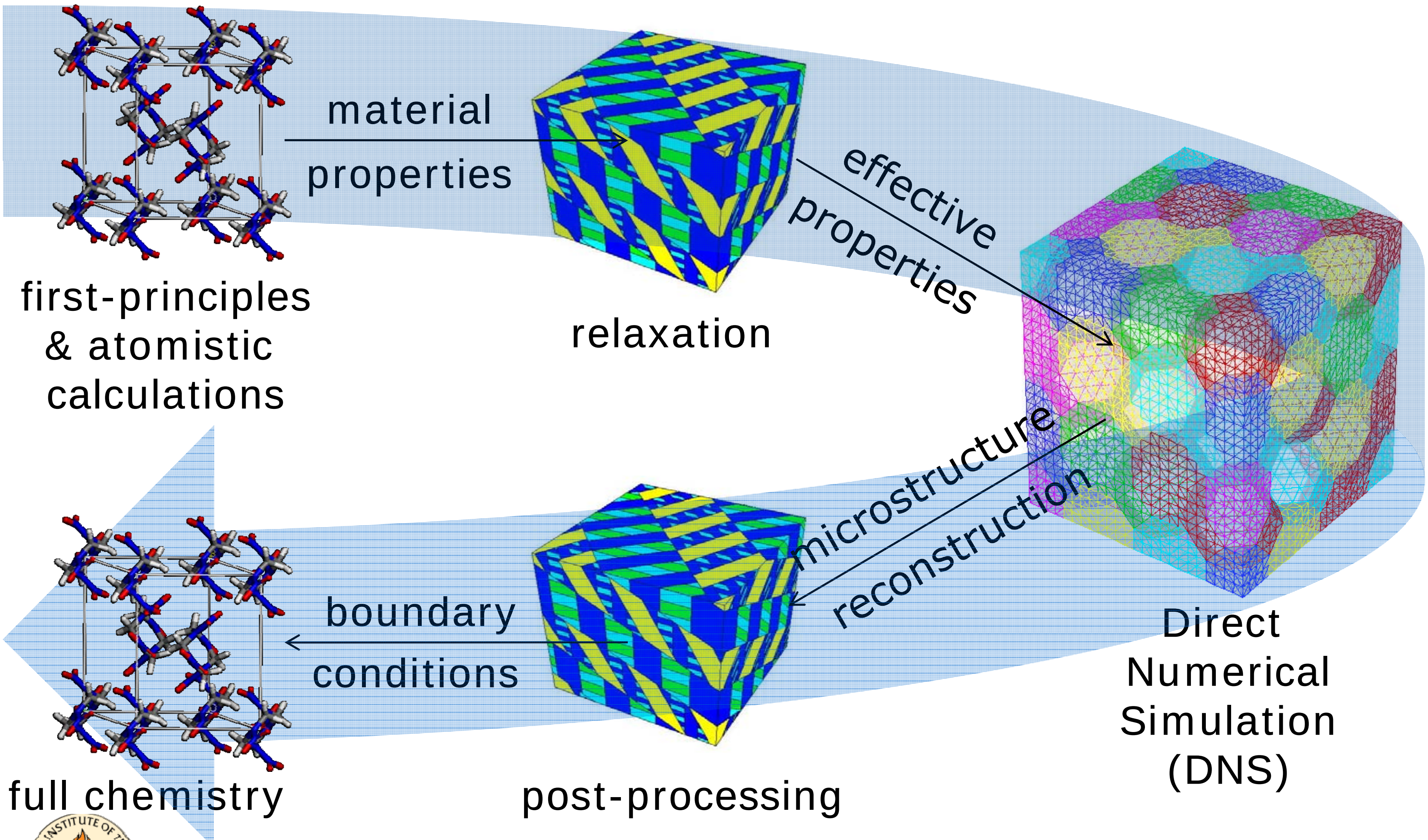
- Can hot spots arise as a result of localized plastic deformation?
- Can small-scale details of the deformation pattern (partially) explain detonation sensitivity?
- Need to predict deformation microstructures, extreme events! (not just average behavior)



SEM image of RDX (Kline *et al*., 2003)

M. J. Cawkwell, T. D. Sewell, L. Zheng, and D. L. Thompson, Phys. Rev. B **78, 8**014107 2008

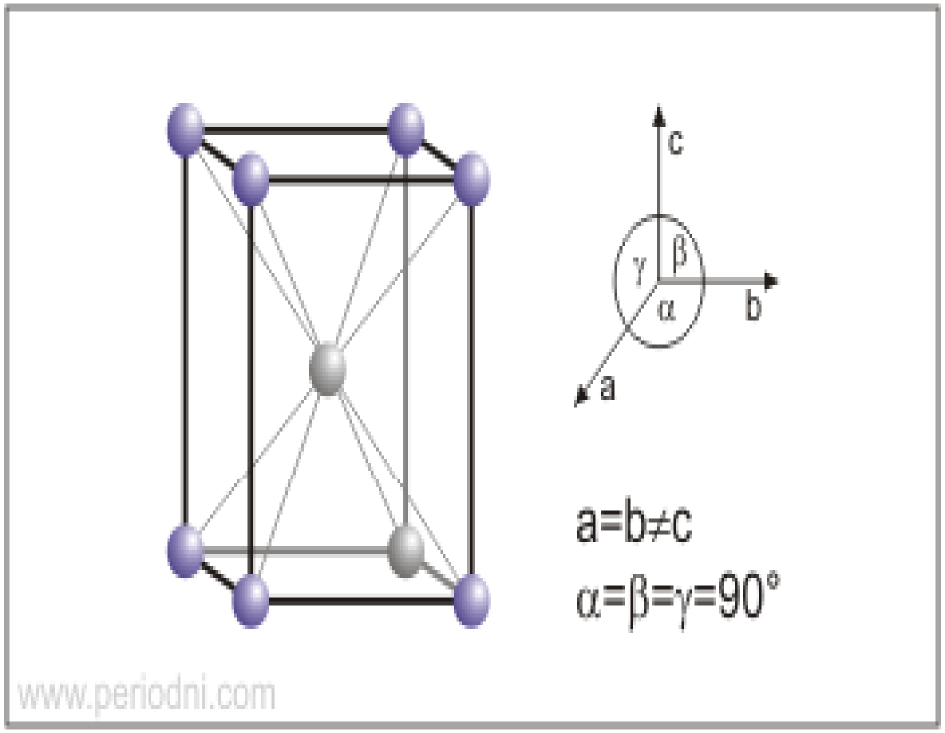
HE initiation – Multiscale modeling



Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

PETN – Elastic constants

Body Centered Tetragonal Lattice



a=b=9.380A and c=6.710A

- Elastic Constants(GPA): (Winey and Gupta, 2001)

