Multiscale modeling of materials: Linking microstructure and macroscopic behavior

M. Ortiz
California Institute of Technology

In collaboration with: E. Gurses, J.J. Rimoli

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Multiscale Modeling & Simulation

- Interest in multiscale modeling and simulation has undergone a notable resurgence over the past decade...
- However, multiscale analysis also enjoys a long tradition in a number of guises, including:
  - *Statistical physics*
  - *Structure-property relations in material science*
  - *Homogeneization*
  - *Micromechanics...*
- Why multiscale modeling and simulation now?
- What is different from previous approaches to the subject?

Multiscale Modeling & Simulation - ASC

- President Clinton in 1993 committed the United States to a global ban on underground nuclear testing, and on Sept. 24, 1996, he signed the Comprehensive Test Ban Treaty at the United Nations
- In the absence of underground testing: use modeling and simulation—requiring unprecedented levels of computing power—to certify the safety and reliability of a reduced U.S. nuclear weapons stockpile
- ASCI is DOE's 10-year, $2 billion program, that was formed to develop the high-resolution, three-dimensional physics modeling needed to evaluate the aging nuclear stockpile

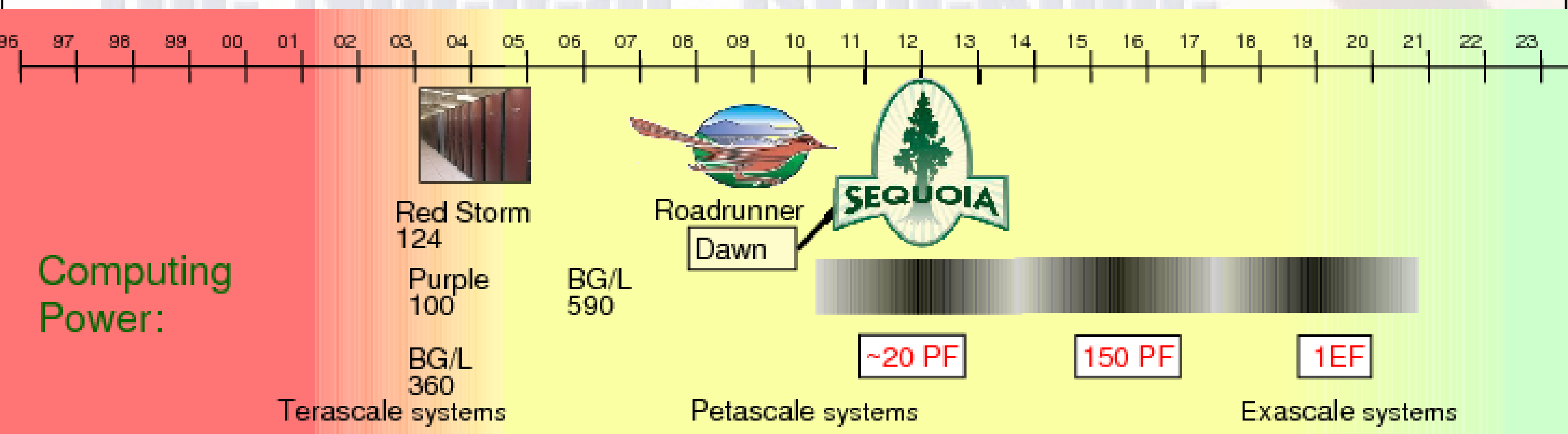
Multiscale Modeling & Simulation

- Present day MM&S emphasizes:
  - *Petascale to exascale massively parallel computing*
  - *High-resolution 4D geometry*
  - *High-fidelity physics, chemistry*
  - *Predictivity (validation, verification, certification)*
- ...with main focus on:
  - *System behavior under extreme dynamical conditions: pressure, temperature, strain rate...*
  - *Complex physics: Deformation microstructures, phase transitions, excited states, chemistry, phenomena far away from equilibrium, failure mechanisms...*
- ...intersects with:
  - *High-performance computing*
  - *Applied physics, materials science*
  - *Probability, uncertainty quantification*

Multiscale Modeling & Simulation - ASC

Purple – 0.1PF/s

BlueGene/L – 0.4



Roadmap to exascale computing

Multiscale Modeling & Simulation
ASC/ASAP → ASC/PSAAP

STANFORD UNIVERSITY
PSAAP

CALIFORNIA INSTITUTE OF TECHNOLOGY 1891
CALTECH PSAAP

PRISM
NNSA Center for Prediction of Reliability, Integrity and Survivability of Microsystems

PURDUE UNIVERSITY

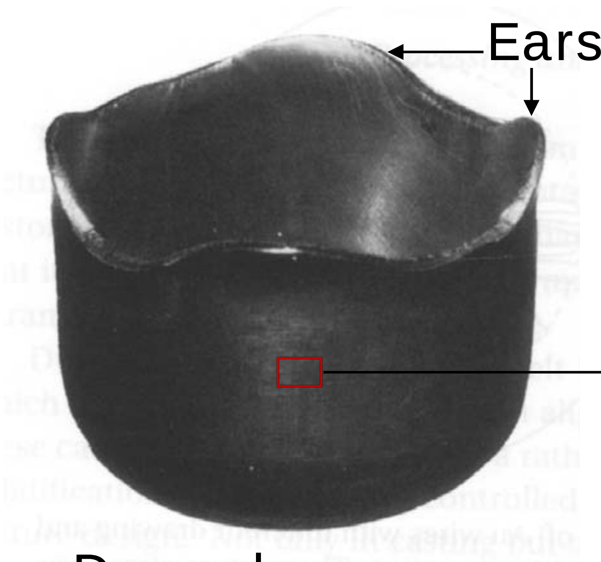
CENTER FOR RADIATIVE SHOCK HYDRODYNAMICS
MICHIGAN

ICES
The Institute for Computational Engineering and Sciences

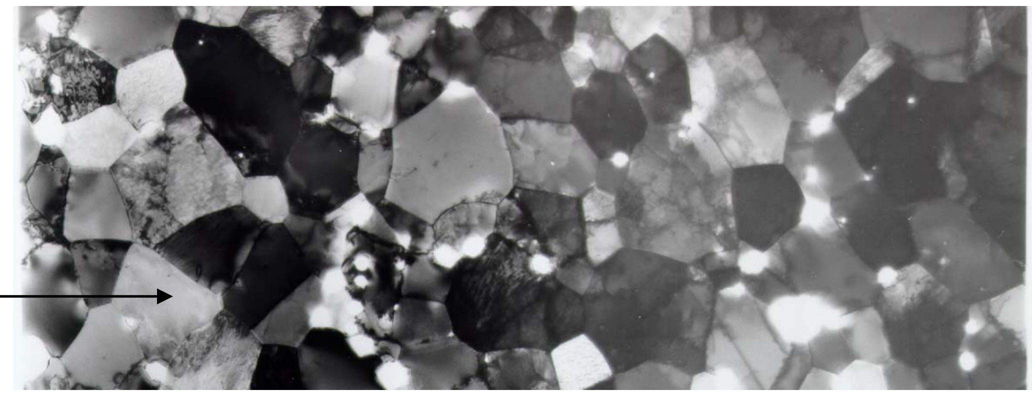
THE UNIVERSITY OF TEXAS AT AUSTIN

ASC/PSAAP Centers

MS&S – Limitations of empirical models



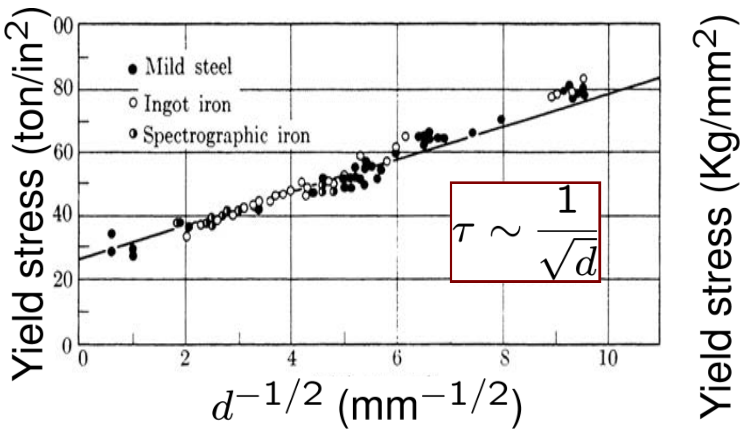
Deep-drawn cup



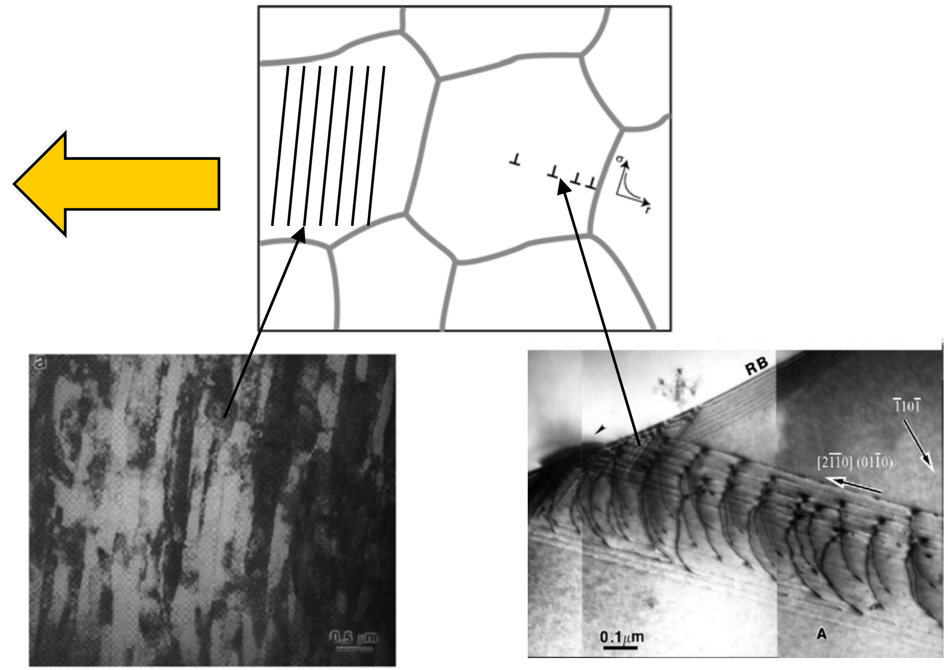
Grain structure of polycrystalline W
(Courtesy of Clyde Briant)

- Conventional engineering plasticity models fail to predict earing in deep drawing
- Prediction of earing requires consideration of polycrystalline structure, texture development

MS&S — Limitations of empirical models



Hall-Petch scaling
(NJ Petch,
J. Iron and Steel Inst.,
174, 1953, pp. 25-28.)



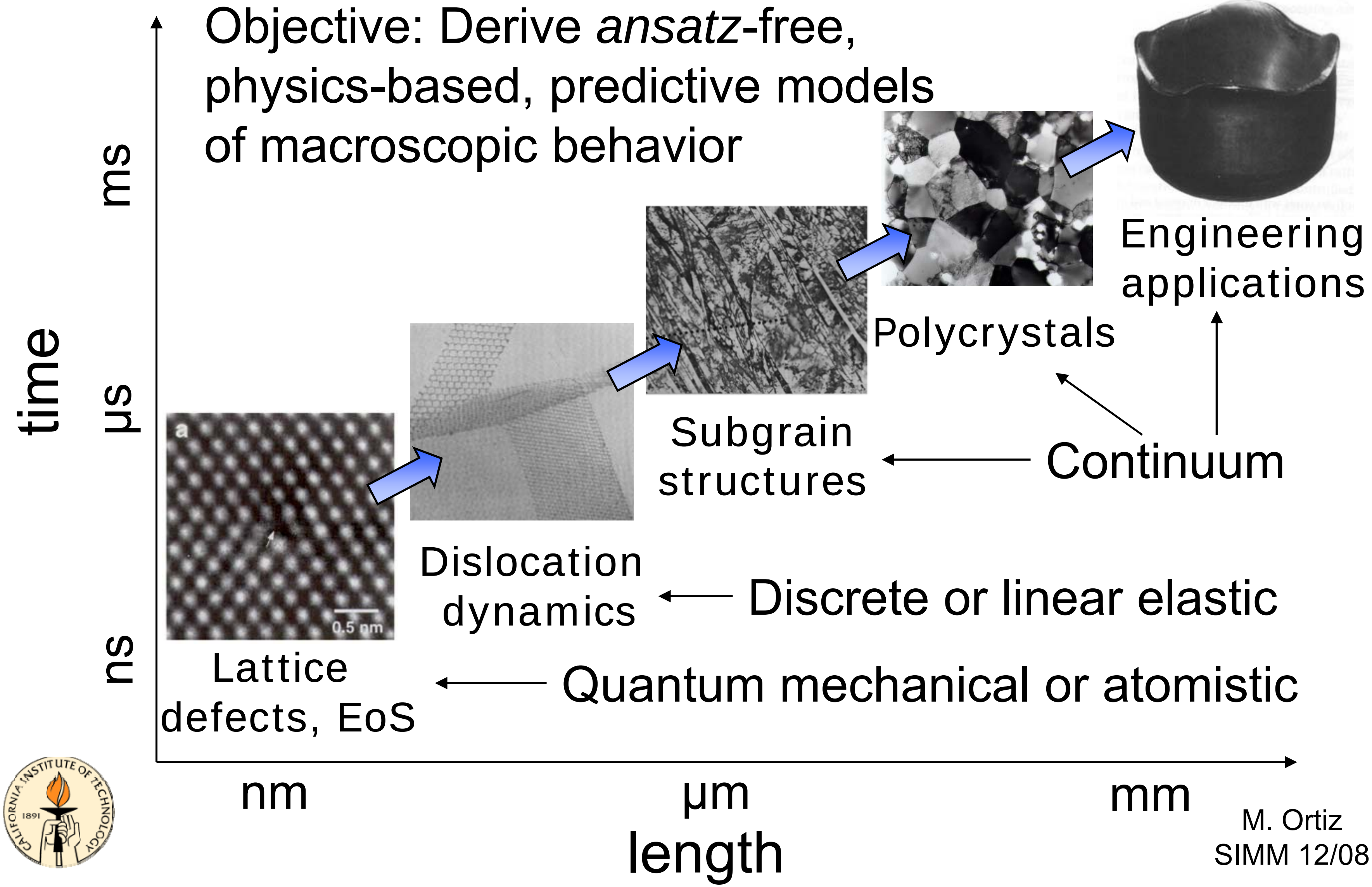
Lamellar structure in shocked Ta (MA Meyers et al´95)

Dislocation pile-up at Ti grain boundary (I. Robertson)

- Conventional plasticity models fail to predict scaling, size effects.

MS&S – Metal plasticity

Objective: Derive *ansatz*-free, physics-based, predictive models of macroscopic behavior



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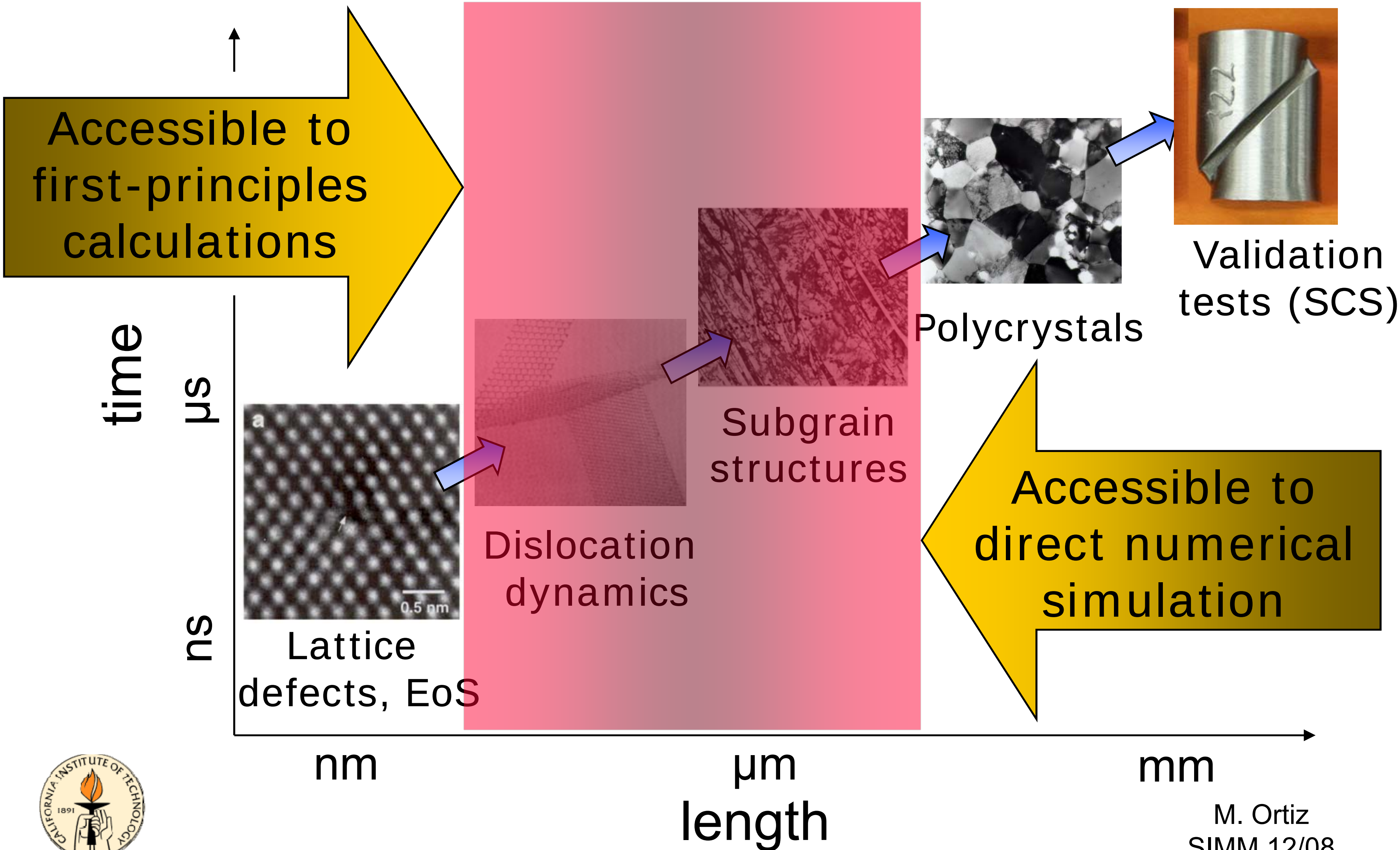
MS&S – Metal plasticity



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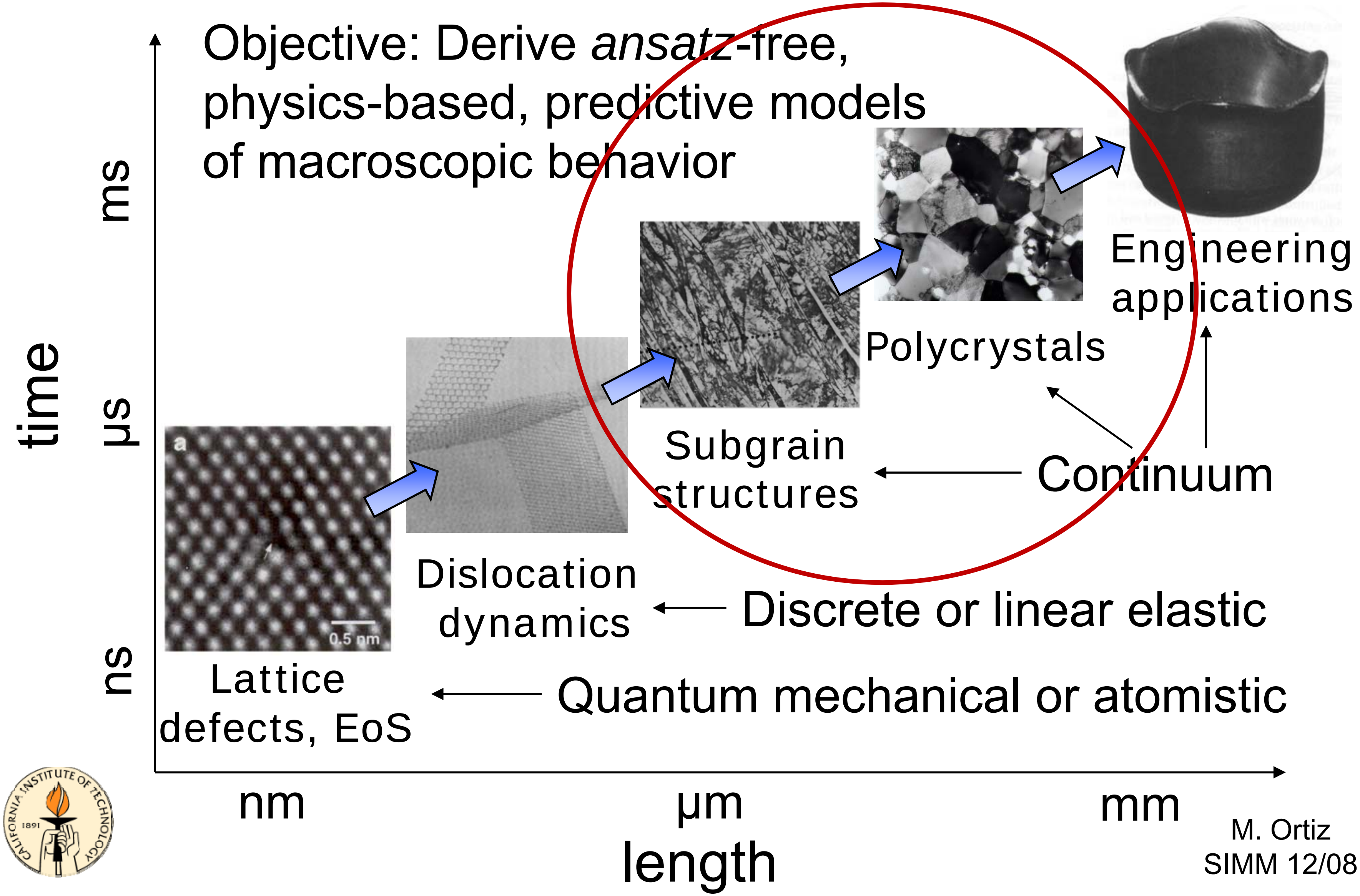
MM&S – Material modeling

- Objective: Derive *ansatz*-free, physics-based, predictive models of macroscopic behavior
- Multiscale model must account for all possible microstructures (no physics lost)
- Multiscale models must yield exact macroscopic behavior (e.g., force-displacement curves...)
- Multiscale model must allow for the *a posteriori* reconstruction of microstructures (no loss of microstructural information)
- Multiscale models must be computationally efficient: Fast Multiscale Models (FMM)
- Static problems: Calculus of variations, relaxation, Gamma convergence, scaling...

