Shock-induced subgrain microstructures in energetic polycrystals

M. Ortiz
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with: E. Gurses, J. Rimoli,

TMS Annual Meeting
Seattle, WA, February 17, 2010

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)

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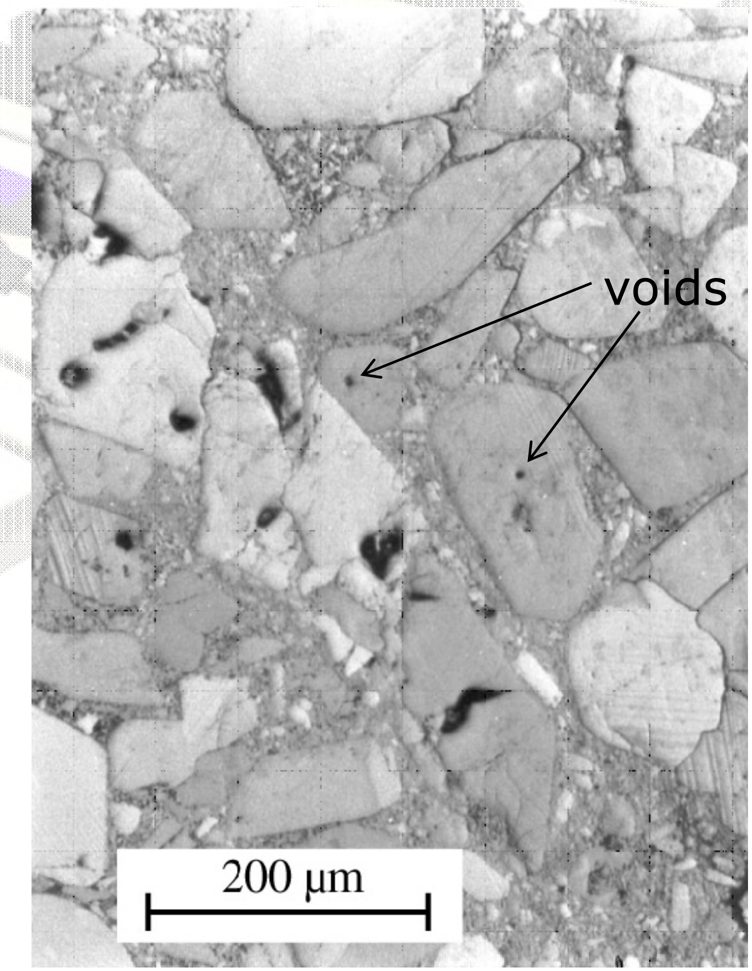
High-Explosives - Initiation

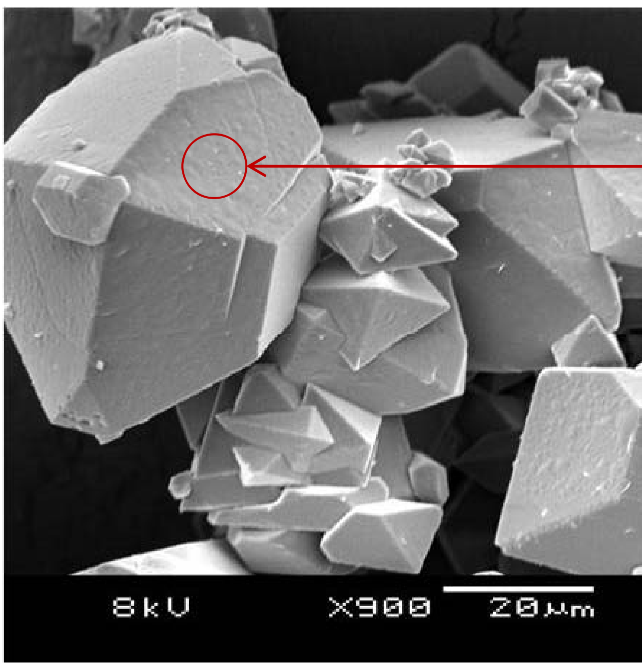
- In high explosives (HE) localized hot spots cause detonation initiation
- The hot spots are often assumed to arise at extended crystal defects such as voids
- Shock-induced void collapse is often modeled at single-crystal level using hydrocodes or continuum (mean-field) single-crystal plasticity



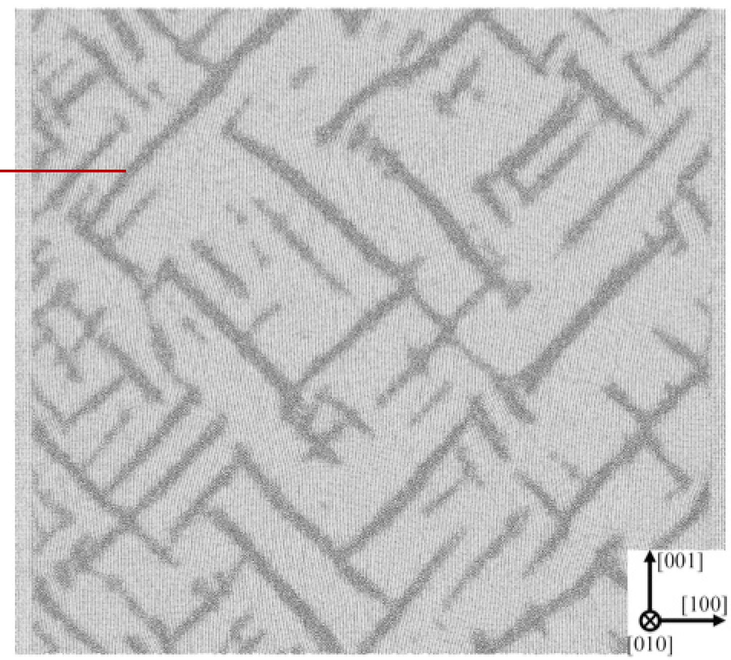
H. Tan, iMechanica, 2008

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)

