Multiscale Modeling of Energetic Materials

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New Frontiers in the Mathematics of Solids
Multiscale Models in Solid Mechanics
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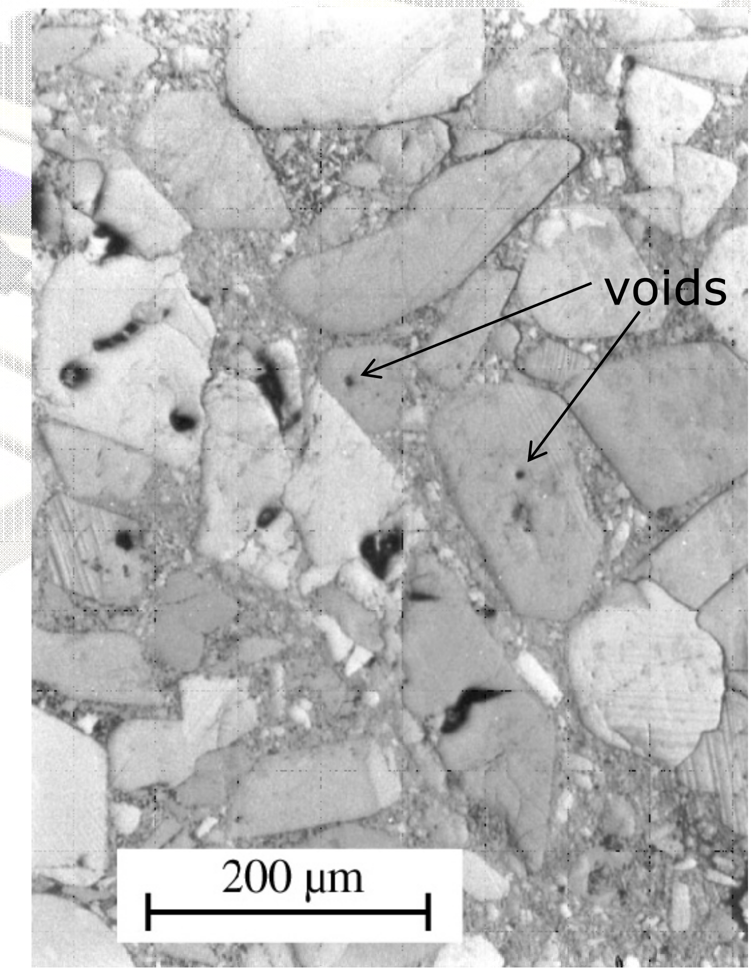
High-Explosives Detonation Sensitivity

- Detonation sensitivity: Ease with which an explosive can be detonated
- What factors determine detonation sensitivity?
  - *Pressure*
  - *Temperature*
  - *Density*
  - *Grain size*
  - *Composition…*

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

High-Explosives - Initiation

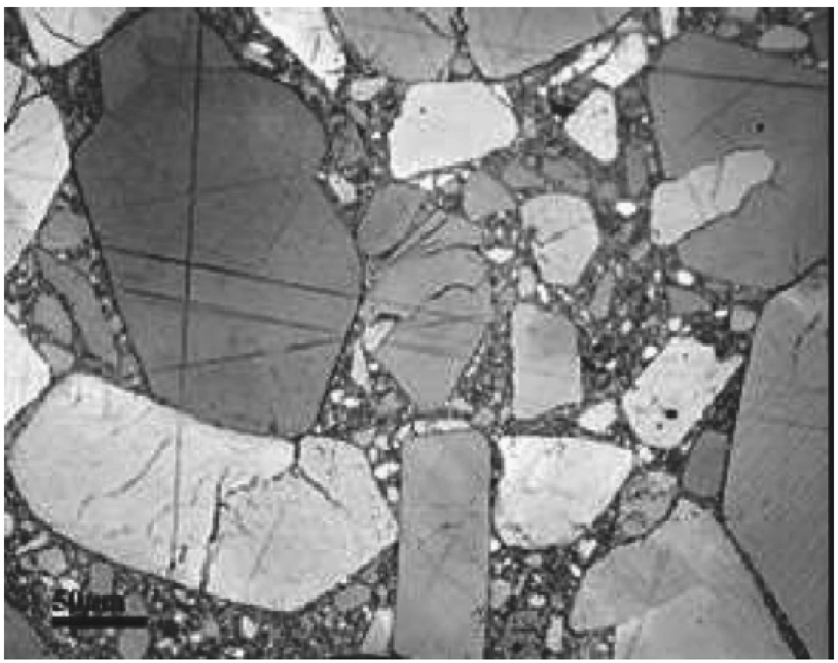
- In high explosives (HE) localized hot spots cause detonation initiation
- The hot spots are often assumed to arise at extended crystal defects such as voids
- Shock-induced void collapse is often modeled at single-crystal level using hydrocodes or continuum (mean-field) single-crystal plasticity



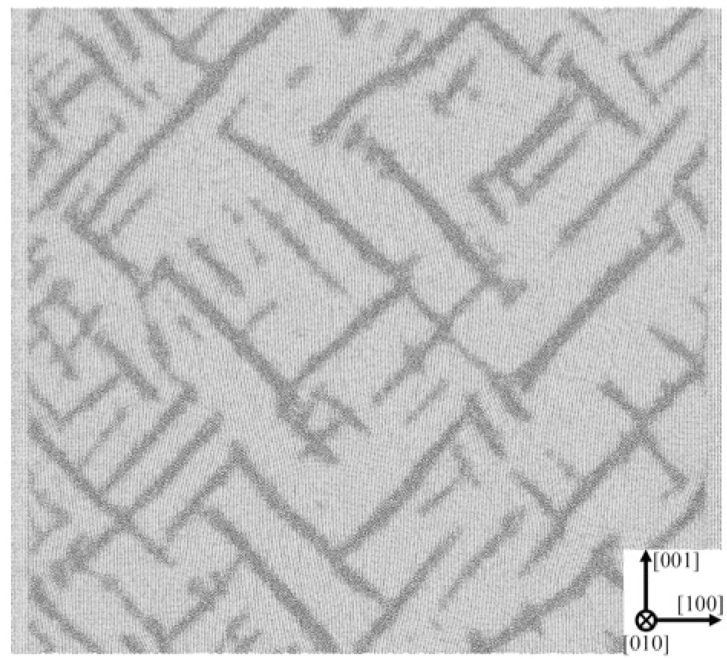
H. Tan, iMechanica, 2008

High-Explosives - Initiation

- But: Hot-spots can be nucleated homogenously due to ***heterogeneous*** plastic deformation (slip line formation) and stress risers such as triple points in the polycrystalline structure



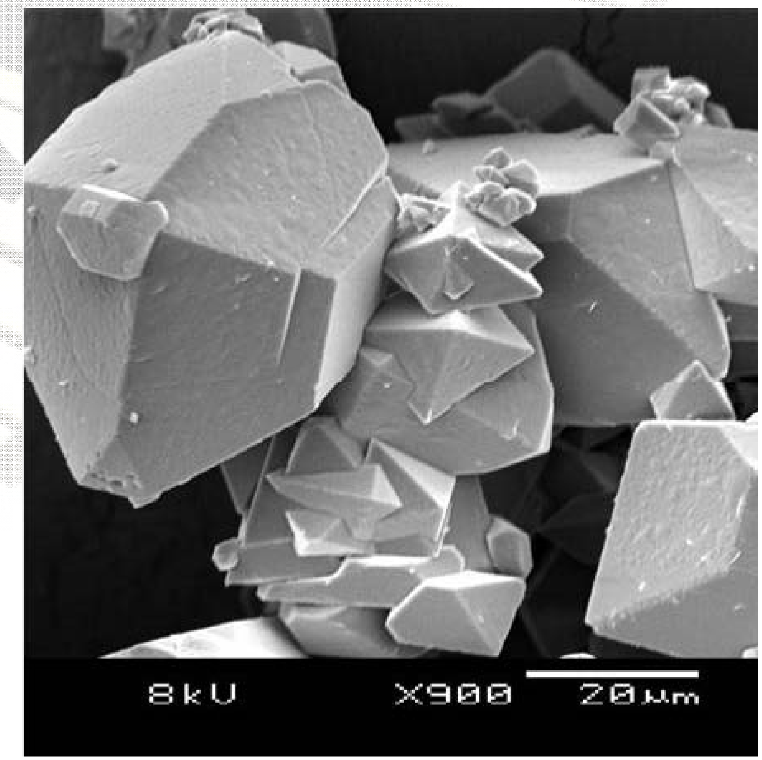
PBX 9501 (C.B. Skidmore, LANL)



Tommy Sewell (2008)

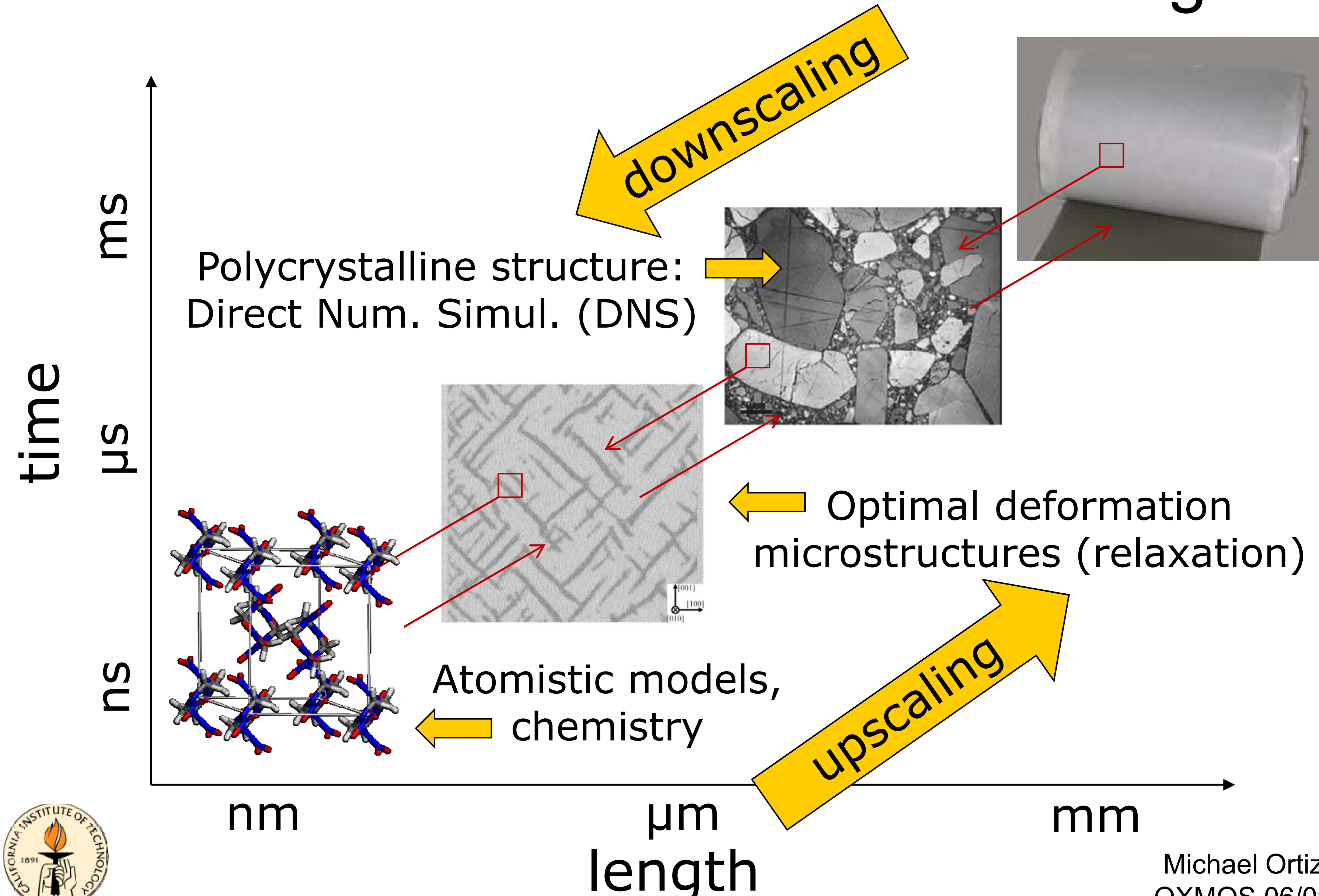
High-Explosives - Initiation

- 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)

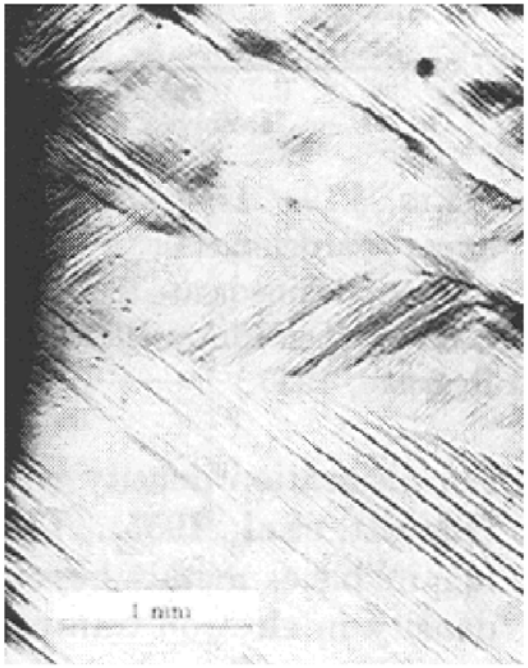


SEM image of RDX (Kline *et al*., 2003)

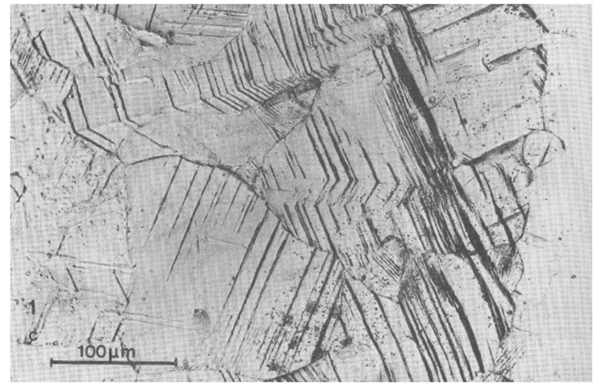
HE initiation – Multiscale modeling



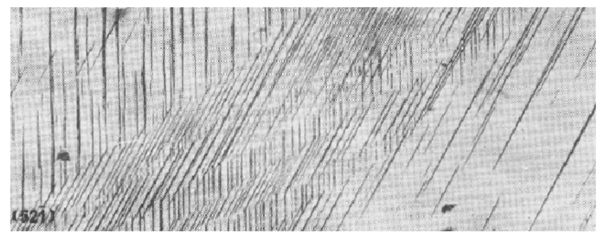
Latent hardening & heterogeneous slip



(Saimoto, 1963)



(Ramussen and Pedersen, 1980)

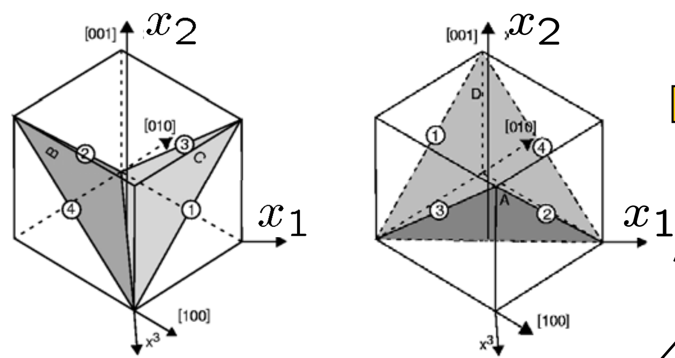


(Jin and Winter, 1984)

- **Latent hardening**: *"These results prove the reality of latent-hardening, in the sense that the slip lines of one system experience difficulty in breaking through the active slip lines of the other one"* (Piercy, G. R., Cahn, R. W., and Cottrell, A. H., *Acta Metallurgica*, **3** (1955) 331-338).