MS&S – Metal plasticity

Objective: Derive *ansatz*-free, physics-based, predictive models of macroscopic behavior



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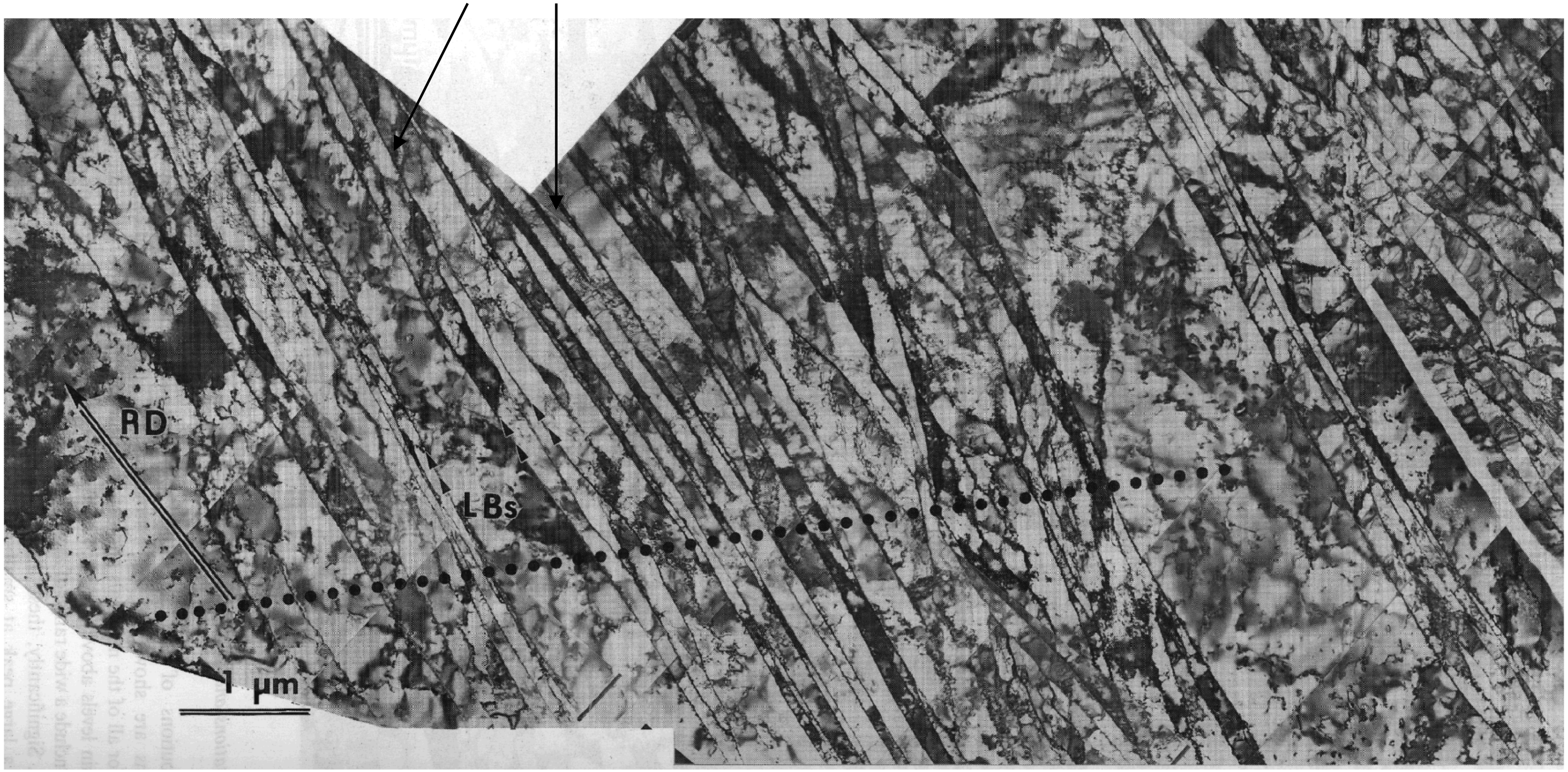
Dislocation structures

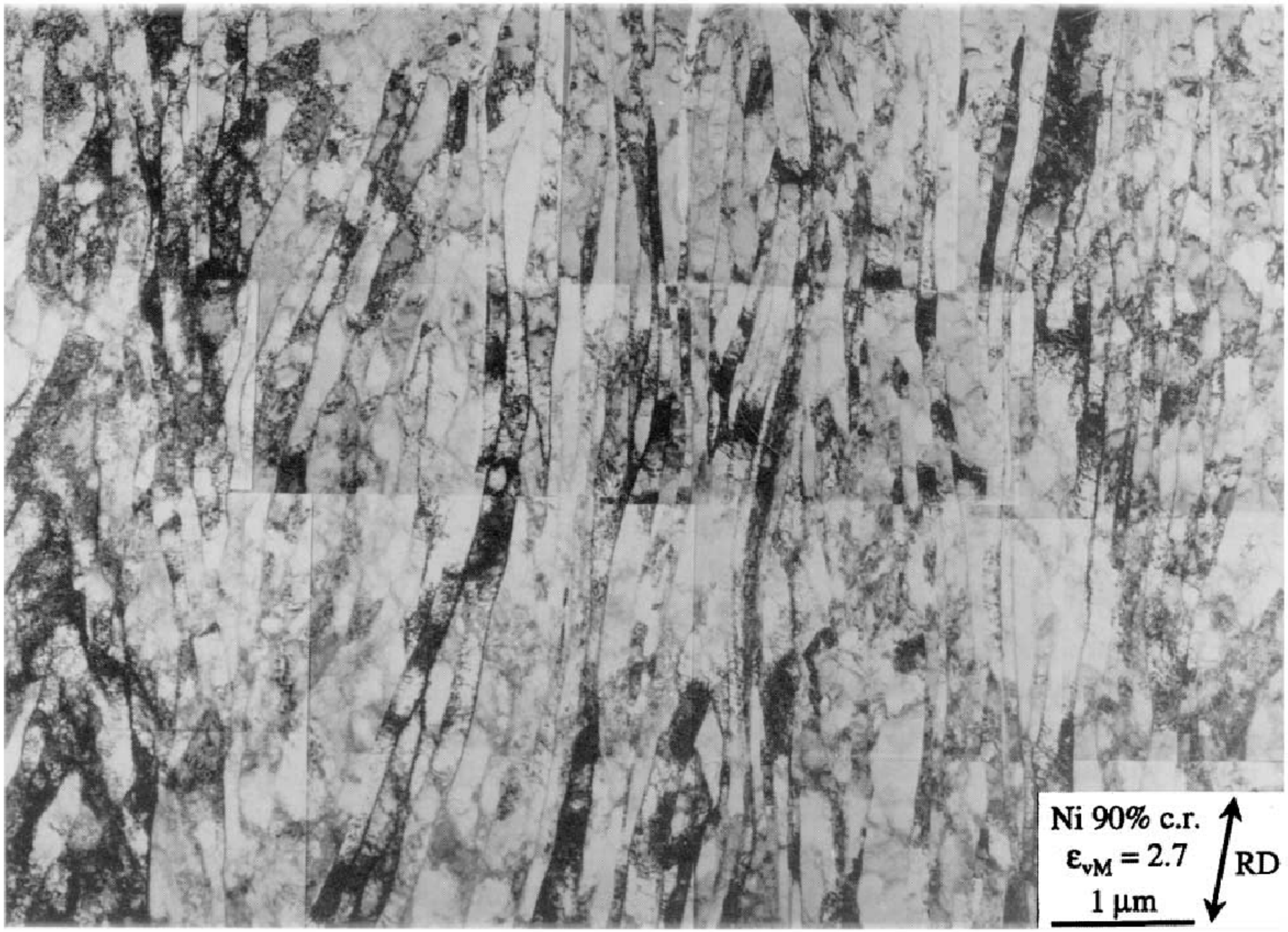
Dislocation walls



Lamellar dislocation structure in 90% cold-rolled Ta

(DA Hughes and N Hansen, Acta Materialia, 44 (1) 1997, pp. 105-112)

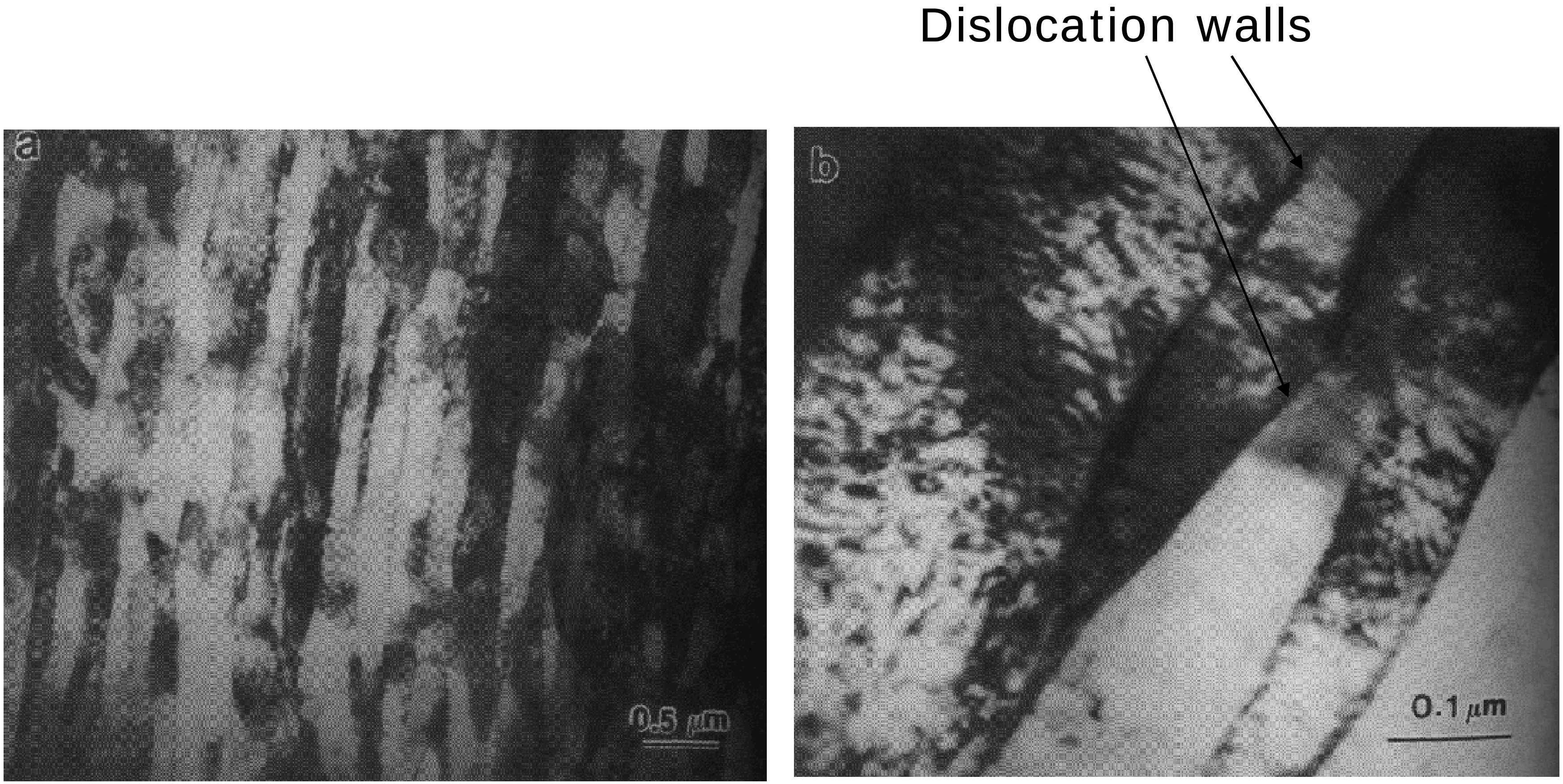
Dislocation structures



Pure nickel cold rolled to 90%

Hansen *et al.* Mat. Sci. Engin. A317 (2001)

Dislocation structures



Lamellar structures in shocked Ta

(MA Meyers et al., Metall. Mater. Trans., 26 (10) 1995, pp. 2493-2501)

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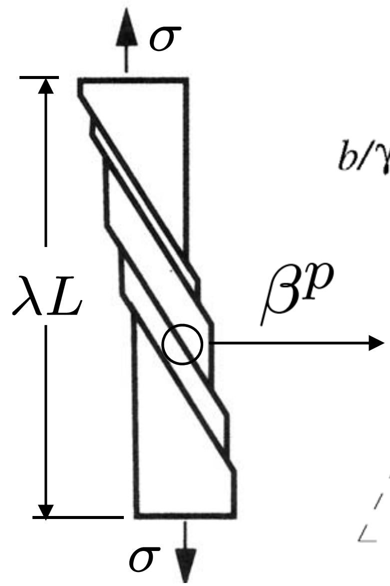
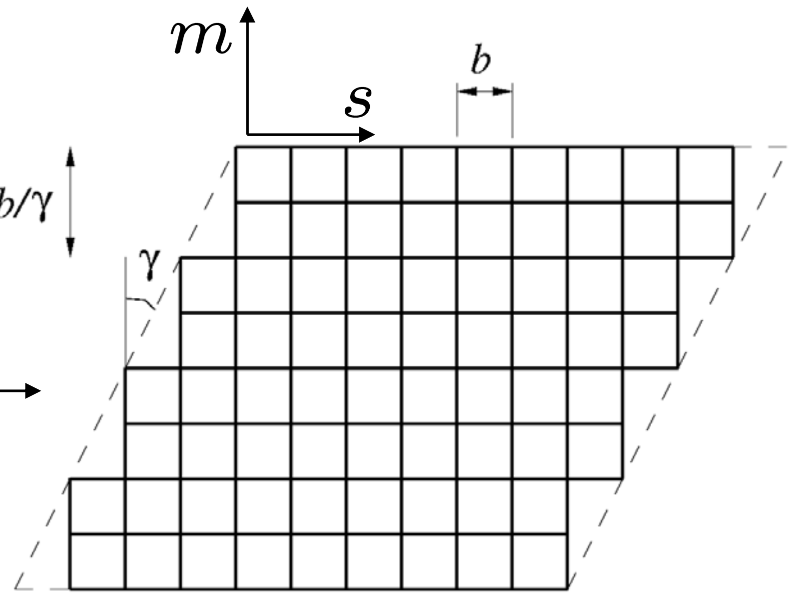
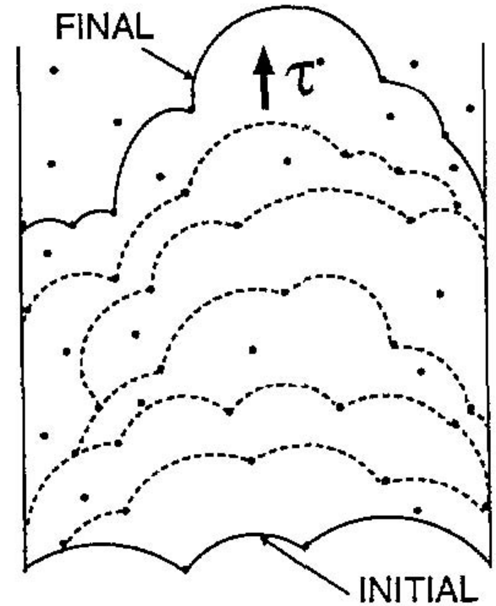
Crystal plasticity – Local







- Incremental flow rule: $\epsilon^p(\gamma) = \sum \gamma s \odot m$
- Pseudo-elastic strain energy density:

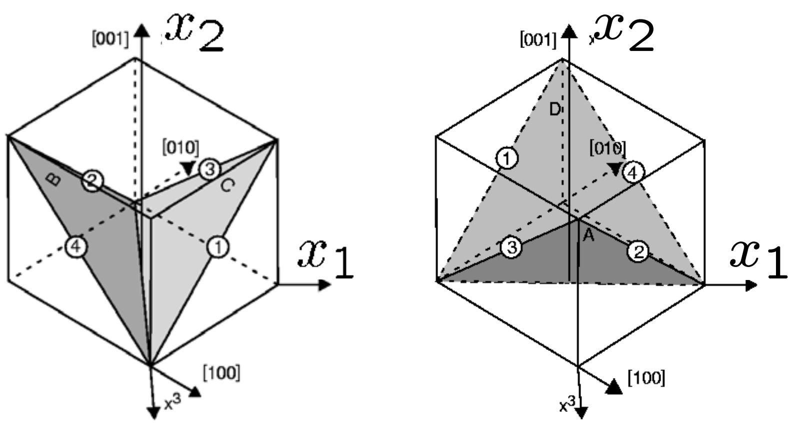
$$W(\epsilon) = \inf_{\gamma > 0} \{W^e(\epsilon - \epsilon^p(\gamma)) + W^p(\gamma)\}$$

- Variational problem (static equilibrium):

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

Non-convexity - Strong latent hardening

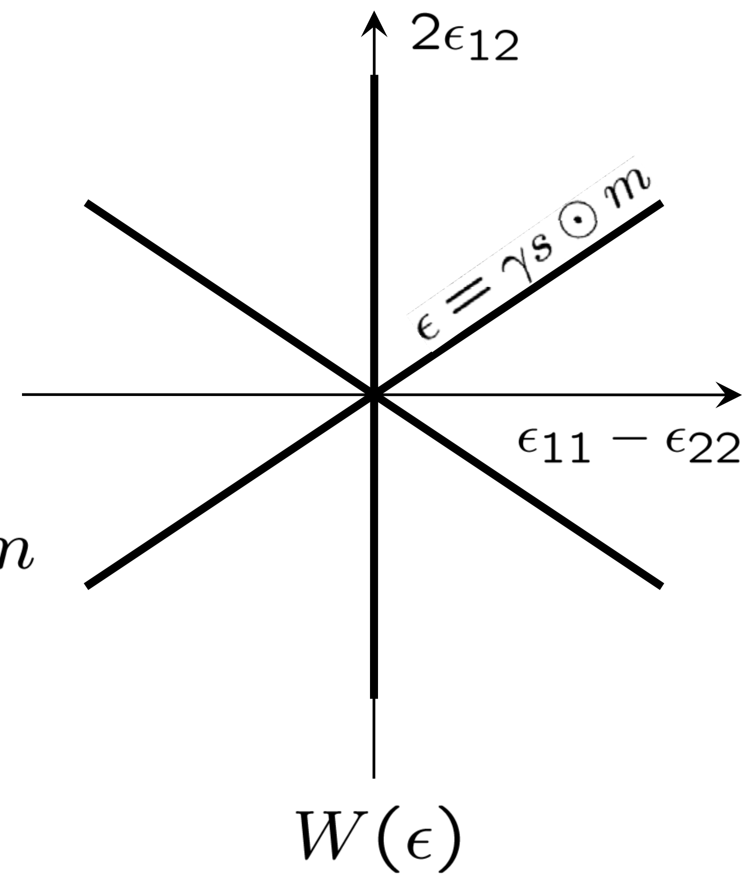
- Example: FCC crystal deforming on $(1\bar{1}0)$-plane



- Rigid-plastic case:

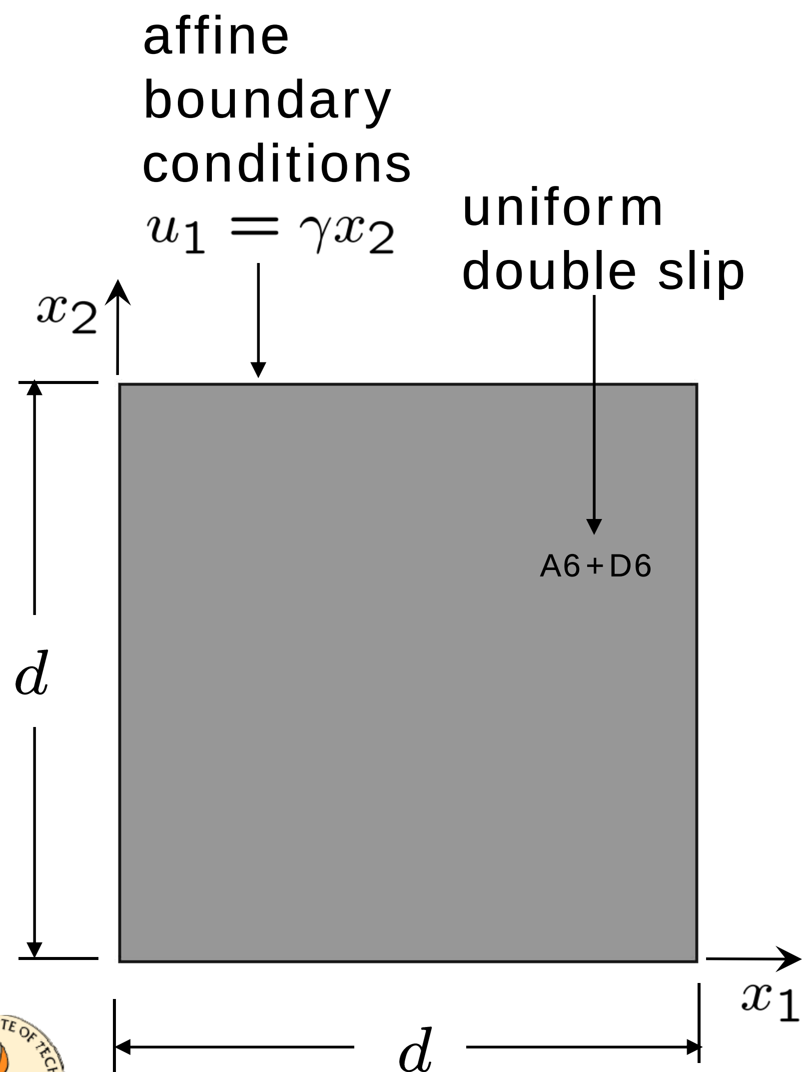
$$W = \begin{cases} 0, & \text{if } \epsilon = \gamma s \odot m \\ +\infty, & \text{otherwise.} \end{cases}$$

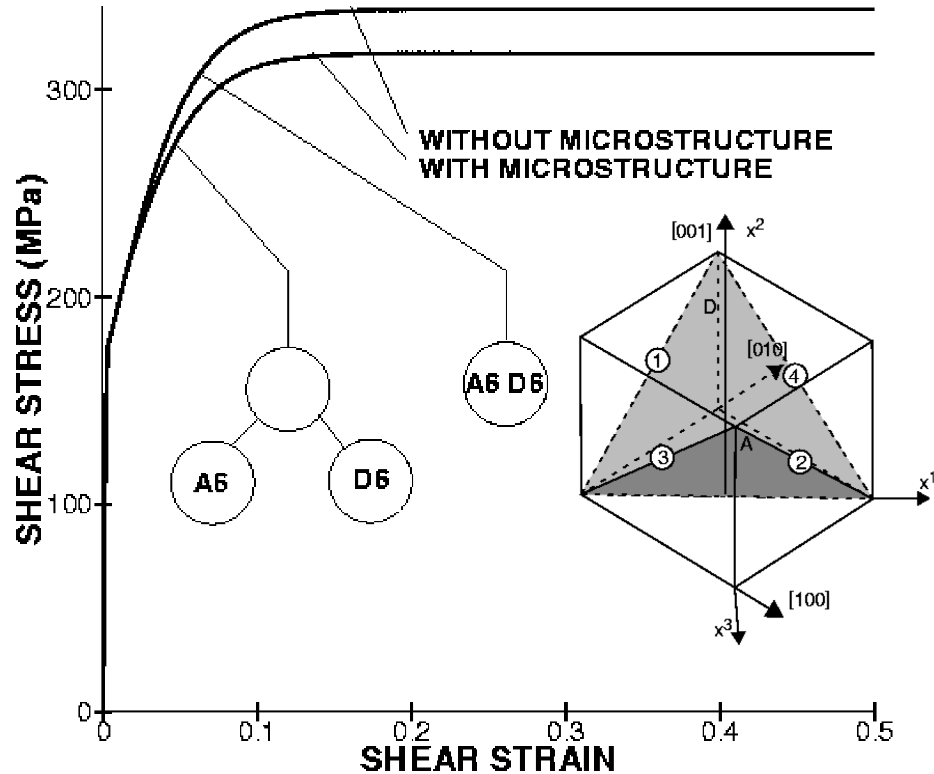
- $W(\epsilon)$ non-convex!