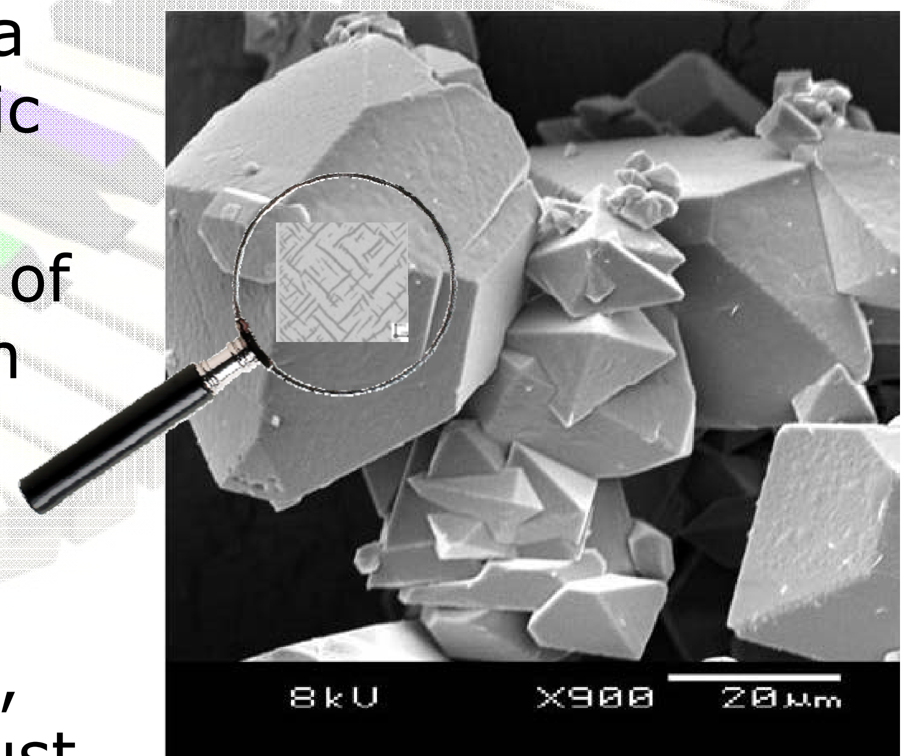


Shear bands in shocked RDX

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