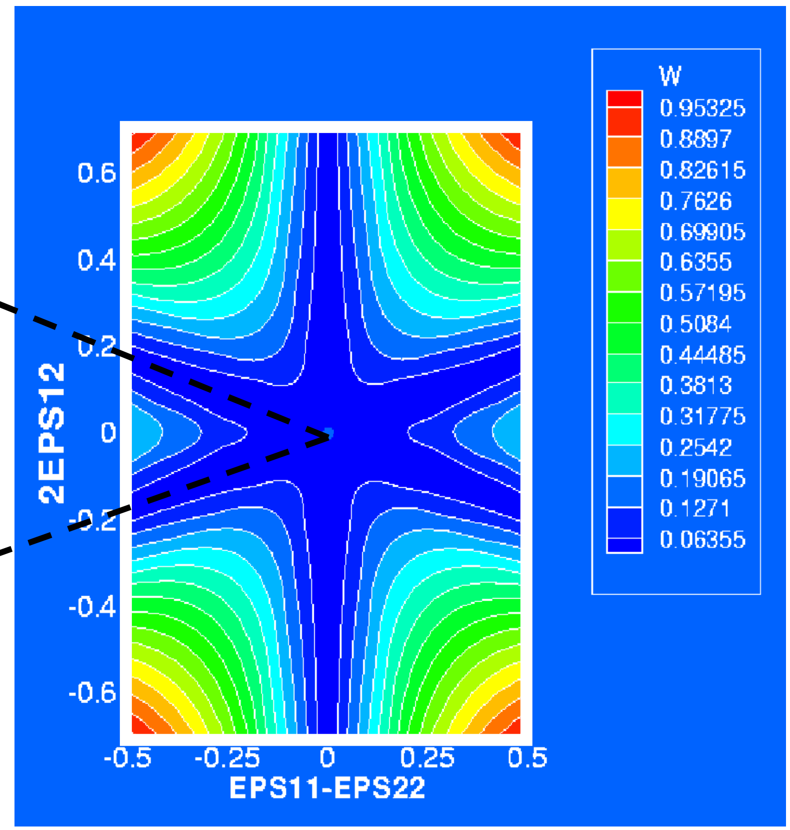
Crystal plasticity – Non-convexity

- Example: FCC crystal deforming on $(1\bar{1}0)$-plane



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

(Single slip)



$W(\nabla u)$

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

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

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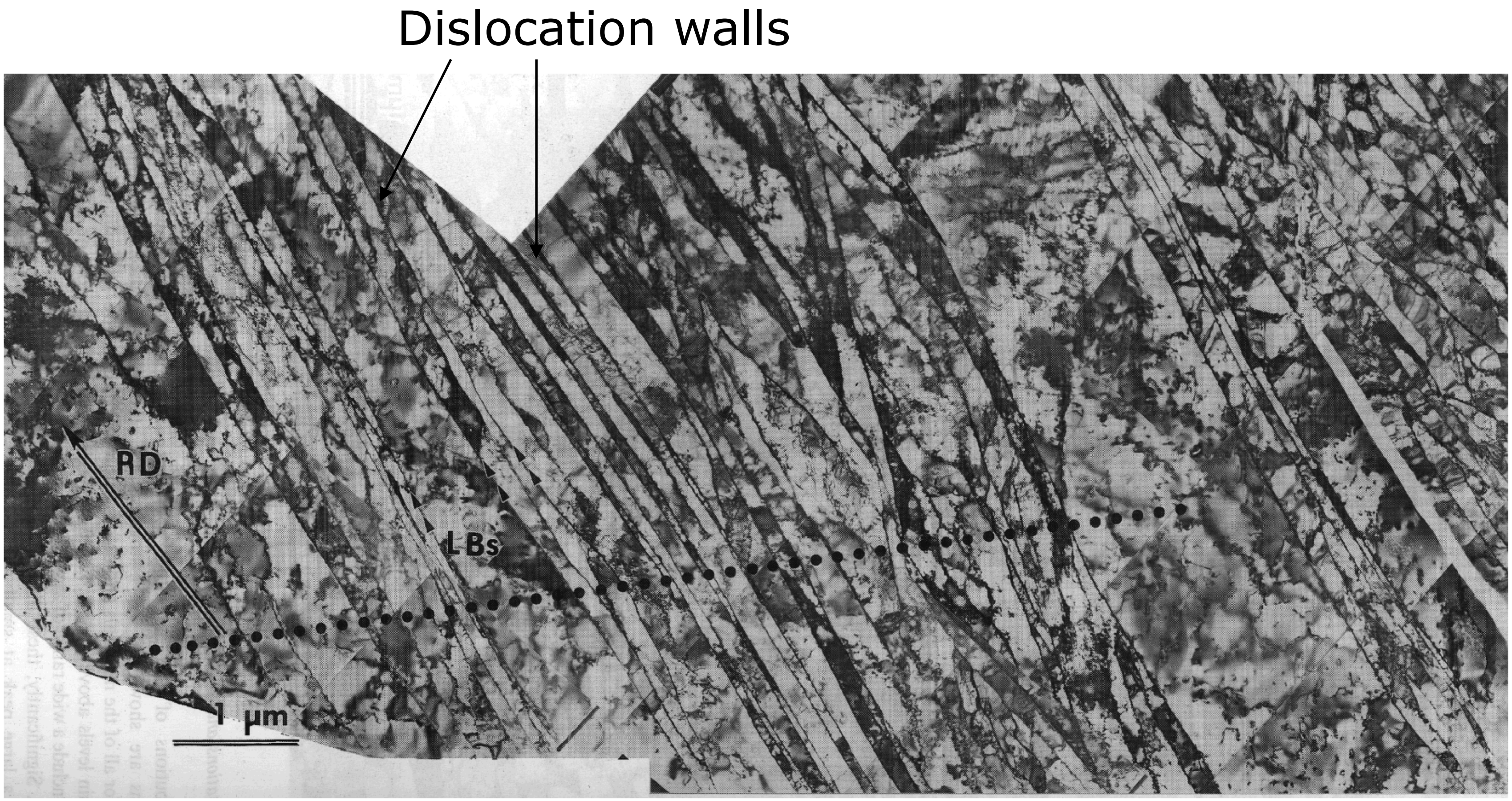
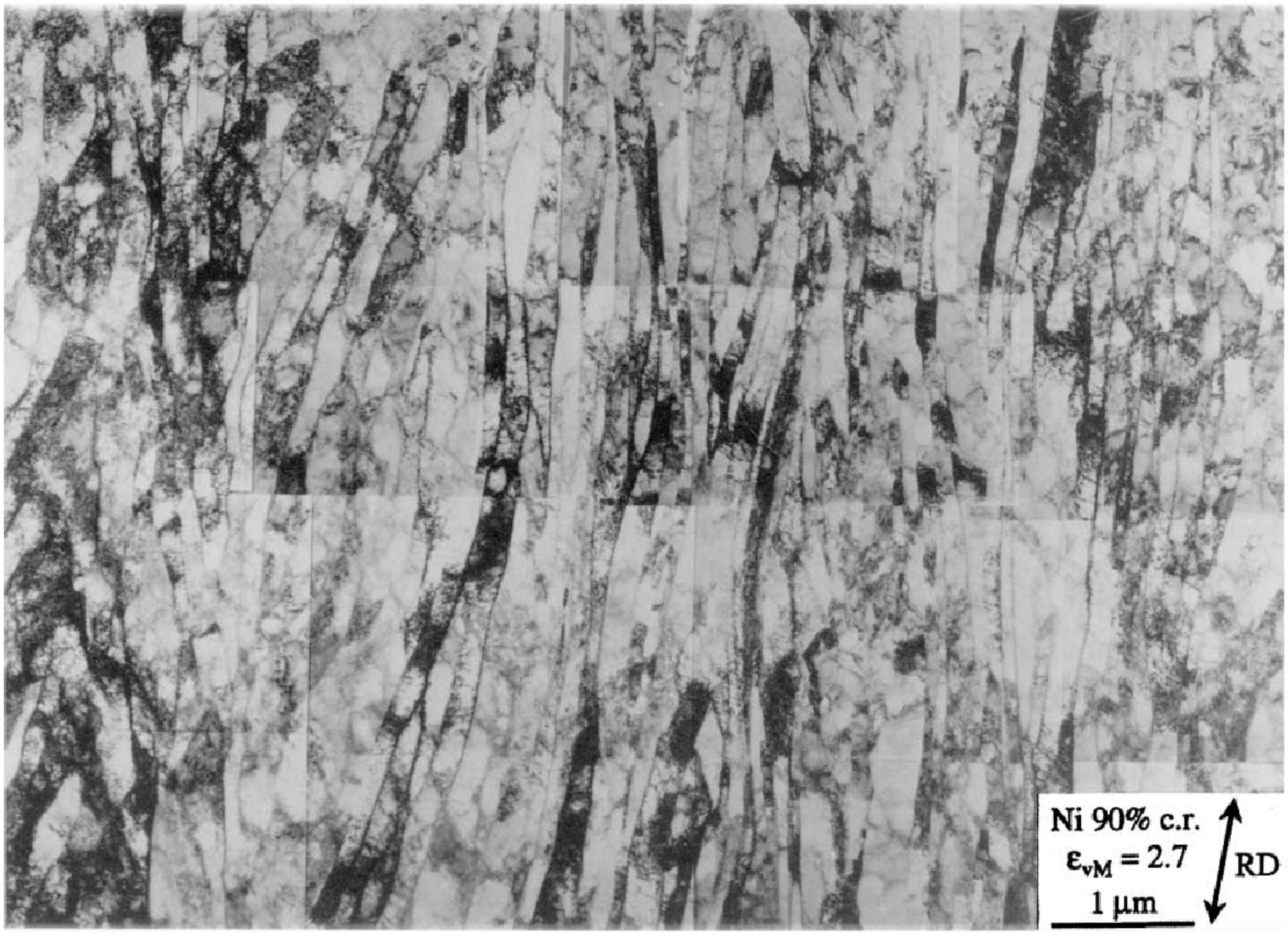
Subgrain dislocation structures



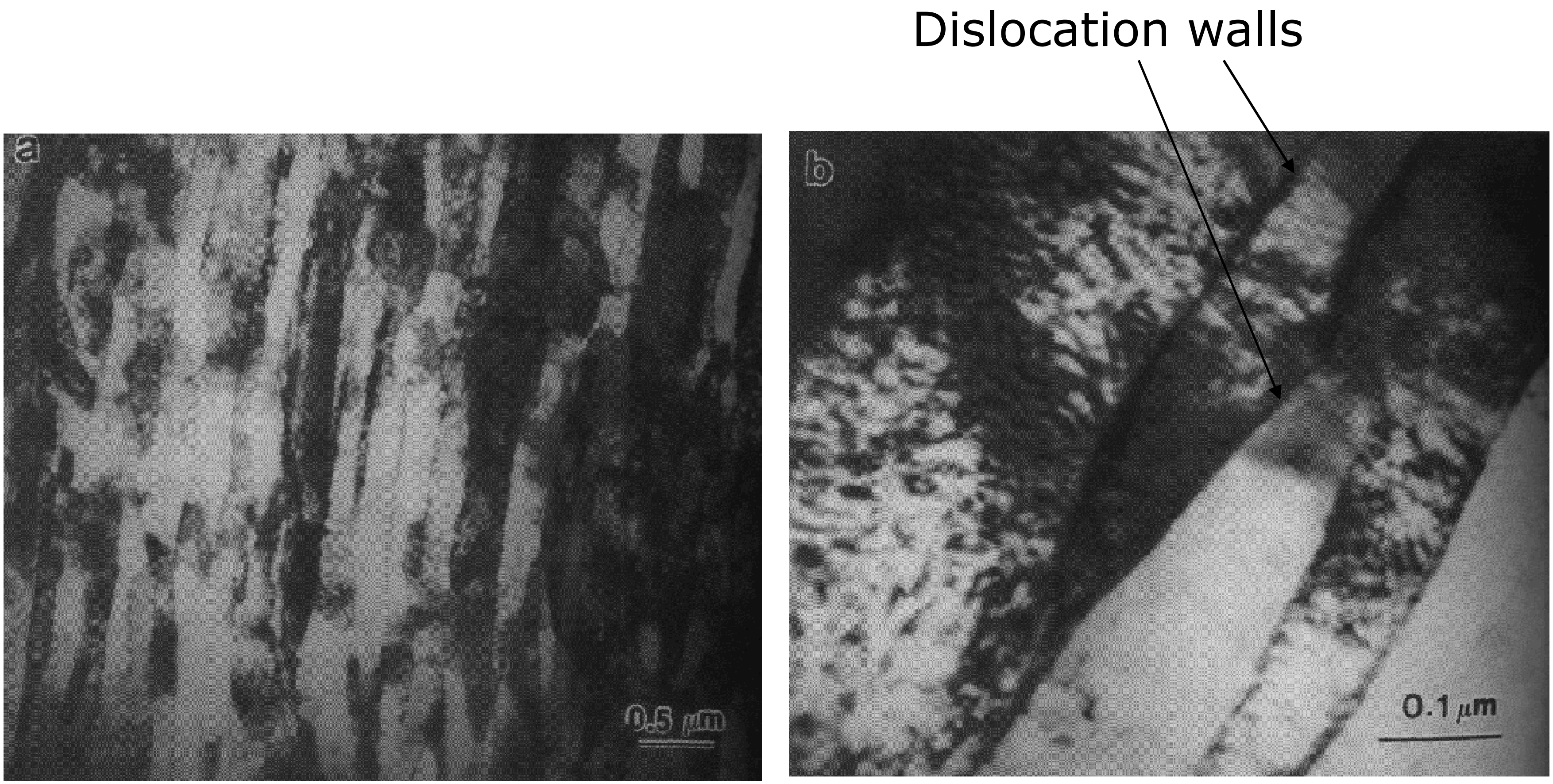
Lamellar dislocation structure in 90% cold-rolled Ta
(DA Hughes and N Hansen, Acta Materialia, 44 (1) 1997, pp. 105-112)

Subgrain dislocation structures



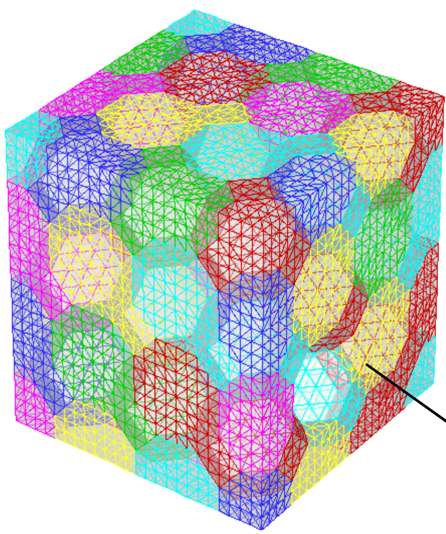
Pure nickel cold rolled to 90%
Hansen *et al.* Mat. Sci. Engin. A317 (2001)

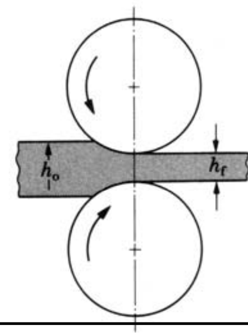
Subgrain dislocation structures

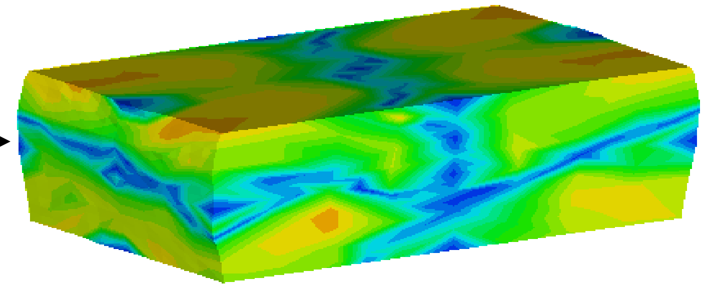


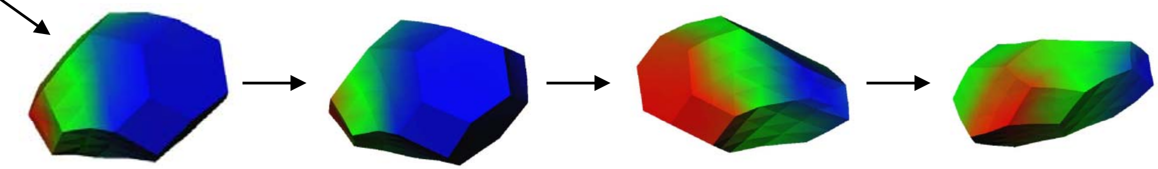
Lamellar structures in shocked Ta
(MA Meyers et al., Metall. Mater. Trans.,
26 (10) 1995, pp. 2493-2501)