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

Strong latent hardening & microstructure

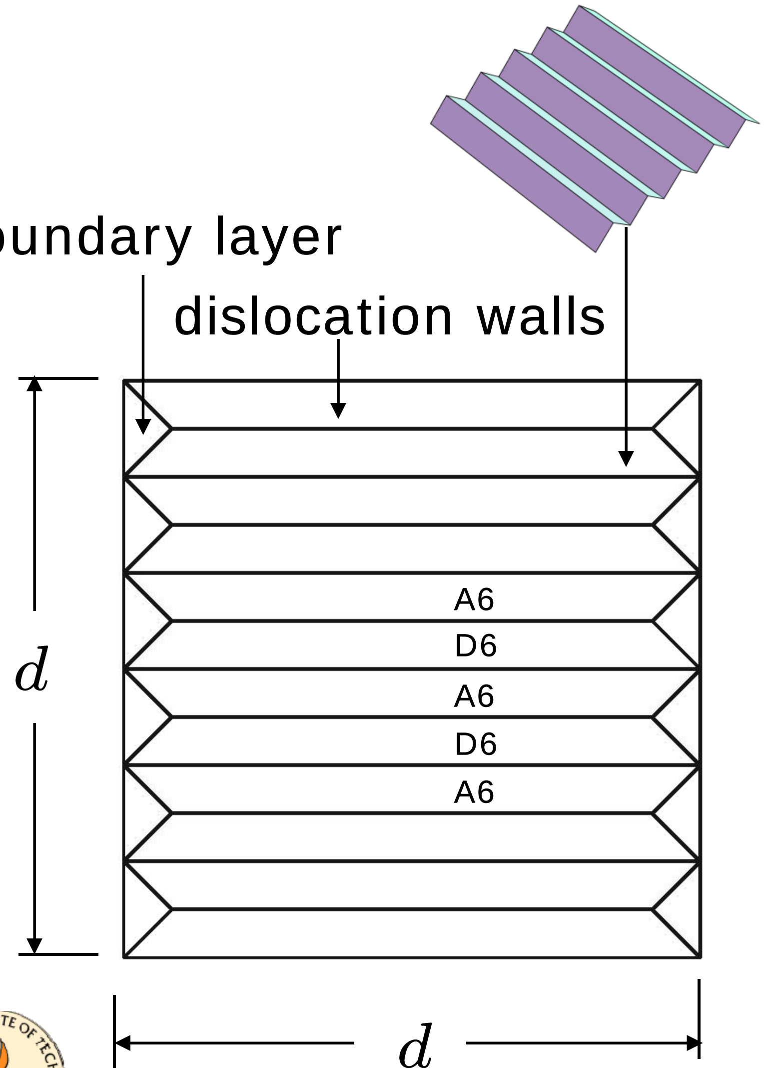


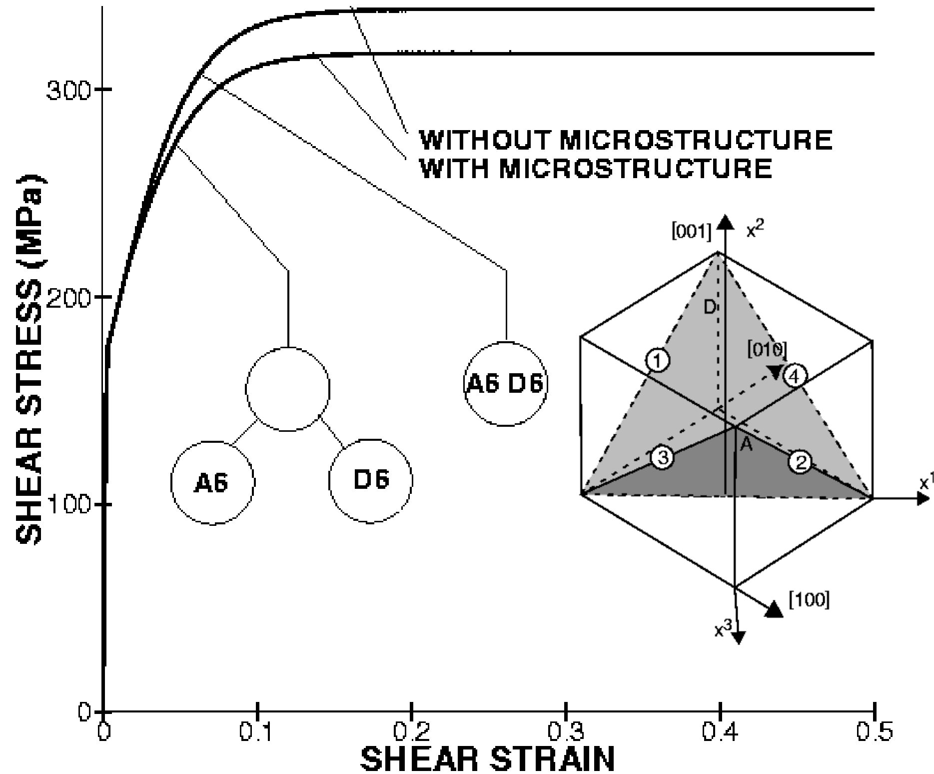


FCC crystal deformed in simple shear on (001) plane in [110] direction

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

Strong latent hardening & microstructure





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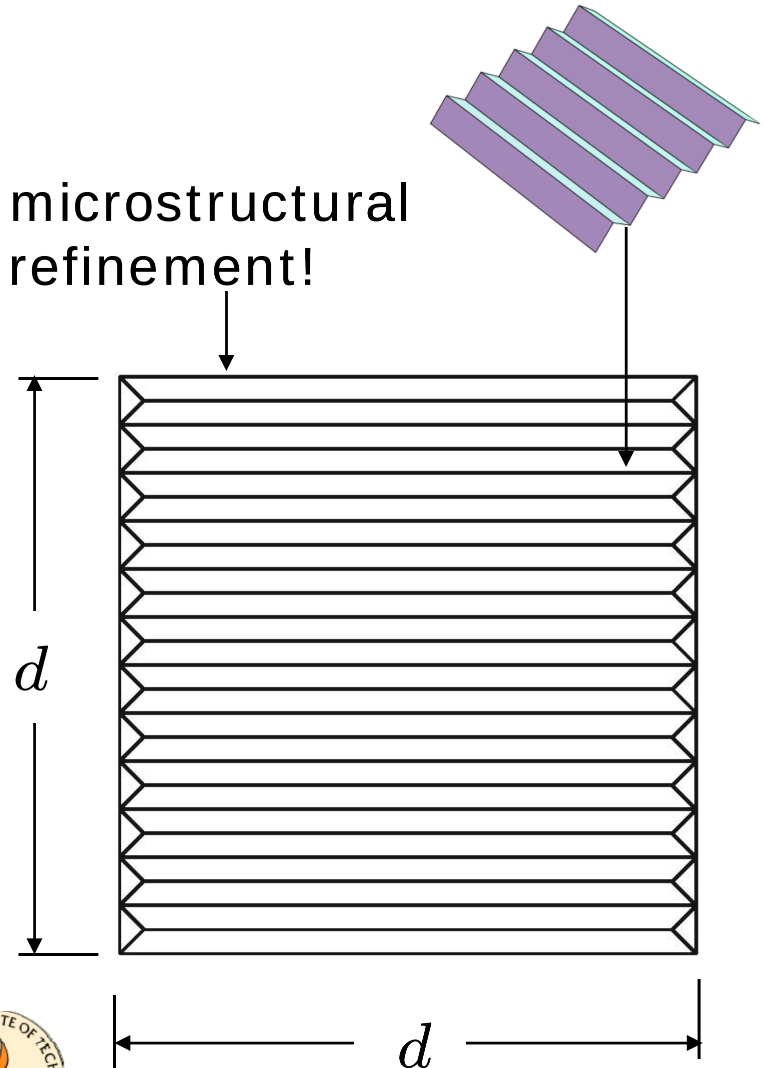
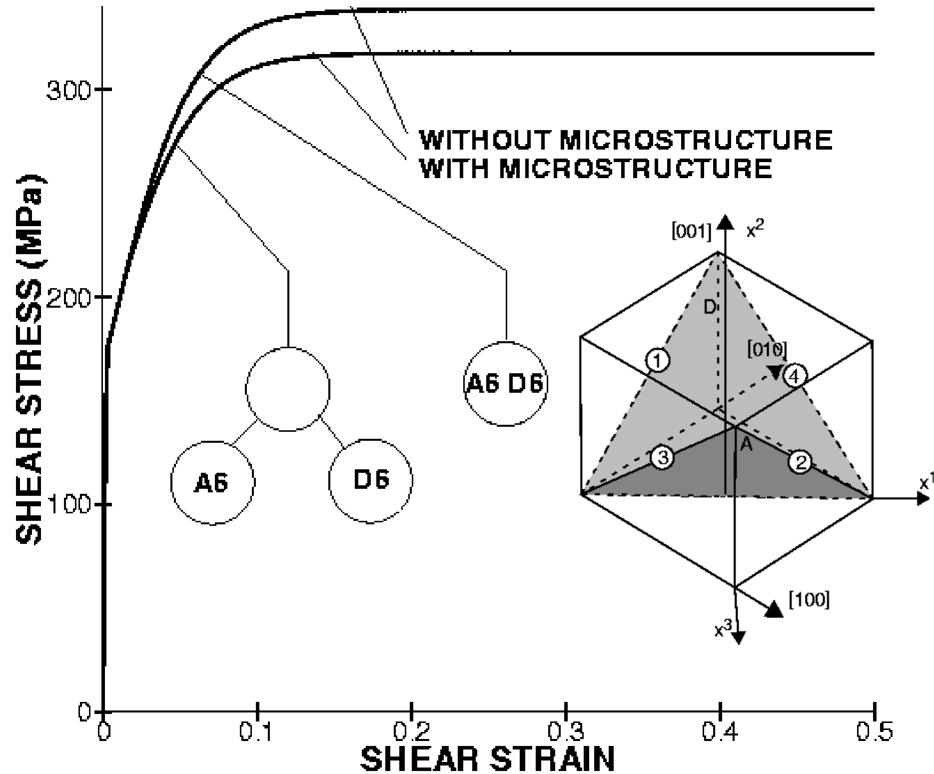
Strong latent hardening & microstructure

microstructural refinement!





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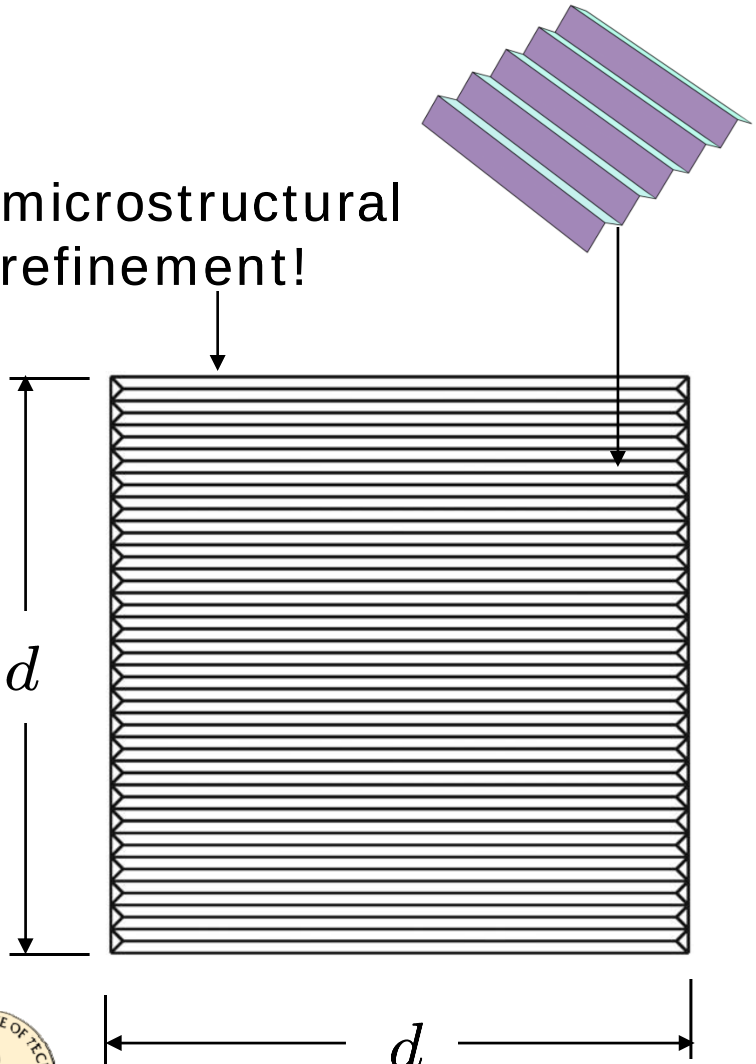

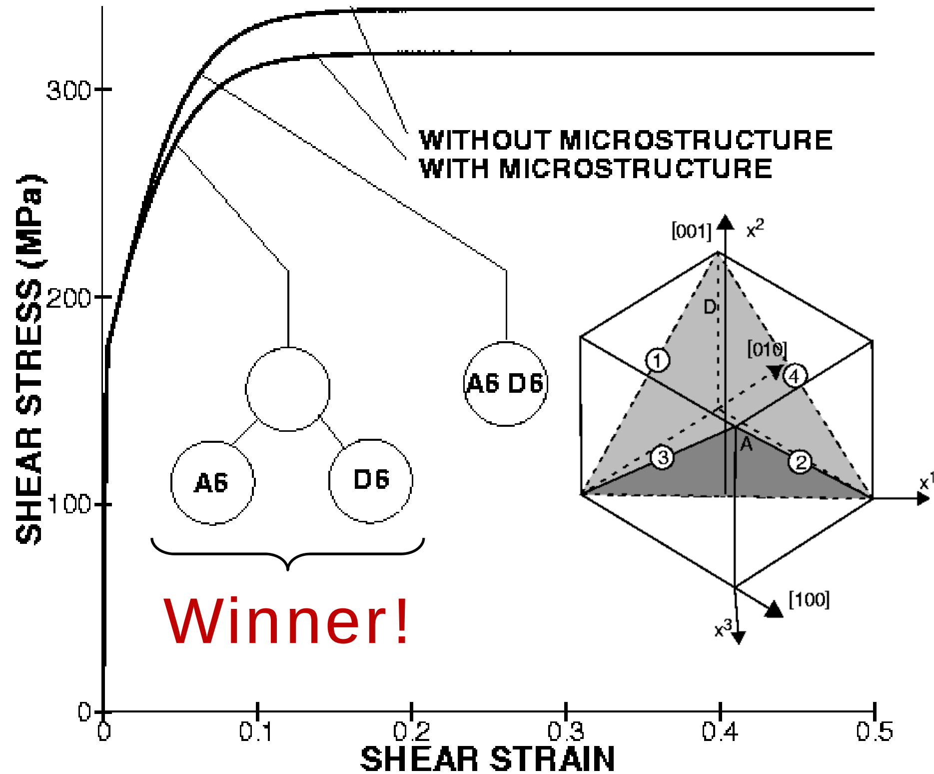

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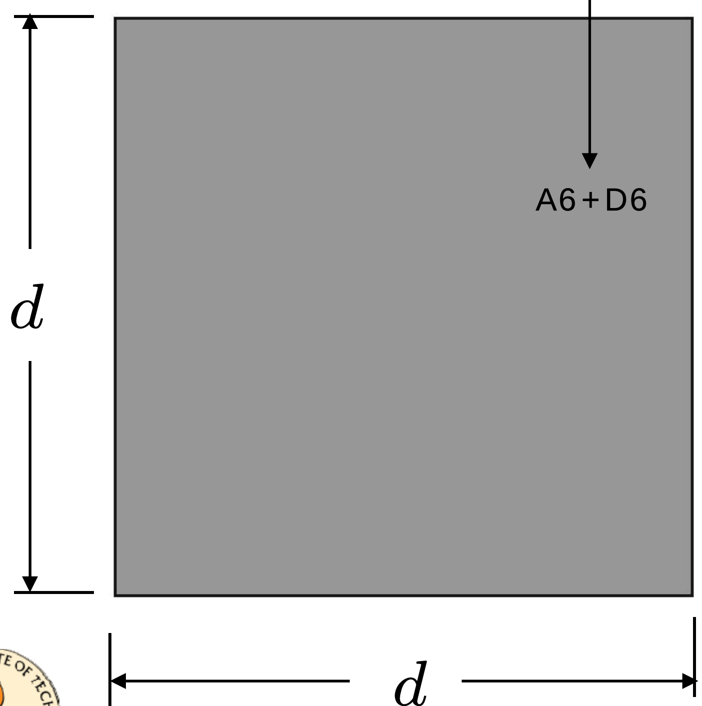
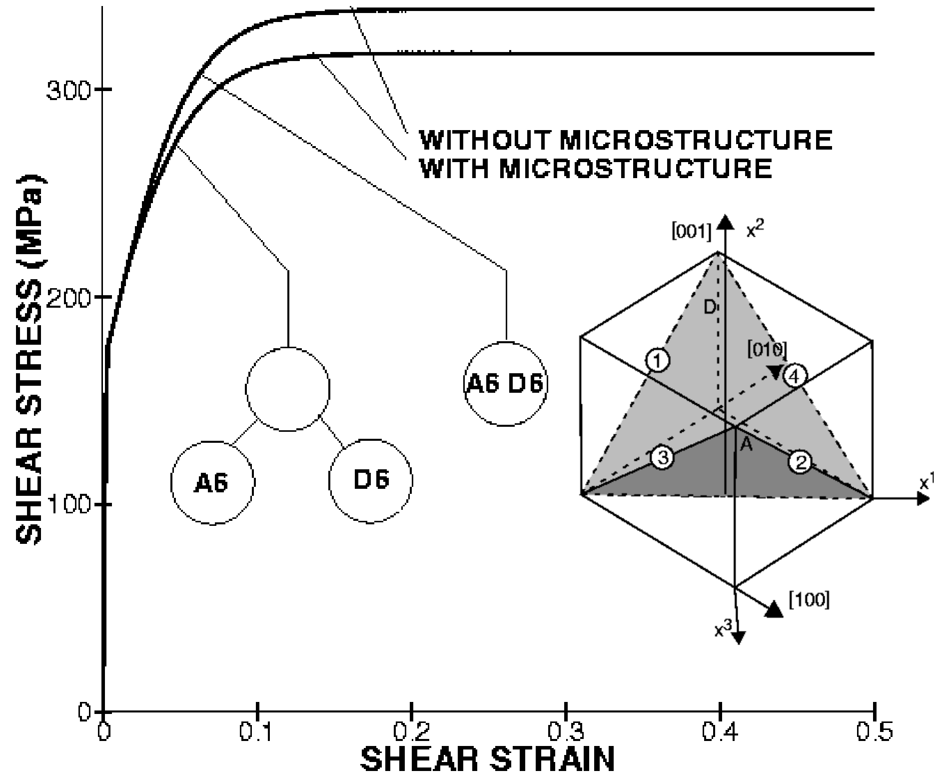
Strong latent hardening & microstructure

NON-EXISTENCE!

Pass to the limit... uniform double slip!





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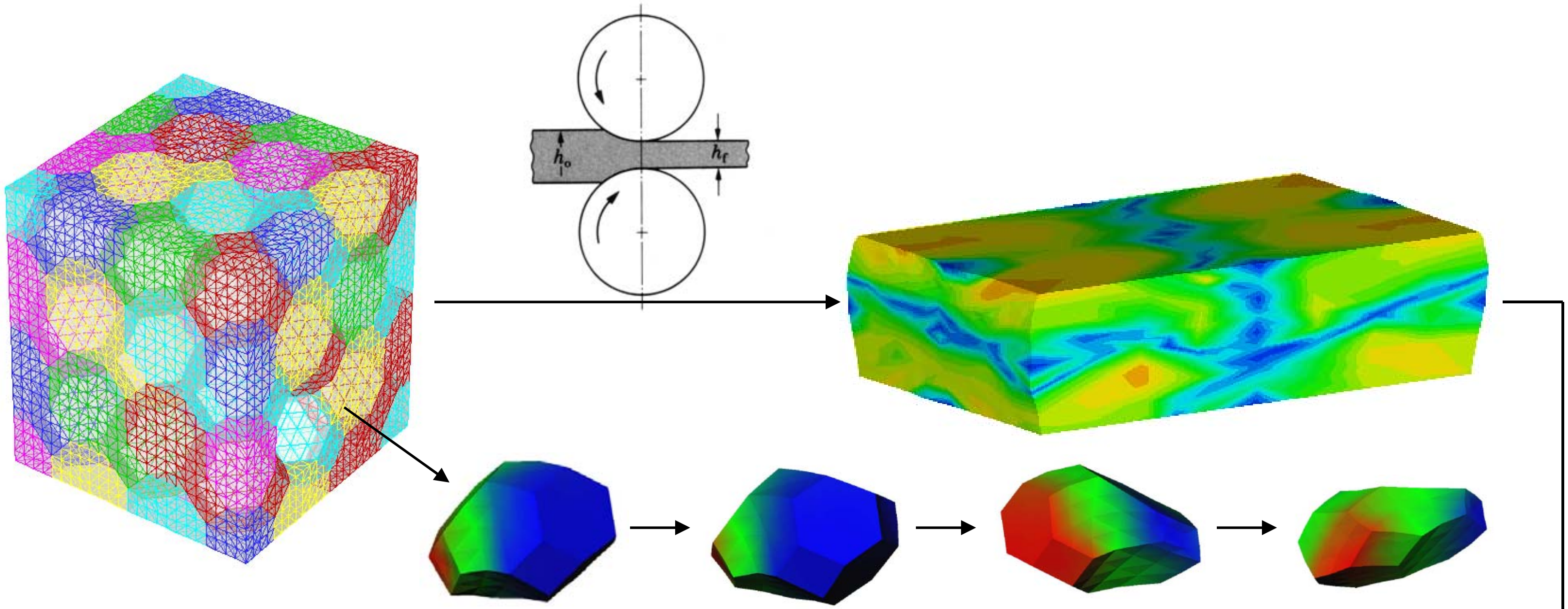
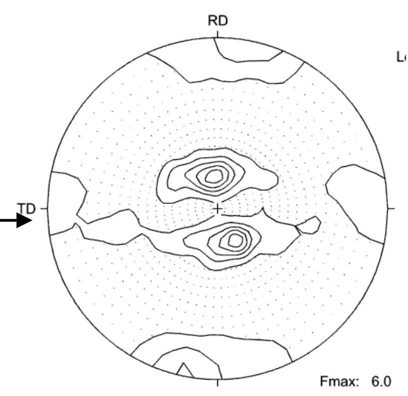
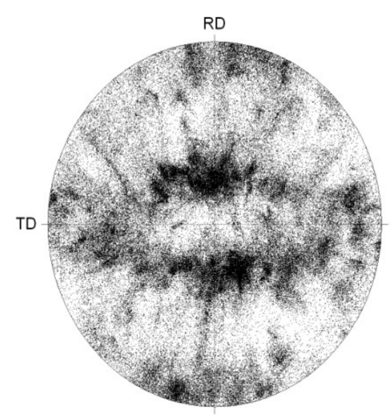
Polycrystals – Limitations of DNS



Cold-rolled @ 42%
polycrystalline Ta

Experimental
cold-rolled texture



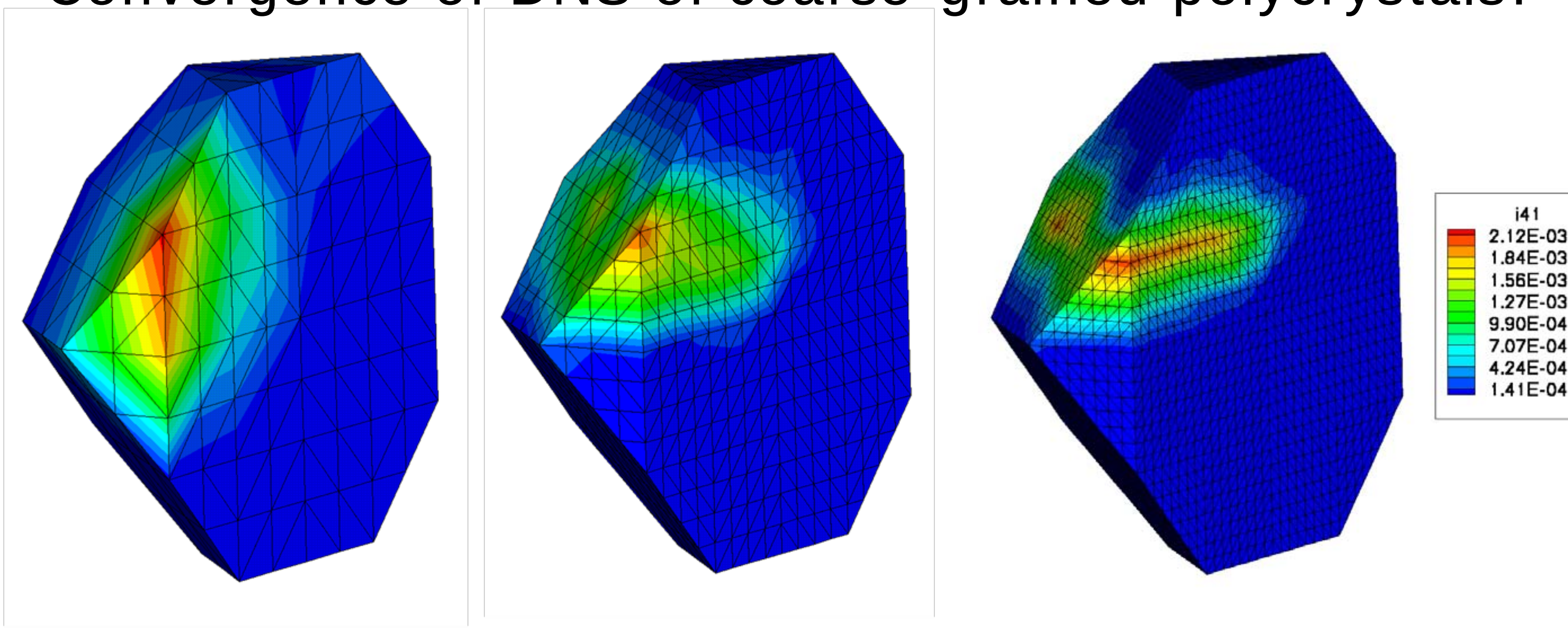


Pole
figure

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

Polycrystals – Limitations of DNS

Convergence of DNS of coarse-grained polycrystals:



Coarse mesh	Intermediate mesh	Fine mesh
192 elmts/grain	1536 elmts/grain	12288 el/grain

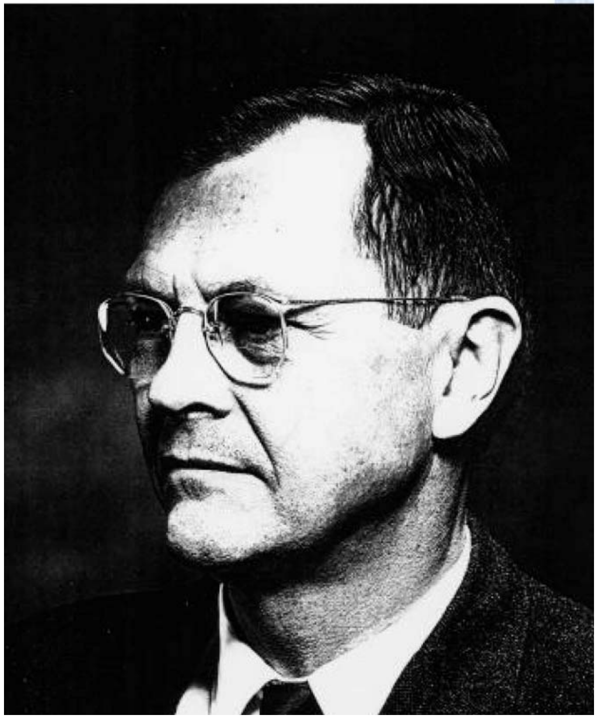
Cold-rolled @ 42% polycrystalline Ta

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

Non-convexity and microstructure

- Strong latent hardening and geometrical softening render the variational problem of crystal plasticity ill-posed...
- Microstructures 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?

Calculus of variations and microstructure



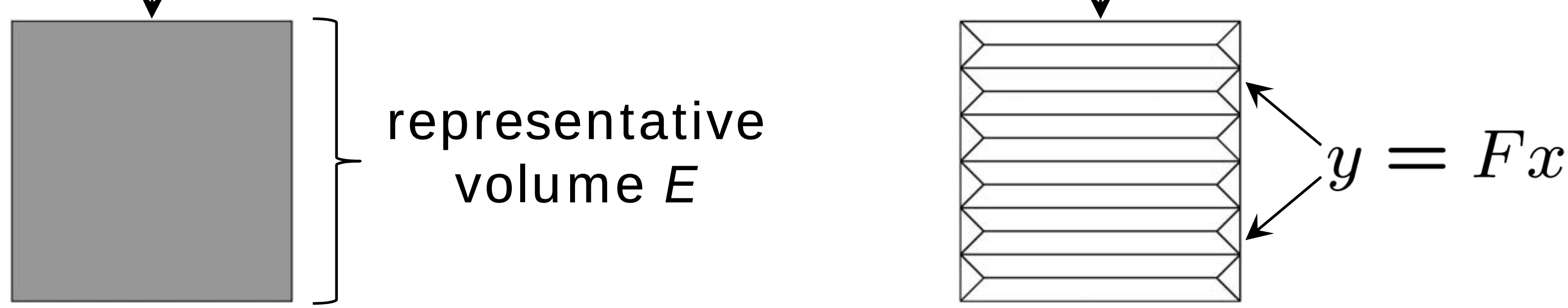
Morrey, C.B. Jr., "Quasi-convexity and the semicontinuity of multiple integrals," *Pacific J. Math*., Vol. 2 (1952) pp. 25-53.

De Giorgi, E., "Sulla convergenza di alcune successioni di integrali del tipo dell'area," *Rend. Mat*., Vol. 8 (1975) pp. 277-294.