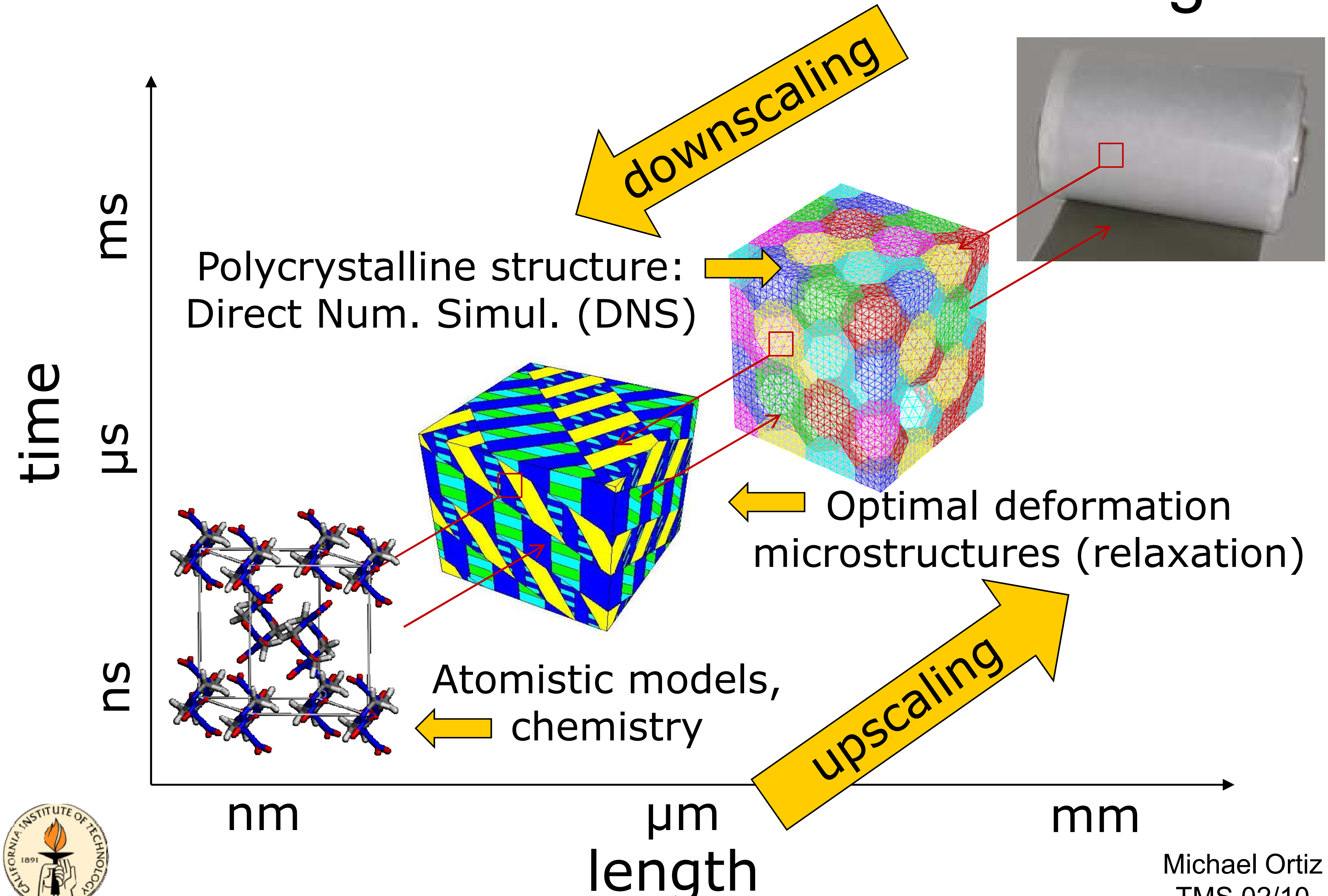
High-Explosives - Initiation

- 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



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