Polycrystals – Limitations of DNS



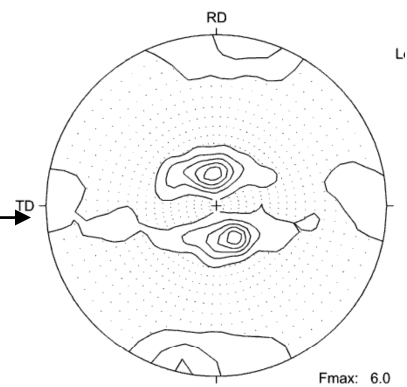


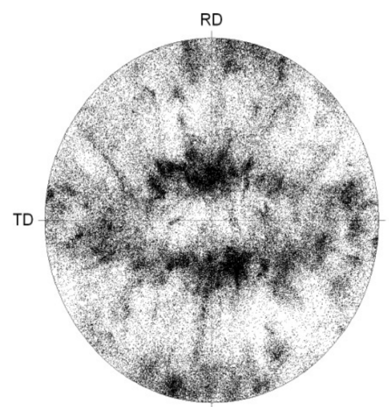




Cold-rolled @ 42% polycrystalline Ta

Experimental cold-rolled texture



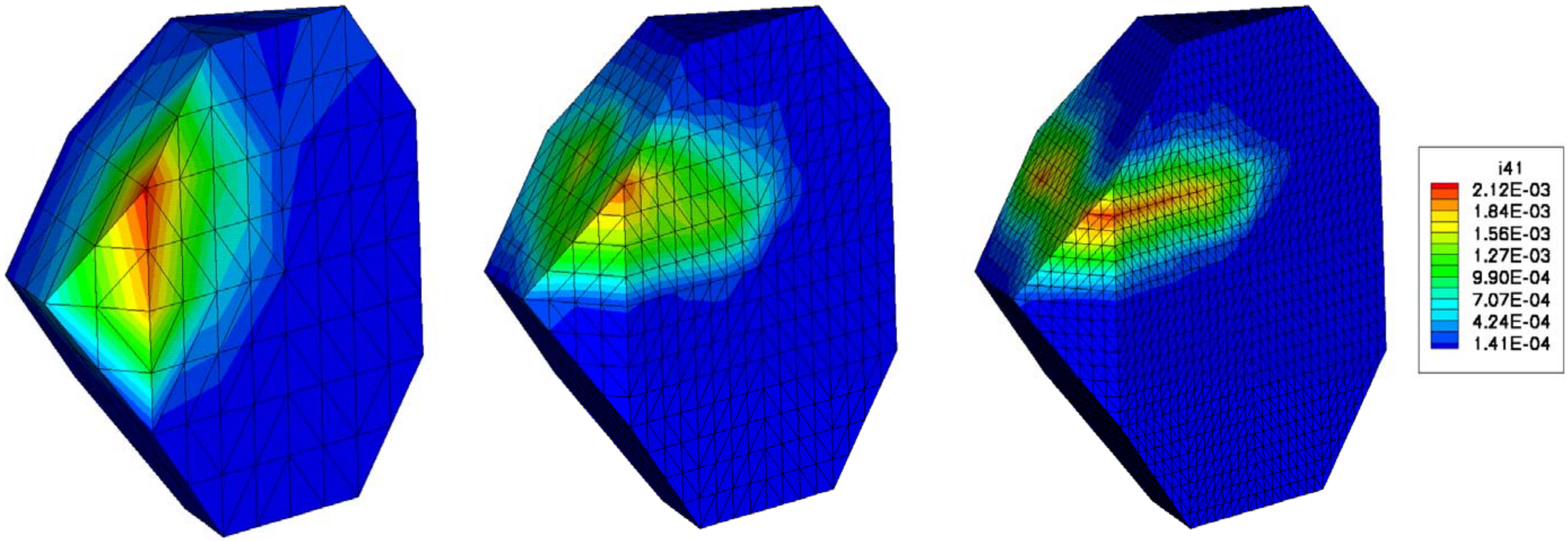


Pole figure

(Zhao, Z. *et al.*, *Acta Mater.*, **55** (2007) 2361-2373)

Polycrystals – Limitations of DNS

Convergence of DNS of coarse-grained polycrystals:



Coarse mesh
192 elmts/grain

Intermediate mesh
1536 elmts/grain

Fine mesh
12288 el/grain

Cold-rolled @ 42% polycrystalline Ta
(Zhao, Z. *et al.*, *Acta Mater*., **55** (2007) 2361-2373)

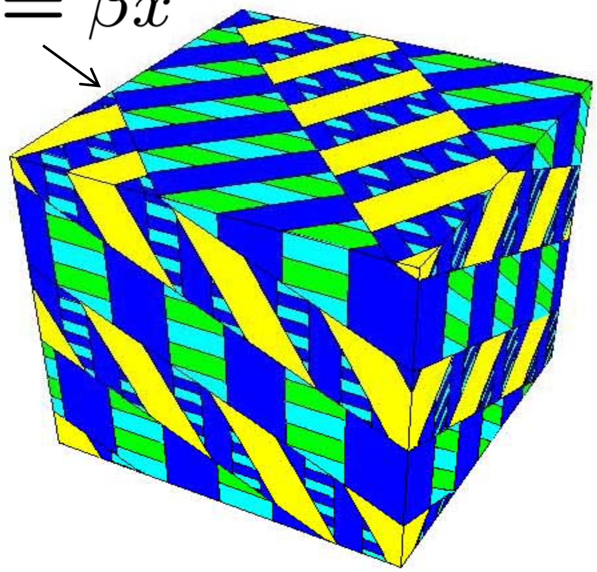
Subgrain dislocation structures

- Strong latent hardening and geometrical softening give rise to subgrain dislocation microstructures almost universally…
- Subgrain dislocation structures beat uniform multiple slip in general, soften the macroscopic response of the crystal, lead to scaling behavior
- Microstructures are much too fine to be resolved numerically by direct numerical simulation
- How to build microstructure into finite element calculations? $\rightarrow$ Multiscale analysis!

Separation of scales - Relaxation

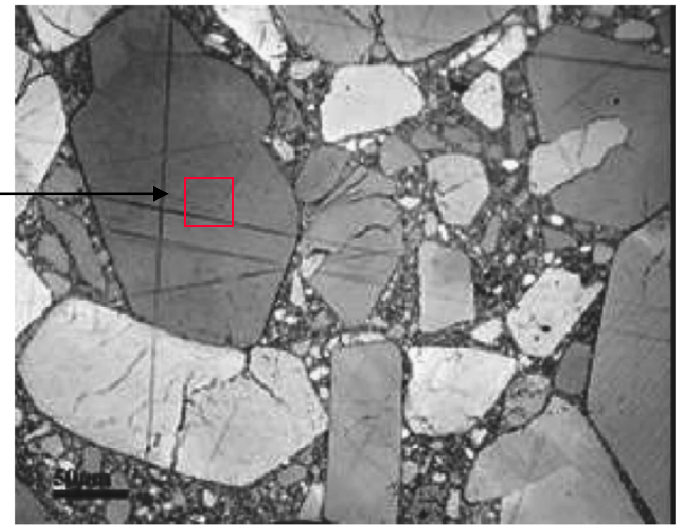
- *W(Du)* ≡ Unrelaxed energy density (non-convex)

$u = \beta x$



$QW(\beta) =$ Minimum energy density

Relaxation



$$\int_\Omega QW(\nabla u)\, dx$$

Relaxed problem

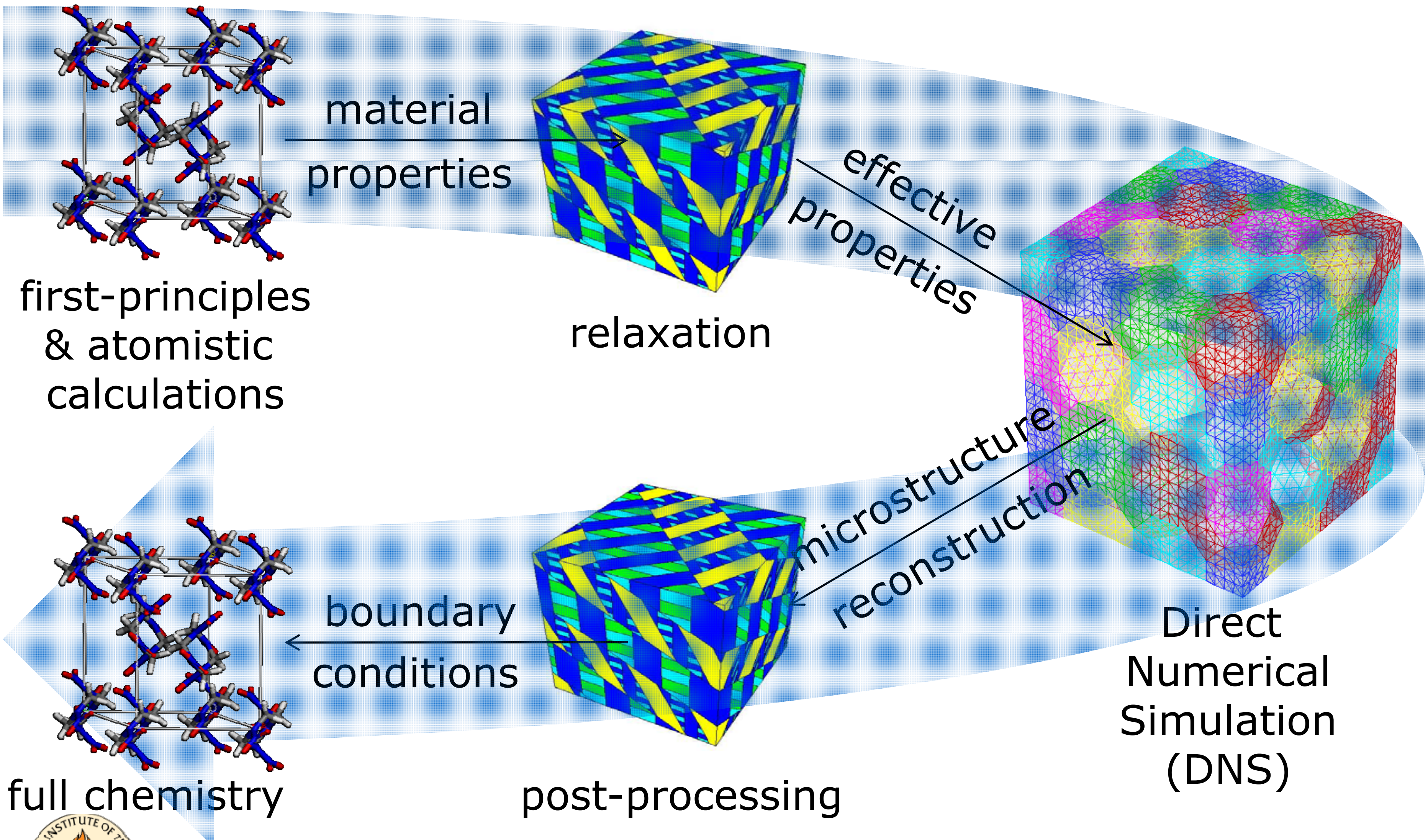
Separation of scales - Relaxation

- Relaxation yields the softest possible macroscopic behavior that can be attained by the formation of microstructure
- All microstructures are accounted for by the relaxed problem (no physics lost)
- Optimal microstructures can be reconstructed from the solution of the relaxed problem (no loss of information)
- Important for HE initiation: Average response is not enough, need to know extremes of deformation (Hot spots!)

Relaxation – Fast Multiscale Models

- Fast Multiscale Models: Use explicitly relaxed constitutive relation (when available) to represent sub-grid behavior (at element level)
- Much faster than concurrent multiscale calculations (on-the-fly generation of sub-grid microstructures, e.g., by sequential lamination)
- Elements equipped with optimal microstructures, exhibit optimal effective behavior
- Convergence of approximations in the sense of Gamma convergence (e.g., Conti, S., Hauret, P. and Ortiz, M., *SIAM Multiscale Model. Simul*., **6** (2007) 135-157)

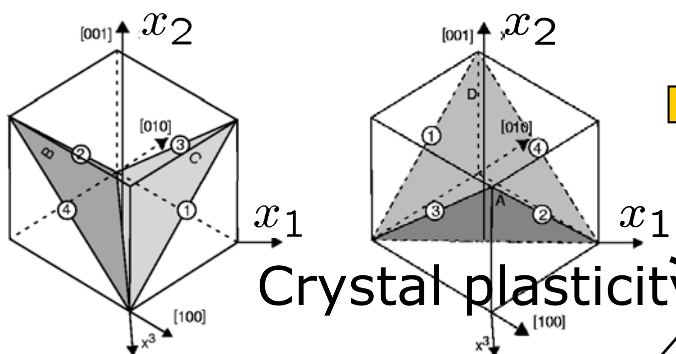
Relaxation – Fast Multiscale Models



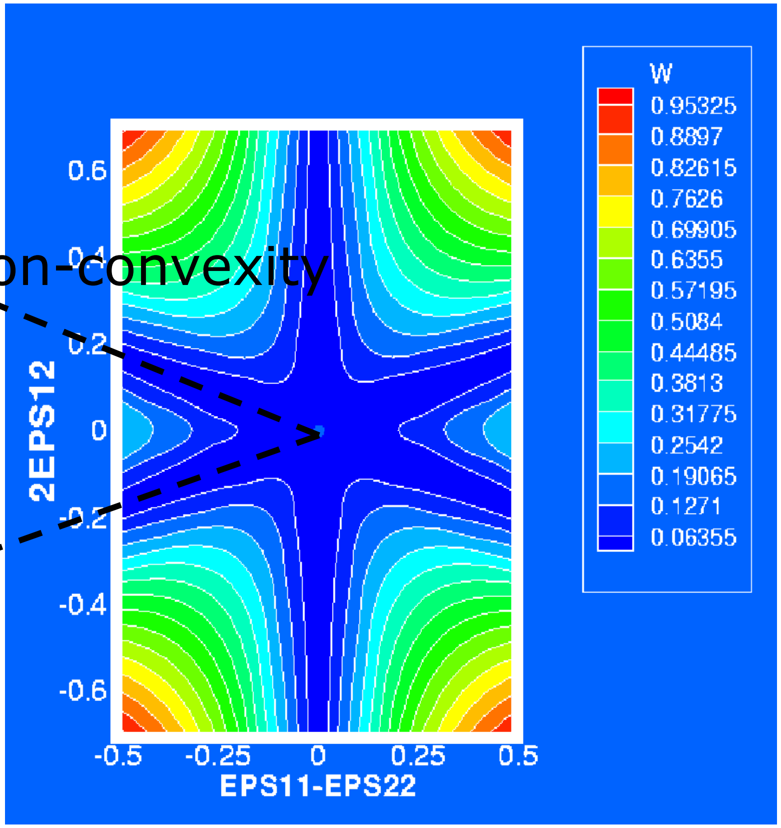
FMM scheme for polycrystalline HE

Application to crystal plasticity

- Example: FCC crystal deforming on $(1\bar{1}0)$-plane



Crystal plasticity → Non-convexity



$W(\nabla u)$

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

(Single slip)

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

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

Crystal plasticity − Relaxation

- Let: $U(\Omega) = \left\{ u \in BD(\Omega, \mathbb{R}^3) : \text{div} u \in L^2(\Omega) \right\}$
- Regression function: $W^\infty(\beta) = \lim_{t \to \infty} \frac{1}{t} W^{**}(t\beta)$

Theorem (Conti and Ortiz, ARMA '05) *Suppose that the set of slip systems is complete. Then, the relaxation of $I(u)$ with respect to the strong L^1 topology is:* $J(u) =$

$$\begin{cases} \int_\Omega W^{**}(\epsilon(u))dx + \int_\Omega W^\infty\left(\frac{E_s u}{|E_s u|}\right) d|E_s u|, & \text{if } u \in U(\Omega) \\ +\infty, & \text{otherwise.} \end{cases}$$