Calculus of variations and microstructure

- *Quasiconvex envelope* of an energy density $W(F)$:

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

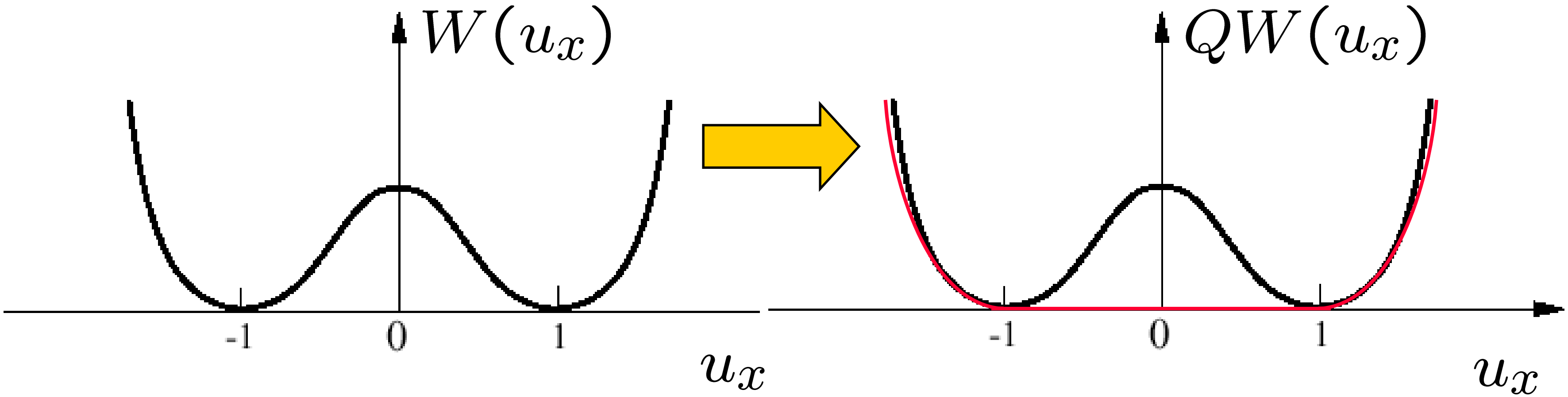


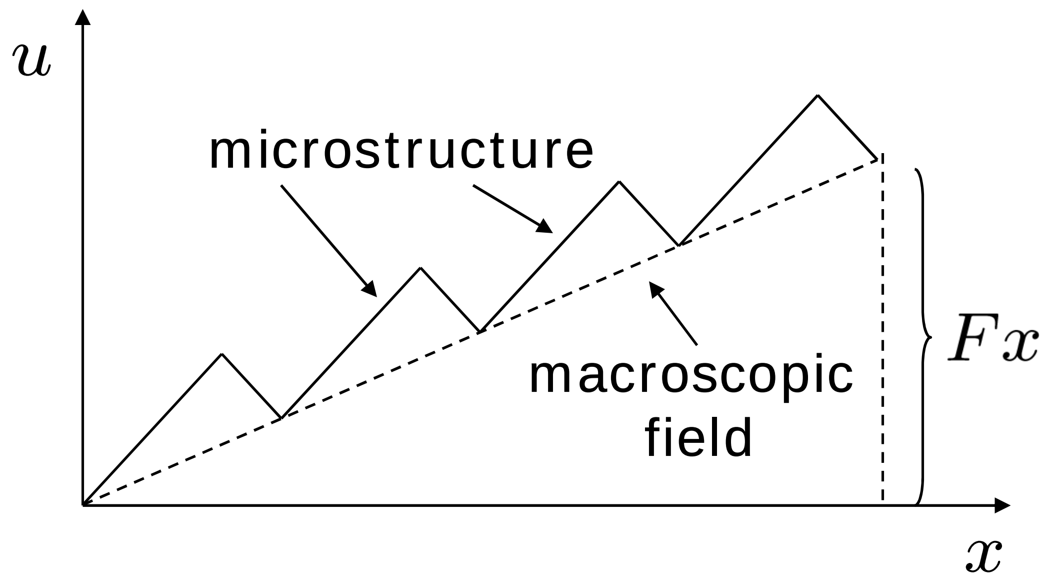
uniform deformation   microstructure

- $QW(F)$ is the largest quasi-convex (stable) energy density majorized by $W(F)$.
- Relaxed problem:

$$\inf_{u \in u_0 + W_0^{1,p}(\Omega)} \int_\Omega QW(\nabla u) dx$$

Calculus of variations and microstructure





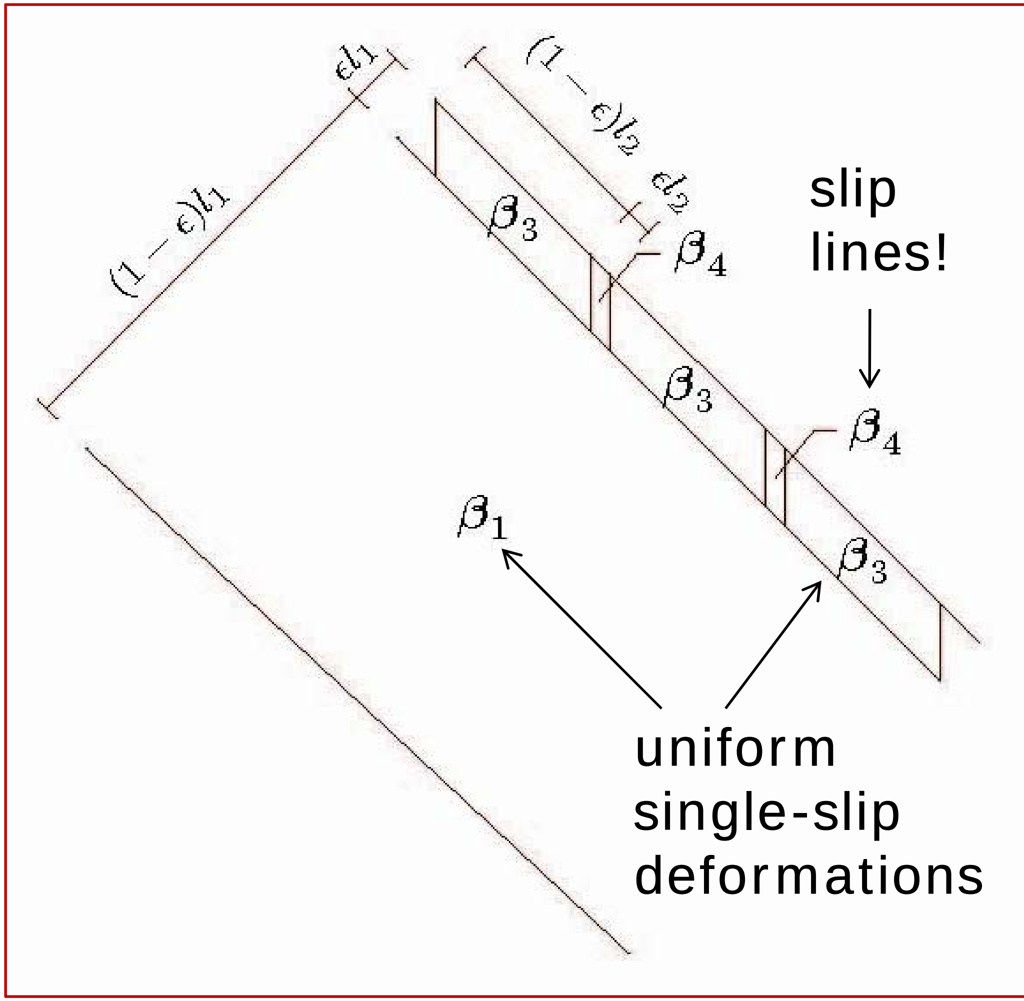
Separation of scales - Relaxation

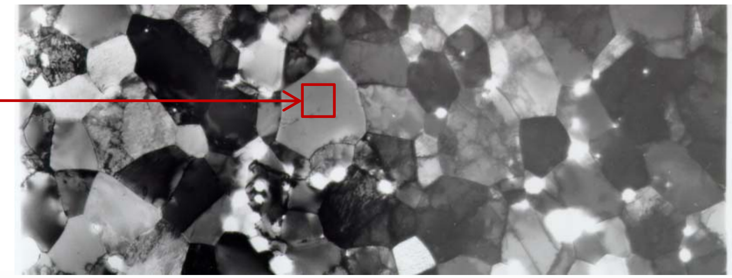
- The relaxed problem is much nicer than the original one, can be solved, e.g., by finite elements
- The relaxed and unrelaxed problems deliver the same macroscopic response (e.g., force-displacement curve)
- All microstructures are accounted for by the relaxed problem (no physics lost)
- All microstructures can be reconstructed from the solution of the relaxed problem (no loss of information)
- Relaxation is the 'perfect' multiscale method!

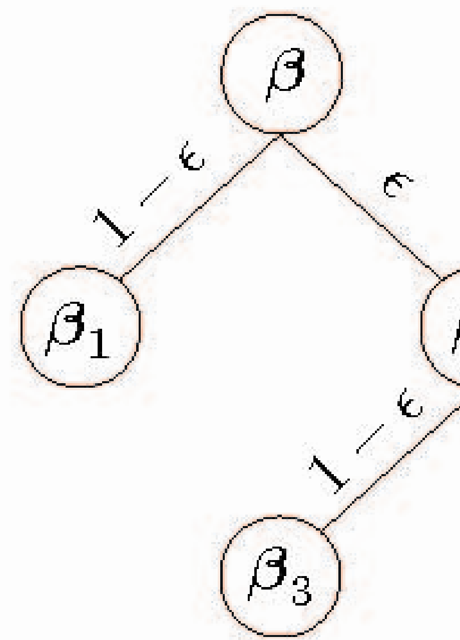
Relaxation as 'exact' multiscale method

- General strategy for computing the relaxation:
  - *Exhibit a microstructure construction that 'beats' uniform deformations over representative volumes*
  - *Prove that the material cannot do better (optimality)*
- Optimality is difficult to prove in general => Exact relaxation is known for few material models:
  - *Small-strain single crystal plasticity (*Conti, S. and Ortiz, M.*, Arch. Rat. Mech. Anal.,* **176** (2005) 103-147*)*
  - *Finite-deformation plasticity in single slip (*S. Conti and F. Theil*, Arch. Rat. Mech. Anal.,* **178** (2005) 125-148*)*
  - *Hierarchical fracture/fragmentation of brittle materials (*Pandolfi, A., Conti, S. and Ortiz, M.*, J. Mech Phys. Solids,* **54** (2006) 1972-2003*)*

Crystal plasticity – Relaxation







hierarchical structure of deformations

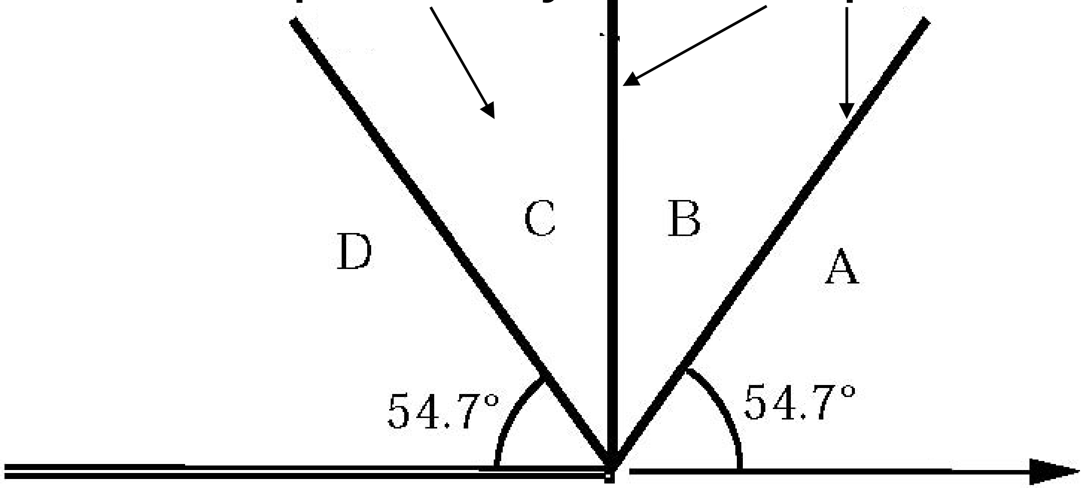
Optimal microstructure construction in double slip

(Conti, S. and Ortiz, M., *Arch. Rat. Mech. Anal.*, **176** (2005) 103-147)

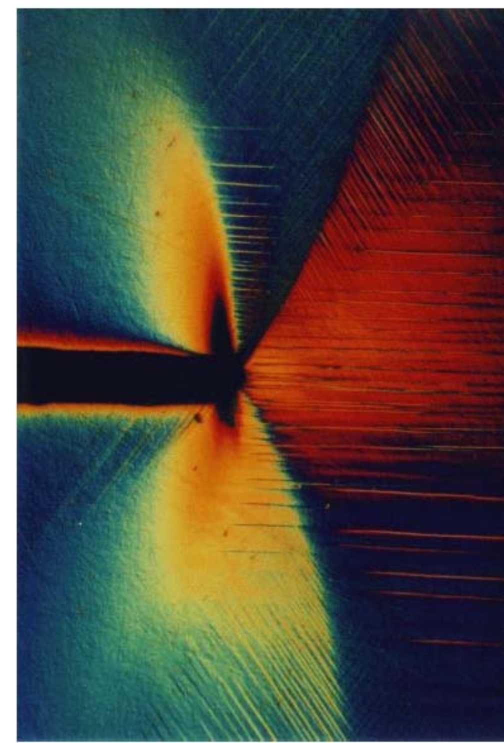
Crystal plasticity – Relaxation

- Relaxed problem:

Minimize: $$\int_\Omega \underbrace{W^{**}(\epsilon(u))dx}_{\text{Ideal plasticity}} + \int_\Omega \underbrace{W^{\infty}\left(\frac{E_s u}{|E_s u|}\right)}_{\text{Slip-line energy}} d|E_s u|$$



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

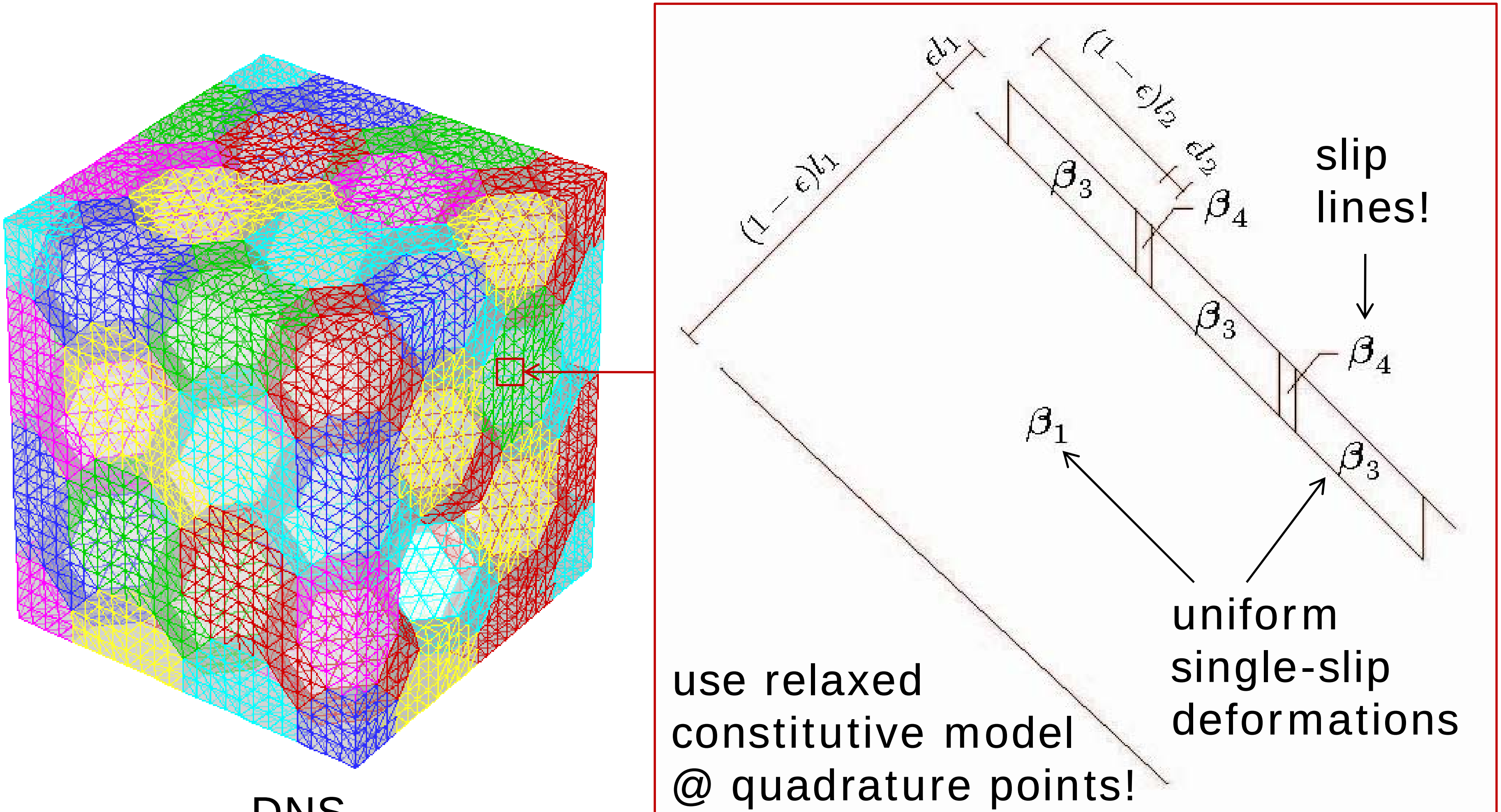


(Crone and Shield, *JMPS*, 2002)

Relaxation – Fast Multiscale Models

- Fast Multiscale Models: Use explicitly relaxed constitutive relation (when available) to represent sub-grid behavior
- 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 (Conti, S., Hauret, P. and Ortiz, M., *SIAM Multiscale Model. Simul*., **6** (2007) 135-157)
- FMM: Optimal element enhancement!

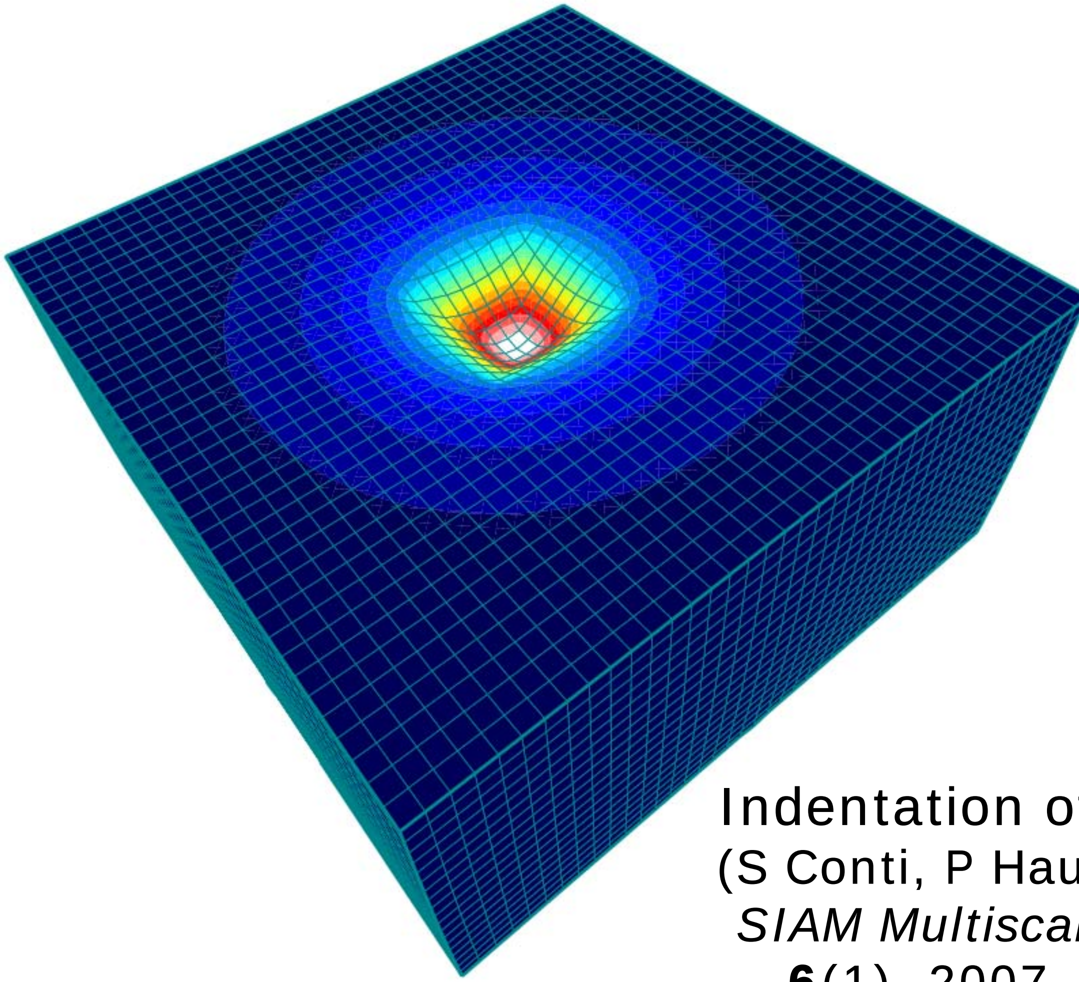
Relaxation – Fast Multiscale Models



DNS

FMM scheme for polycrystal

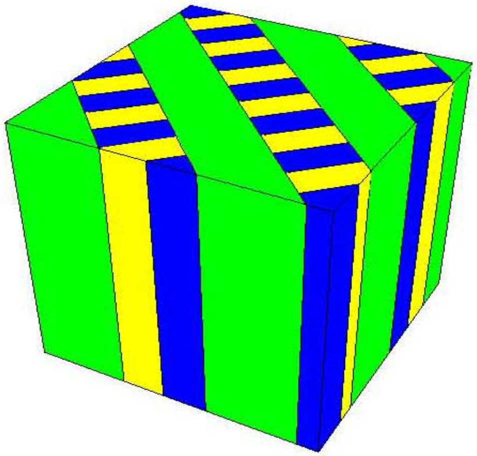
Fast Multiscale Models – Indentation

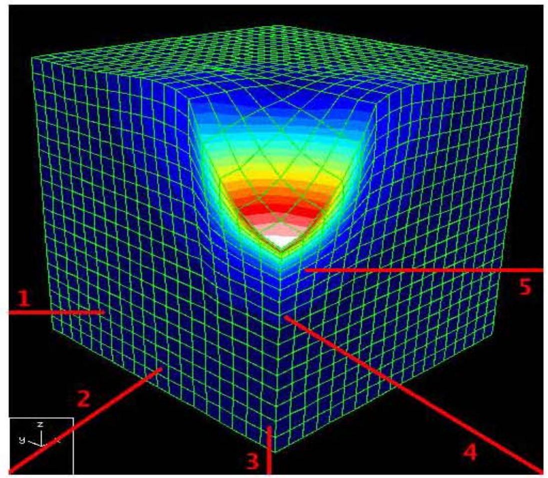


Indentation of [001] copper
(S Conti, P Hauret and M Ortiz,
SIAM Multiscale Model. Simul.
6(1), 2007, pp. 135–157)

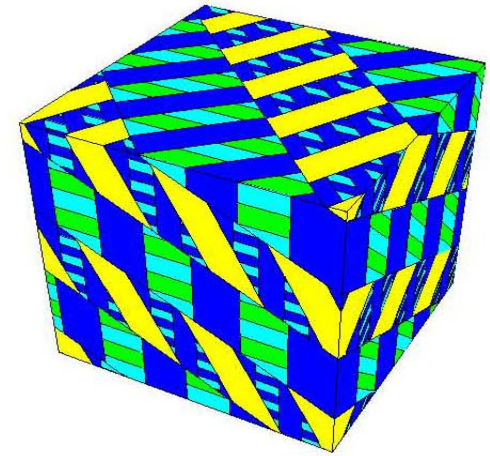
Fast Multiscale Models – Indentation

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

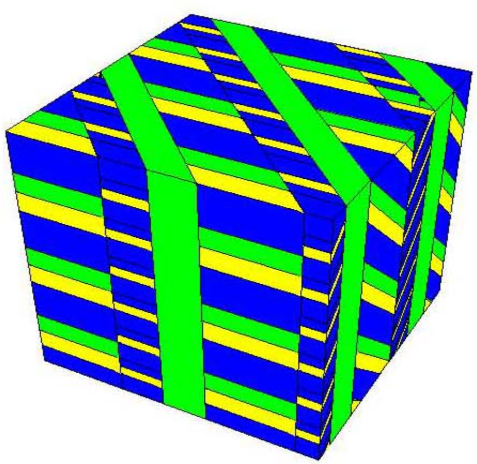




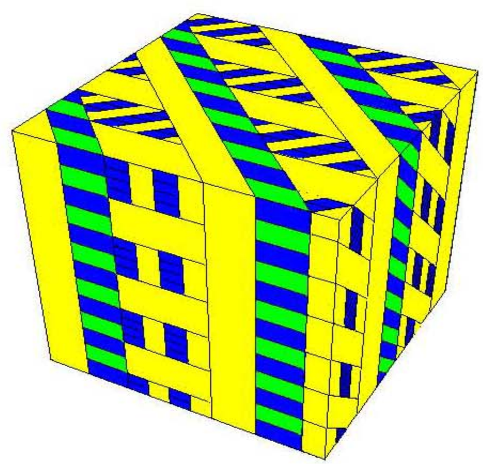
rank 4/14, $|\gamma|_\infty$ = 0.43



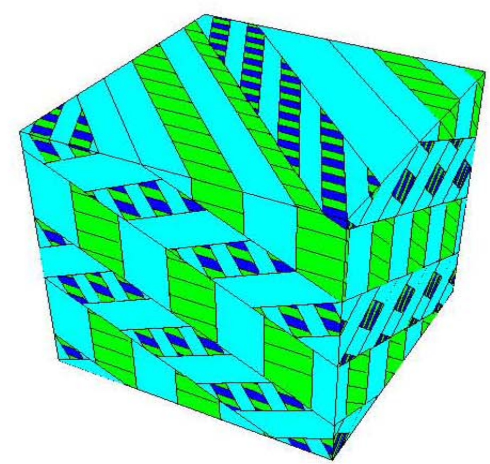
rank 4/12, $|\gamma|_\infty$ = 0.02



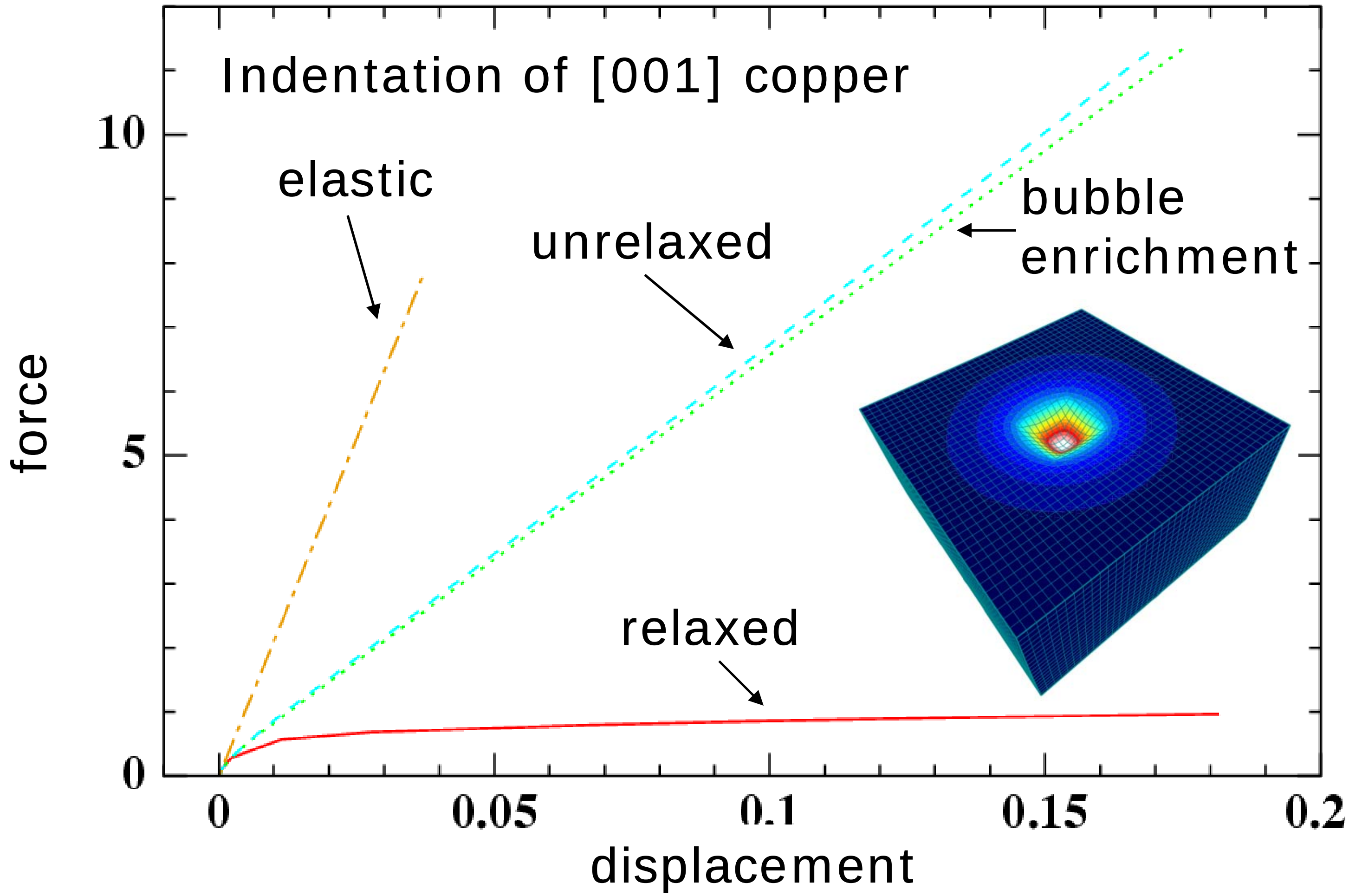
rank 4/6, $|\gamma|_\infty$ = 0.026



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



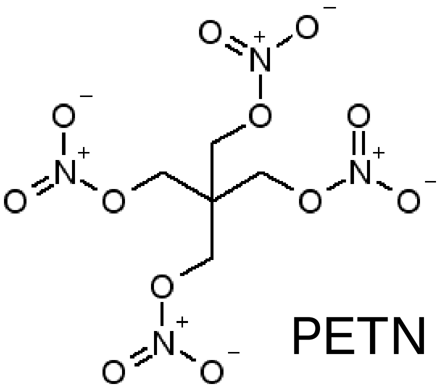
Fast Multiscale Models – Indentation



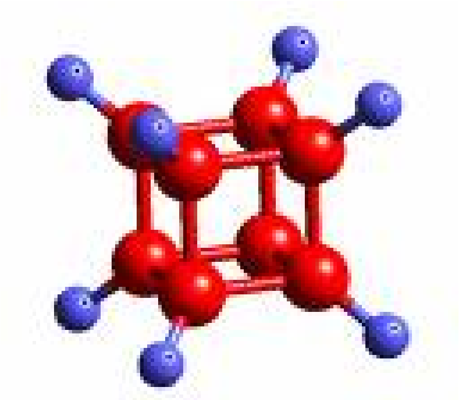
(S Conti, P Hauret and M Ortiz, *SIAM Multiscale Model. Simul.* **6**(1), 2007, pp. 135–157)