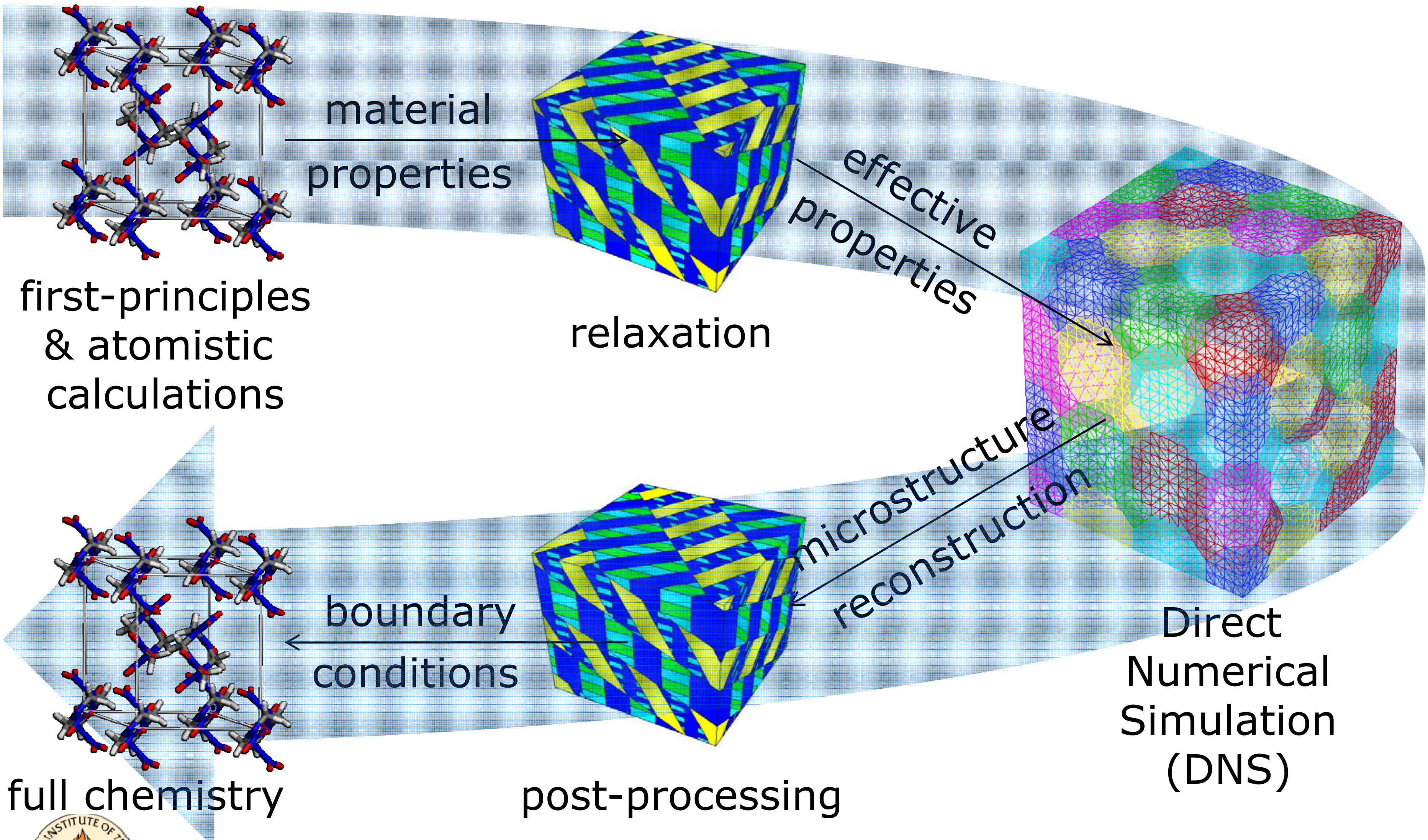
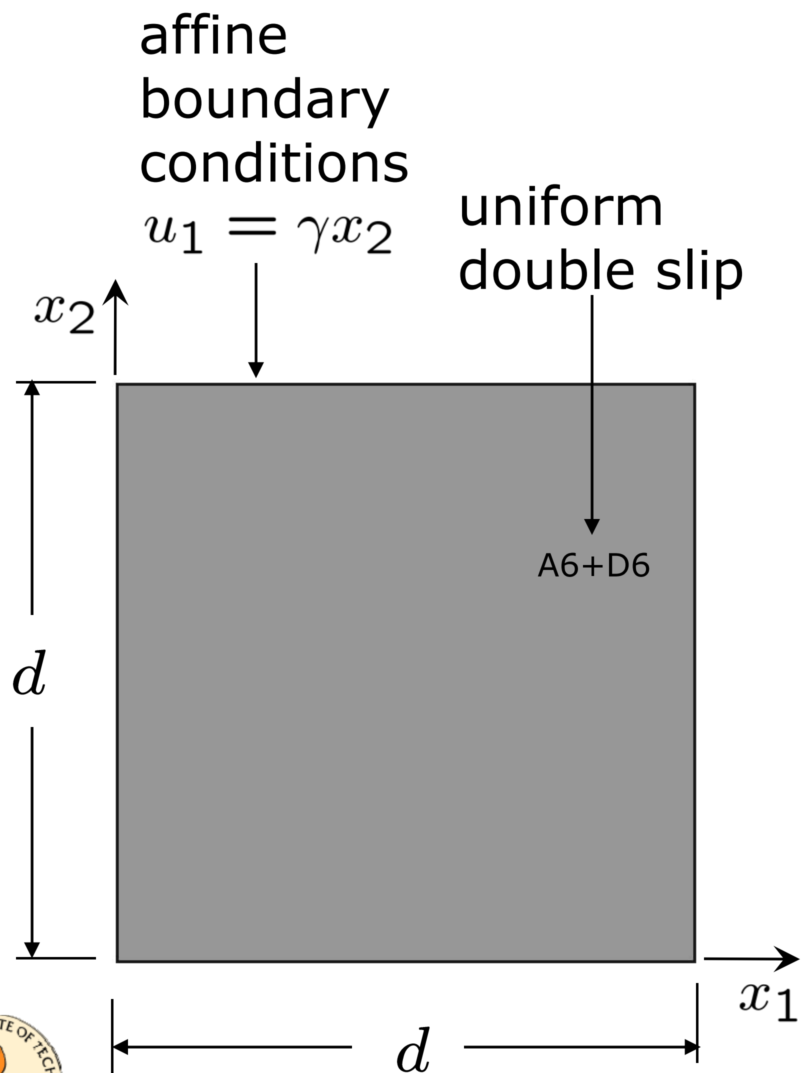
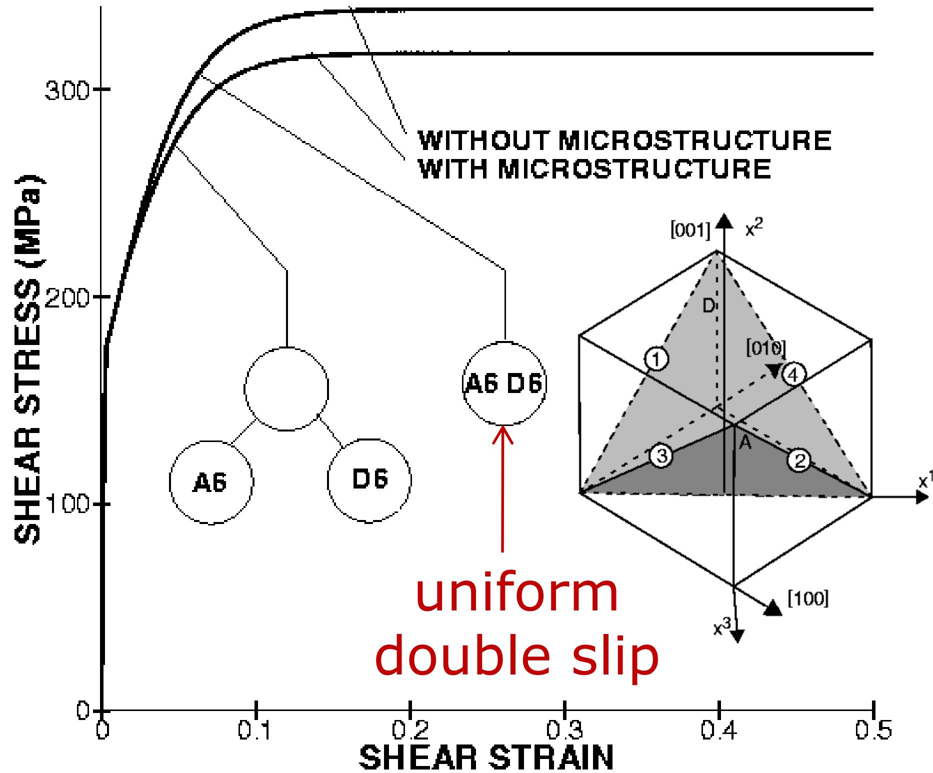