Crystal plasticity − Relaxation

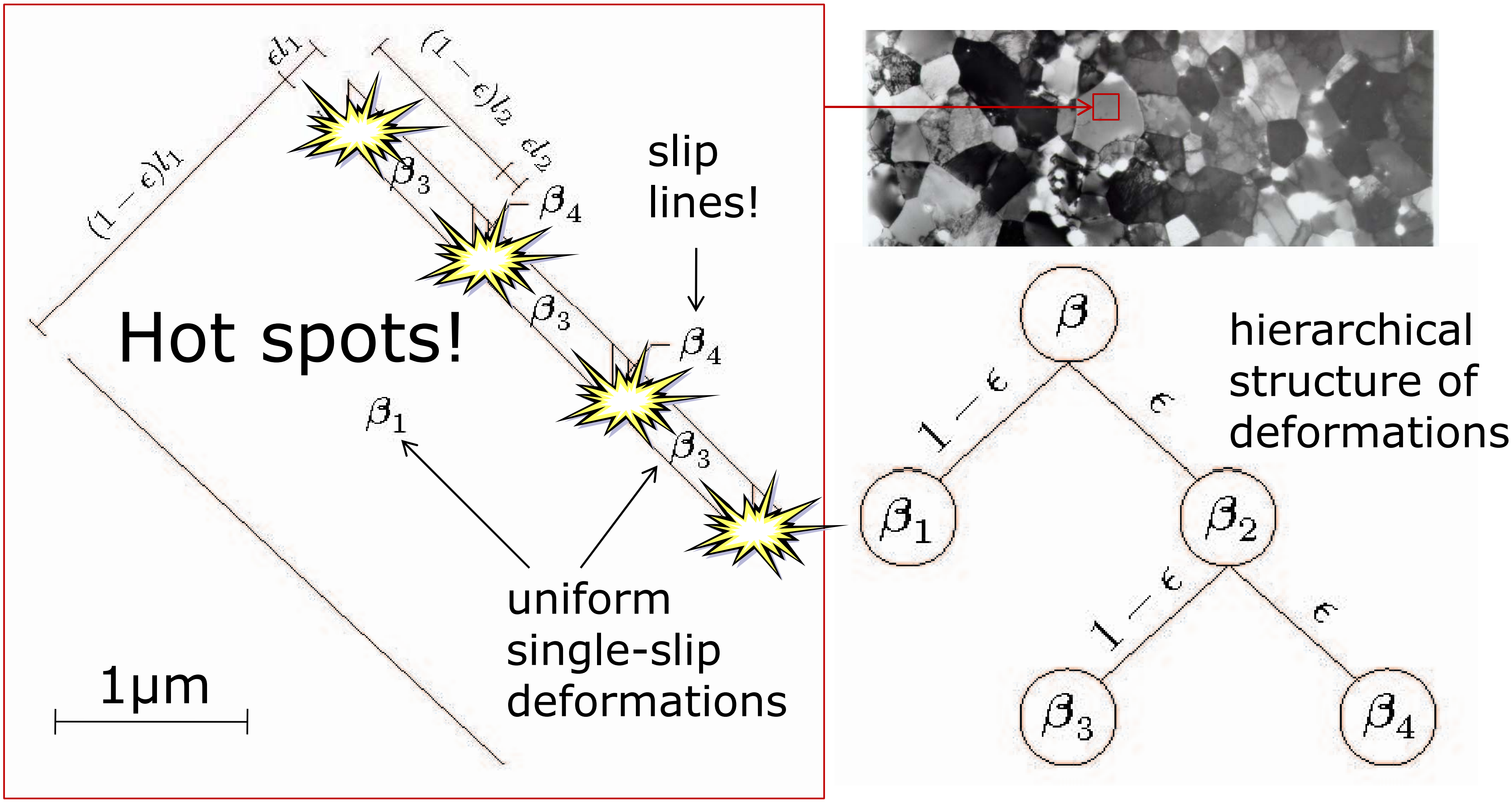
- Proof: Match upper & lower bounds, $W^{\mathrm{qc}} = W^{**}$.
- Lower bound: $J(u)$ convex functional of measure Eu, $J(u) \leq I(u)$.

Lemma *Let $\mathcal{S}$ be a complete set of slip systems. For any $\beta \in \mathbb{R}^{3\times3}$ and any $\epsilon > 0$ there is a laminate ν (of finite order) such that*

$$\langle \nu, \mathrm{Id} \rangle = \beta \qquad \textit{and} \qquad \langle \nu, W \rangle \leq W^{**}(\beta) + \epsilon\,.$$

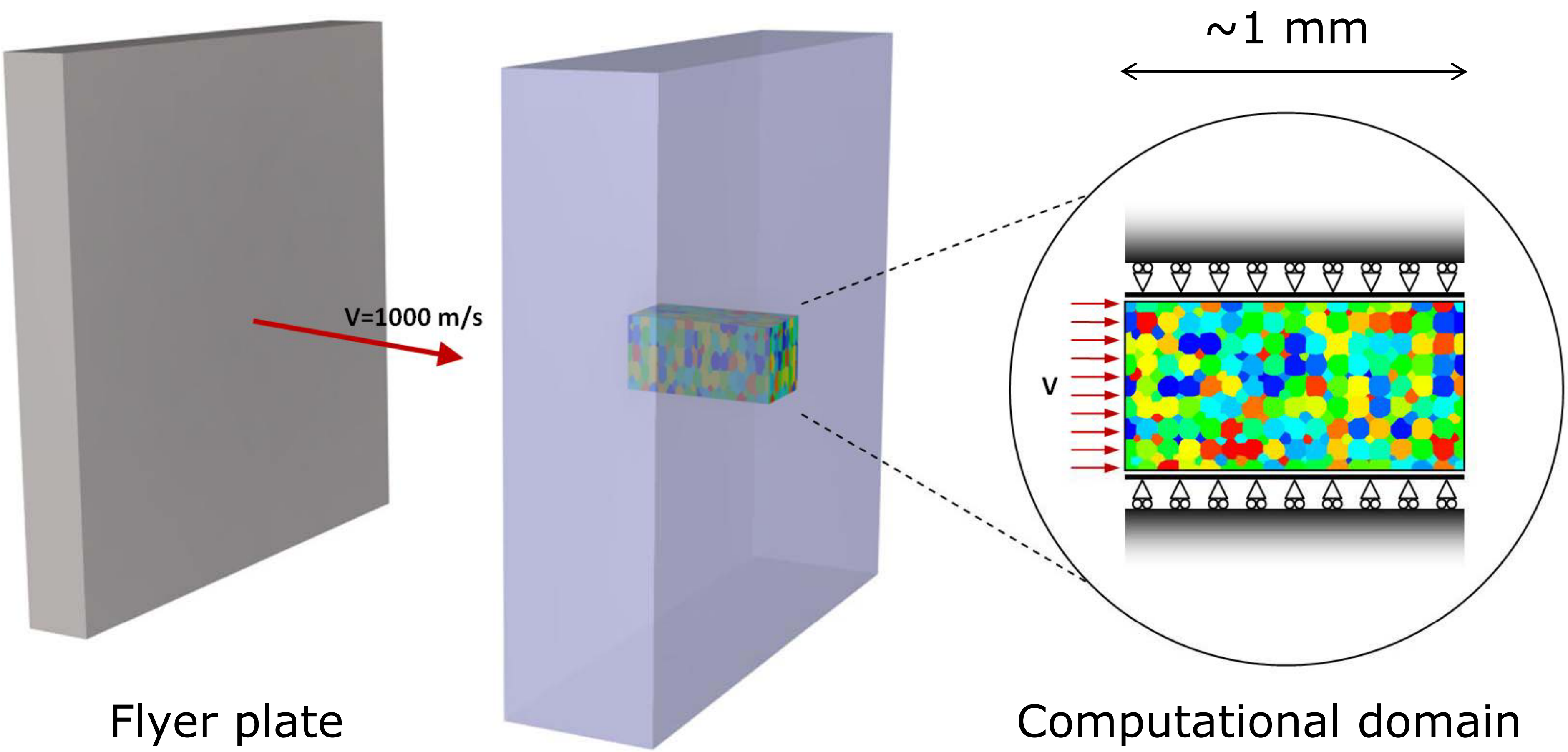
- Some of the deformations in the laminate may become unbounded as $\epsilon \to 0$ and become slip lines in the limit.

Crystal plasticity – Relaxation



Optimal microstructure construction in double slip
(Conti, S. and Ortiz, M., *Arch. Rat. Mech. Anal.*, **176** (2005) 103-147)

Fast Multiscale Models – HE detonation



Flyer plate

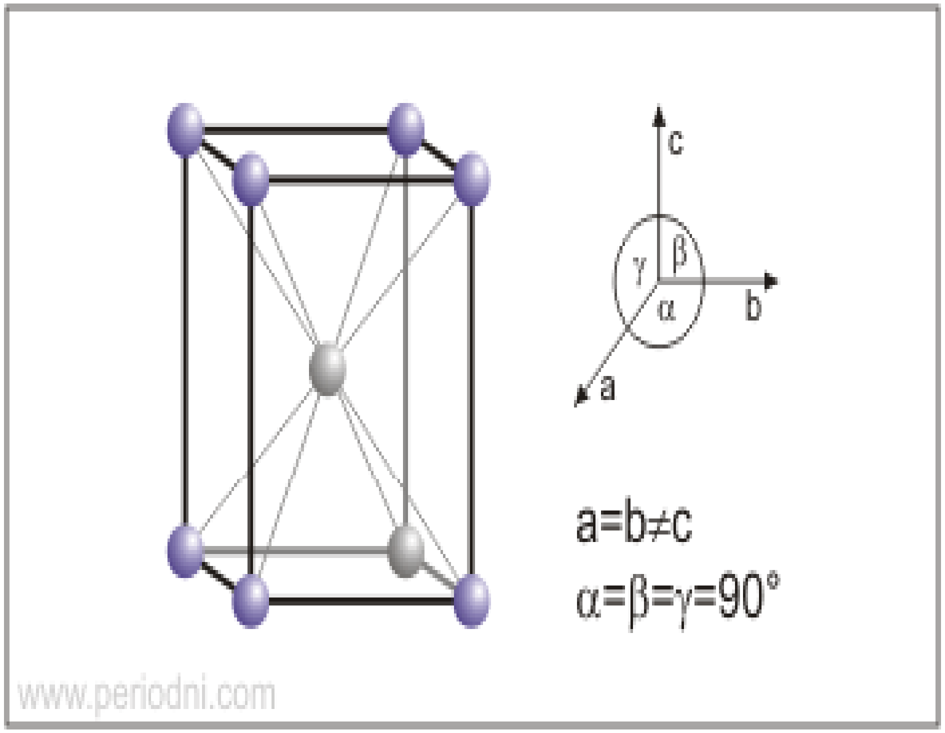
Computational domain

HE target plate

Plate-impact configuration

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

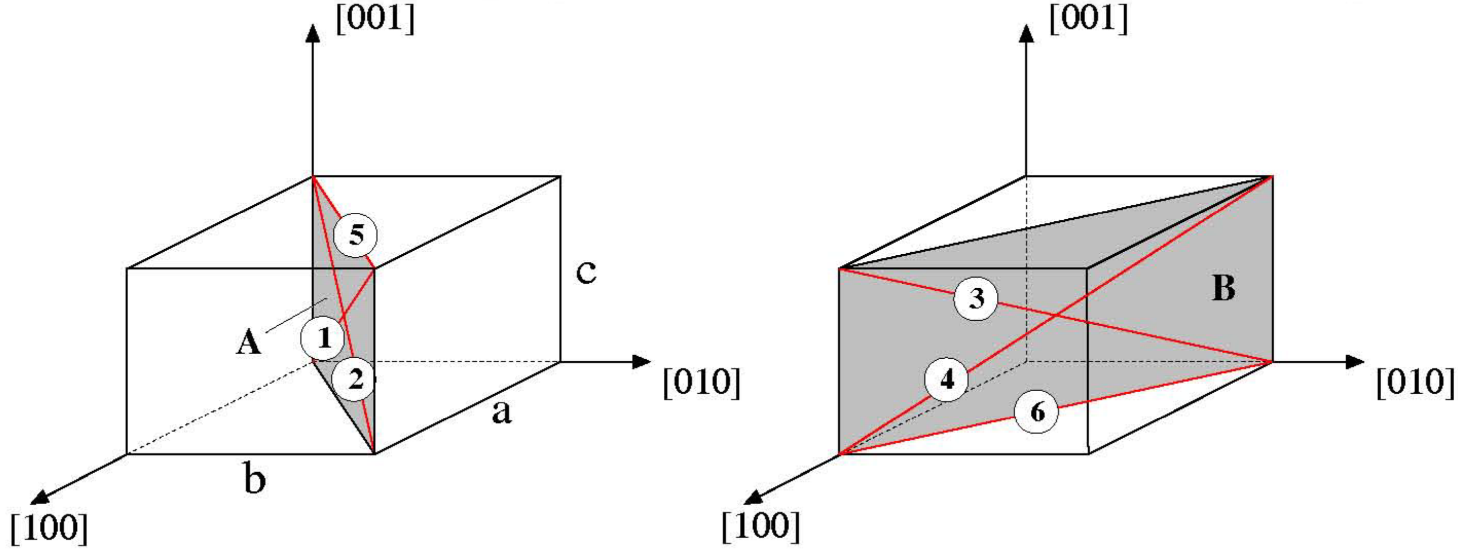
- Elastic constants assumed to decrease linearly with temperature, vanish at melting:

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

- 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

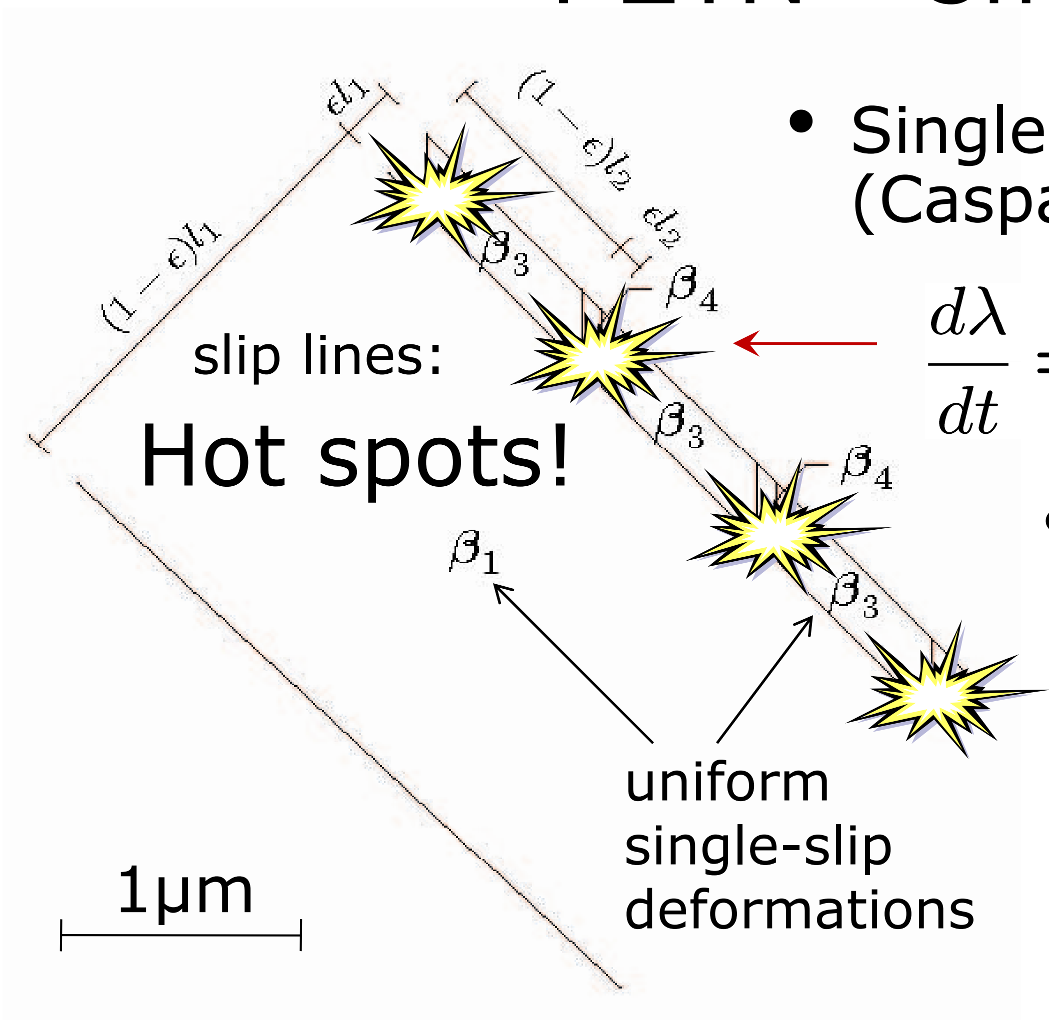


$a = b = 9.380Å \qquad c = 6.710Å$

- $\tau_c(\theta)$ 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

PETN – Chemistry



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

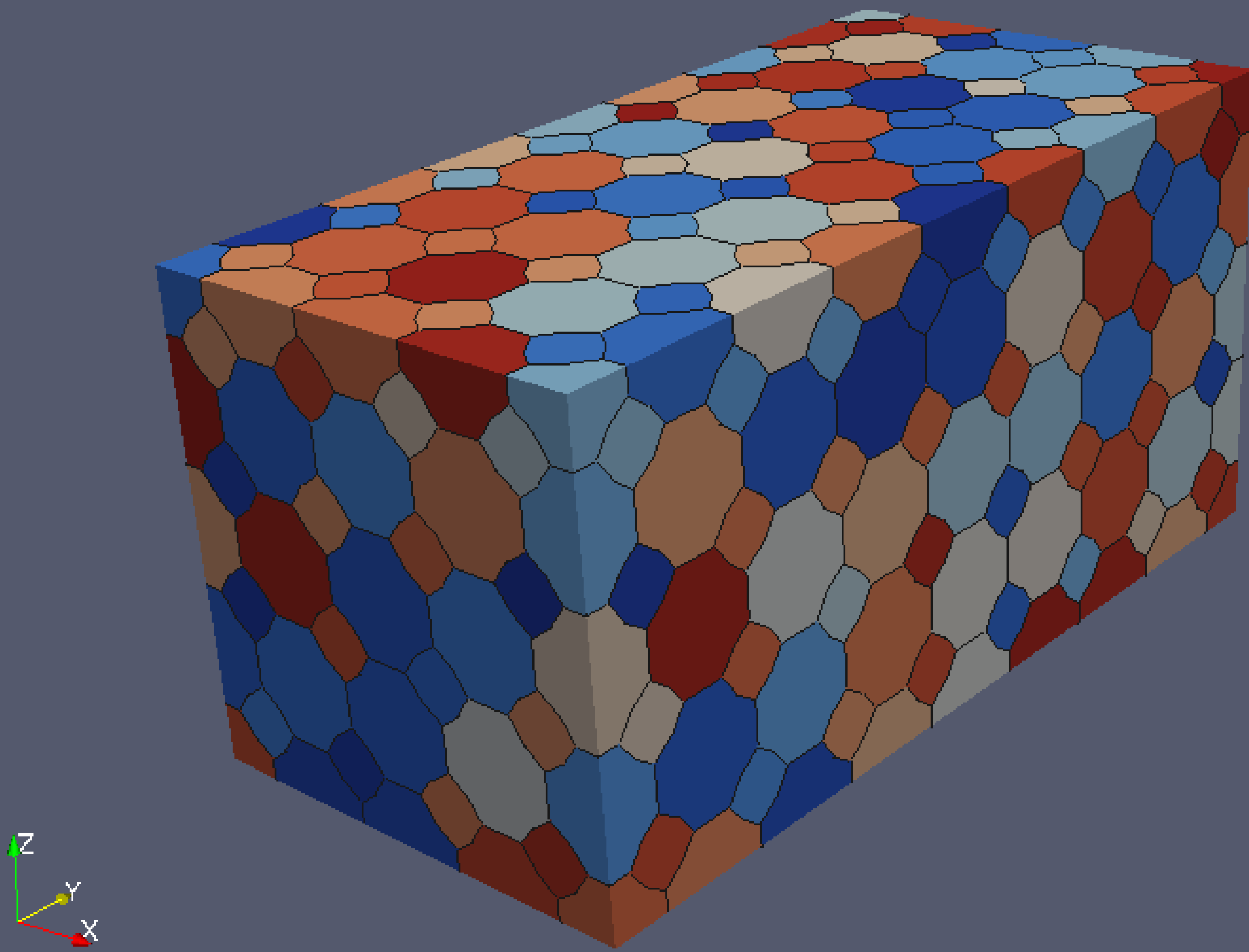
$$\frac{d\lambda}{dt} = Z(1-\lambda)\exp\left(-\frac{ER}{\theta}\right)$$

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

R	8.314 J/mol/K
E	196.742×10^3 J/mol
Z	6.3×10^{19} s^{-1}

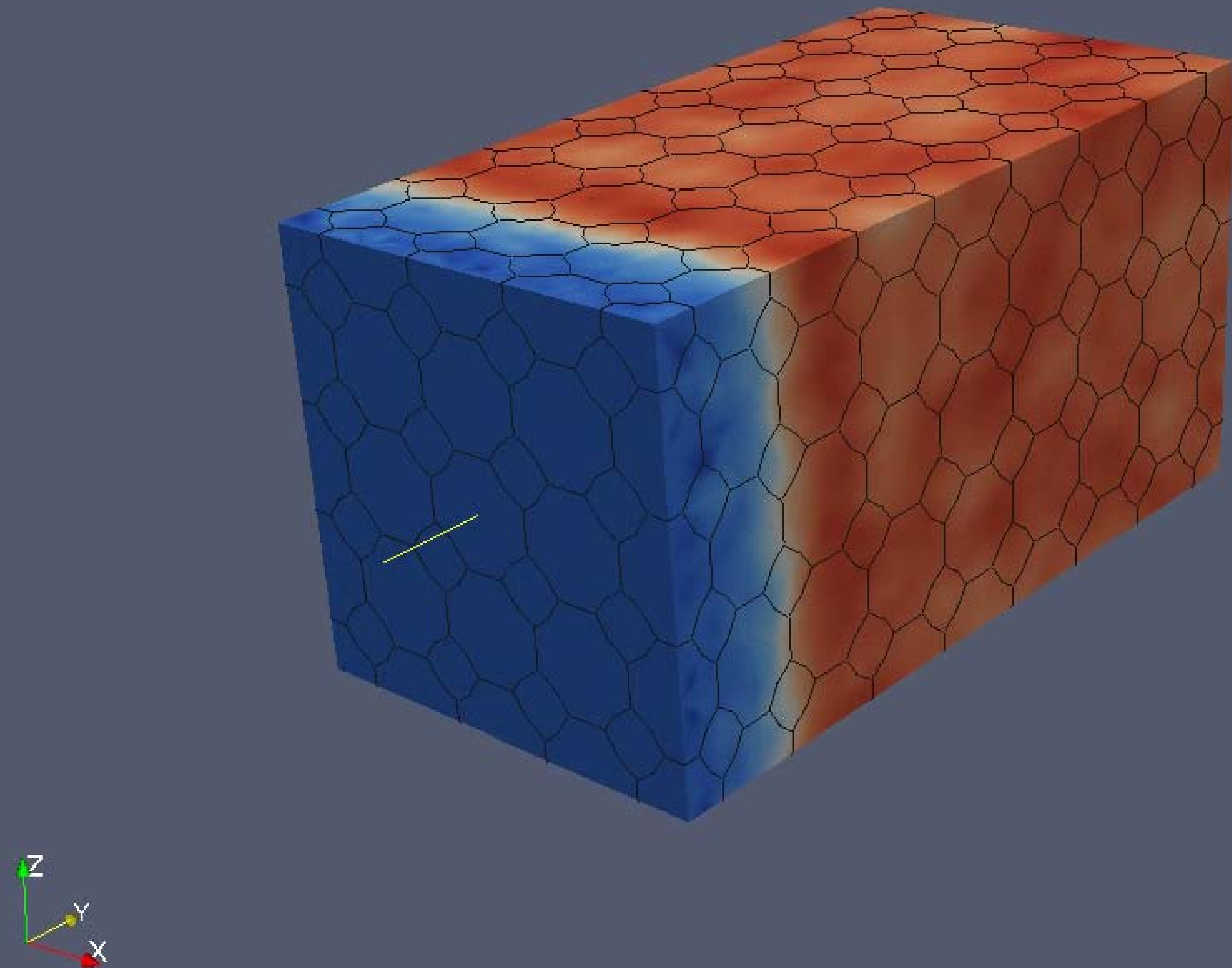
- Temperature computed assuming adiabatic heating, full conversion of plastic work to heat, heat capacity