Fast Multiscale Models
High-Explosives Detonation Initiation

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



PETN



M. Ortiz
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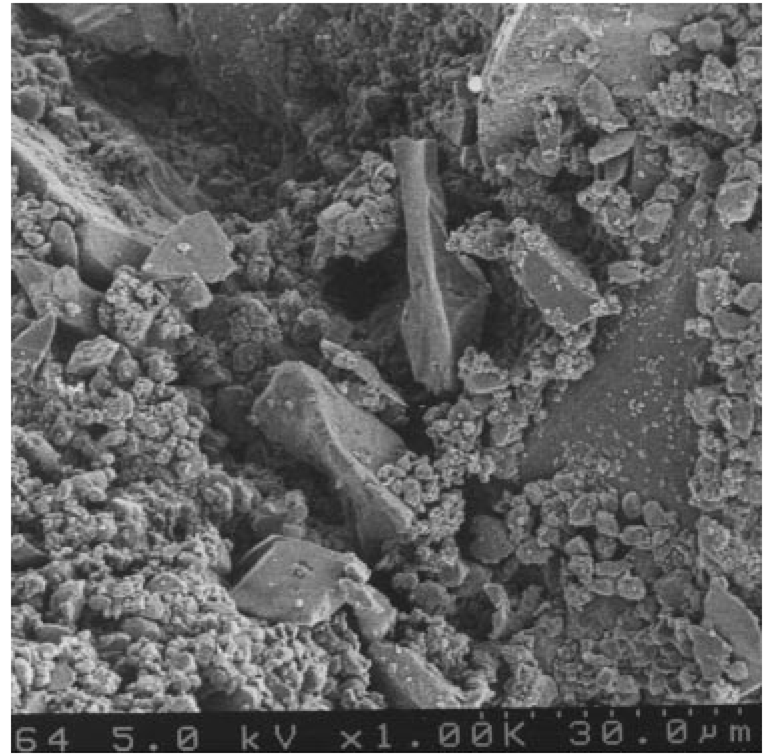
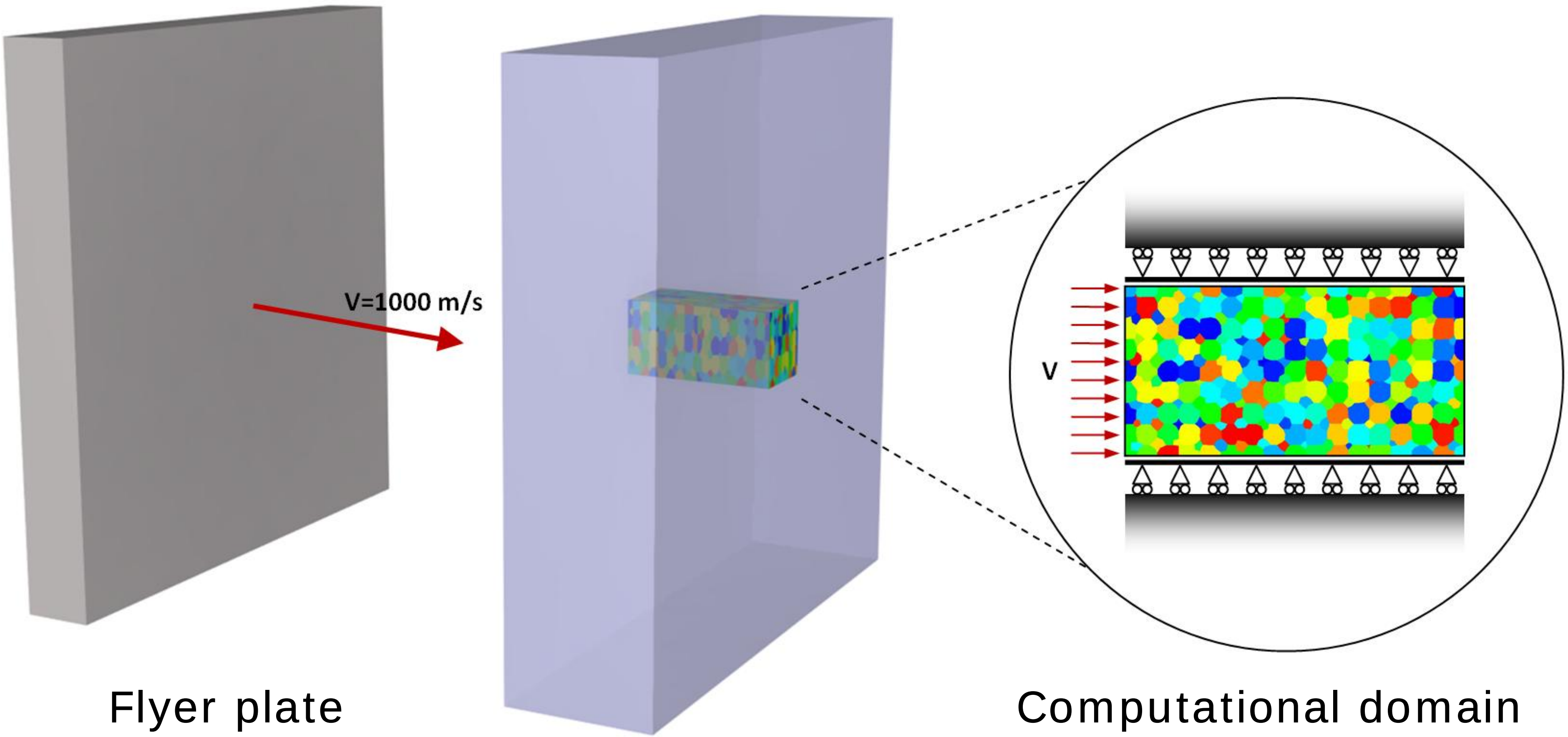
High-Explosives Detonation Initiation

- In high explosives (HE) localized hot spots cause detonation initiation
- Some hot spots may arise as a result of localized plastic deformation
- Heterogeneity and defects act as stress risers and promote localization
- Need to predict defor-mation microstructures, extreme events! (not just average behavior)



Polycrystalline structure of high-explosive (LLNL S&TR June 1999)