Information flow for polycrystalline HE

Strong latent hardening & microstructure

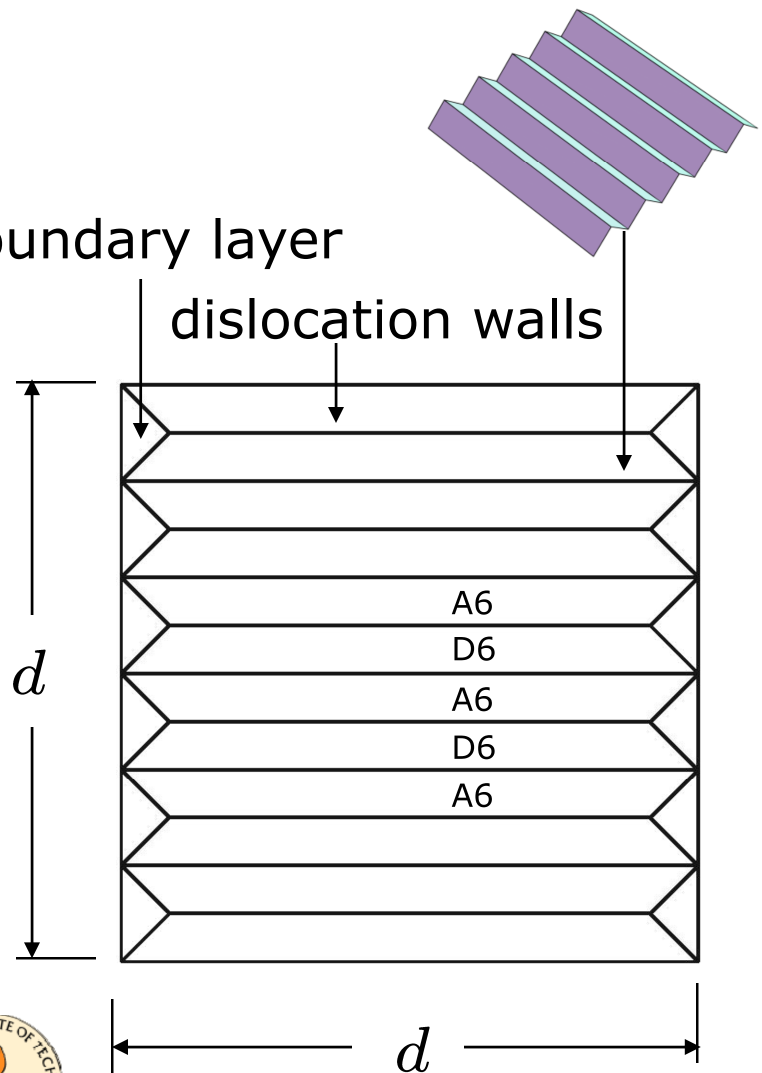


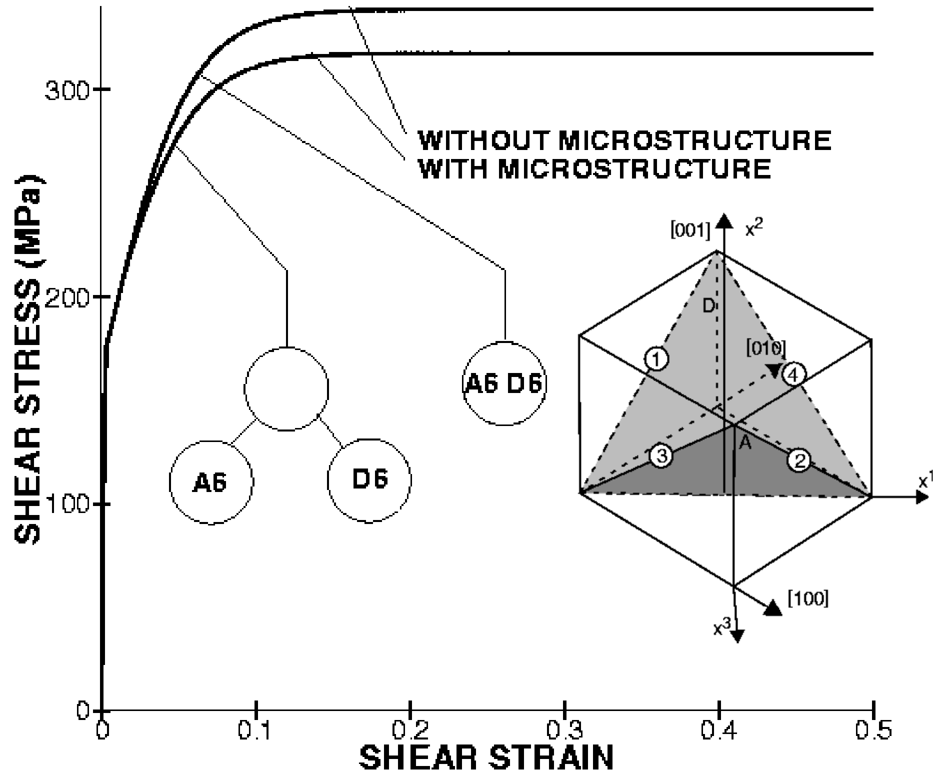


FCC crystal deformed in simple shear on (001) plane in [110] direction

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

Strong latent hardening & microstructure





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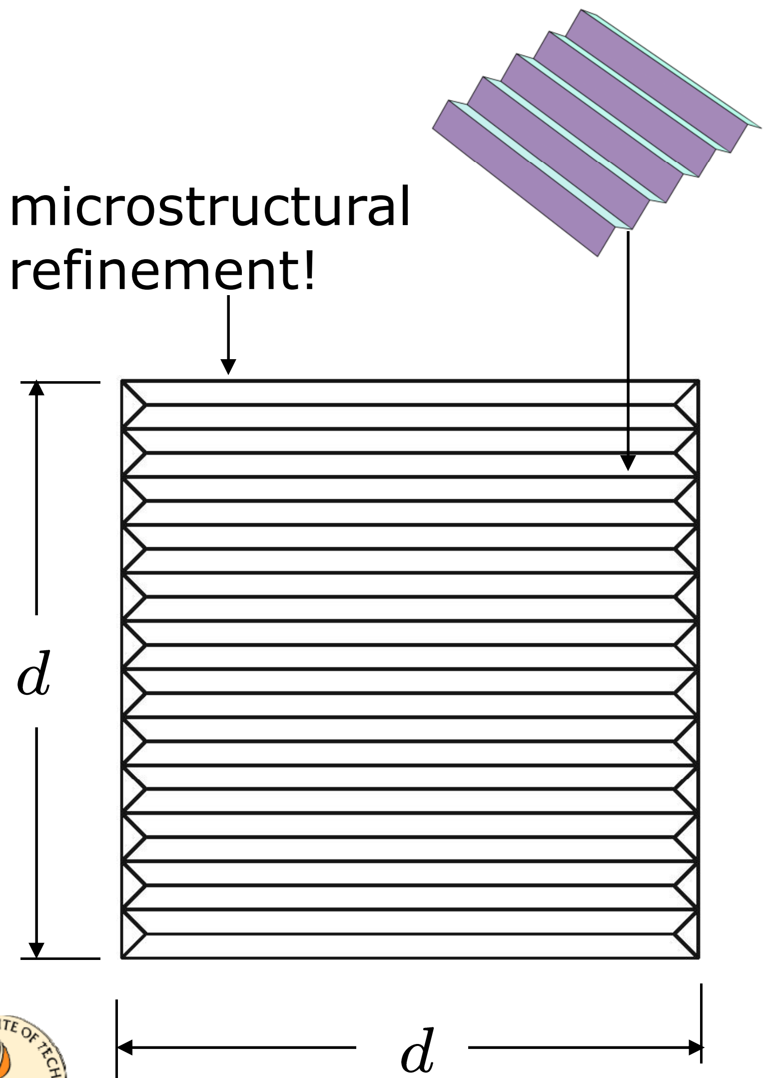