High-Explosives Detonation Initiation

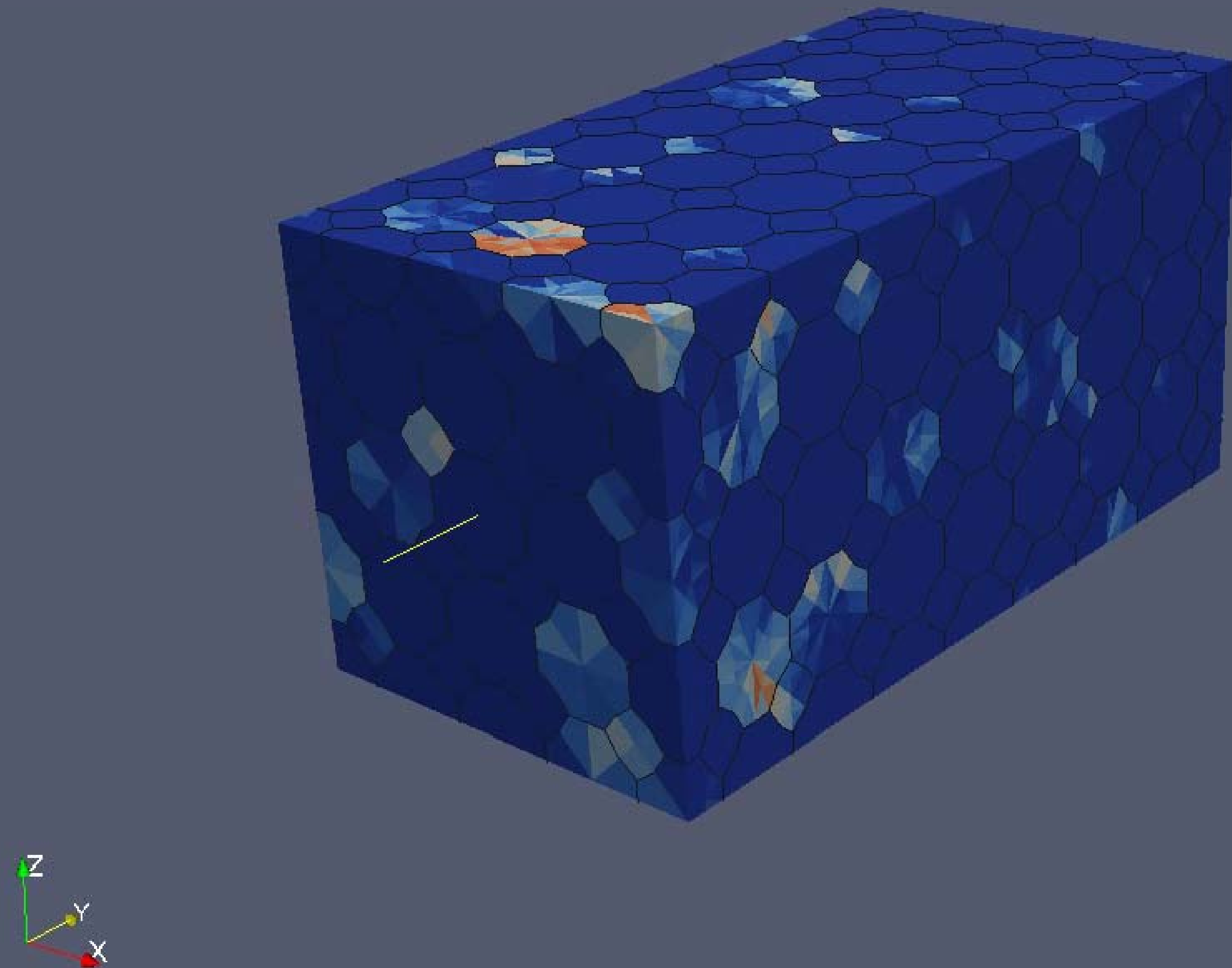


Polycrystal model and grain boundaries

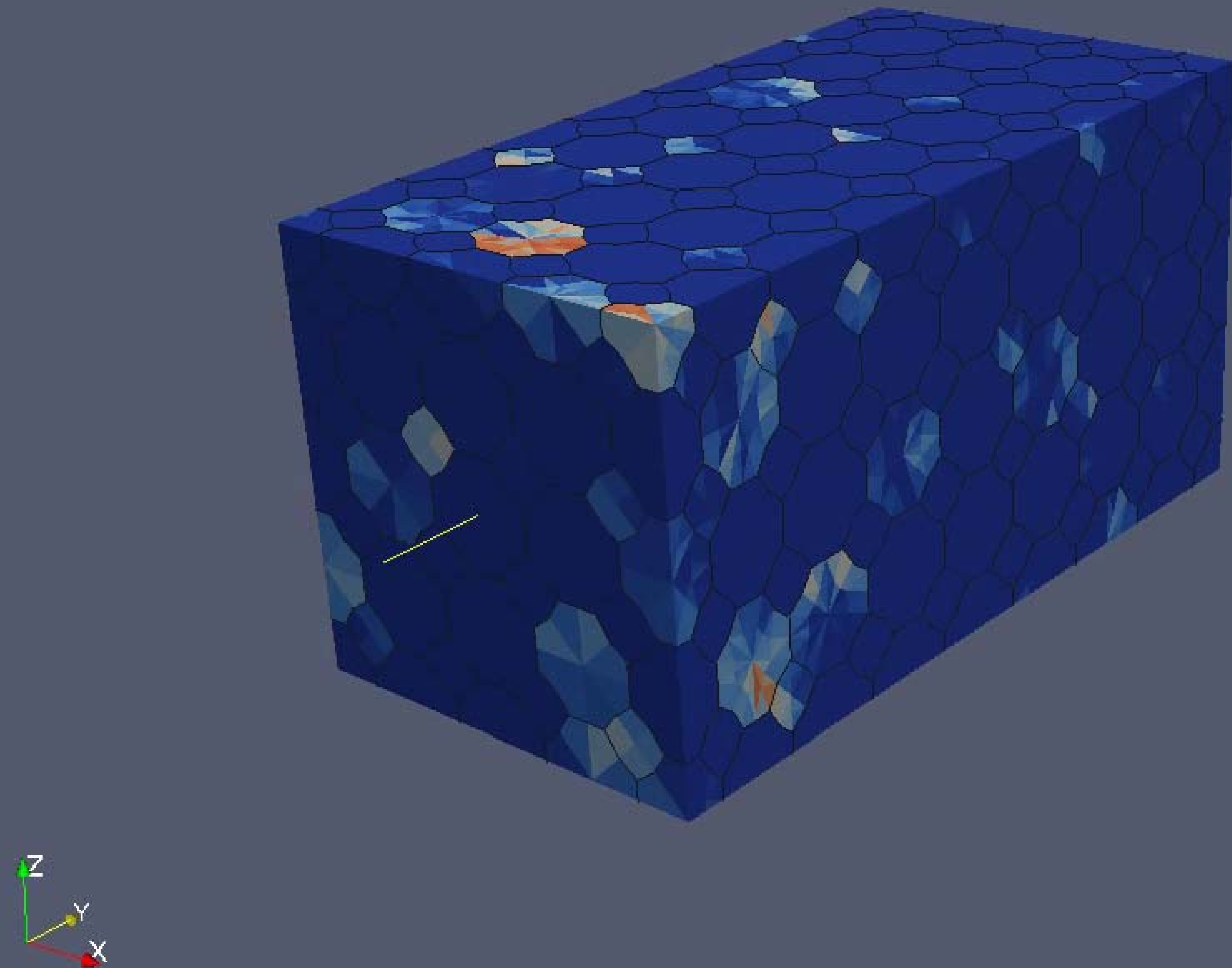
PETN plate impact - Velocity



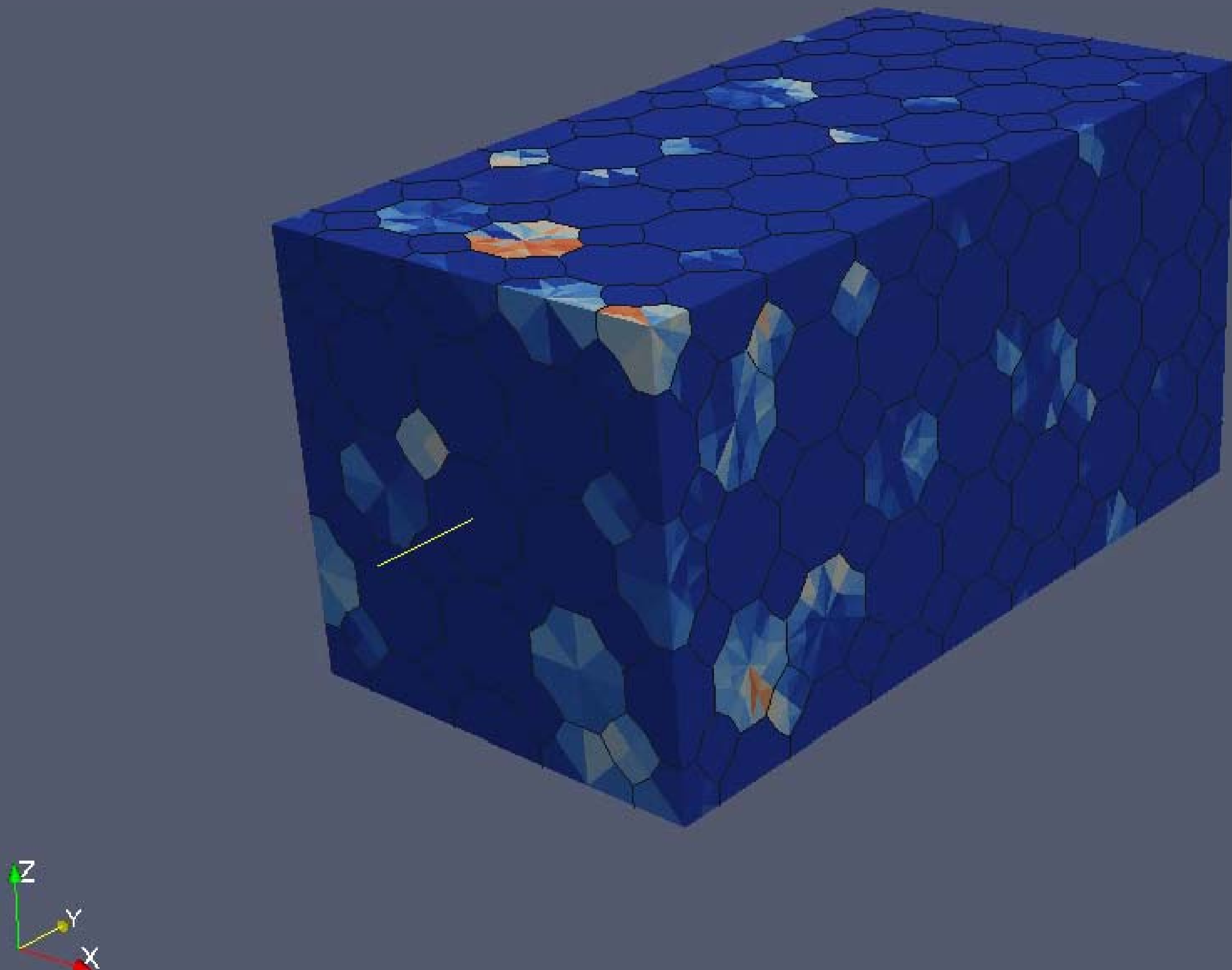
PETN plate impact - temperature



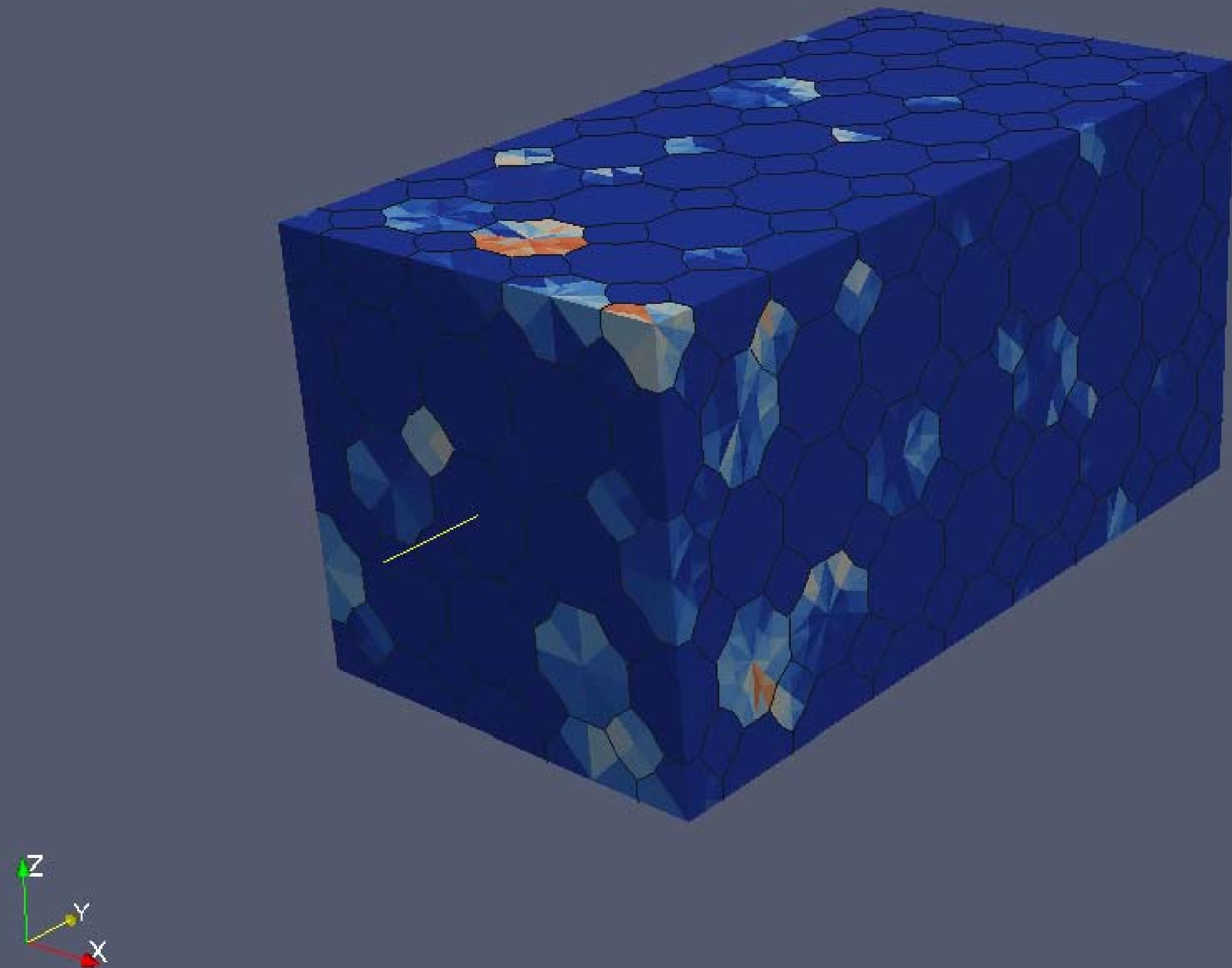
PETN plate impact - temperature



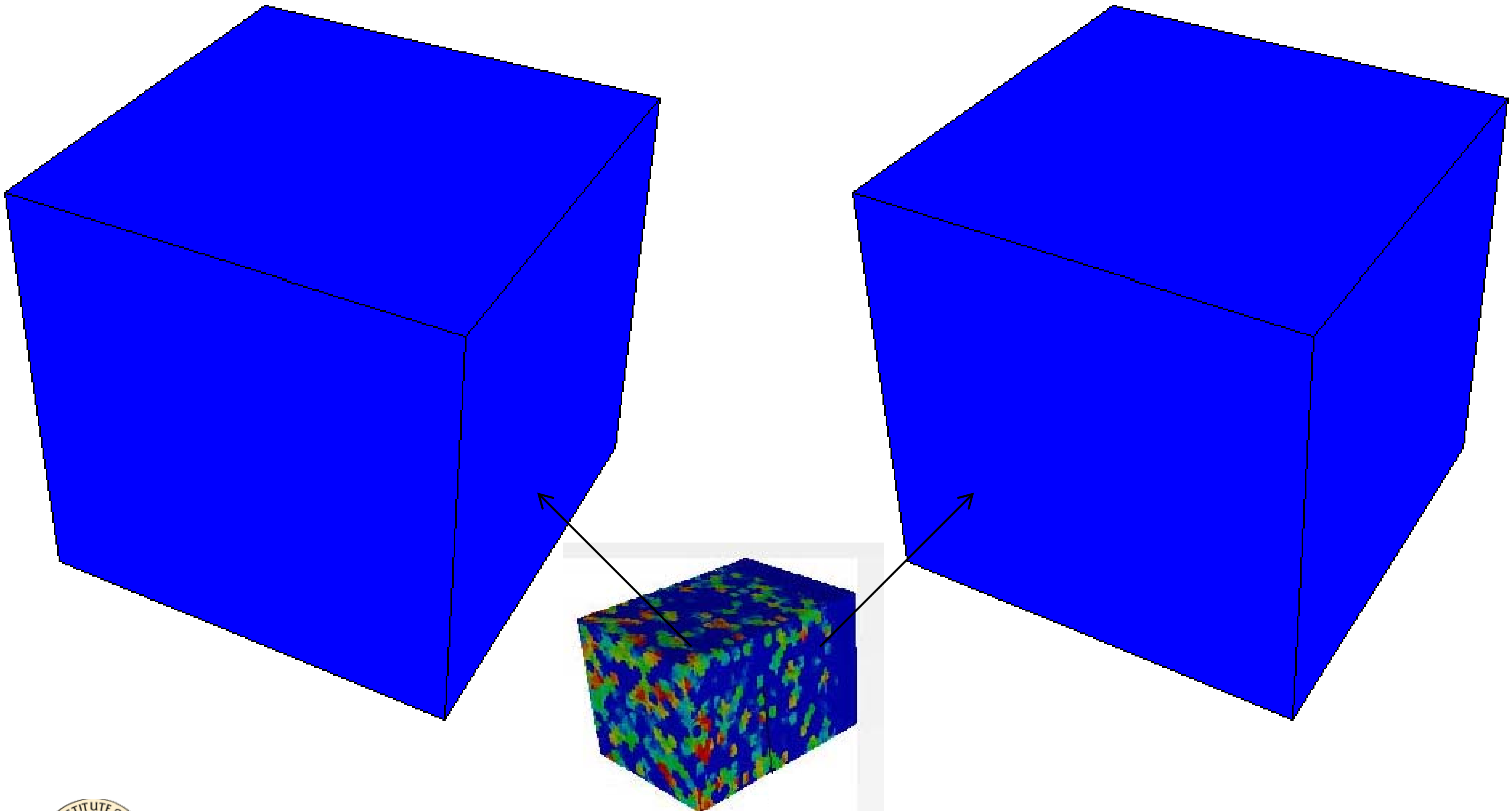
PETN plate impact - temperature



PETN plate impact - temperature



PETN plate impact – Subgrain microstructures



Microstructure evolution at selected material points

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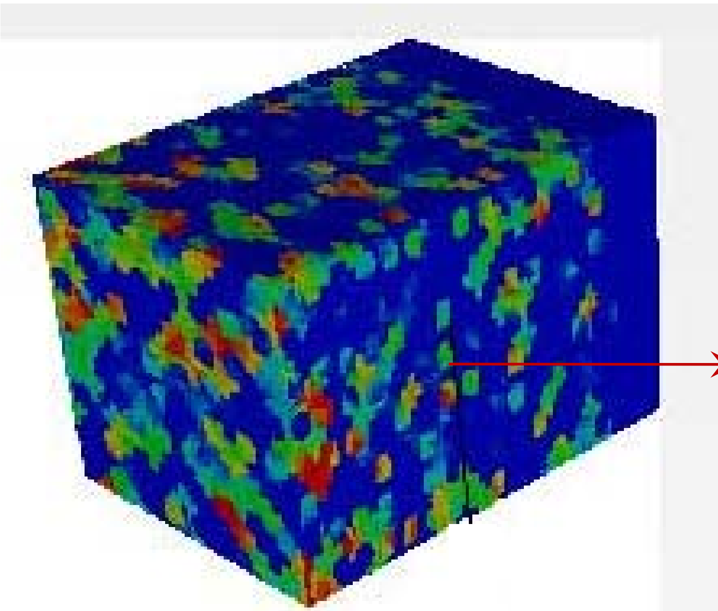
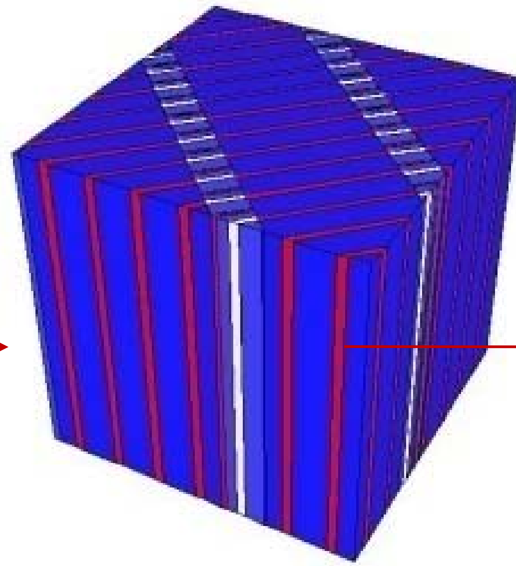
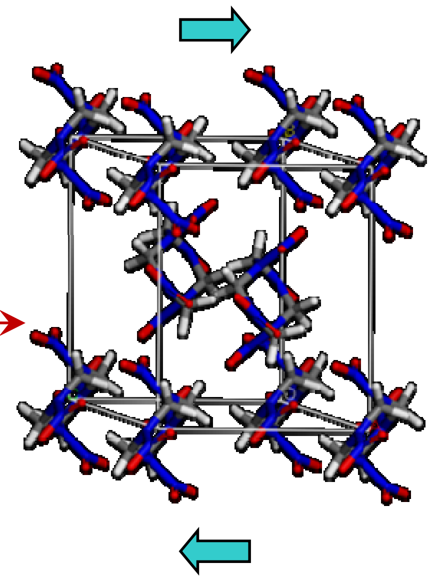
PETN plate impact – Hot-spot analysis