Fast Multiscale Models – HE detonation



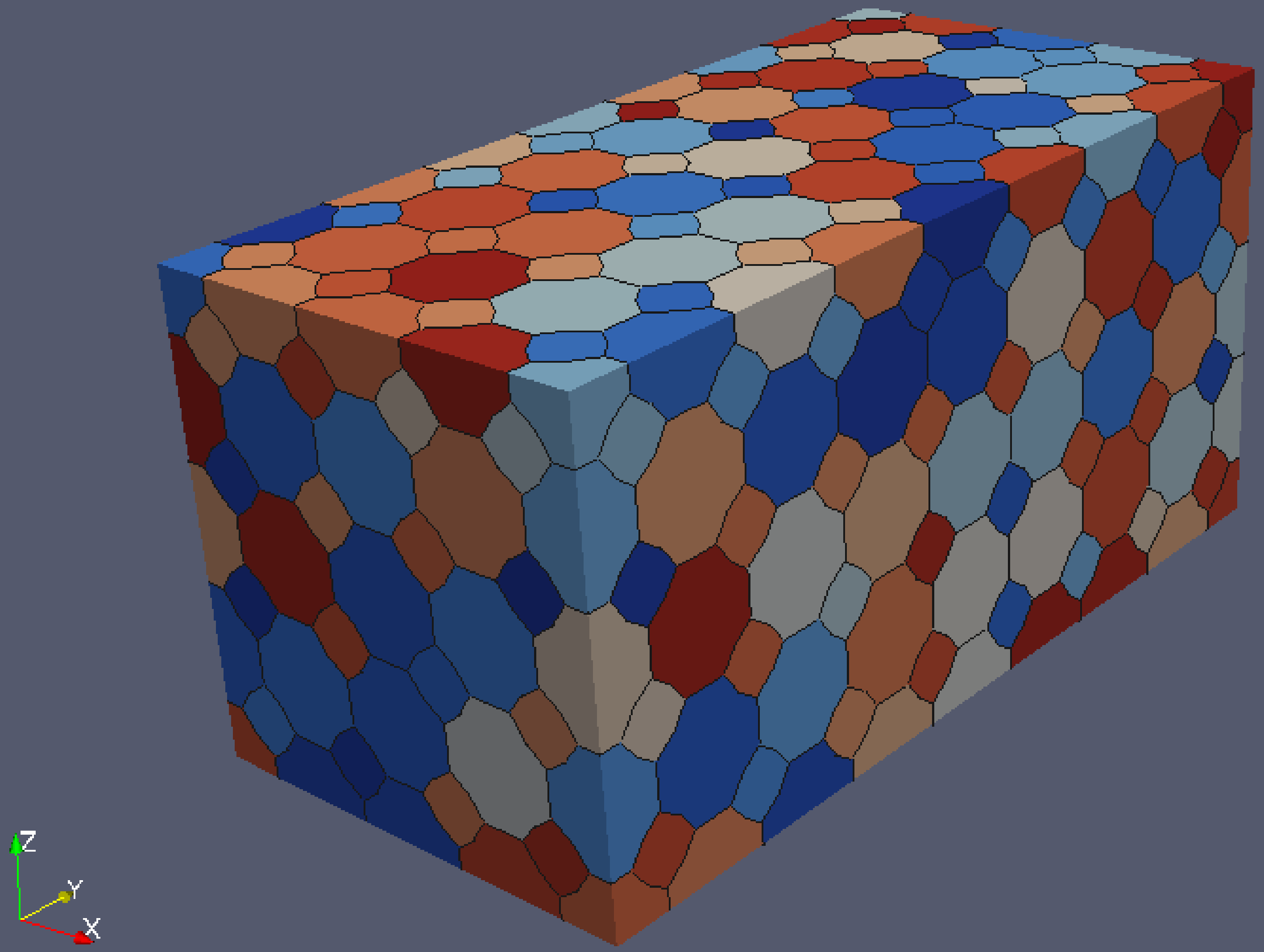
Flyer plate

Computational domain

HE target plate

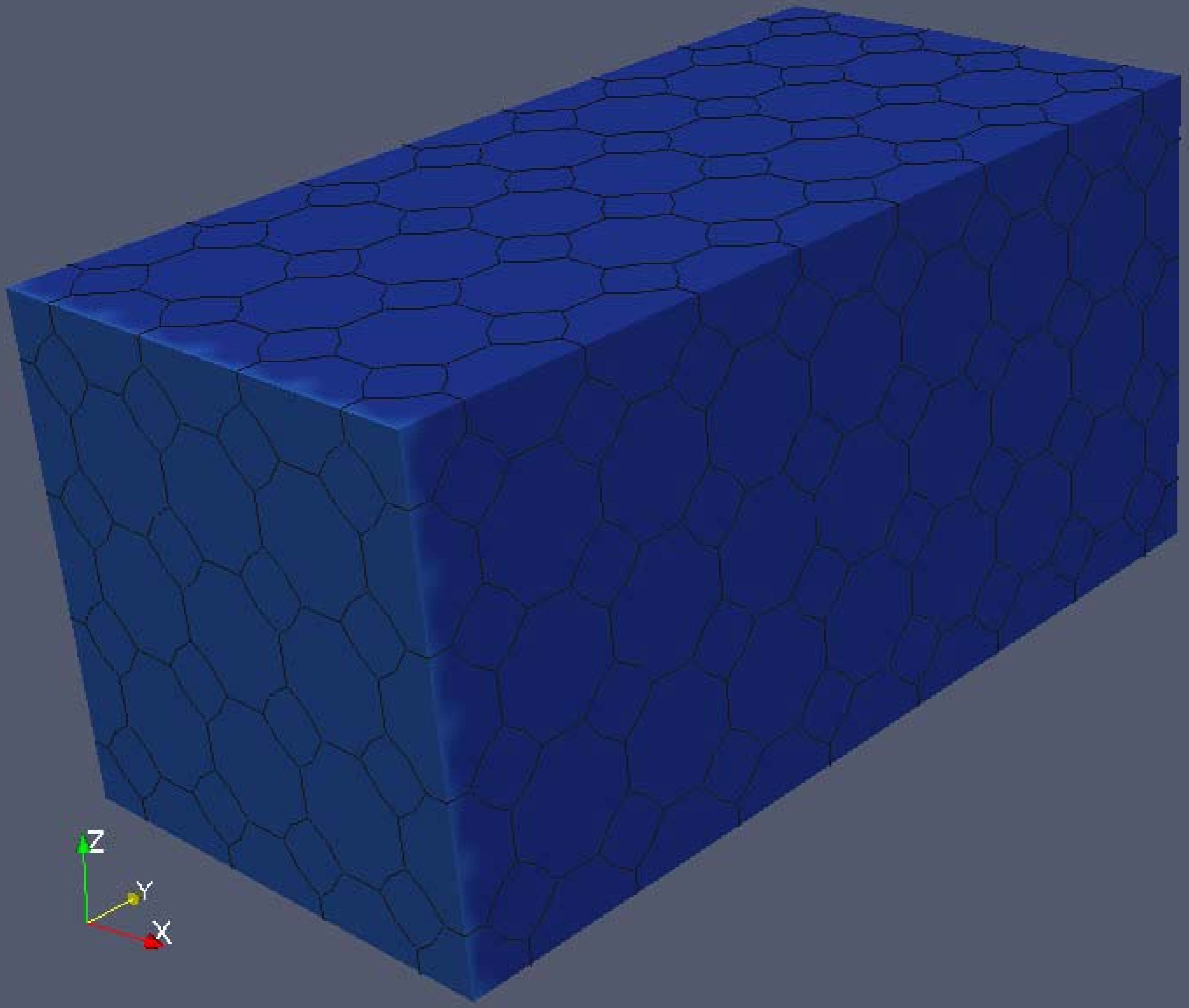
Plate-impact configuration

High-Explosives Detonation Initiation

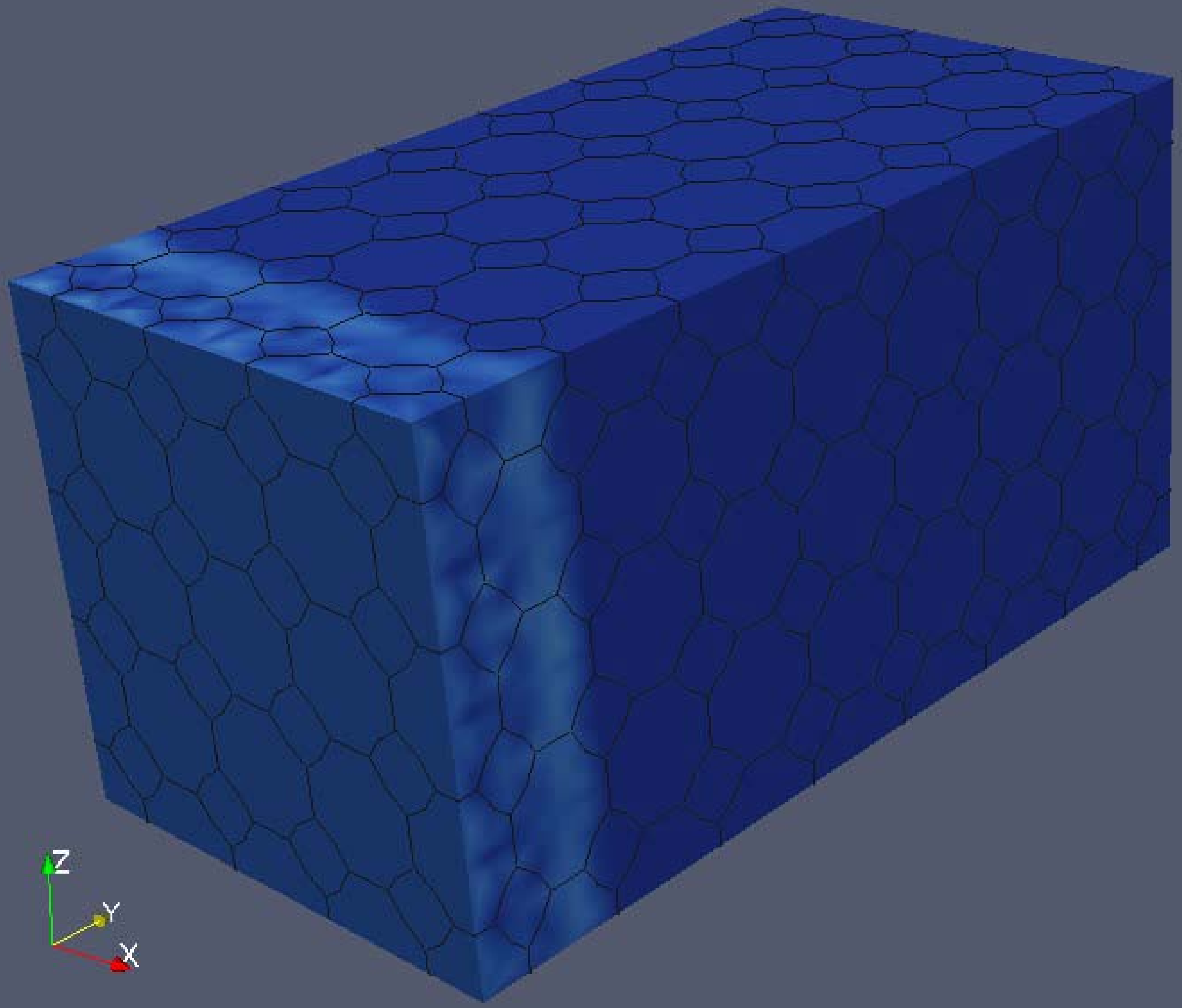


Polycrystal model and grain boundaries

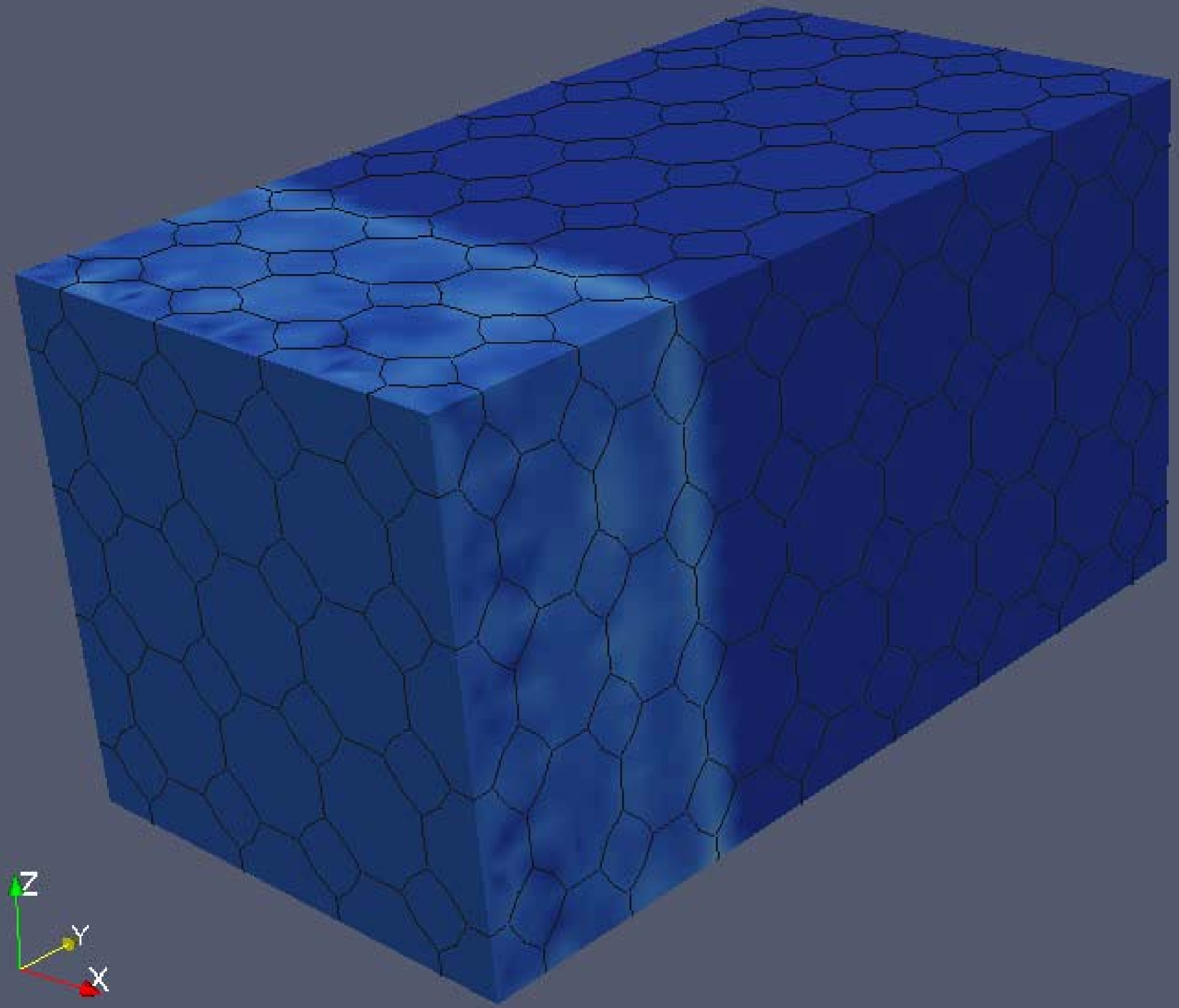
PETN plate impact - Velocity



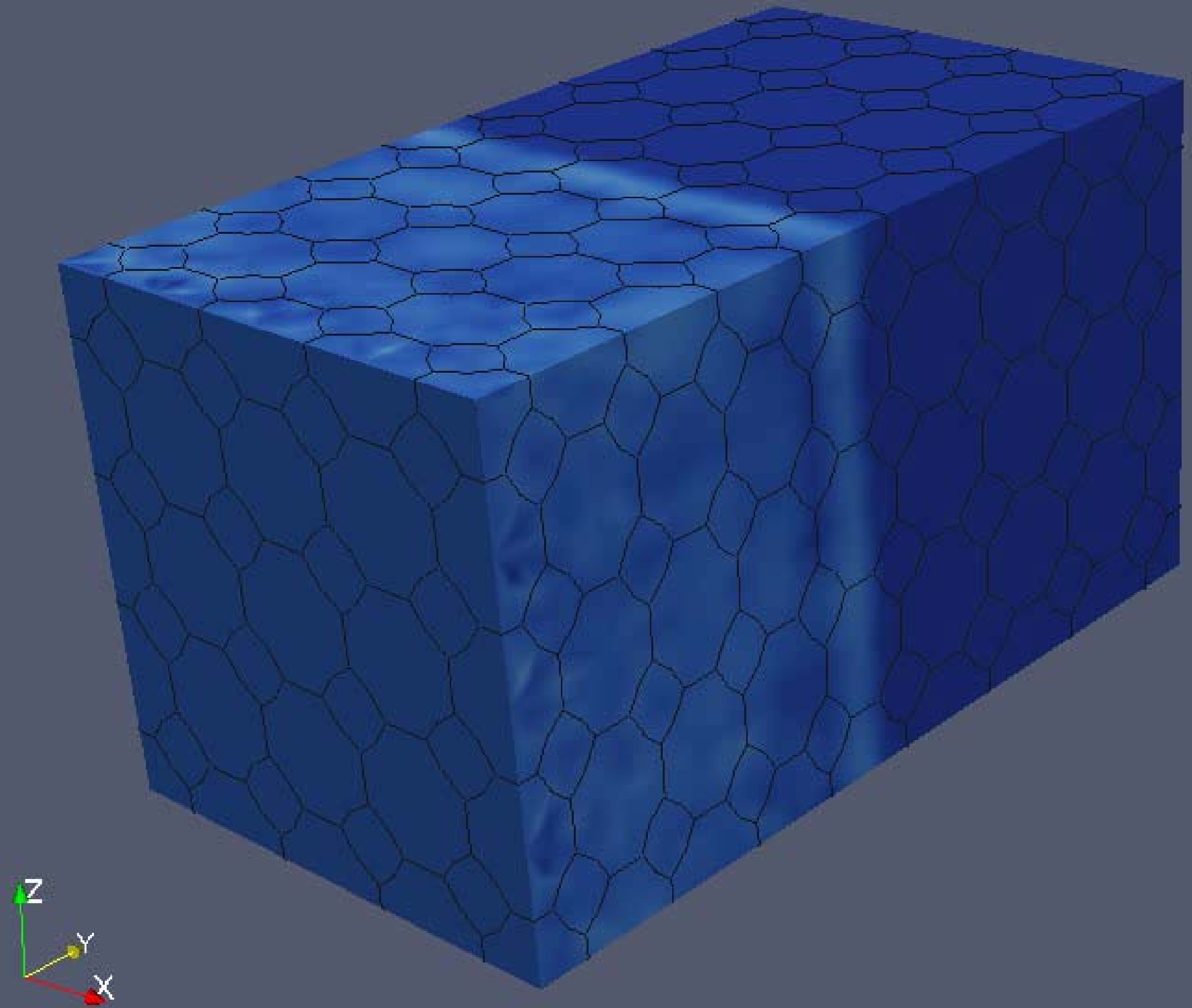
PETN plate impact - Velocity



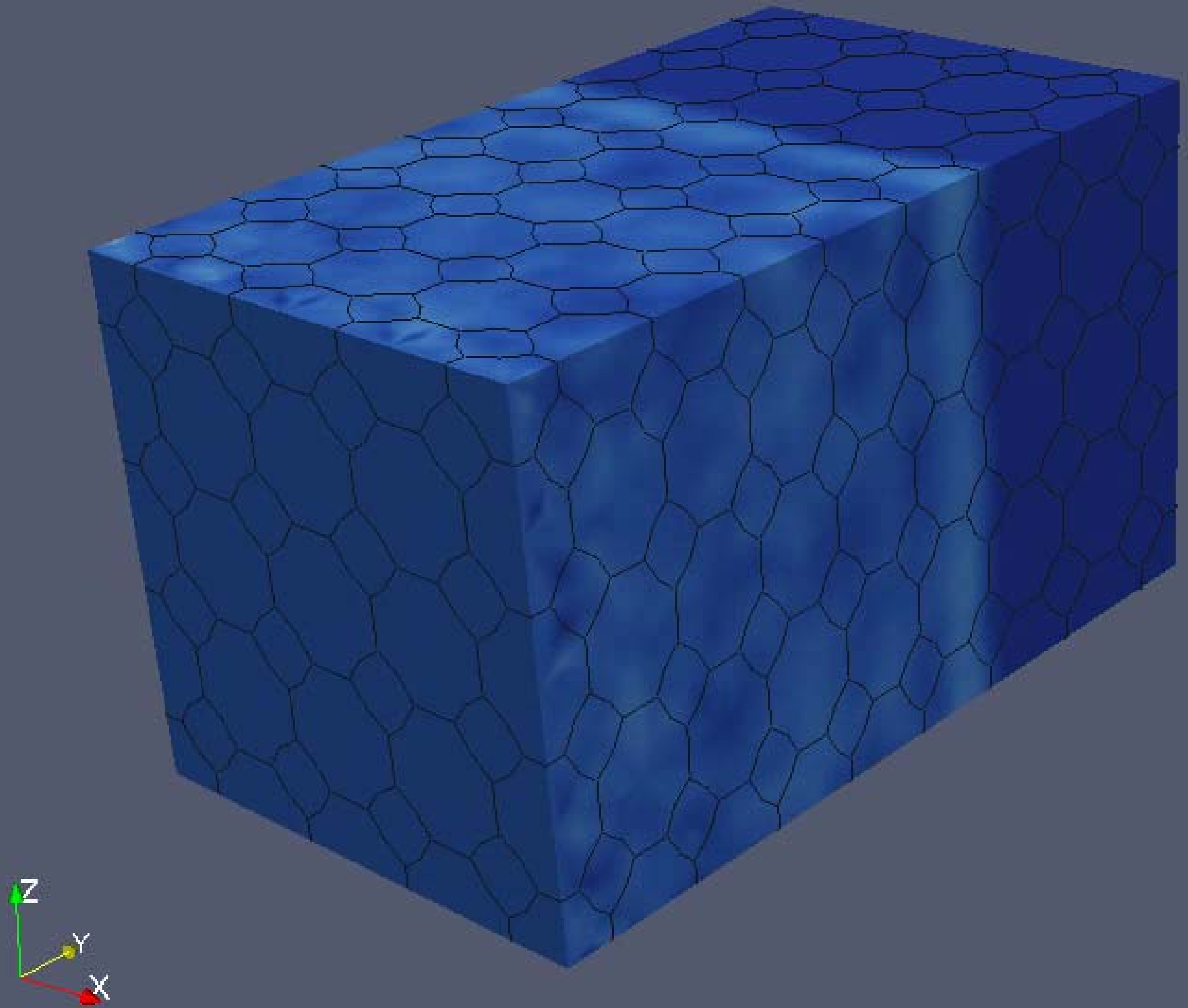
PETN plate impact - Velocity



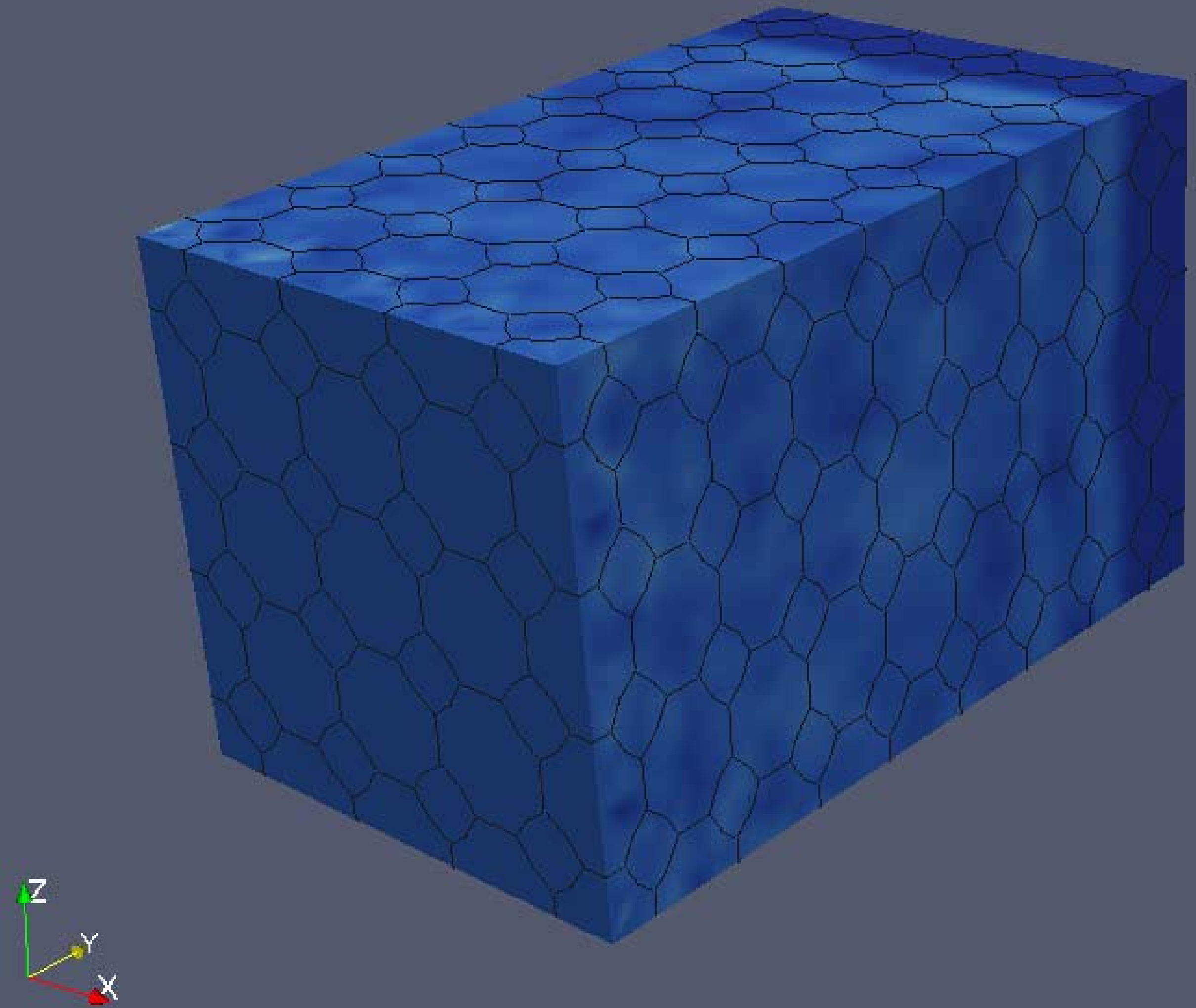
PETN plate impact - Velocity



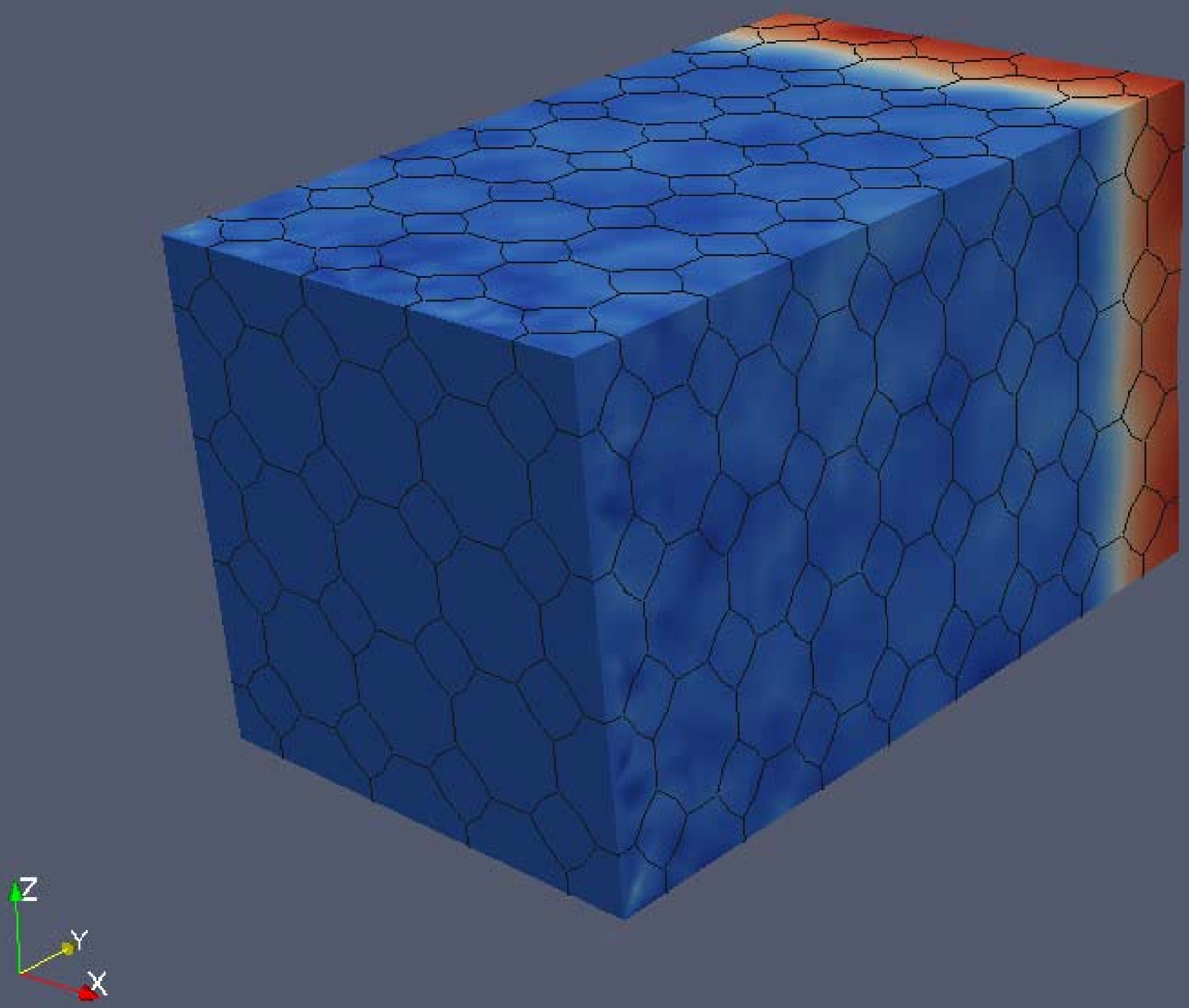
PETN plate impact - Velocity



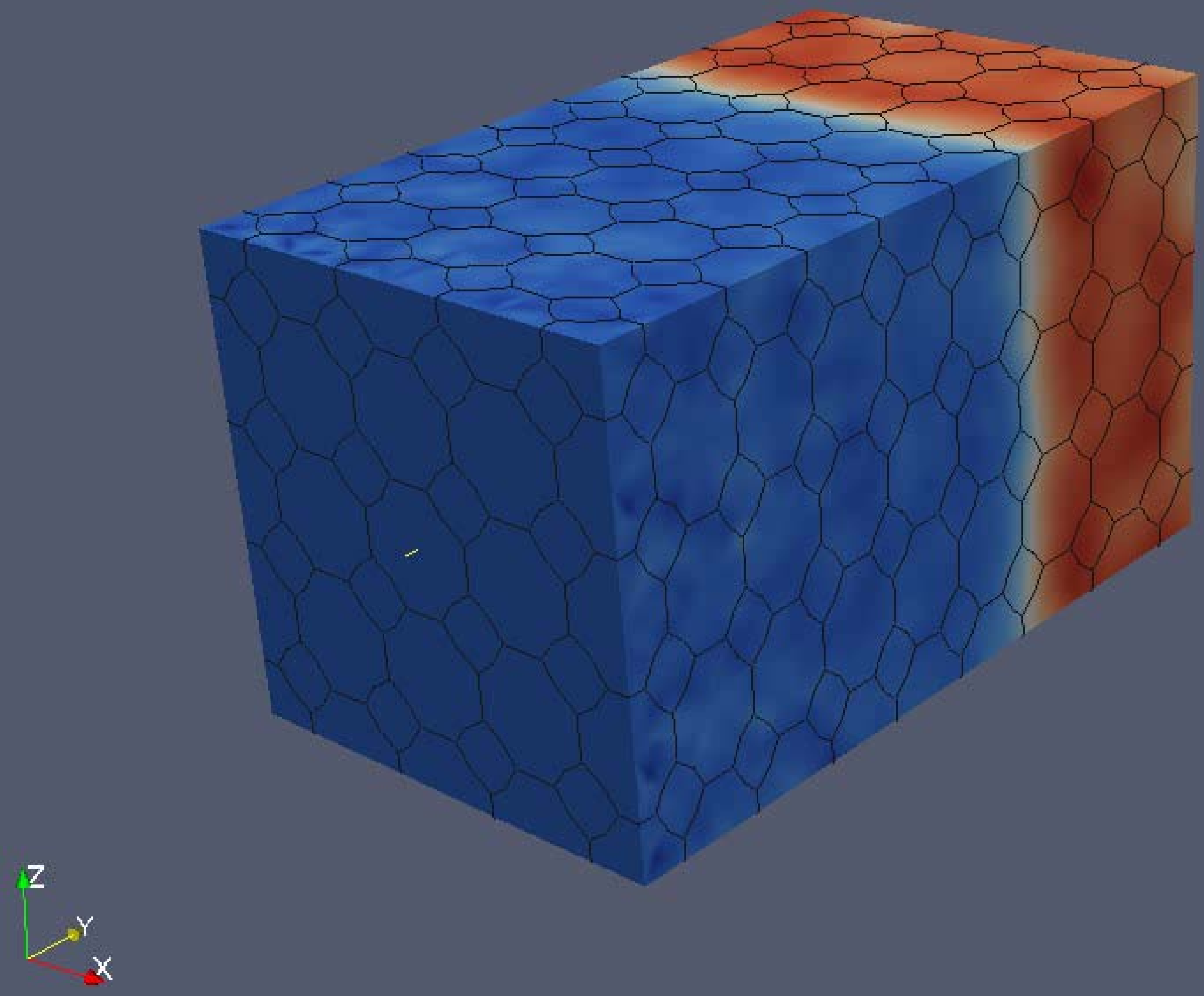
PETN plate impact - Velocity



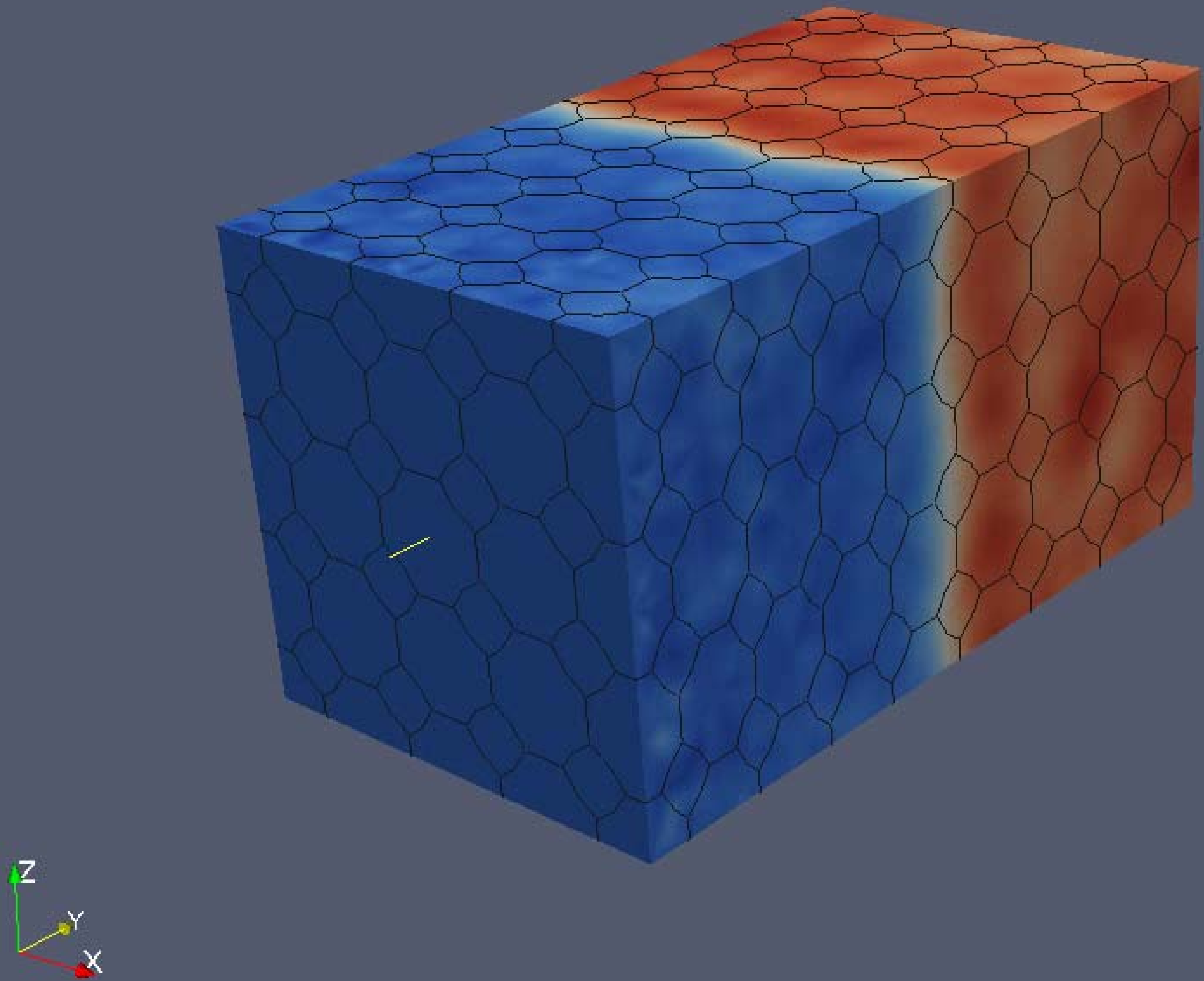
PETN plate impact - Velocity



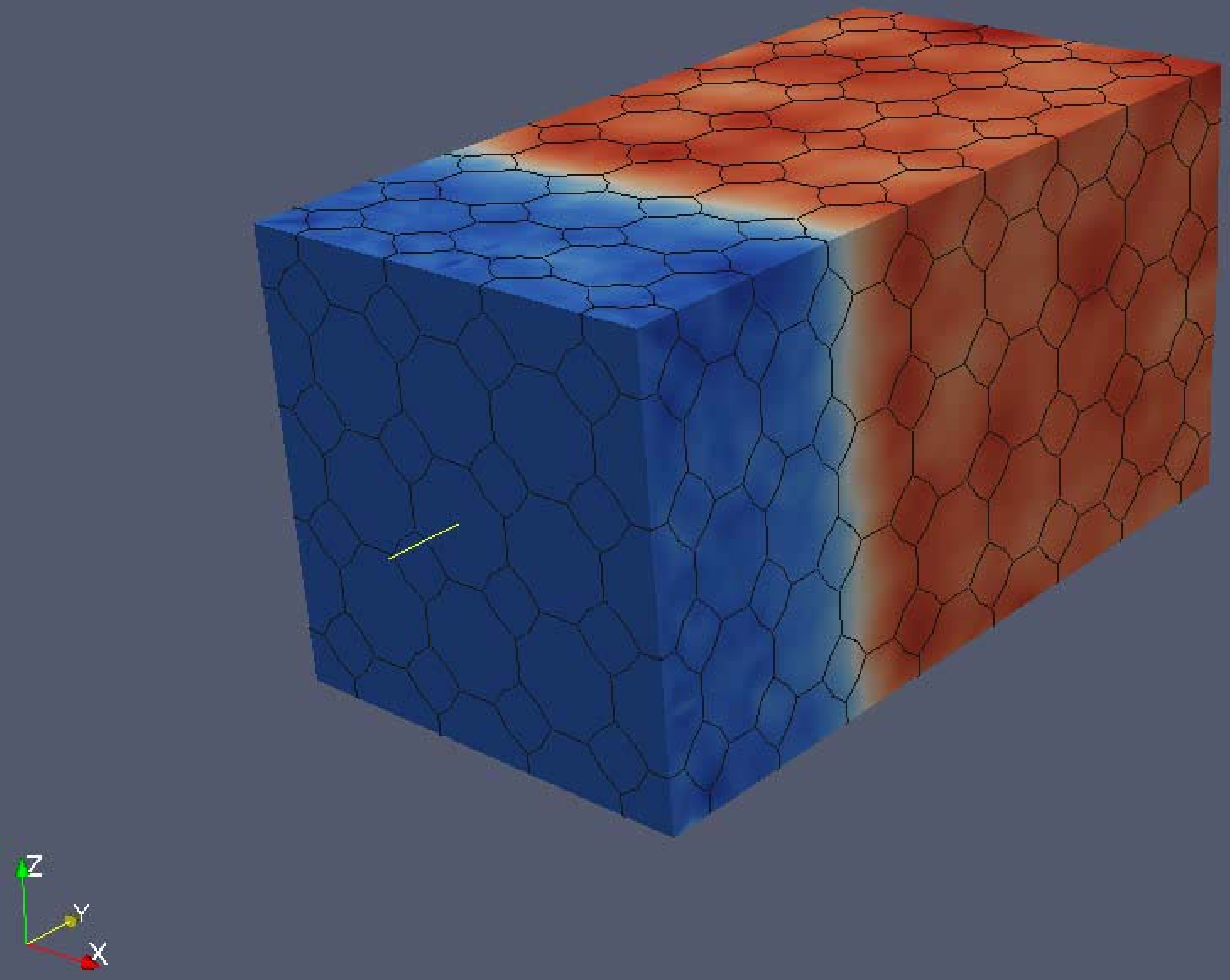
PETN plate impact - Velocity



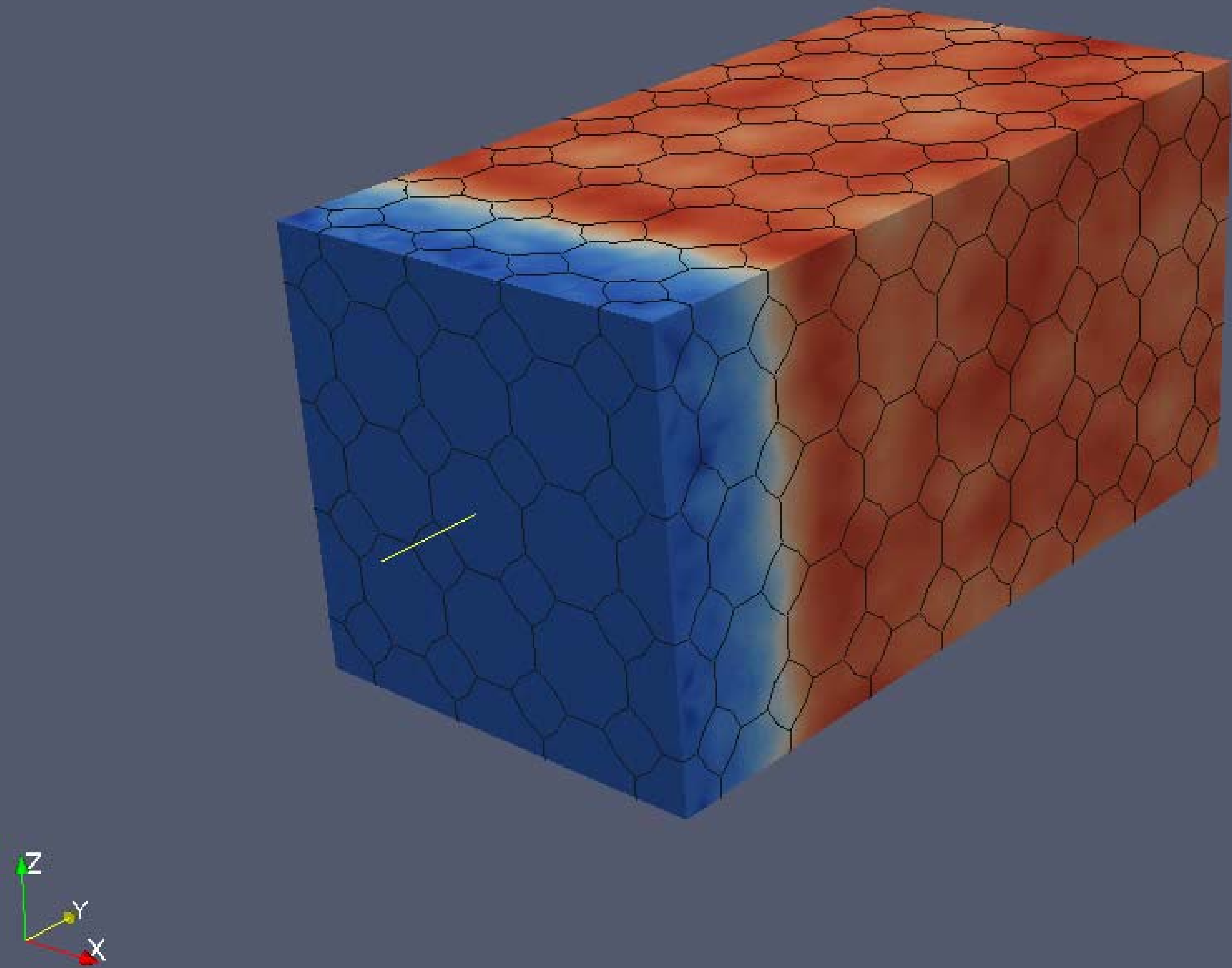
PETN plate impact - Velocity



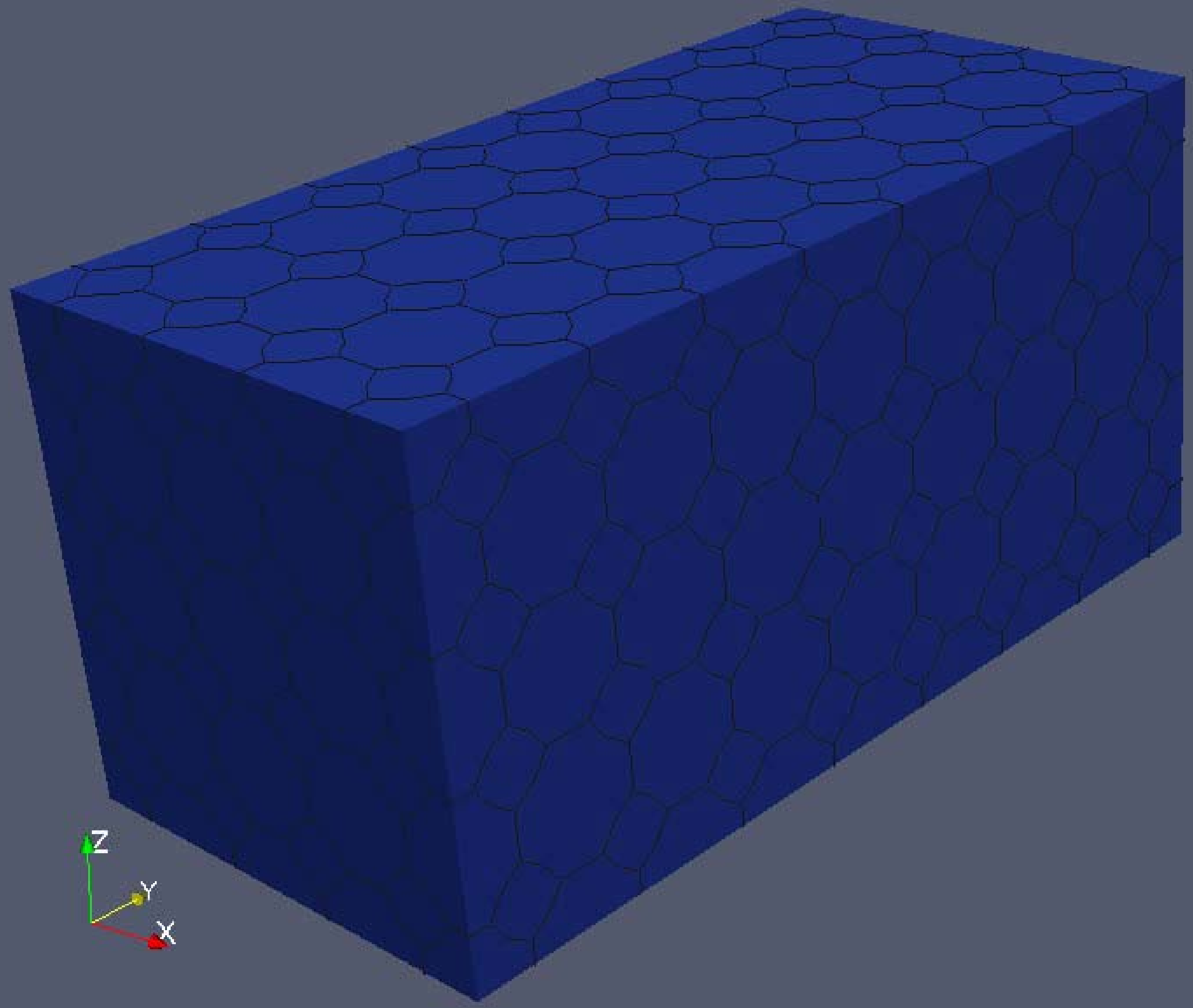