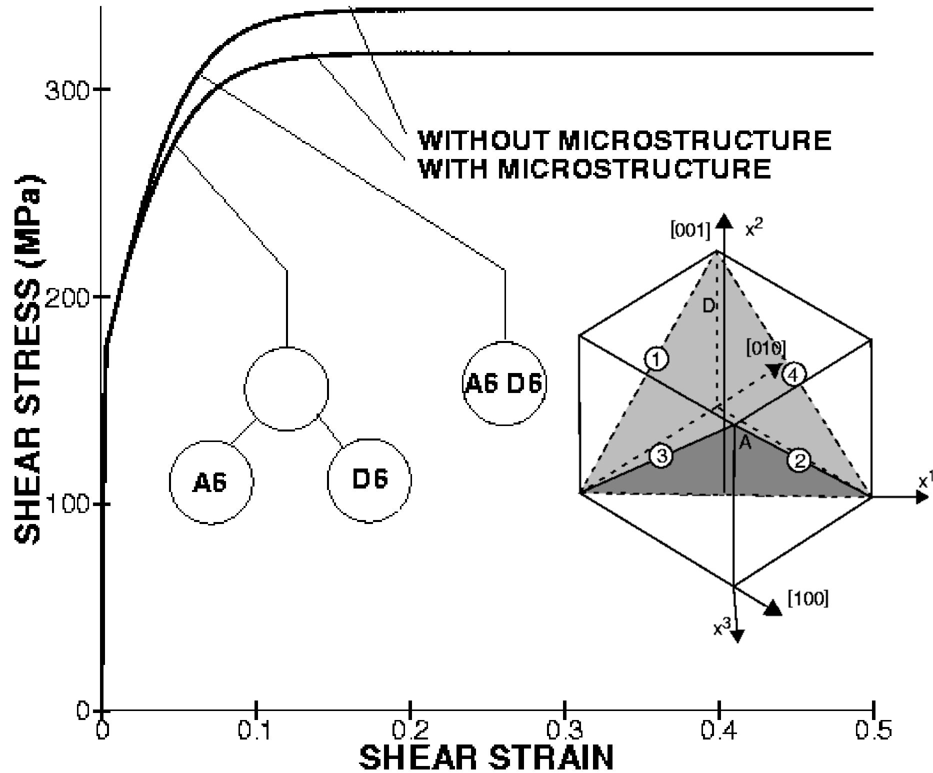

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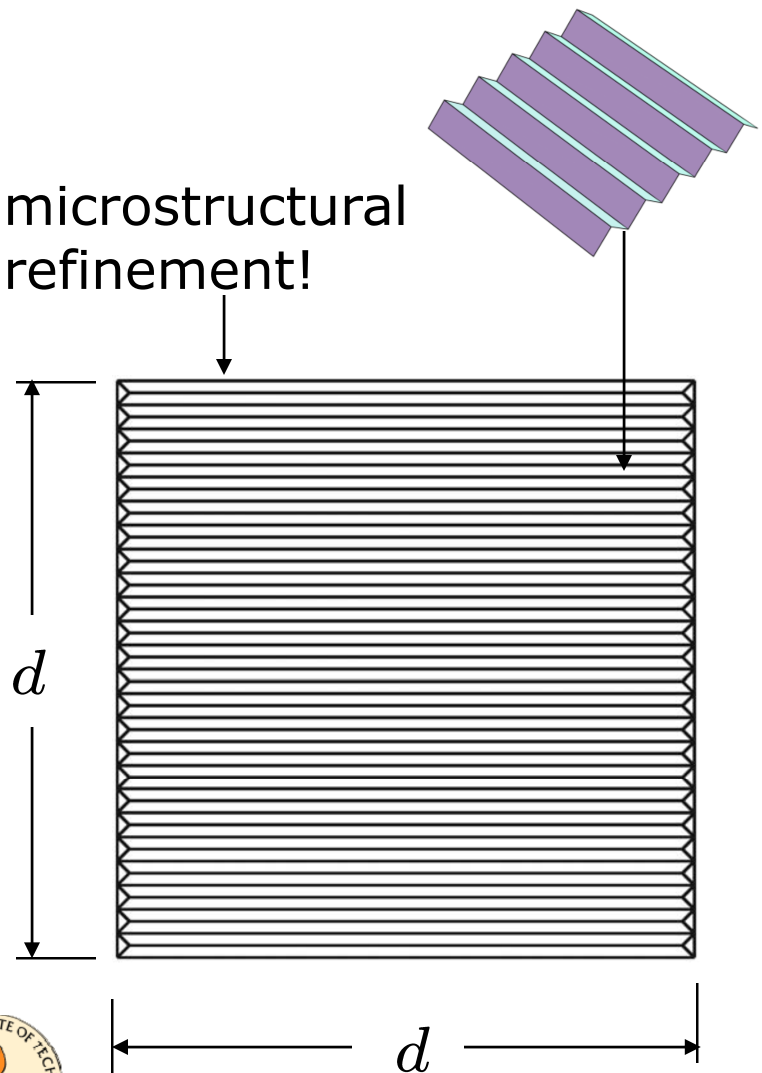