  C_{11}=17.22 C_{33}=12.17
  C_{44}=5.04 C_{66}=3.95
  C_{12}=5.44 C_{13}=7.99

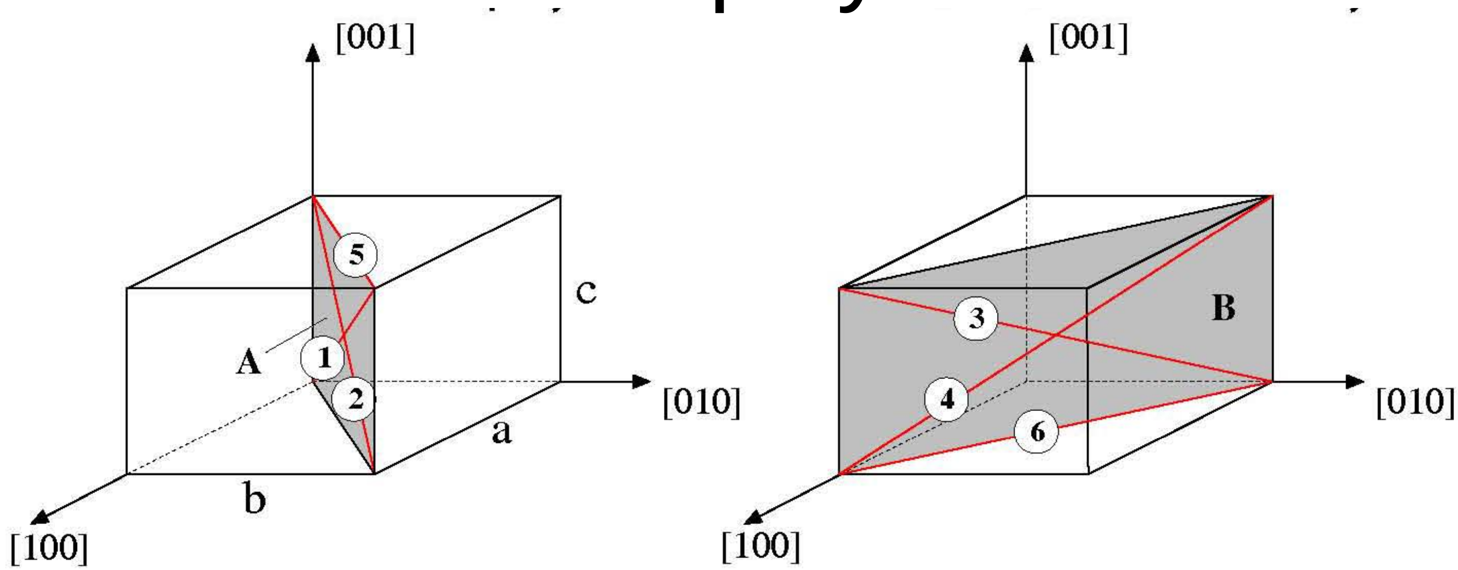
- Elastic constants assumed to decrease linearly with temperature, vanish at melting:

$$C_{ij}(\theta, p) = \frac{\theta - \theta_{\text{melt}}(p)}{\theta_0 - \theta_{\text{melt}}(p)}$$

- Menikoff and Sewell (2002): $\theta_{\text{melt}}(p) = \theta_{\text{melt}}(p_0)\left(1 + a\frac{\Delta V}{V_0}\right)$

  where a = 2(Γ-1/3), Γ ~ 1.2 = Grüneisen constant

PETN – Slip systems



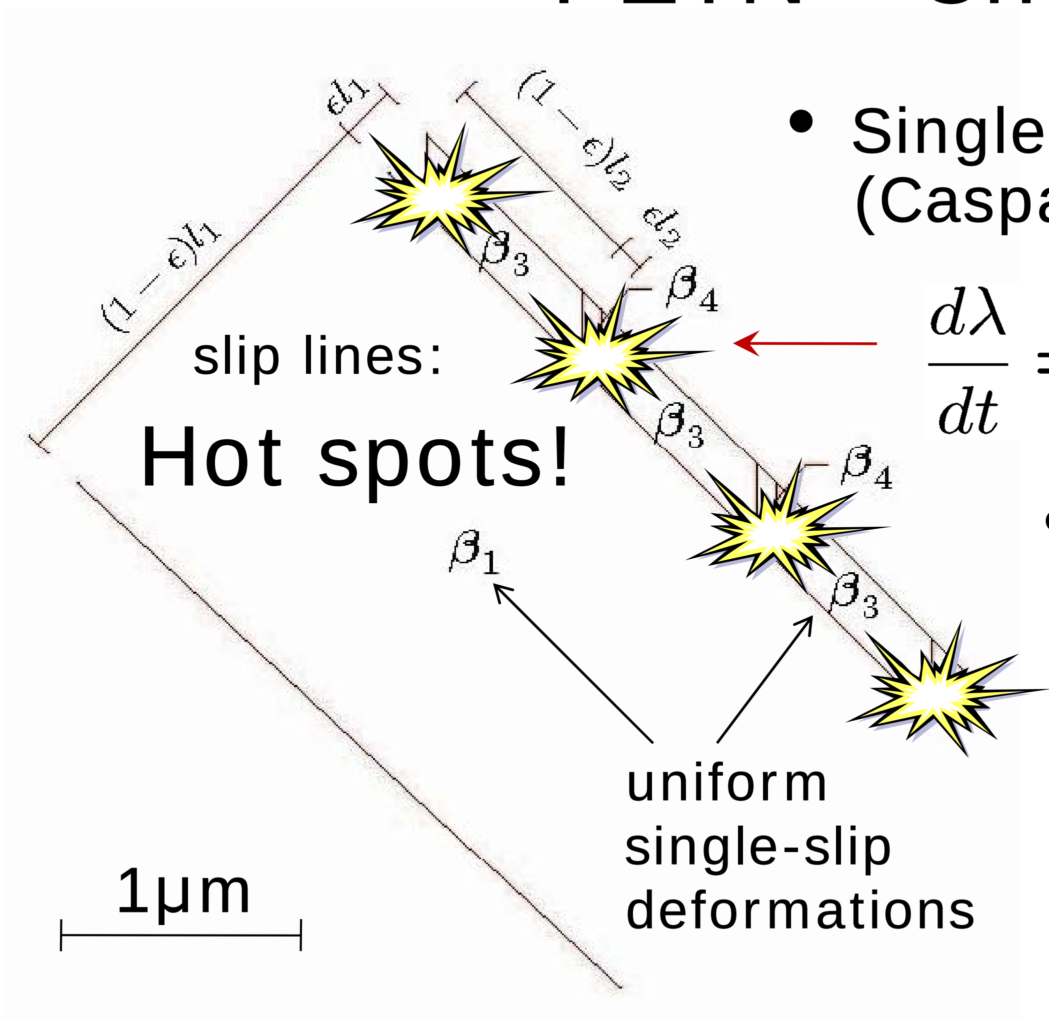
a = b = 9.380Å c = 6.710Å

- $\tau_c\,(\theta)$ fitted to data of Amuzu *et al*. (1976) and:

Slip System	B3	B4	A1	A2	B6	A5
s^α	$\pm[1\bar{1}1]$	$\pm[1\bar{1}\bar{1}]$	$\pm[111]$	$\pm[11\bar{1}]$	$\pm[1\bar{1}0]$	$\pm[\bar{1}\bar{1}0]$
m^α	(110)	(110)	$(1\bar{1}0)$	$(1\bar{1}0)$	(110)	$(1\bar{1}0)$
τ_c [GPa]	1.0	1.0	1.0	1.0	2.0	2.0

P. Xu, S. Zybin, S. Dasgupta, and W. A. Goddard III, private communication

PETN – Chemistry



- Single-step reaction kinetics (Caspar *et al*., 1998):