direct numerical simulation of polycrystalline PETN

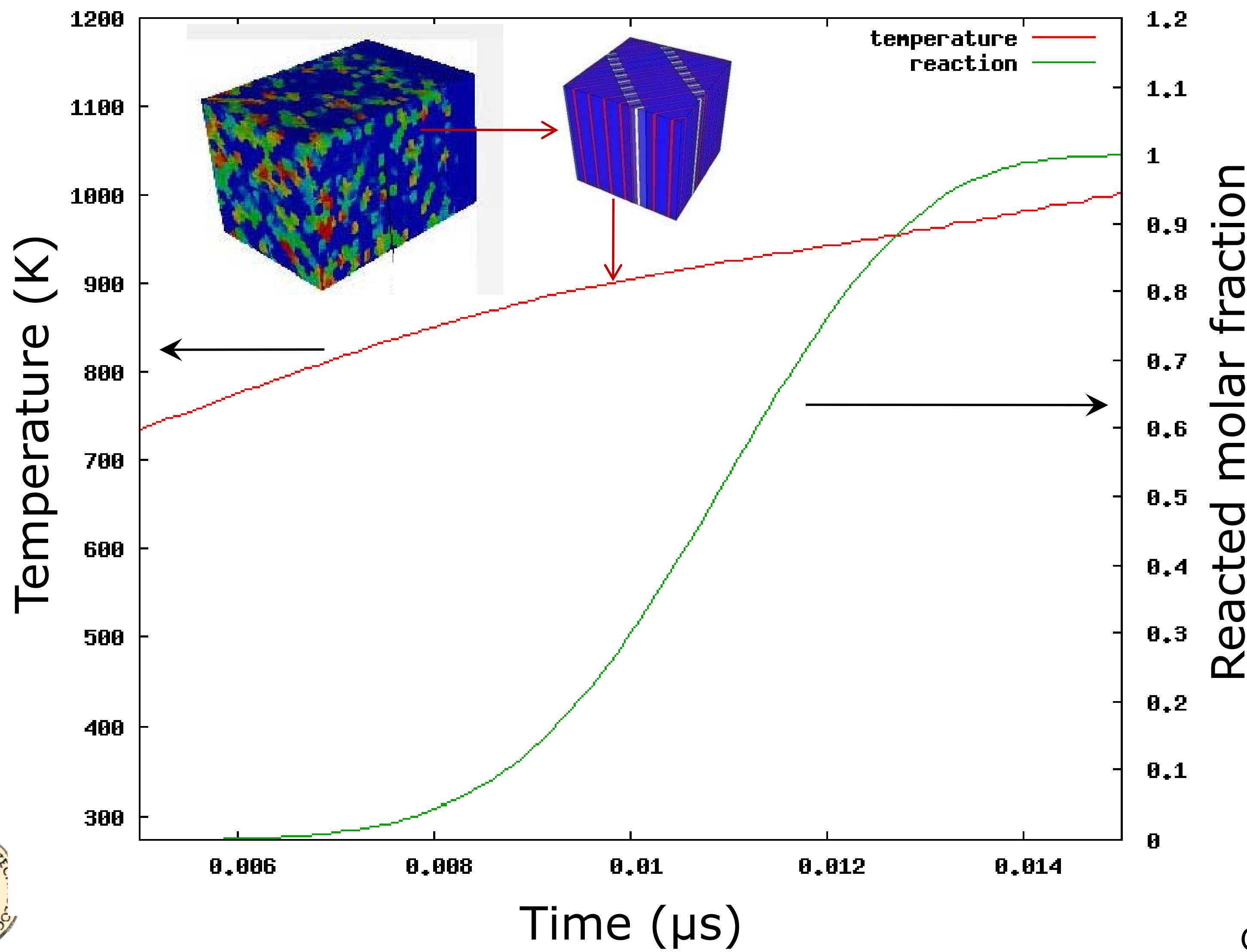


reconstructed microstructure at selected material points



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

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



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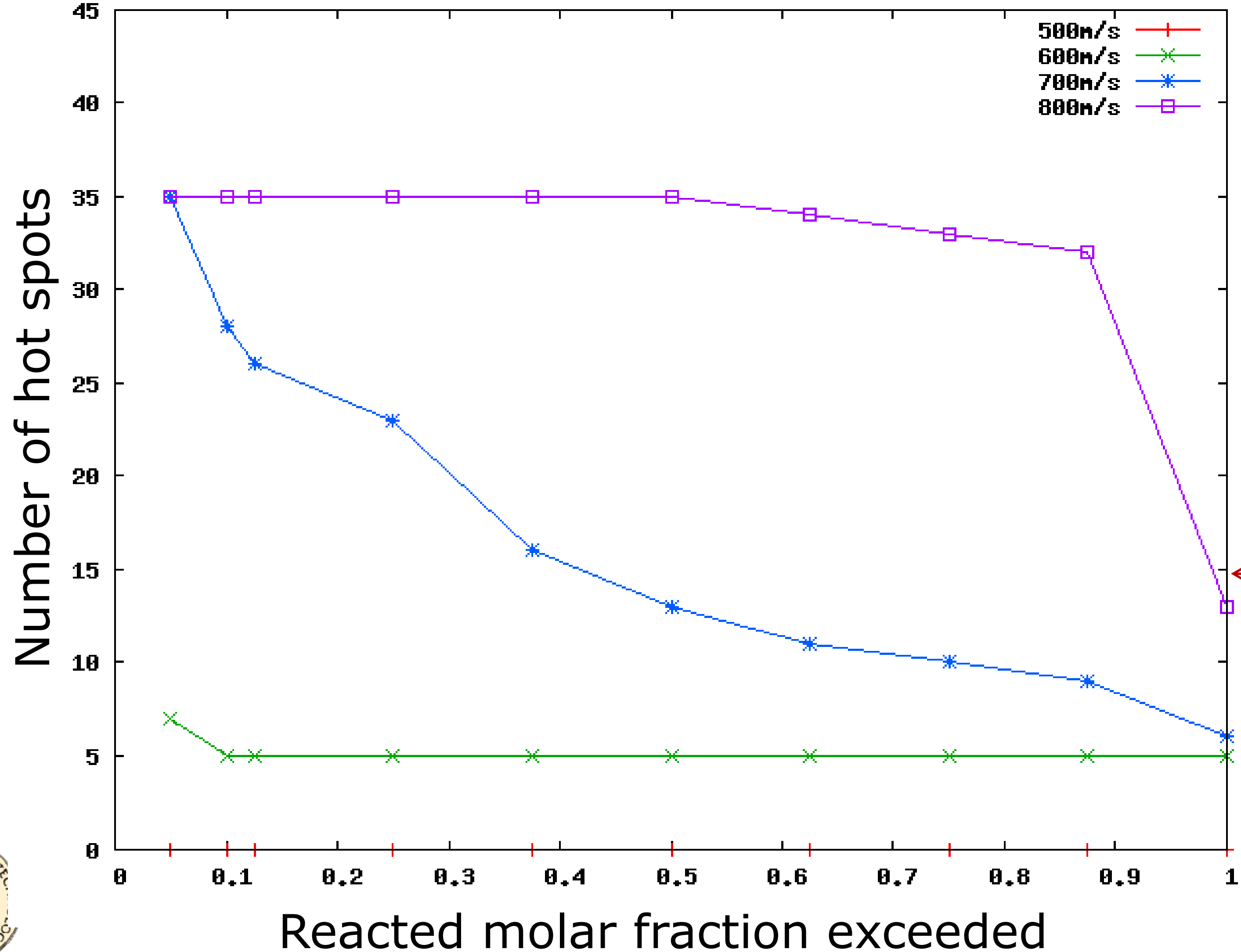
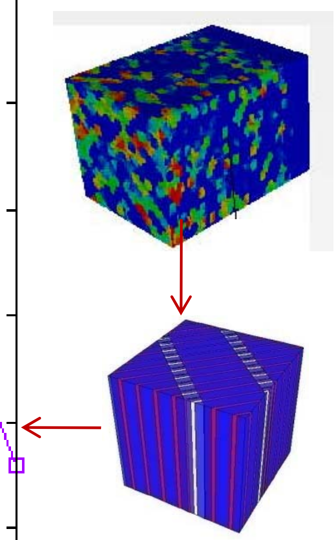
PETN plate impact - Number of hot spots





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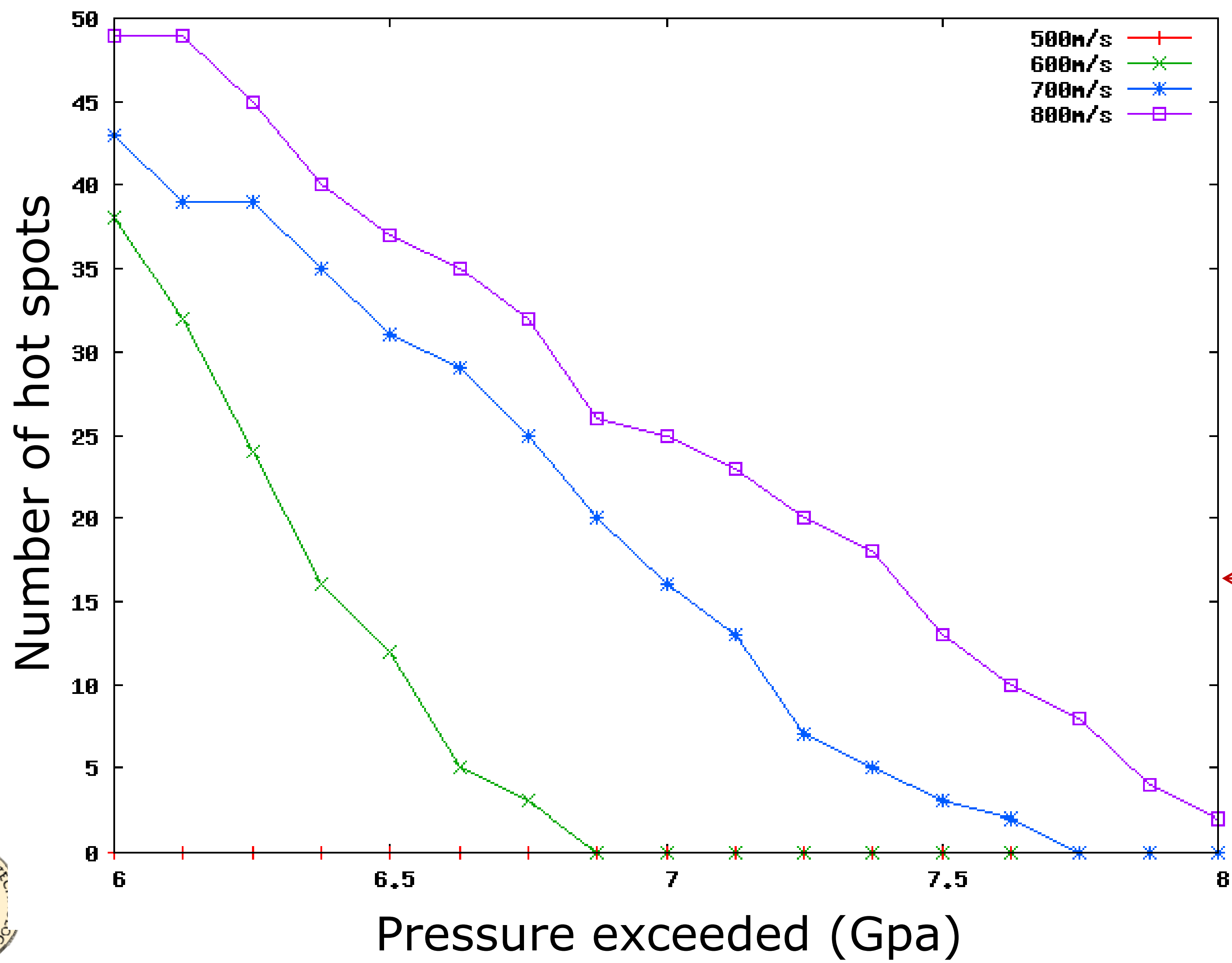
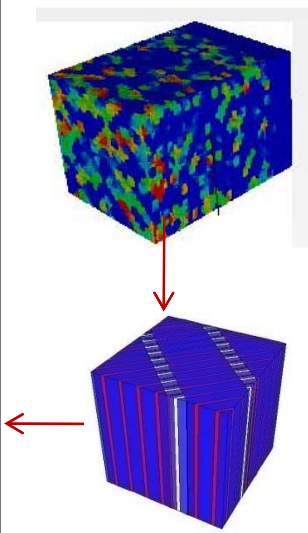
PETN plate impact - Number of hot spots





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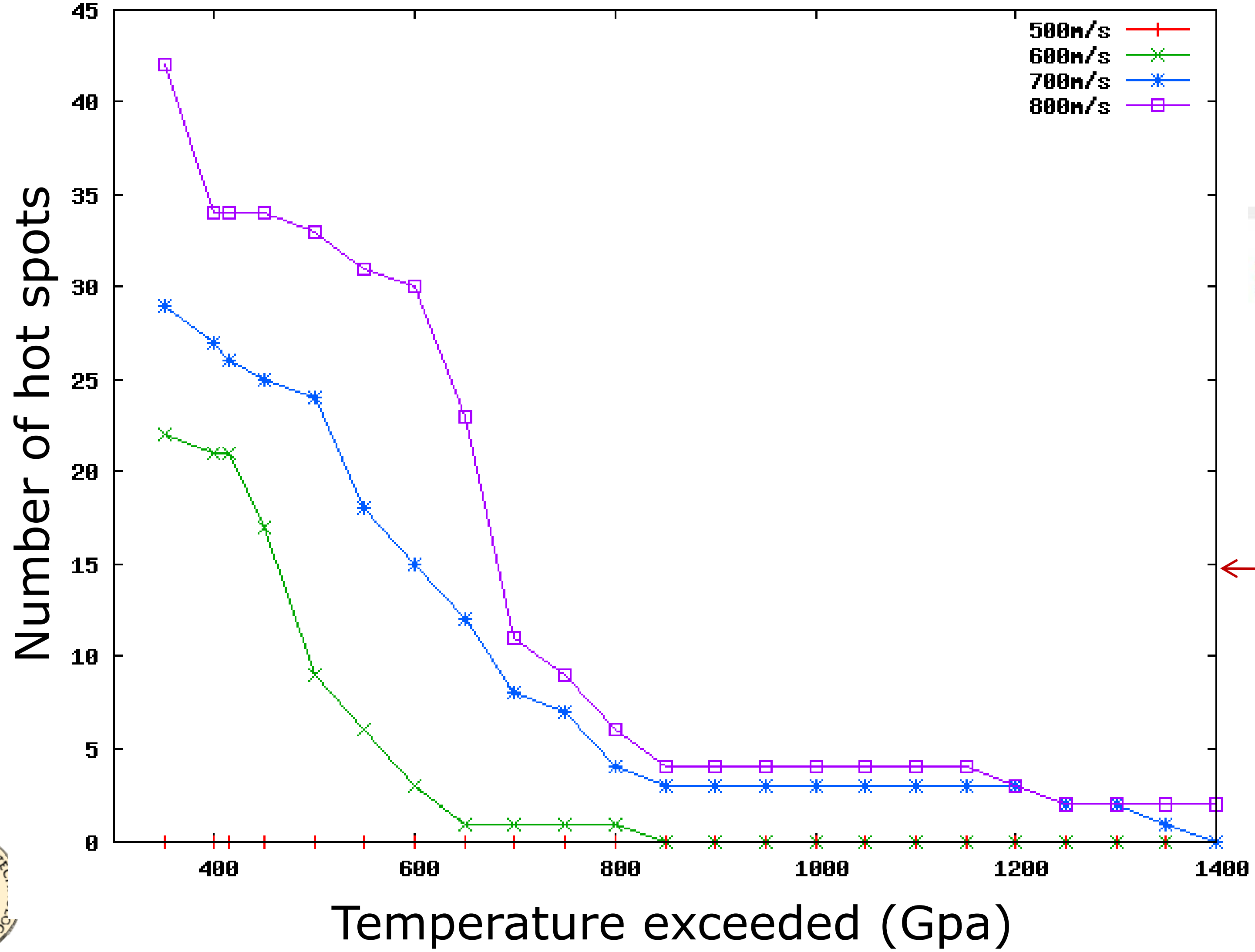
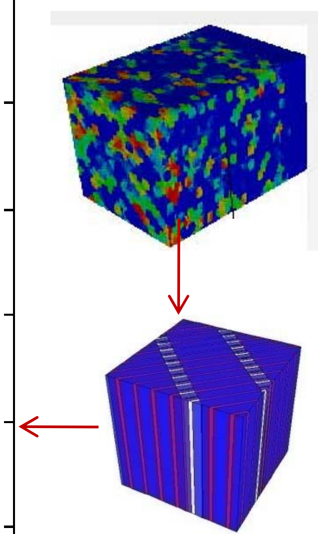
PETN plate impact - Number of hot spots