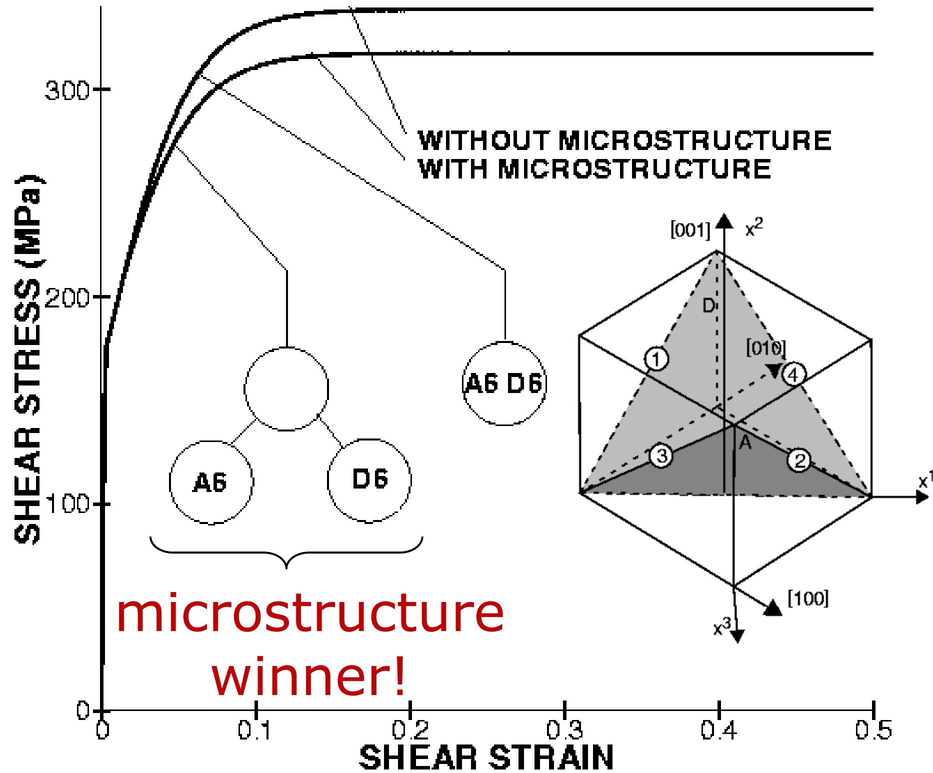

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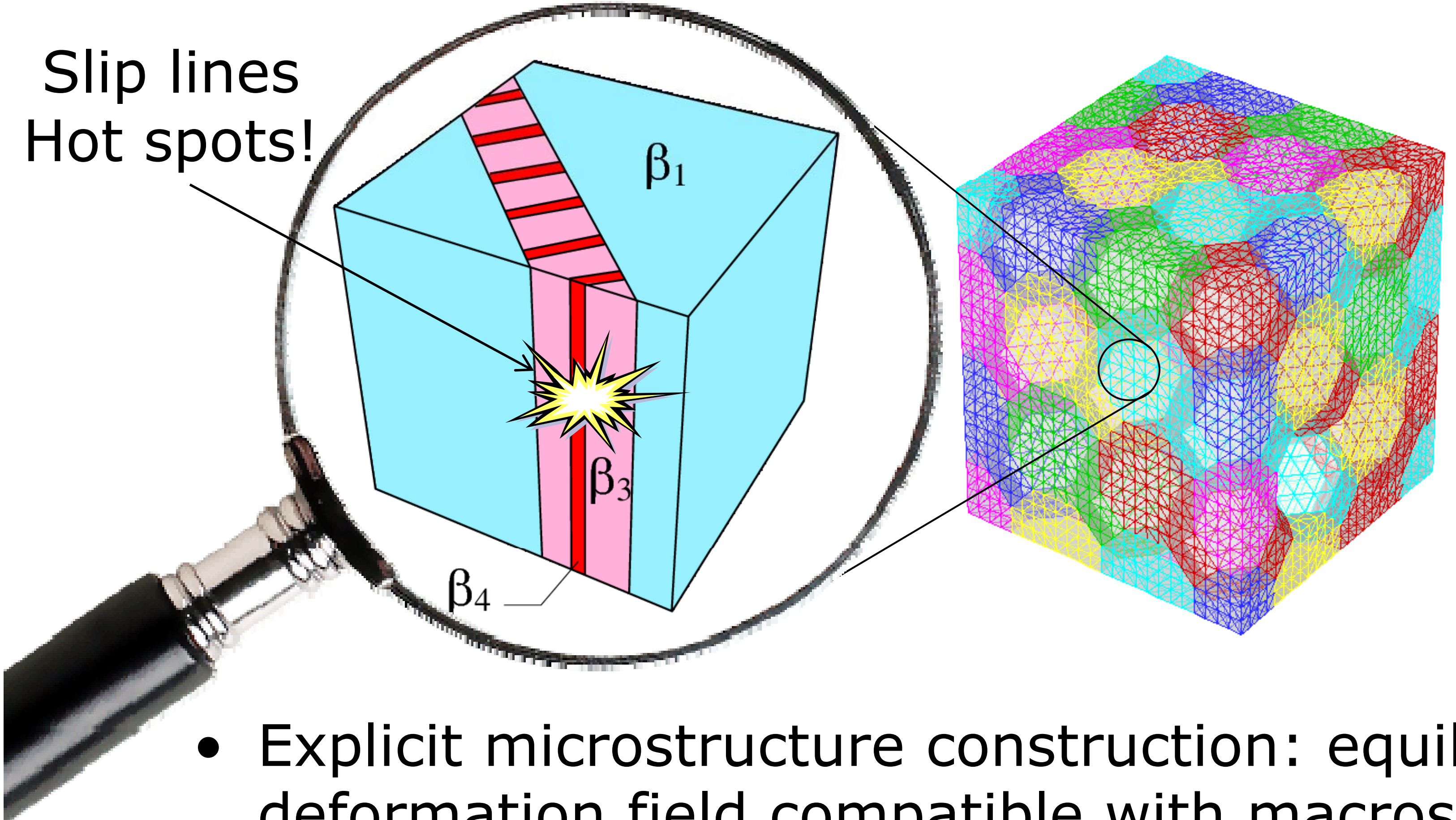
(M Ortiz, EA Repetto and L Stainier
JMPS, **48**(10) 2000, p. 2077)