PETN plate impact - Velocity



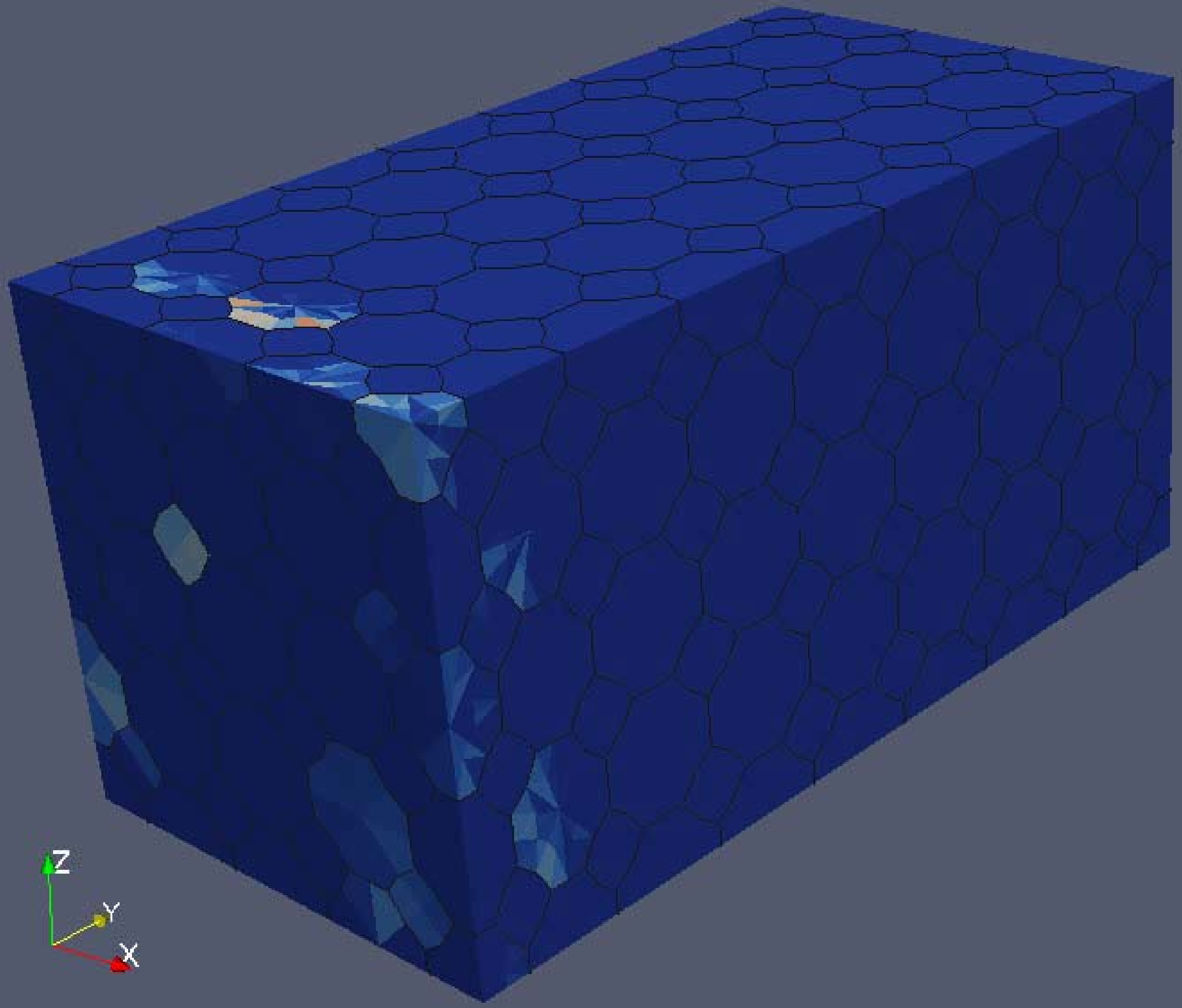
PETN plate impact - Velocity



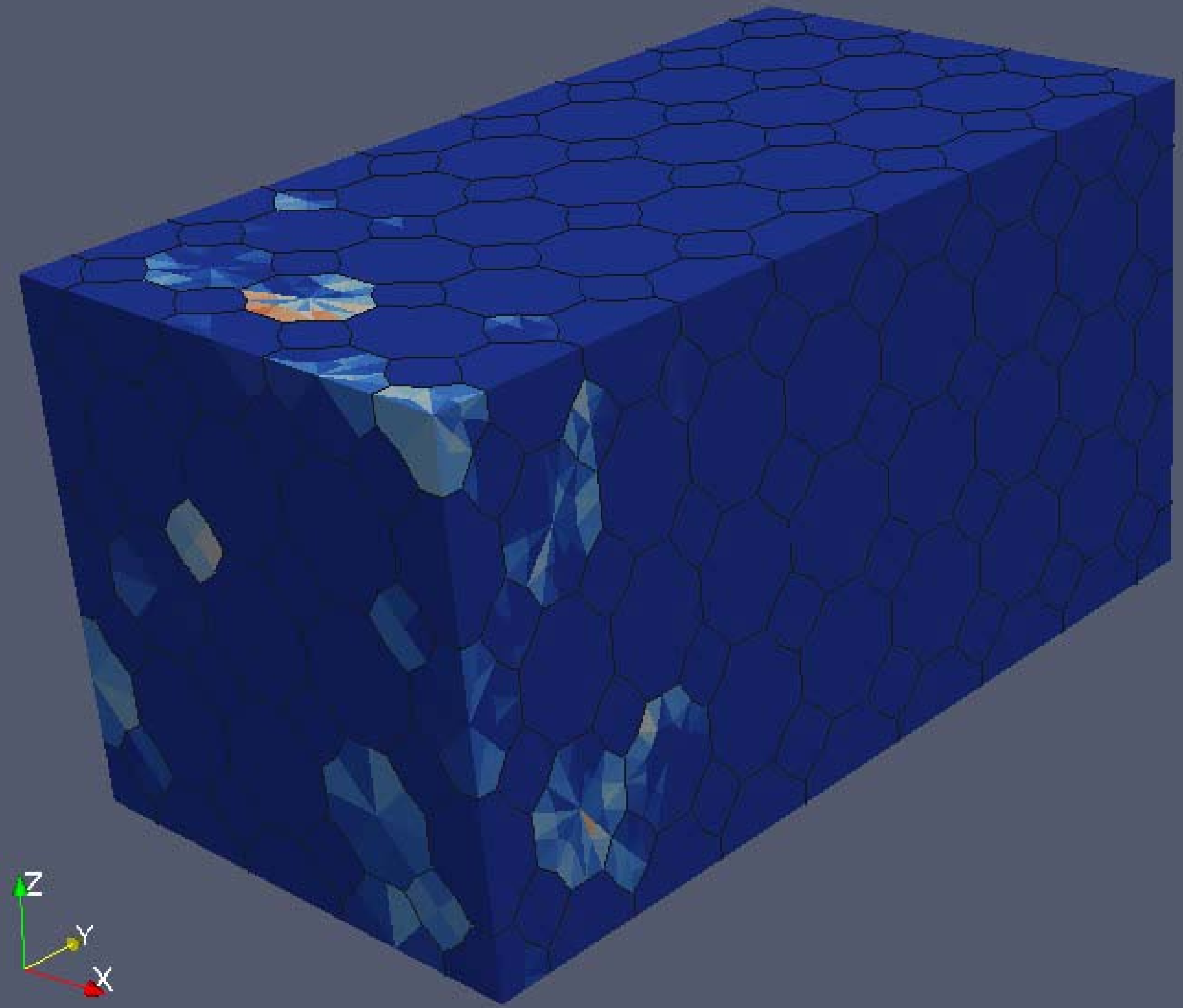
PETN plate impact - Temperature



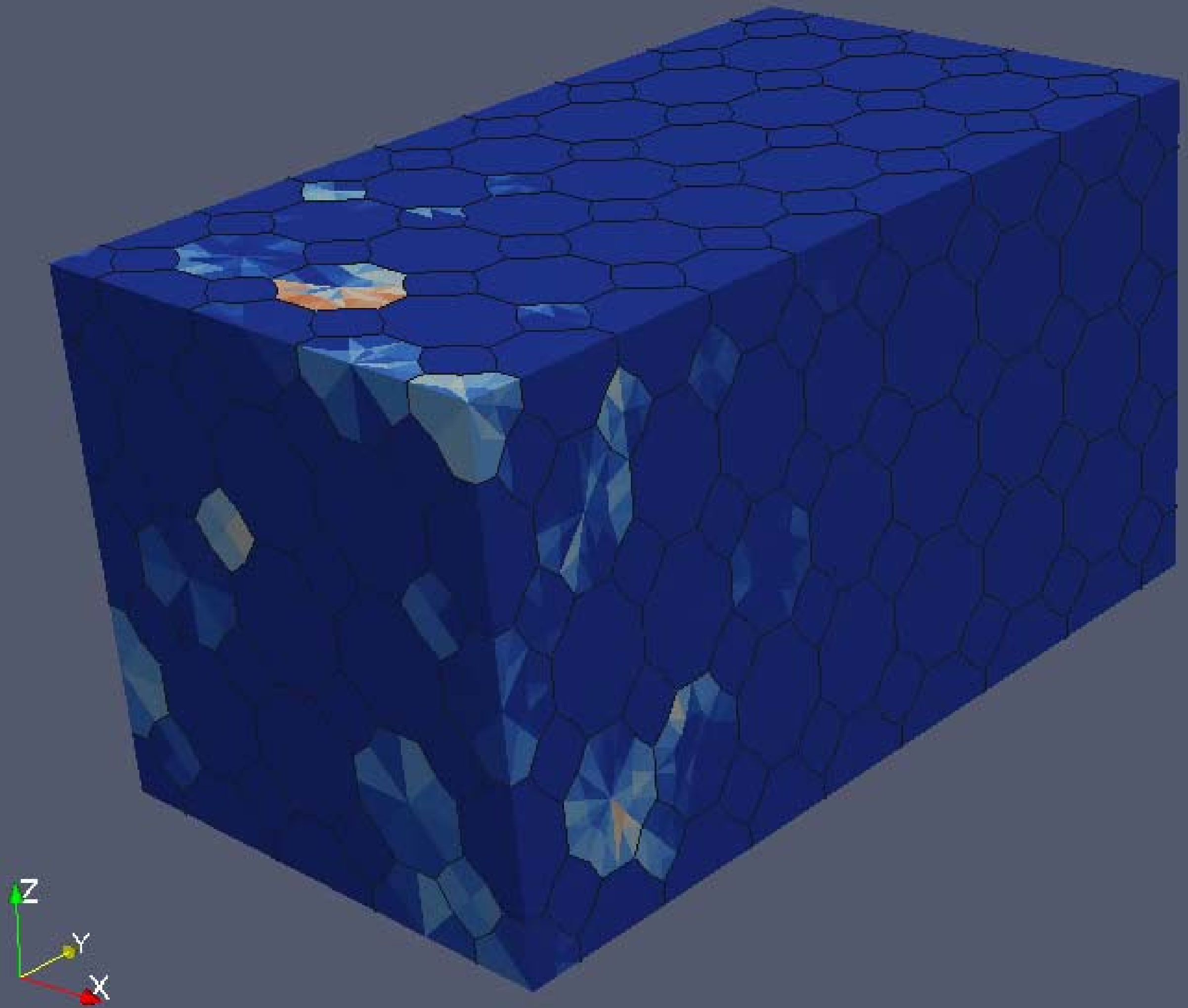
PETN plate impact - Temperature



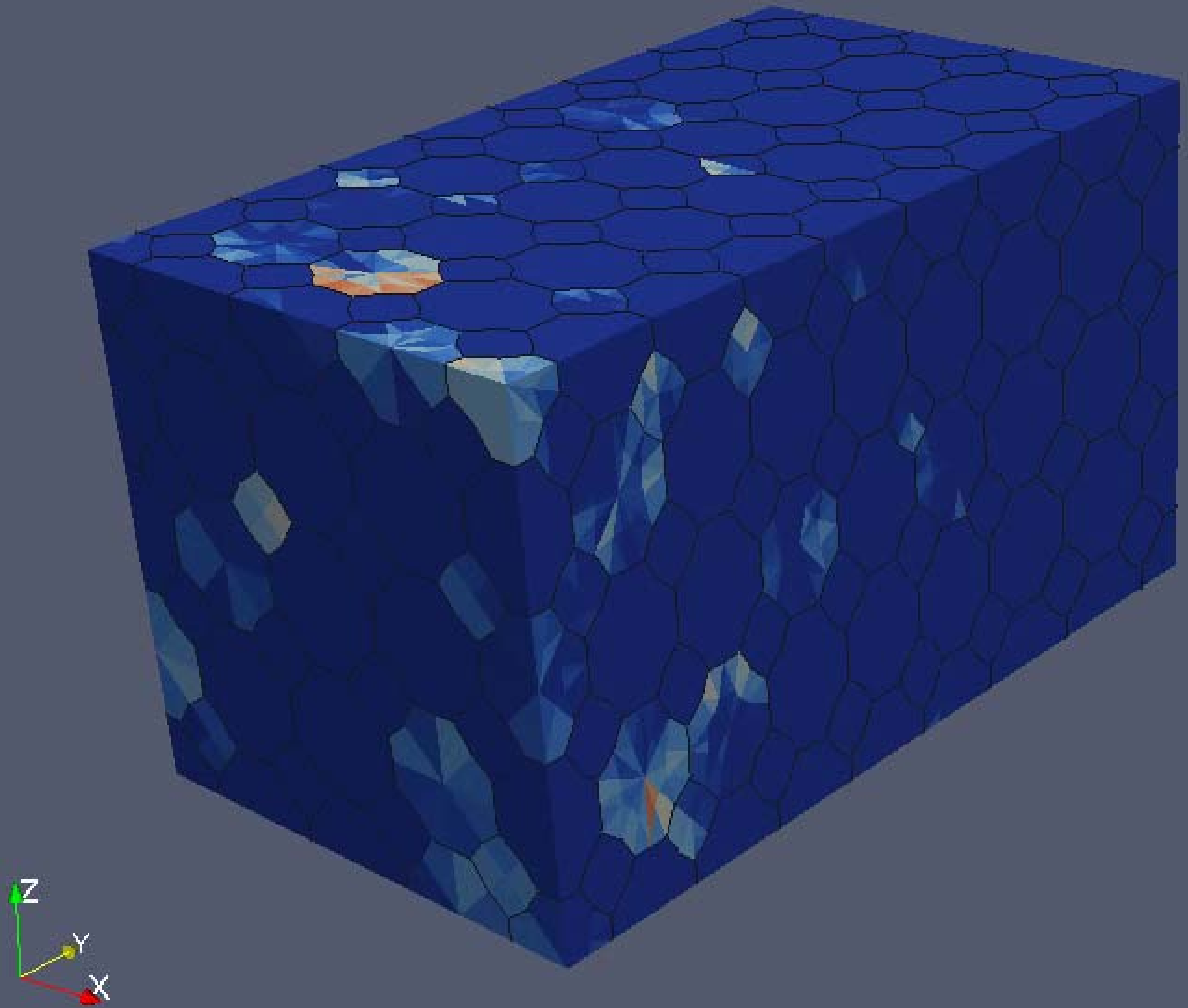
PETN plate impact - Temperature



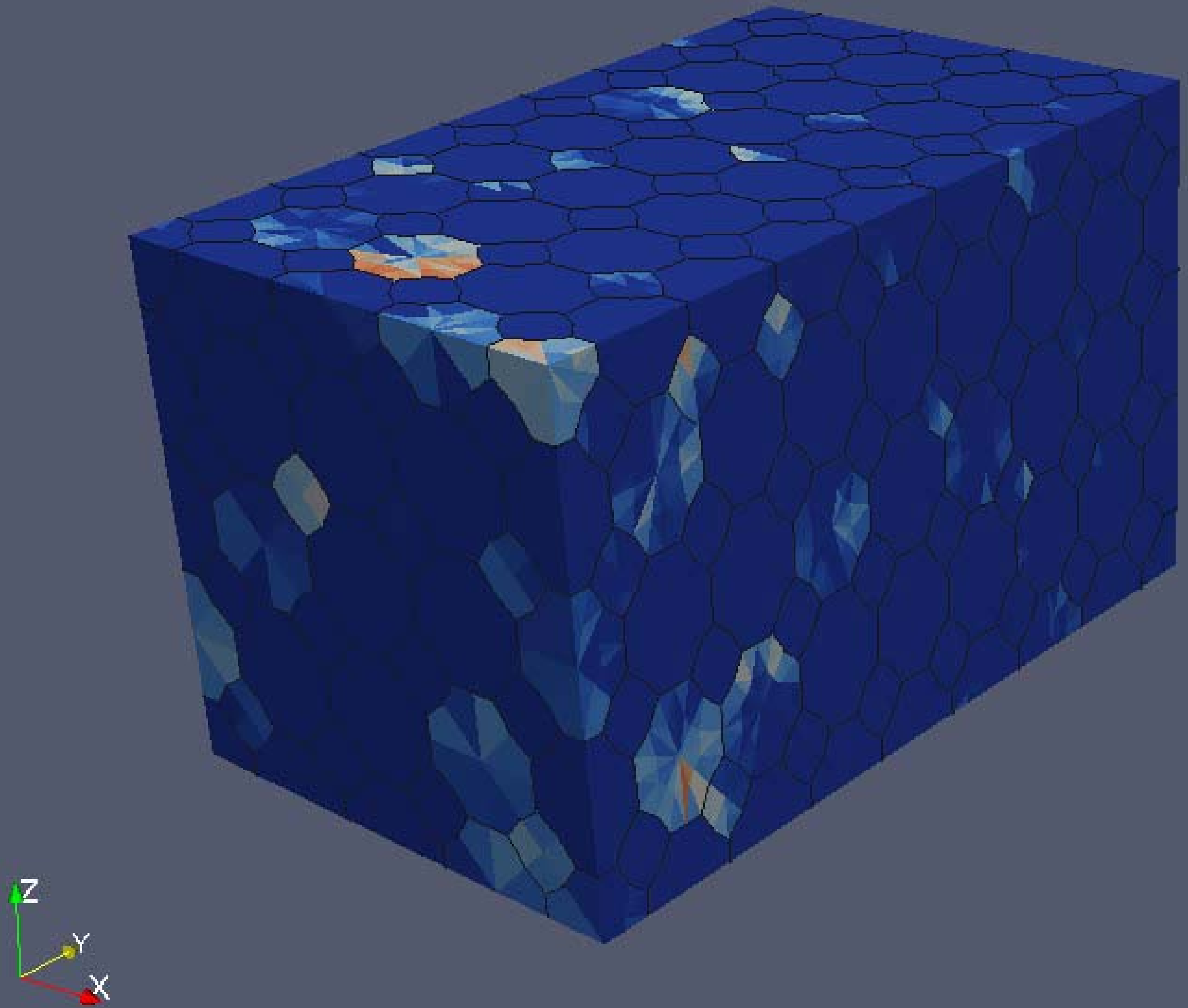
PETN plate impact - Temperature



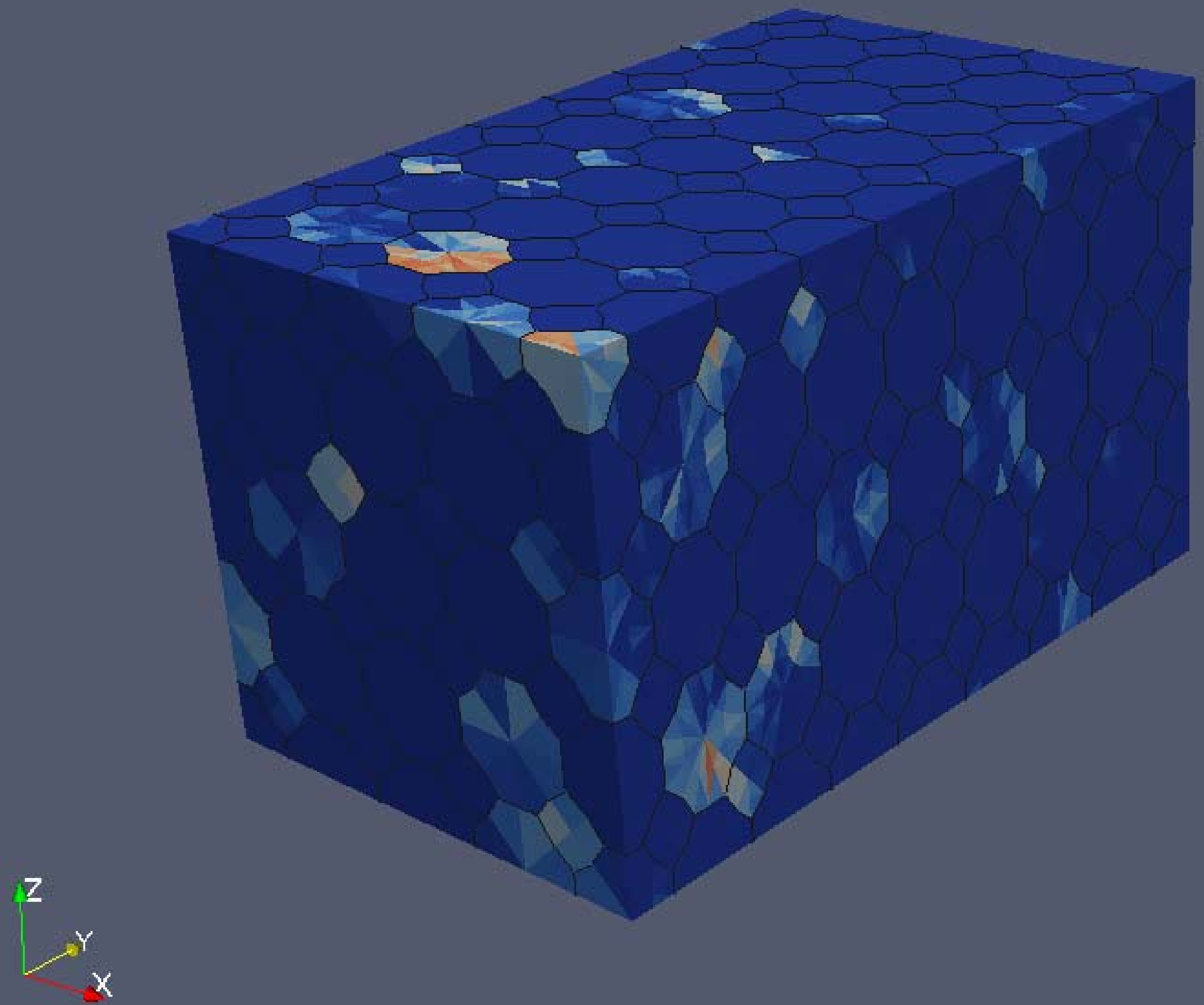
PETN plate impact - Temperature



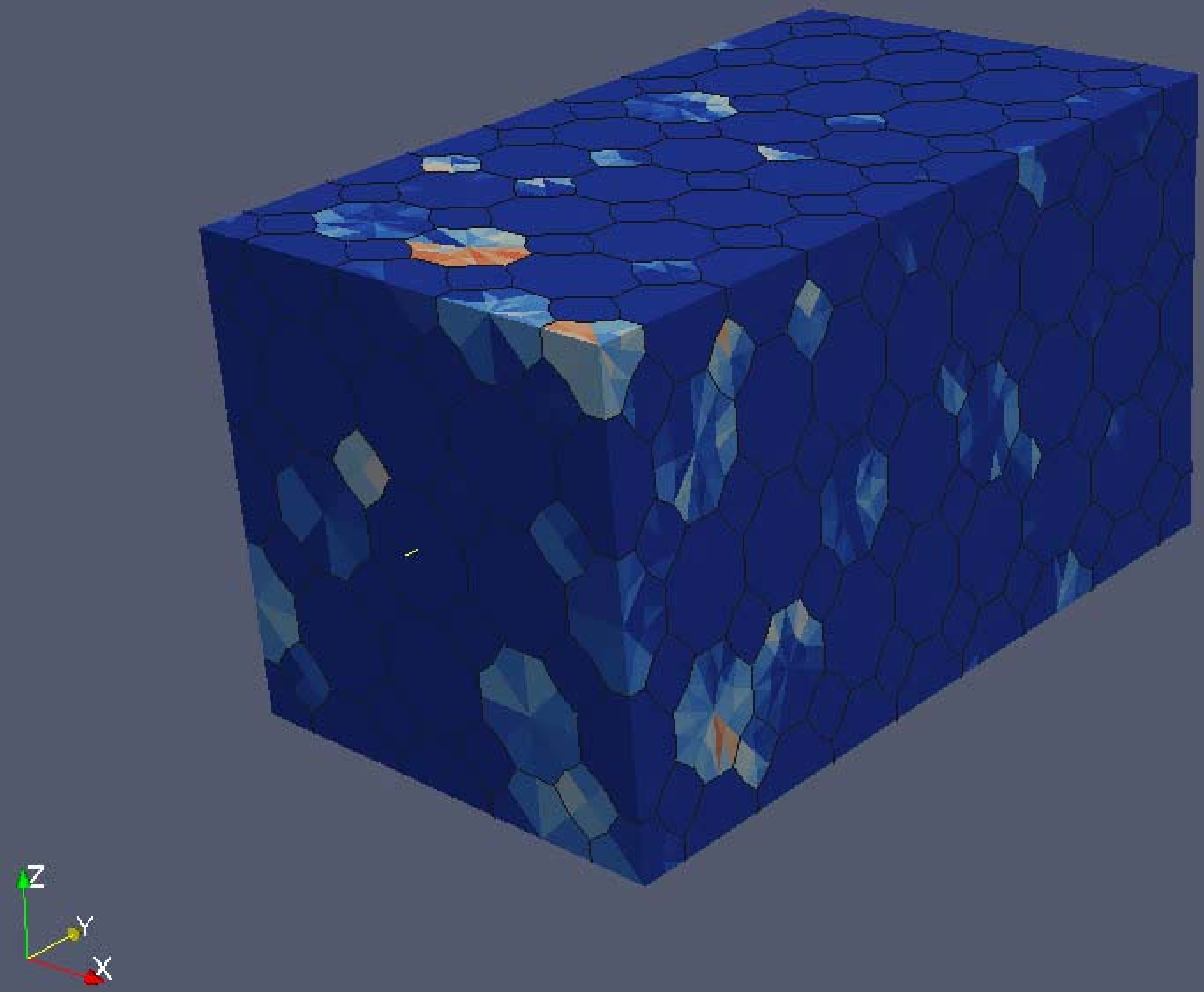
PETN plate impact - Temperature



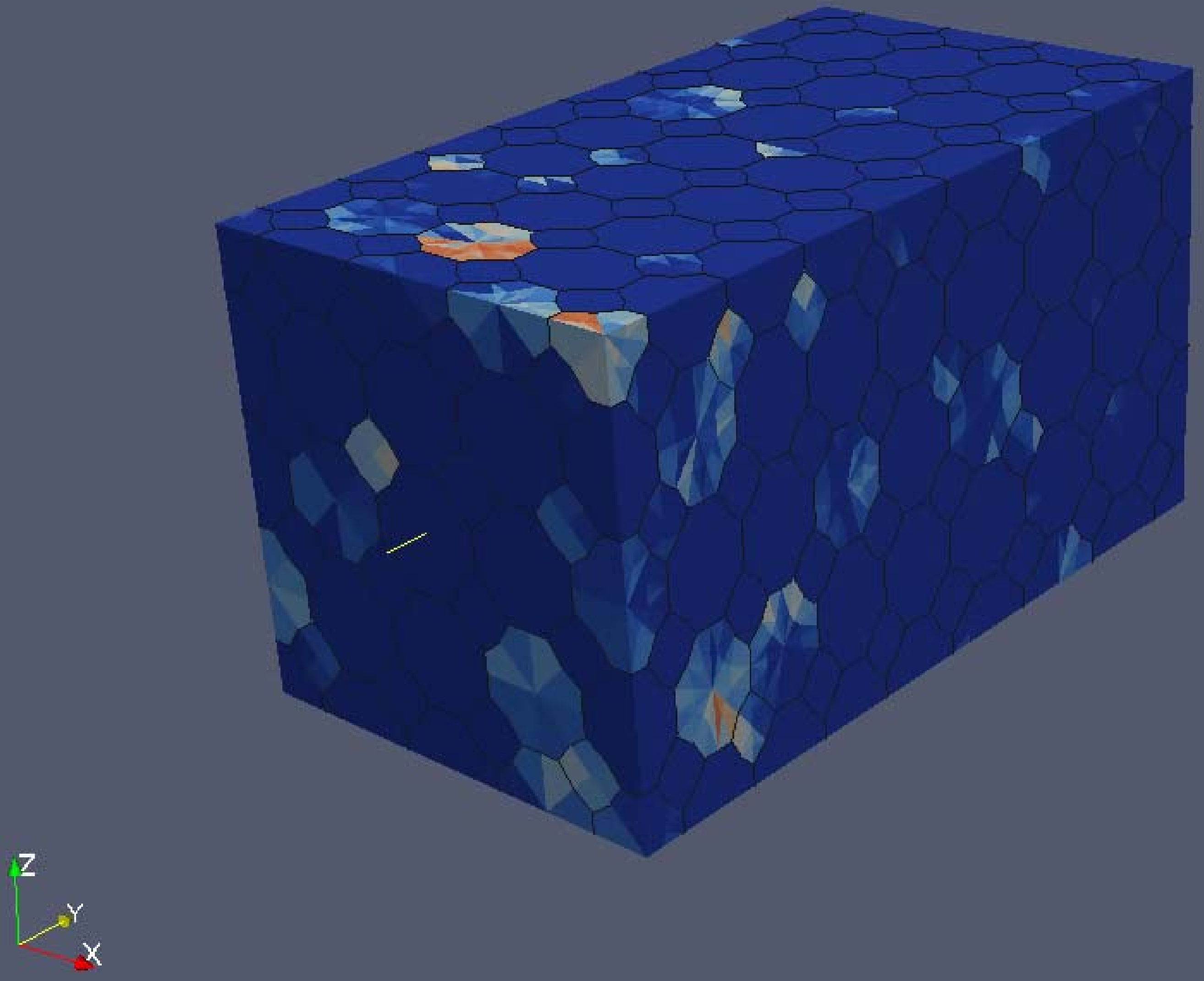
PETN plate impact - Temperature



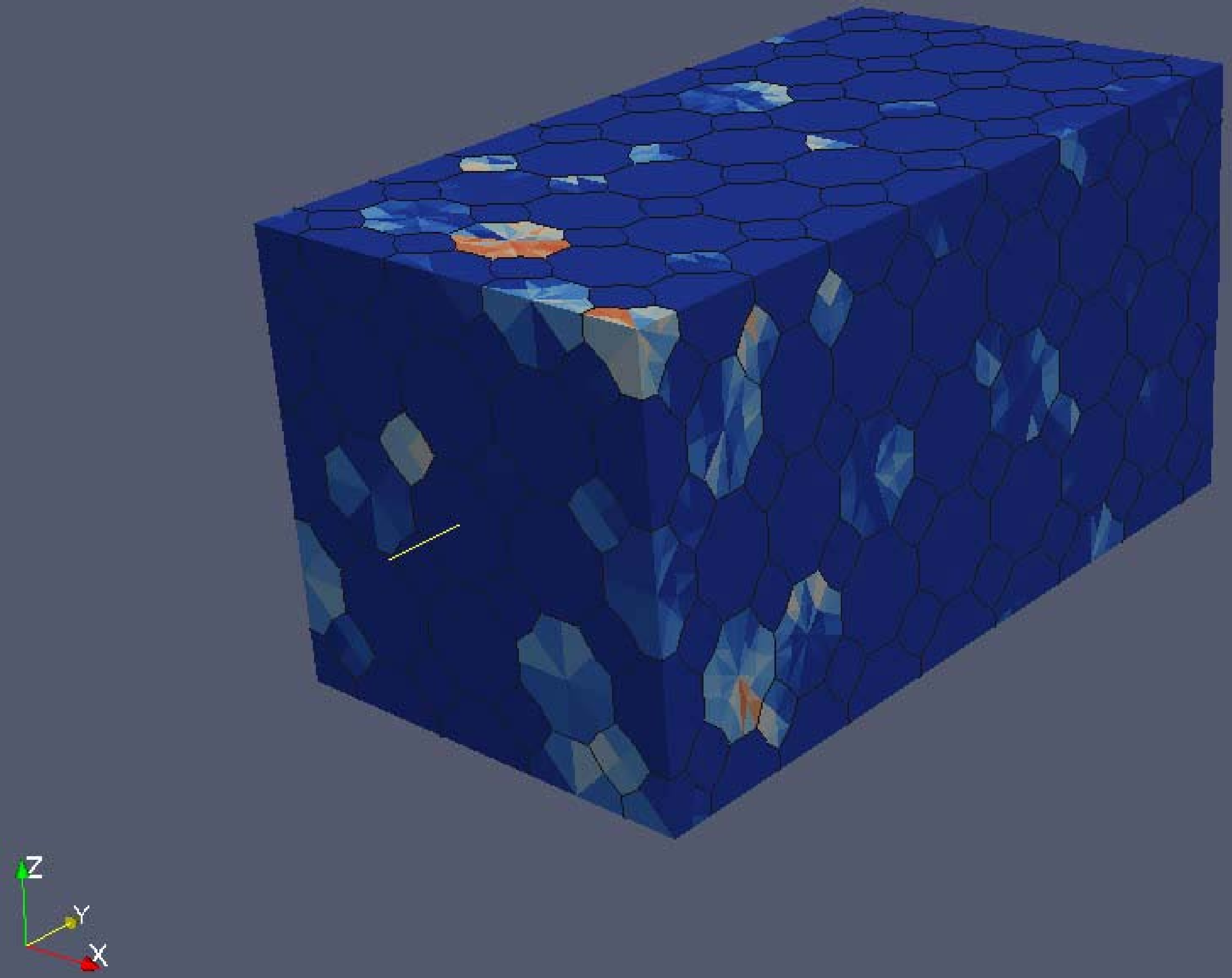
PETN plate impact - Temperature



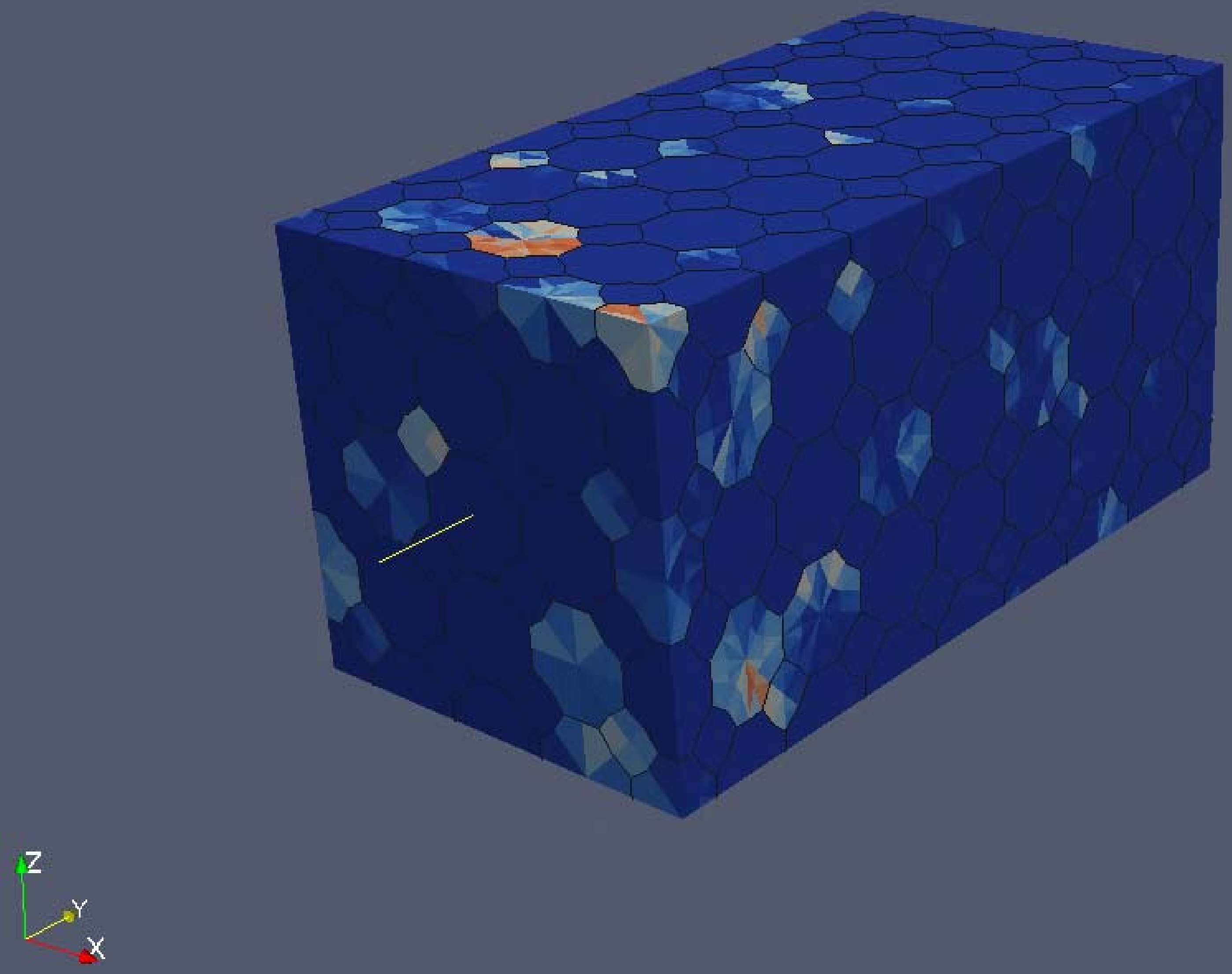
PETN plate impact - Temperature



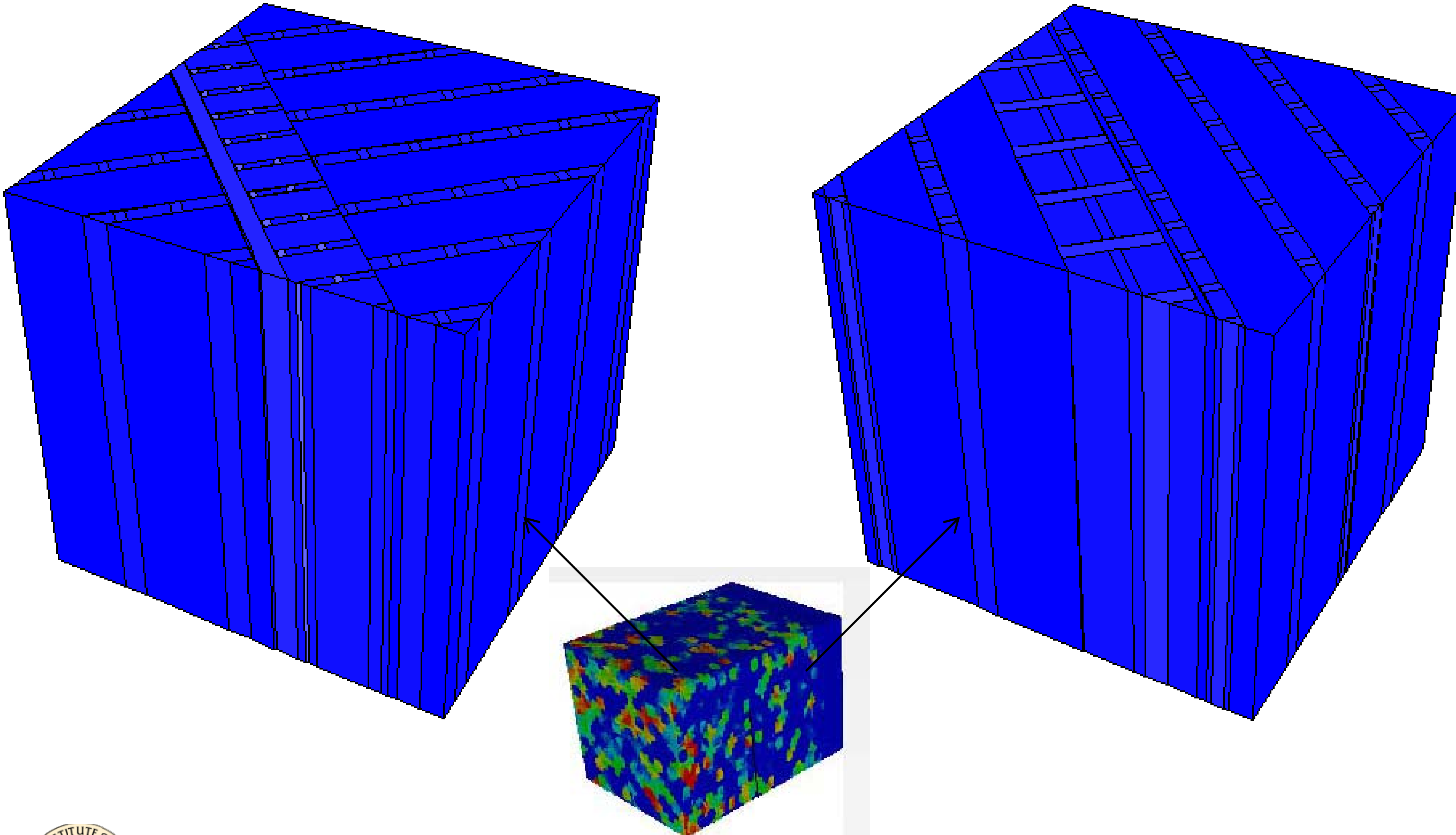
PETN plate impact - Temperature



PETN plate impact - Temperature



Fast Multiscale Models – HE detonation



Microstructure evolution at selected material points

M. Ortiz
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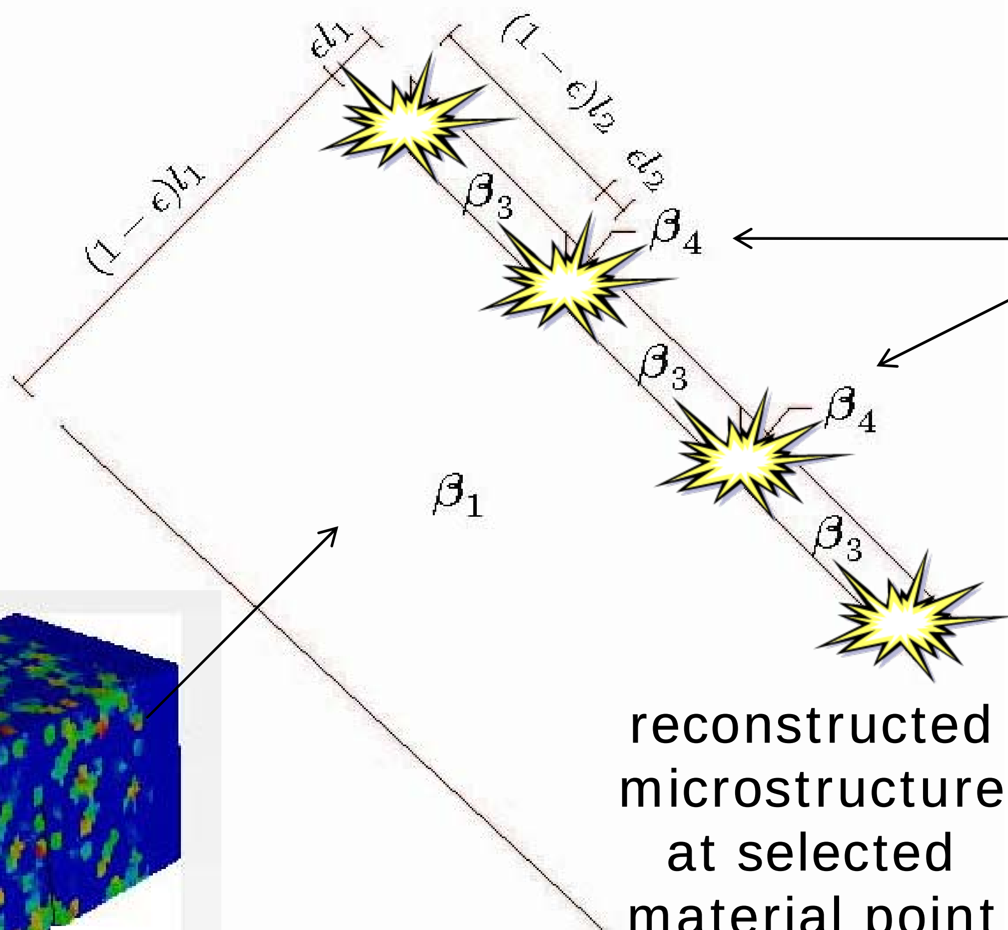