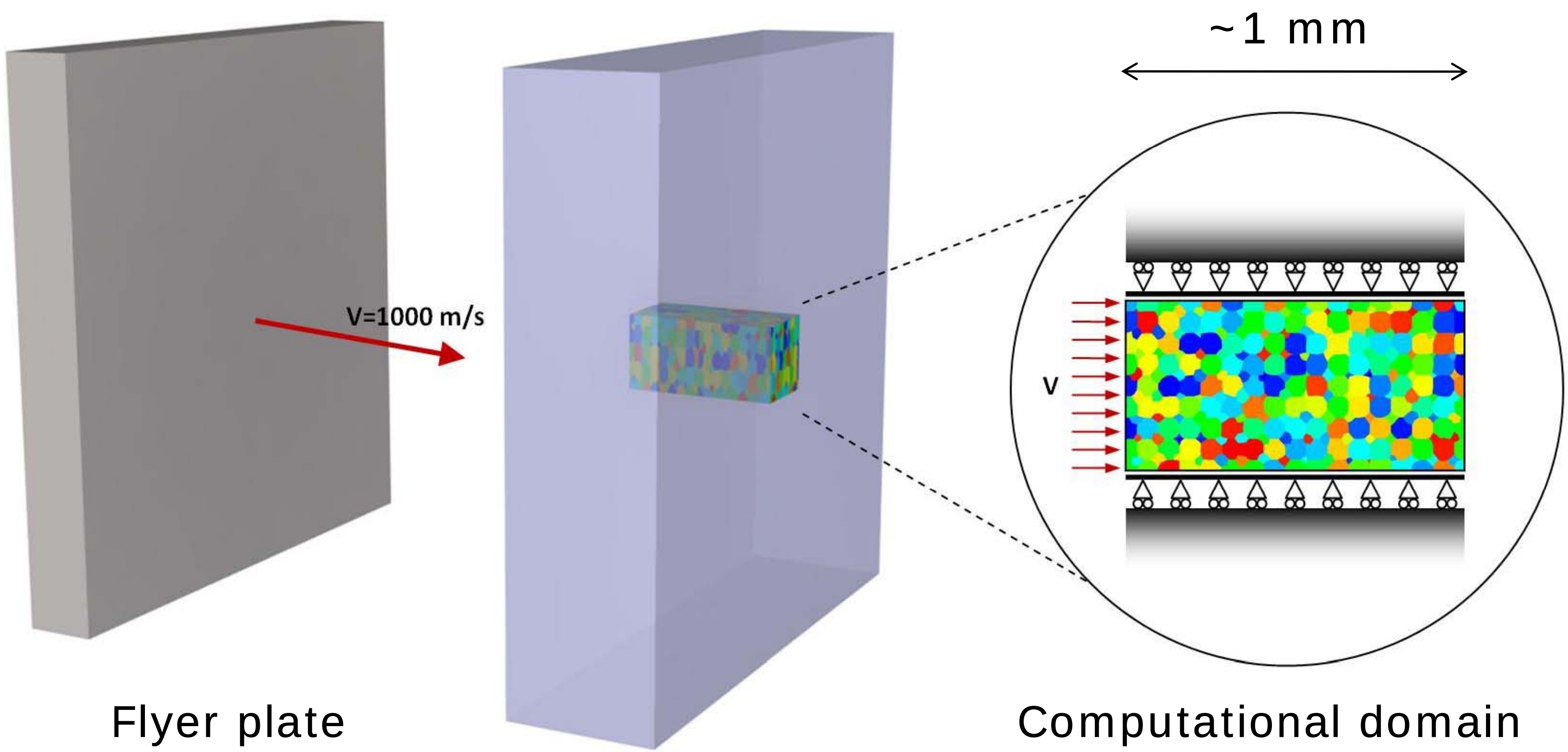
$$\frac{d\lambda}{dt} = Z(1-\lambda)\exp\left(-\frac{ER}{\theta}\right)$$

- Activation energy E and rate constant Z from Rogers (1975):

R	8.314 J/mol/K
E	$196.742\text{x}10^3$ J/mol
Z	6.3 $\text{x}10^{19}$ s^{-1}

- Temperature computed assuming adiabatic heating, full conversion of plastic work to heat, heat capacity