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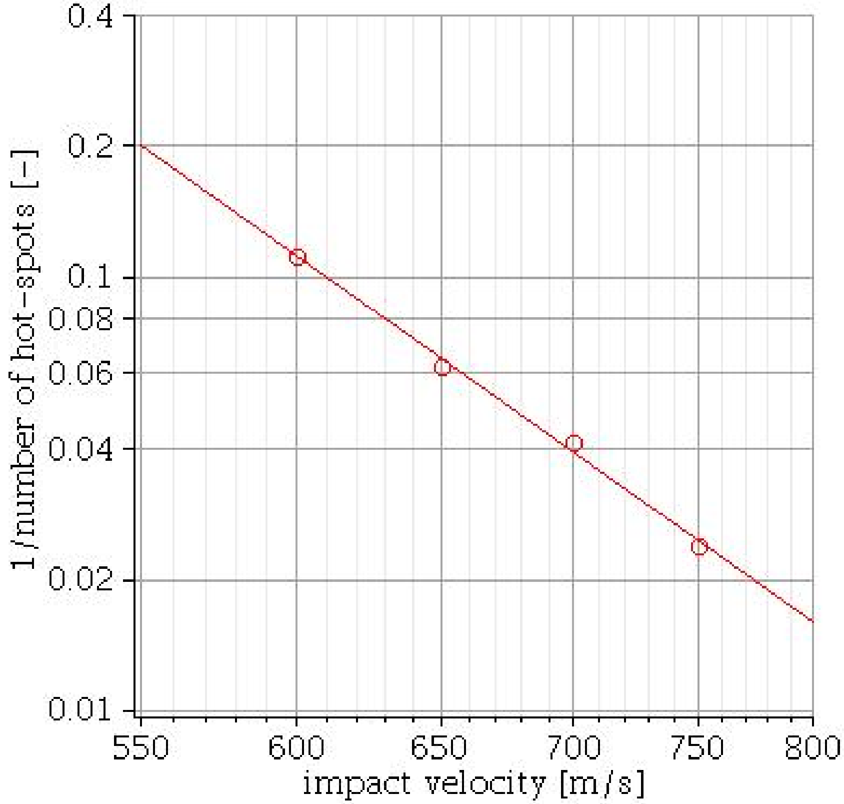
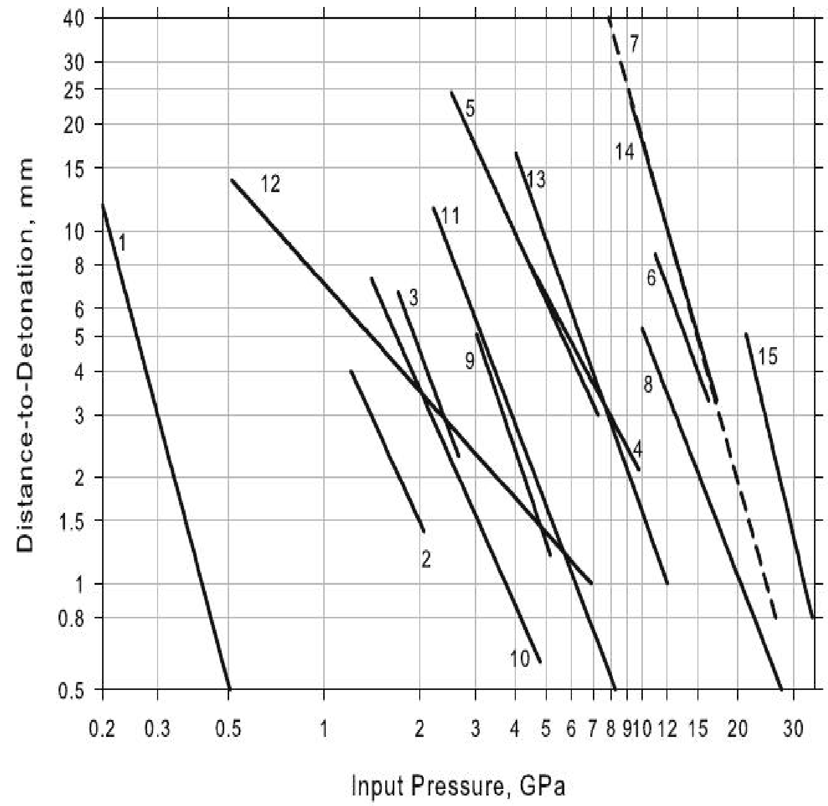
PETN plate impact – pop-plots



Multiscale model



Sheffield and Engelke [2009]

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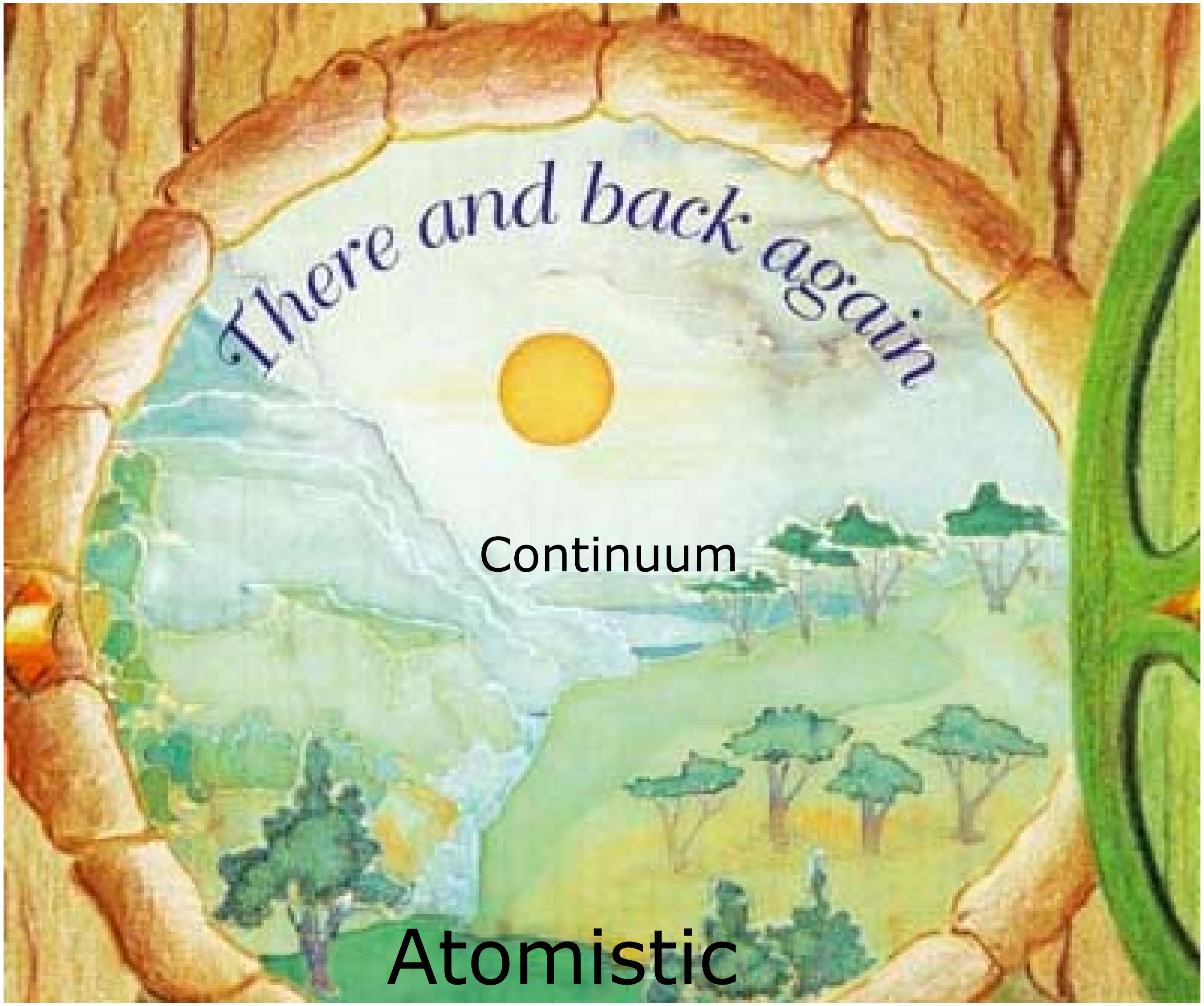
Concluding remarks

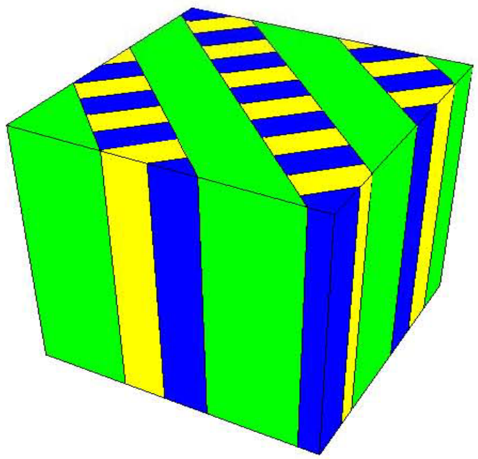
- Multiscale scheme bridges:
  - *Macroscopic scale*
  - *Polycrystalline structure*
  - *Subgrain heterogeneous slip*
- Calculations are based on relaxed model → Can simulate large samples over long times
- Subgrain deformation microstructures reconstructed *a posteriori* → B.C. for detailed atomistic calculations including chemistry
- Limitations of present capability:
  - *Static relaxation: Need relaxation theory that accounts for kinetics and inertia*
  - *Linearized kinematics: Need relaxation of crystal plasticity at large strains*

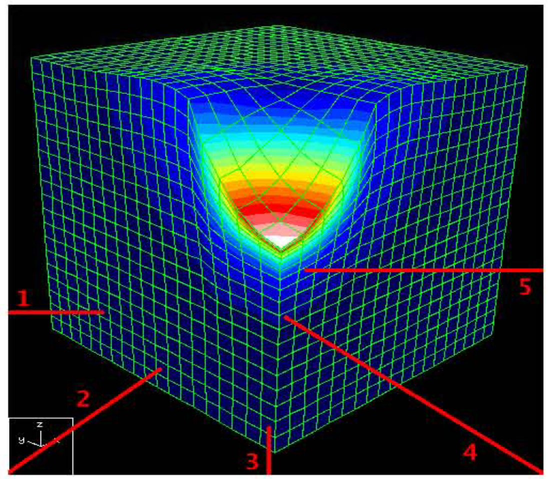
Atomistic to Continuum (and back again)



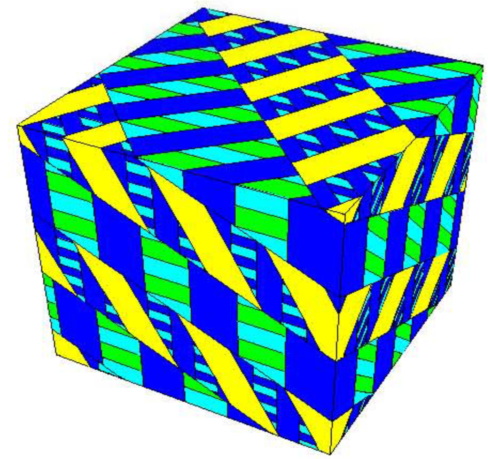
Relaxation – Fast multiscale models

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

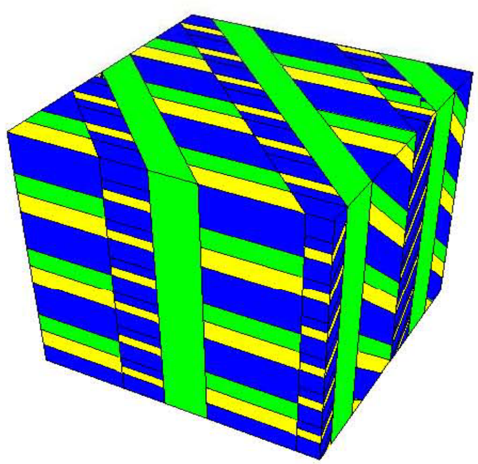




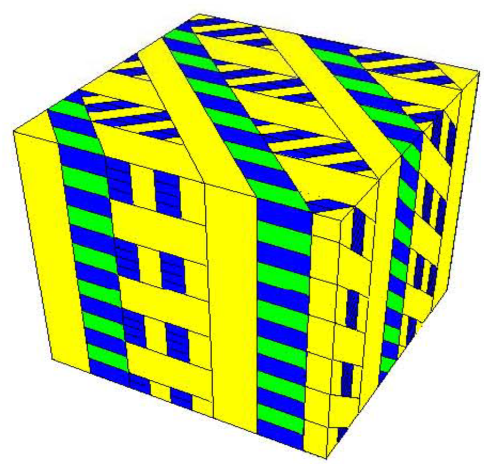
rank 4/14, $|\gamma|_\infty$ = 0.43



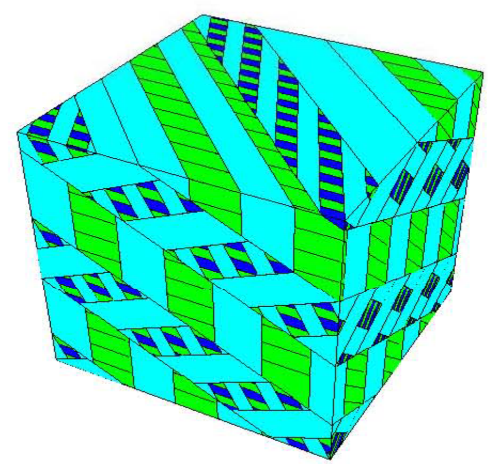
rank 4/12, $|\gamma|_\infty$ = 0.02



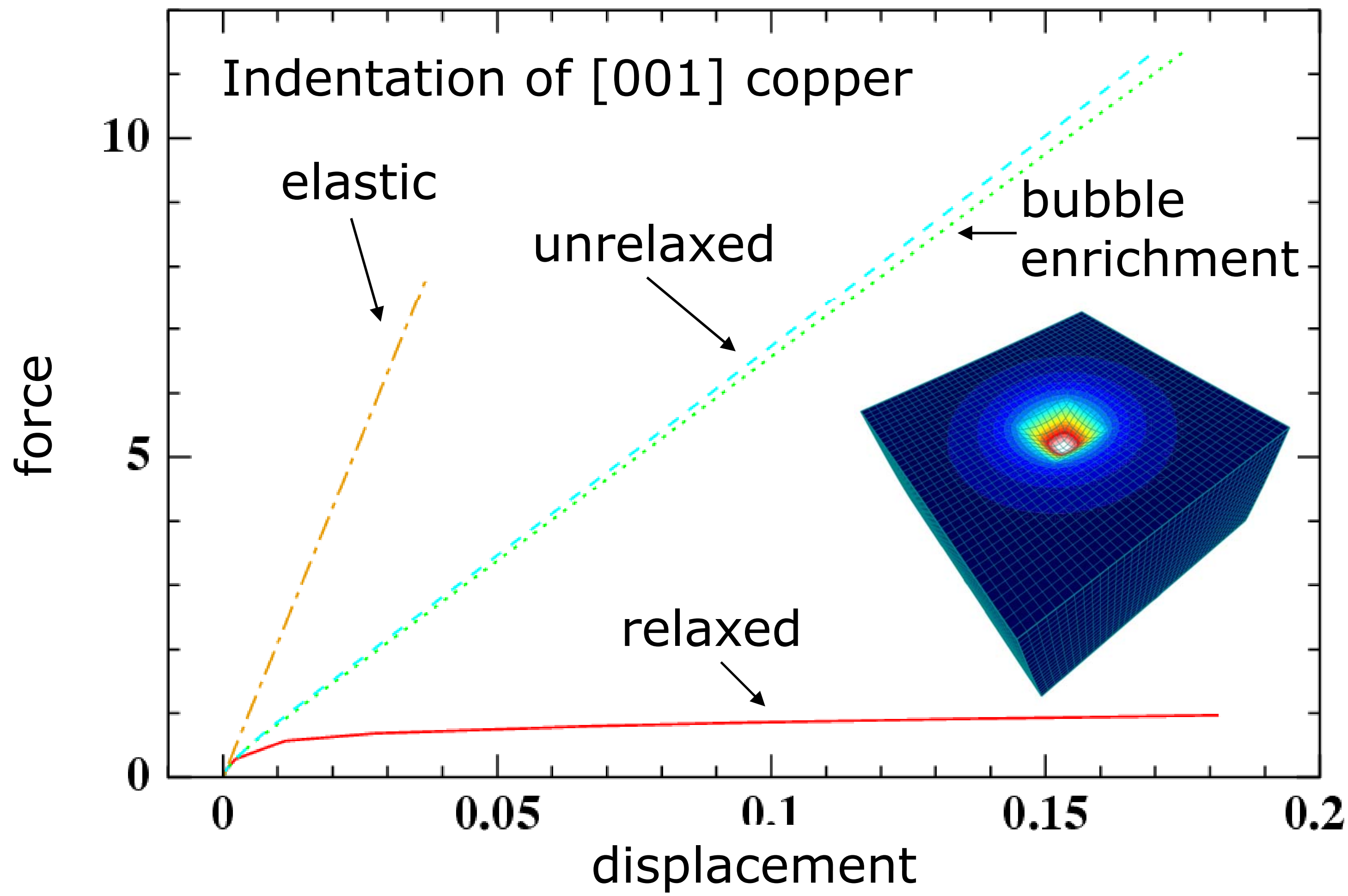
rank 4/6, $|\gamma|_\infty$ = 0.026



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



Relaxation – Fast multiscale models



(S Conti, P Hauret and M Ortiz, *SIAM Multiscale Model. Simul.* **6**(1), 2007, pp. 135–157)