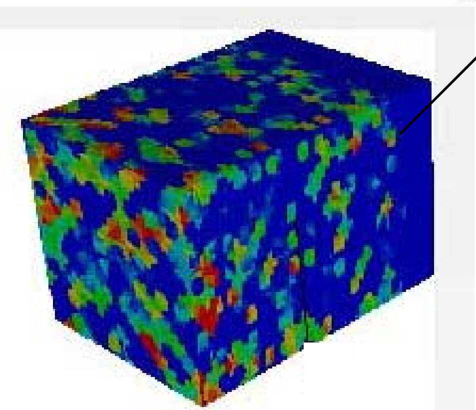
High-Explosives Detonation Initiation



high deformation, deformation rate, temperature

Hot spots!

boundary conditions for full-chemistry analysis



reconstructed microstructure at selected material point

Plate impact simulation hot spot analysis

MM&S - Outlook

- Present standard theory in the Calculus of Variations covers well static problems with strict separation of scales
- Open problems:
  - *Frustration: Lengthscale cutoff, branching microstructures, non-local behavior, scaling...*
  - *Microstructural evolution: Non-proportional paths, unloading, cyclic loading...*
  - *Relaxation of crystal plasticity with finite kinematics*
  - *Dynamics: Micro-inertia, heating rates, phonon drag...*
  - *Finer scales: Dislocation dynamics, crystalization, defect core structure, quantum-mechanical accuracy...*
  - *Larger scales: Fast Mulsticale Models of polycrystals...*
  - *Other multiscale phenomena: ductile fracture, fragmentation...*