PETN – Plate impact test



Flyer plate

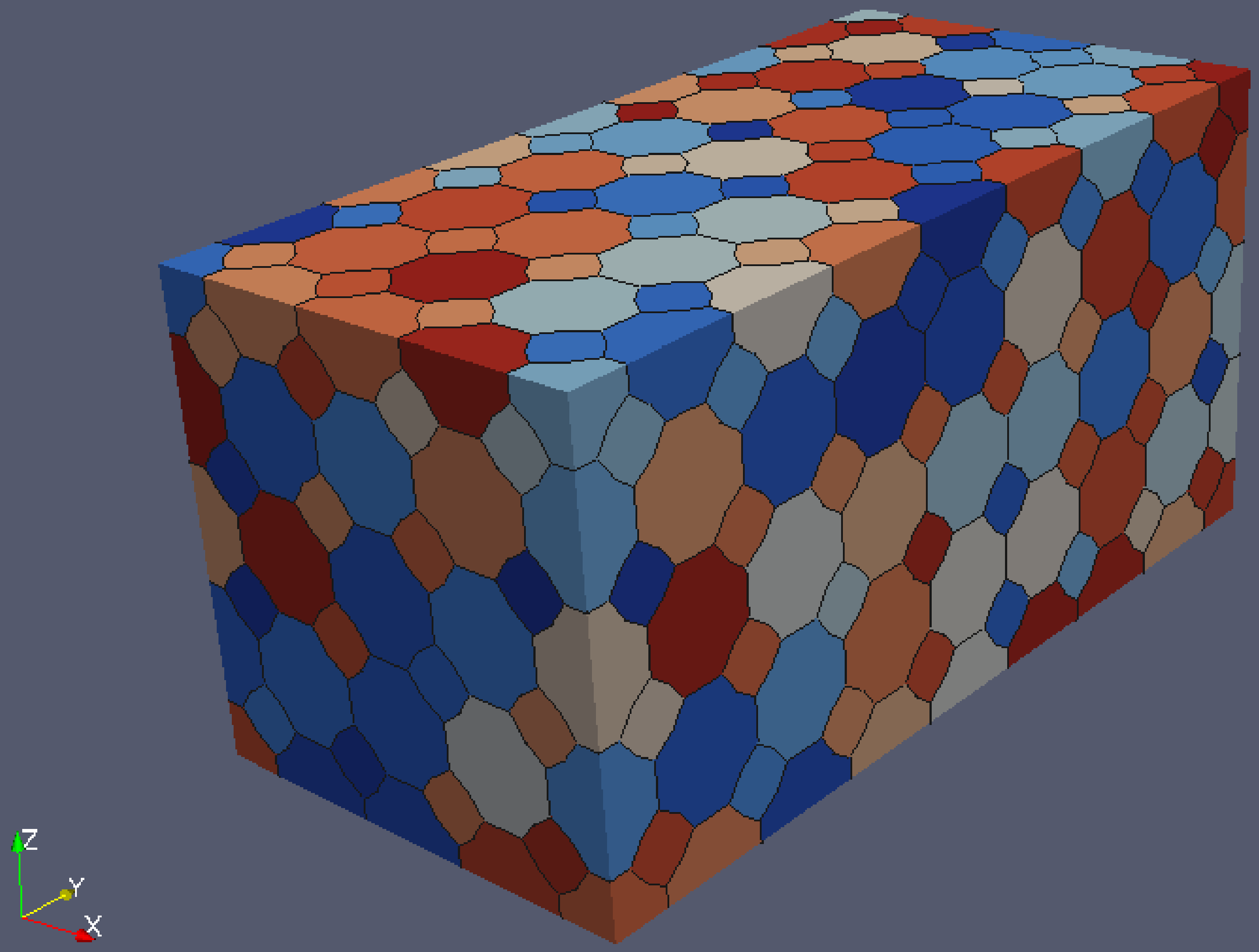
Computational domain

PETN target plate

Plate-impact configuration

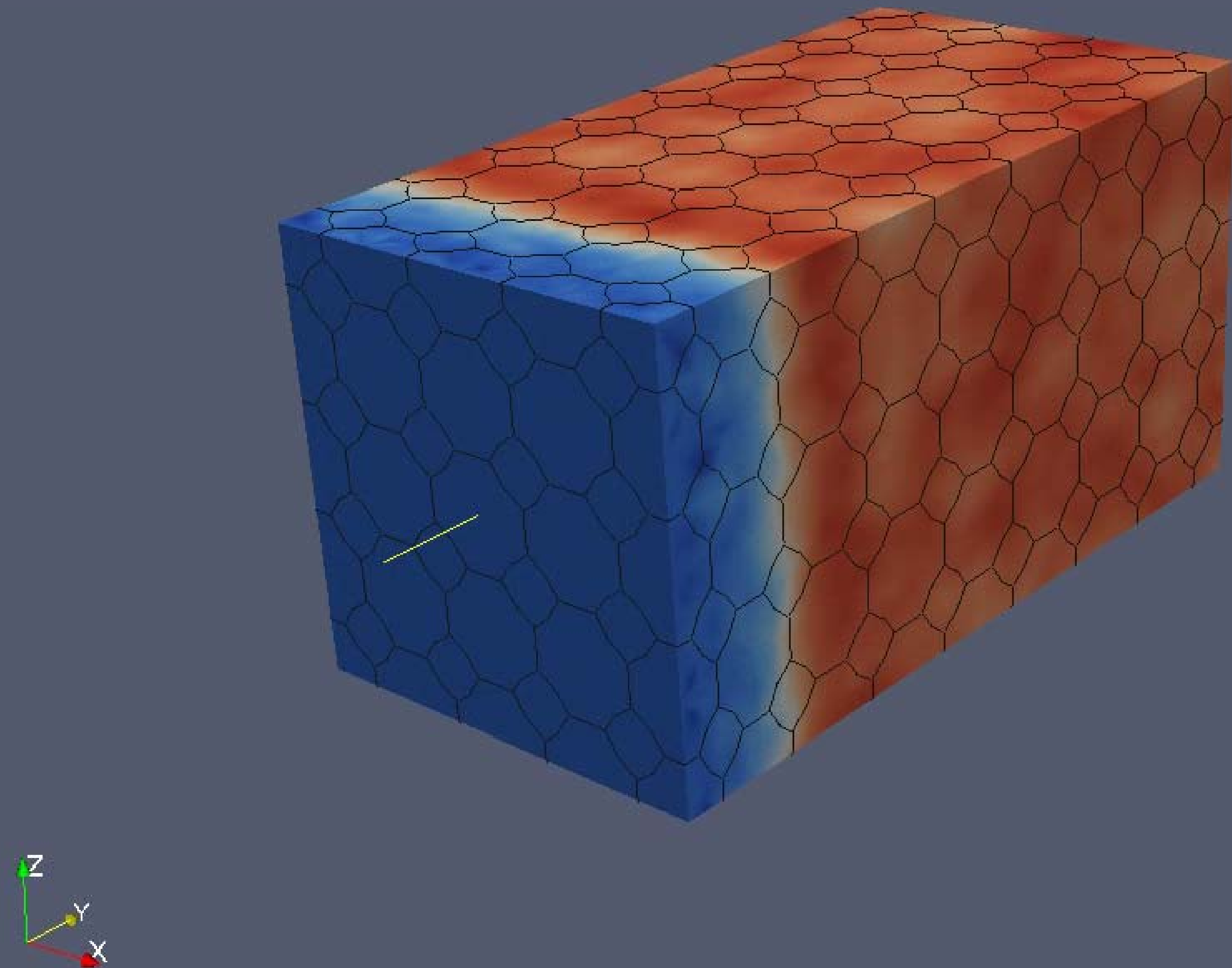
Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

High-Explosives Detonation Initiation

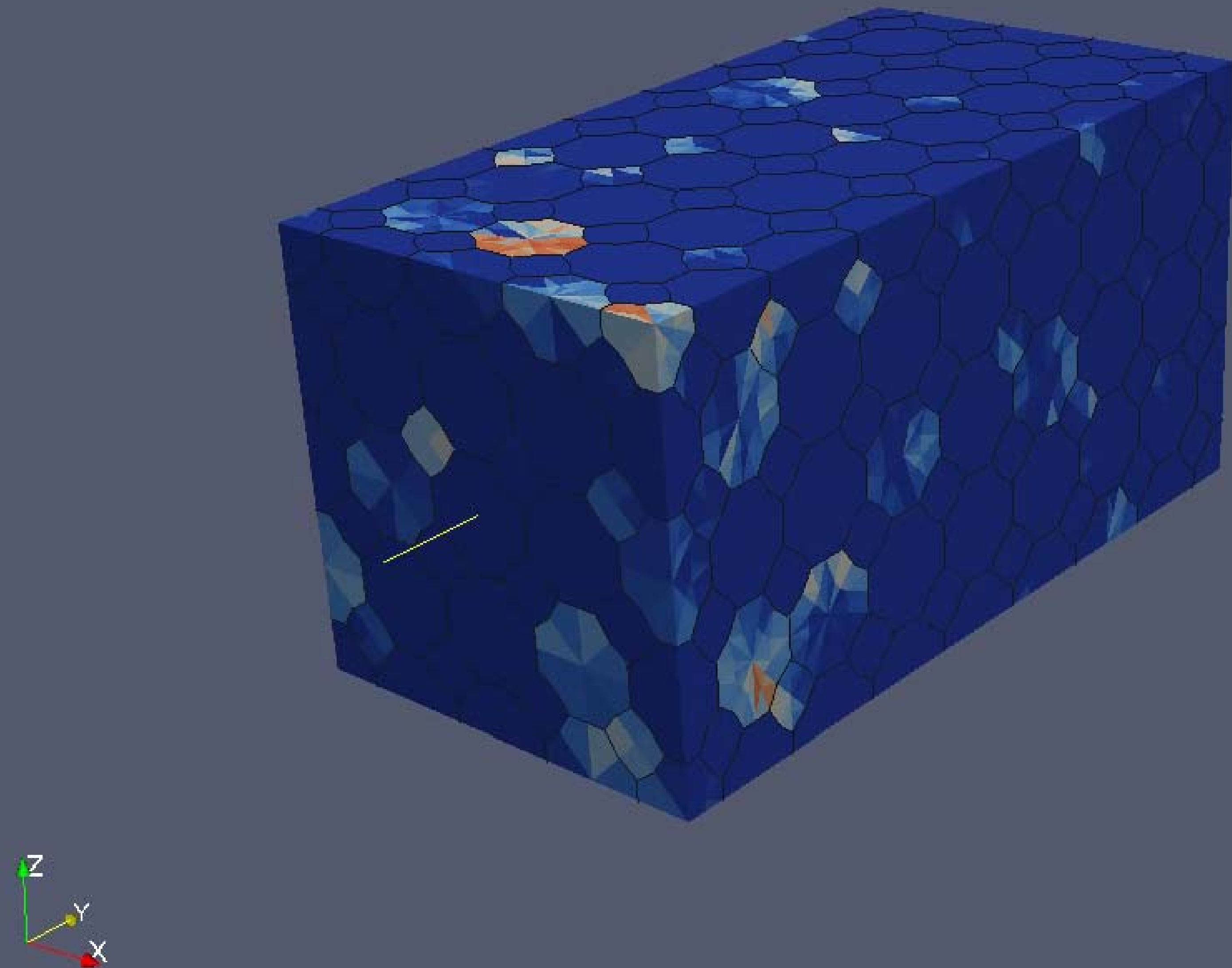


Polycrystal model and grain boundaries

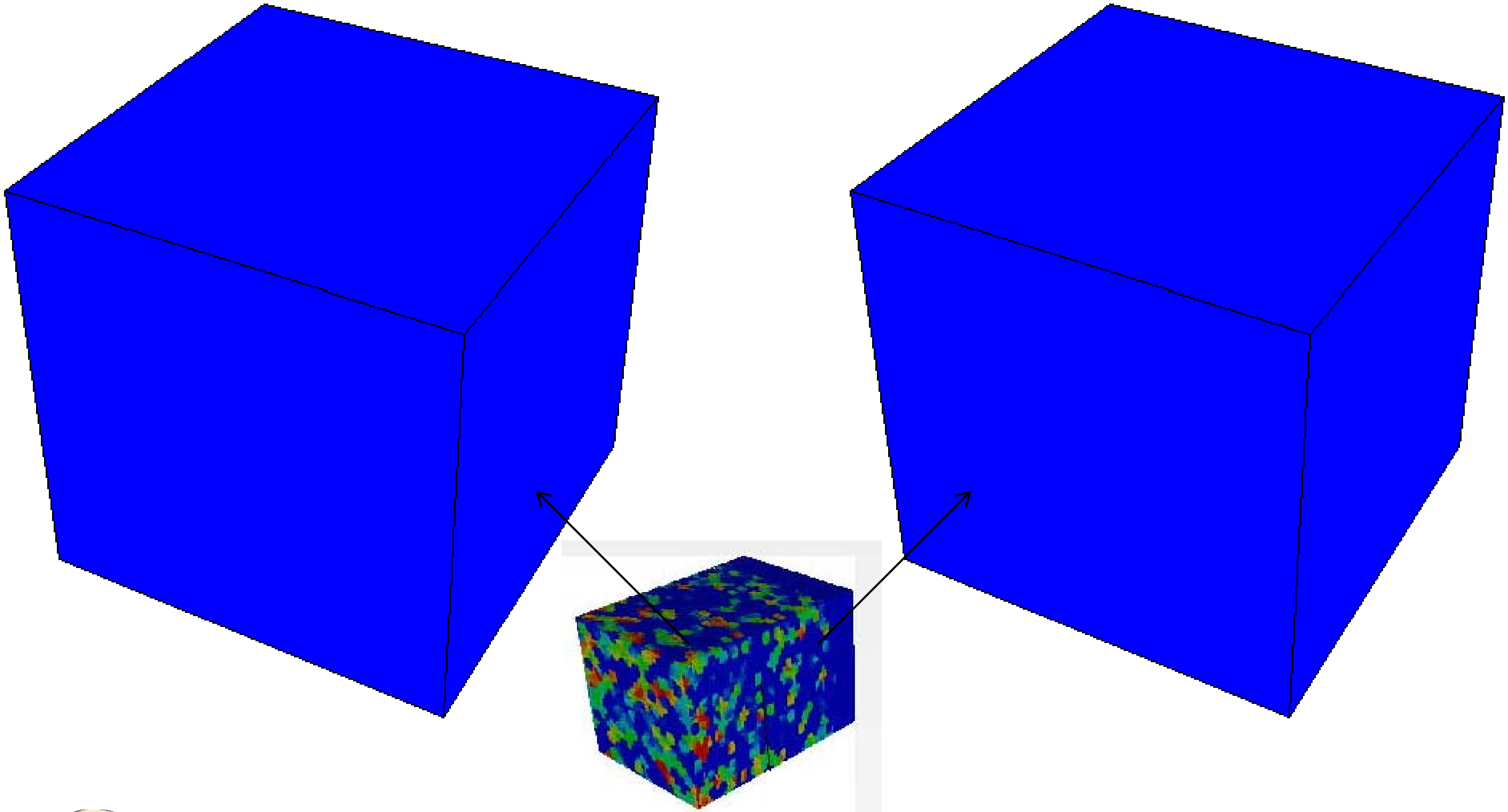
PETN plate impact - Velocity



PETN plate impact - temperature



PETN plate impact – Subgrain microstructures

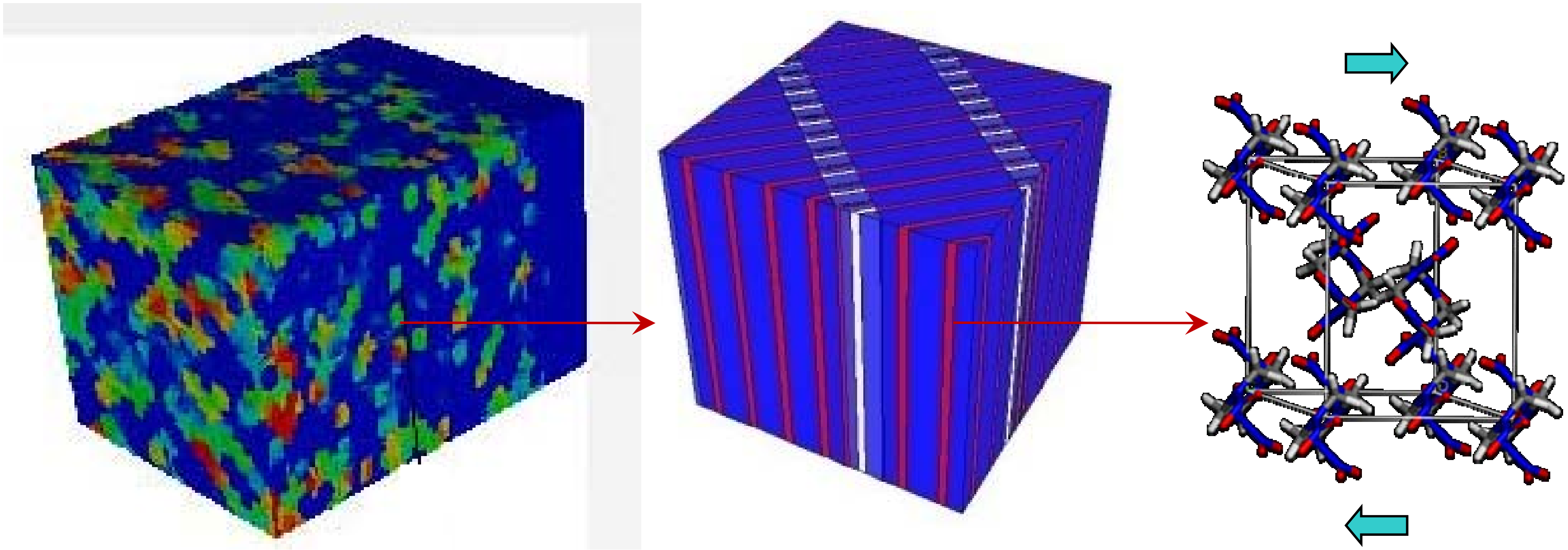


Microstructure evolution at selected material points

Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

Michael Ortiz
MMM2010

PETN plate impact – Hot-spot analysis



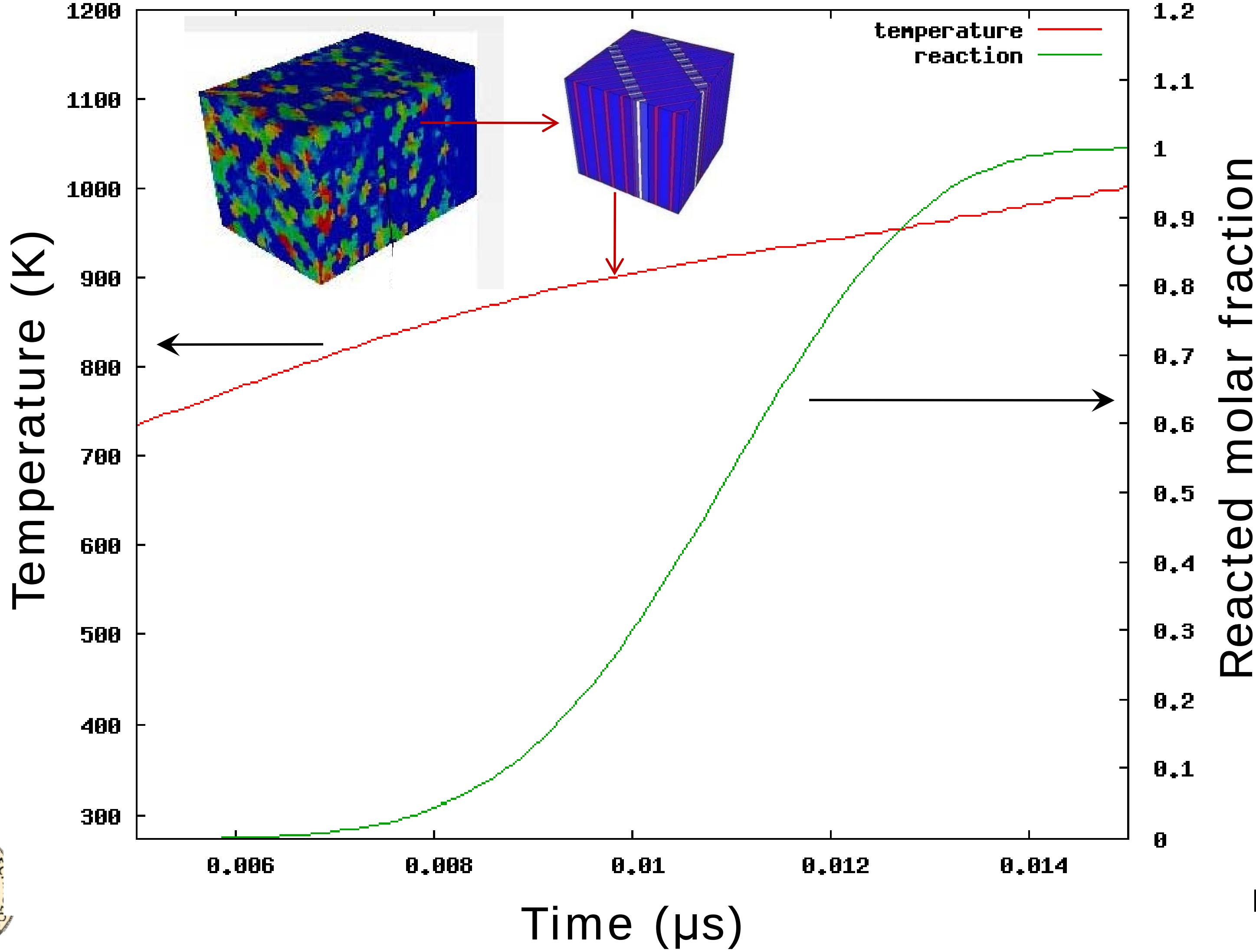
direct numerical simulation of polycrystalline PETN

reconstructed microstructure at selected material points

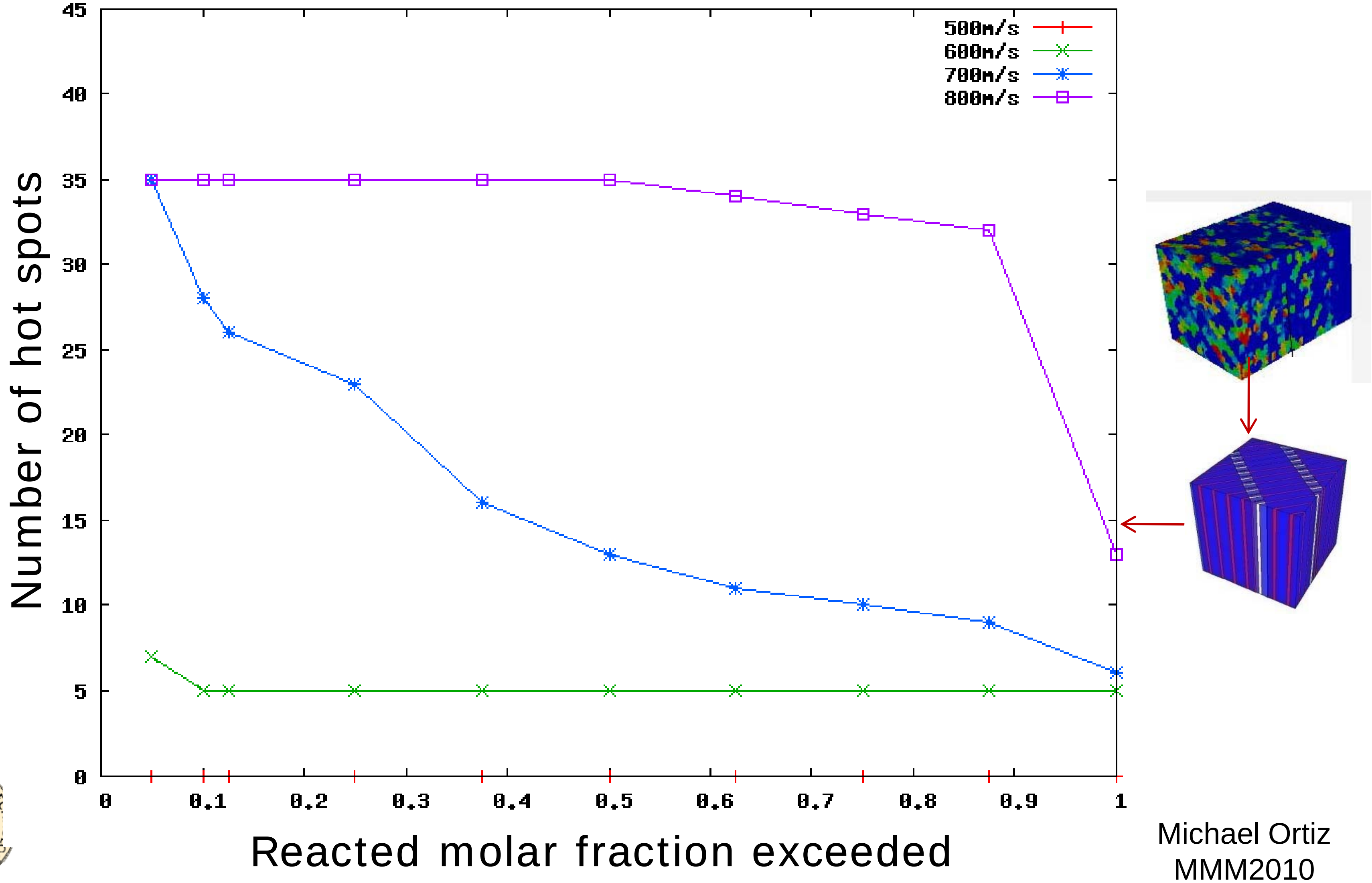
chemical analysis of hot-spots with B.C. from microstructure

Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

PETN plate impact - temperature and reaction evolution at selected hot spot



PETN plate impact - Number of hot spots



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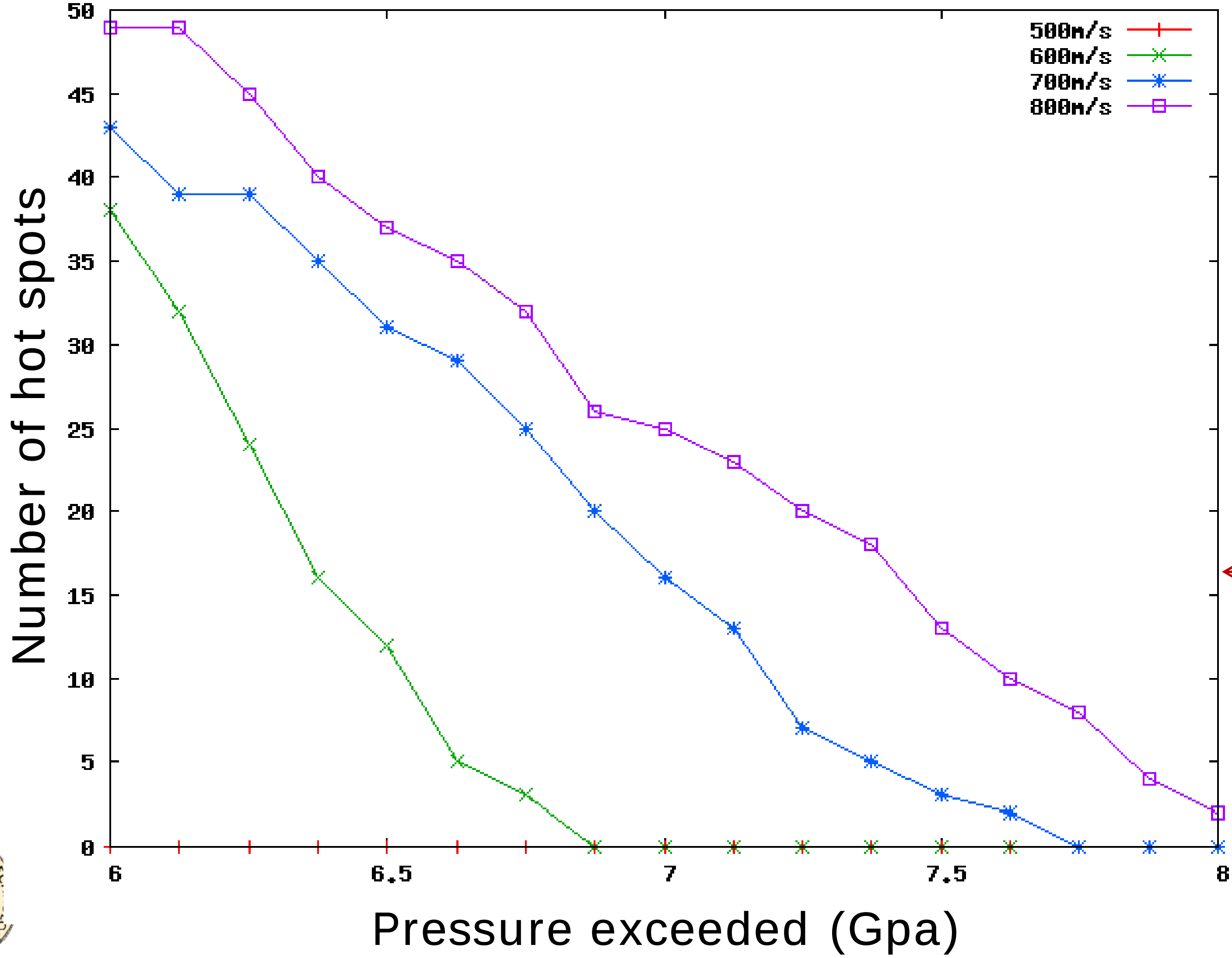
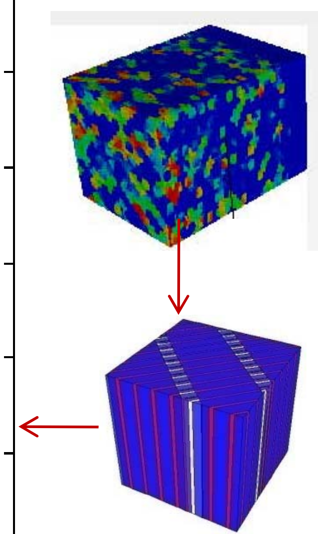
PETN plate impact - Number of hot spots





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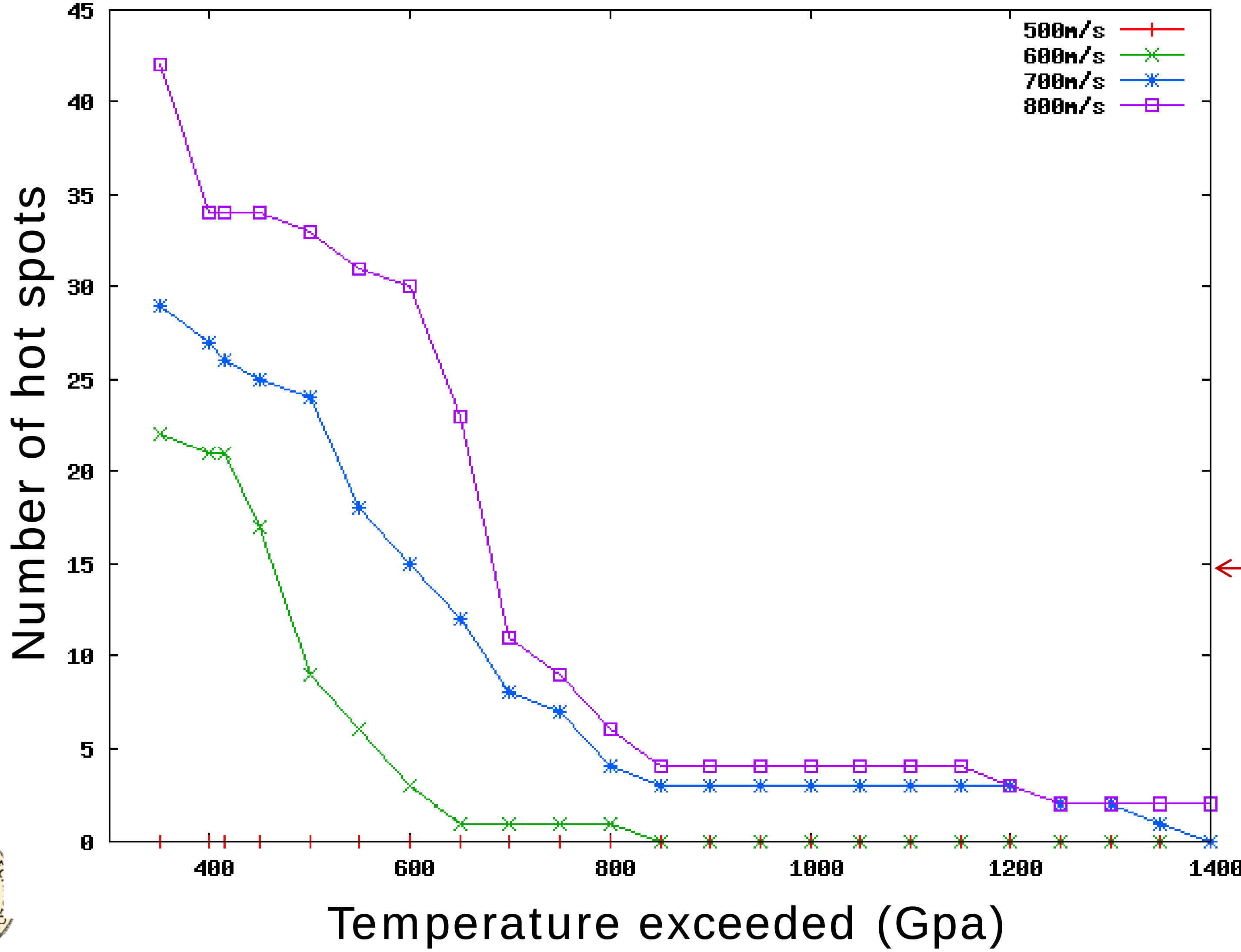
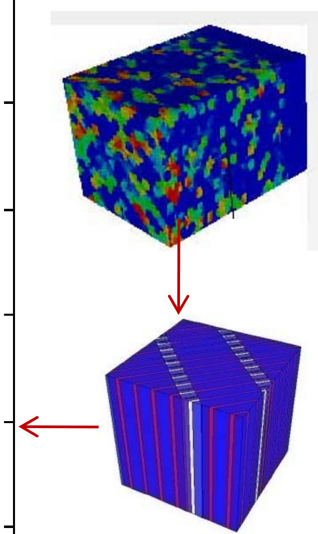
PETN plate impact - Number of hot spots





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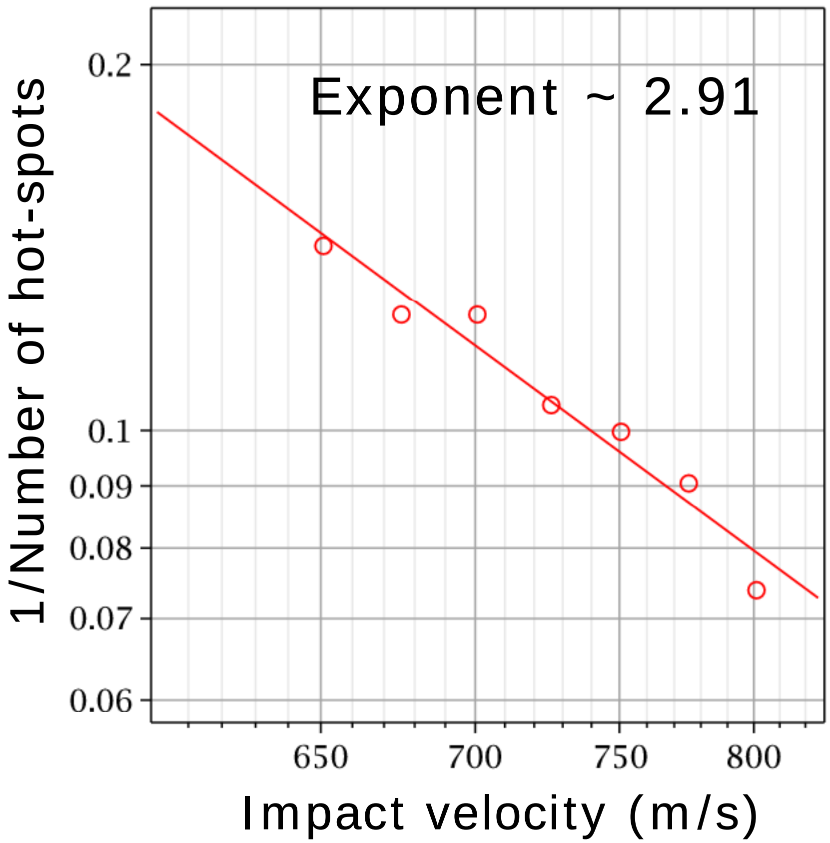
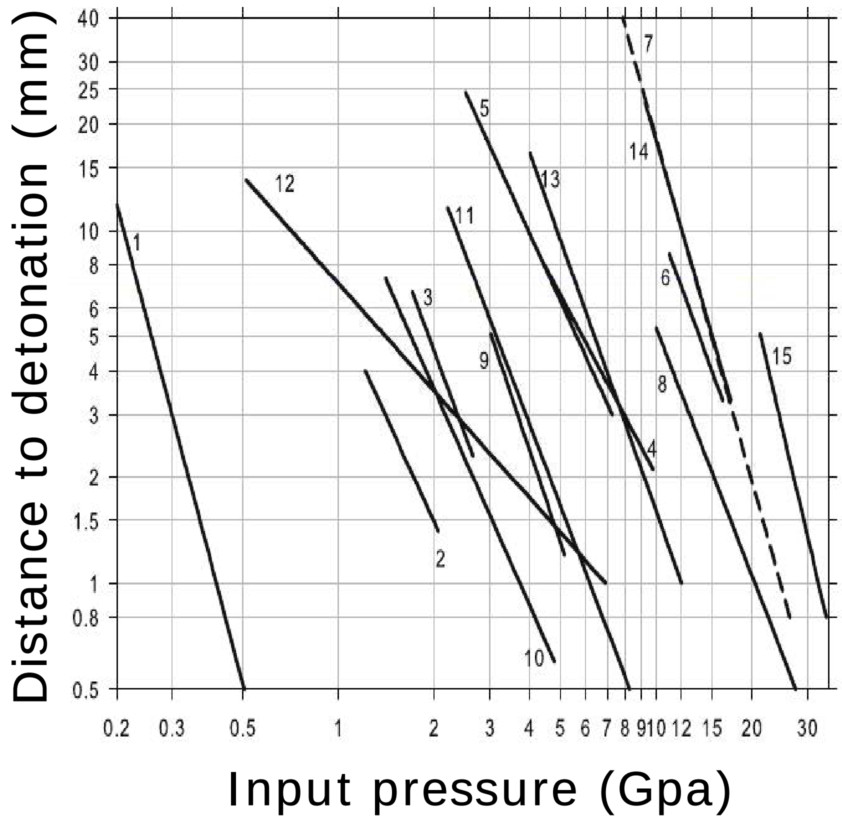
PETN plate impact – pop-plots

Impact velocity (m/s)





Multiscale model

S.A. Sheffield and R. Engelke (2009)

Experimental exponent ~ 2.01–2.58

Rimoli, J.J. and MO, *Phys. Rev. E,* 2010

Michael Ortiz
MMM2010

Concluding remarks

- Relaxation: Optimal theory of Multiscale Analysis with a clear sense of 'convergence': Exactness of macroscopic response for all applied loadings
- Relaxation eliminates fine-scale microstructural features from consideration in macroscopic calculations, but provides a 'return option': The optimal microstructures can be reconstructed at *post-processing* stage
- Return option is important when the extreme values of the solution, and not just averages, are of concern: failure, nucleation, initiation...
- Application to HE initiation would not have been possible without relaxation scheme...

Micro to Macro (and back again)