Strong latent hardening & microstructure

Sir Alan H. Cottrell
ScD HonLLD FRS

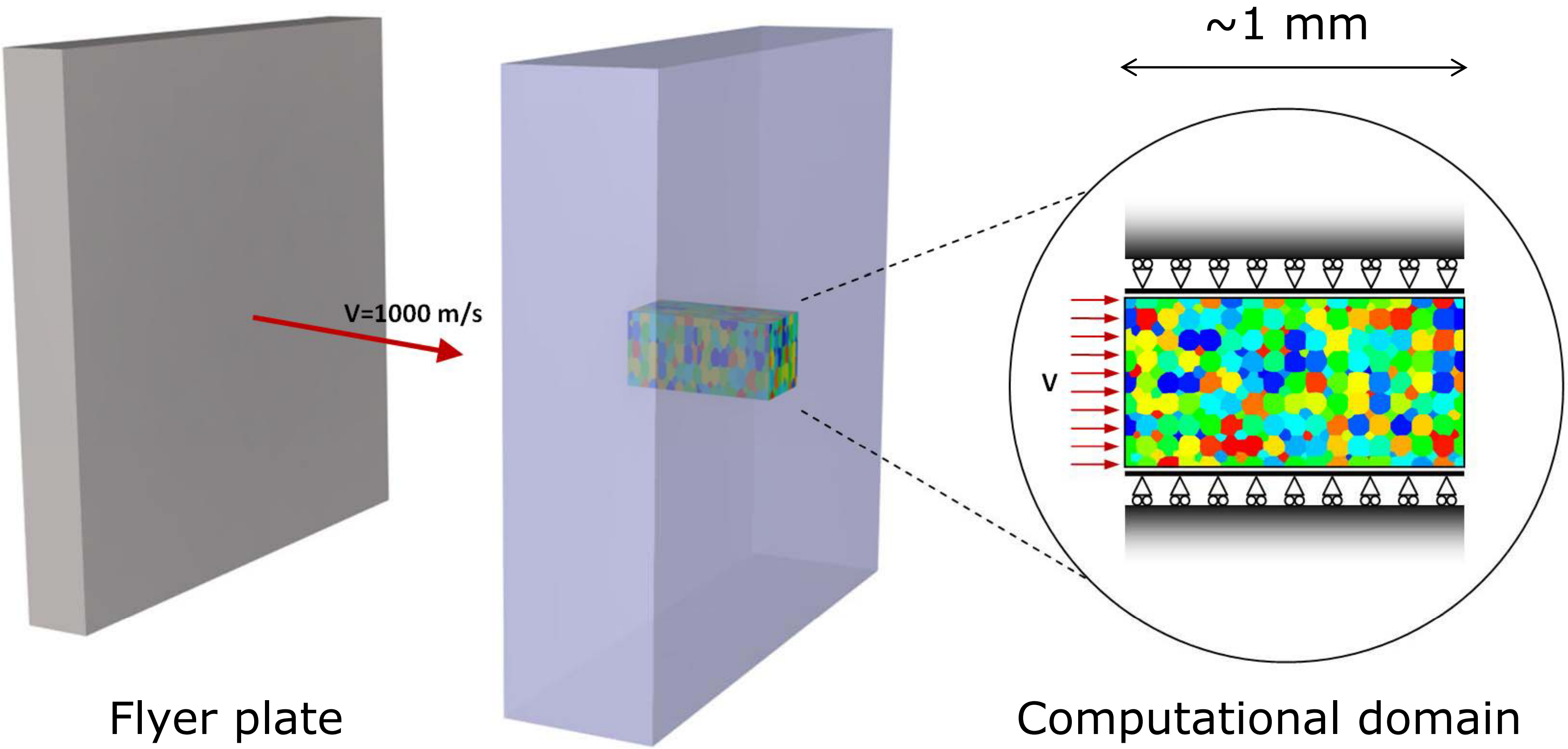
- *"These results prove the reality of latent-hardening, in the sense that the slip lines of one system experience difficulty in breaking through the active slip lines of the other"* (Piercy, G.R., Cahn, R.W. and Cottrell, A.H., *Acta Metallurgica*, **3** (1955) 331-338).
- Sub-grain microstructures are *universal* in plastically deformed single crystals

Crystal plasticity – Relaxation



- Explicit microstructure construction: equilibrium deformation field compatible with macroscopic deformation, single slip in each variant!
- Optimality: Conti, S. and Ortiz, M., *ARMA*, **176** (2005) 103-147

PETN – Plate impact test



Flyer plate

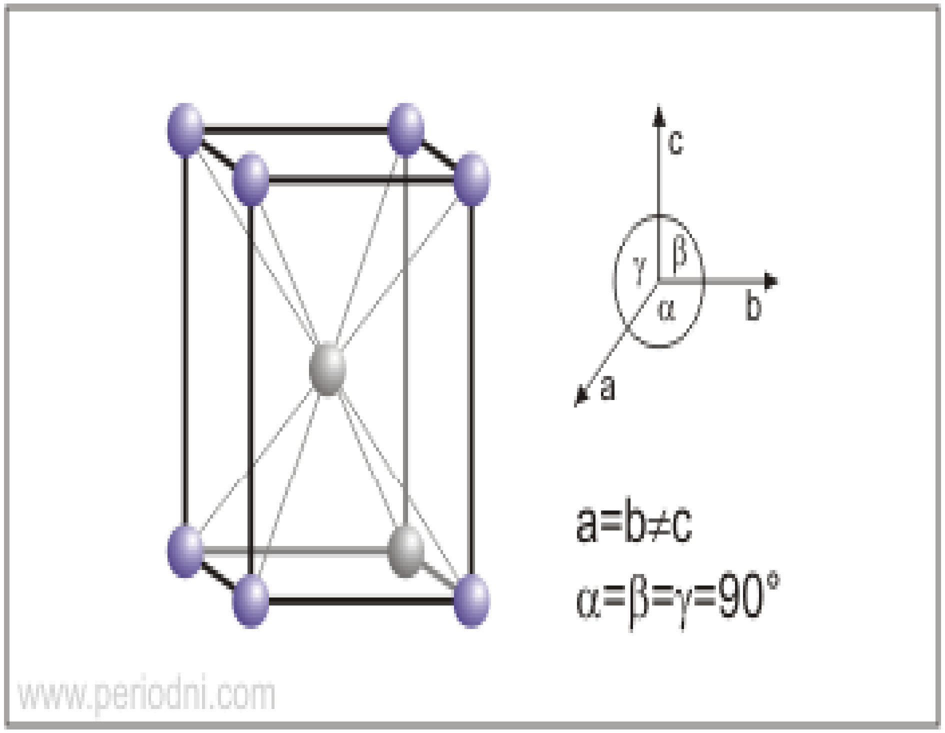
PETN target plate

Computational domain

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

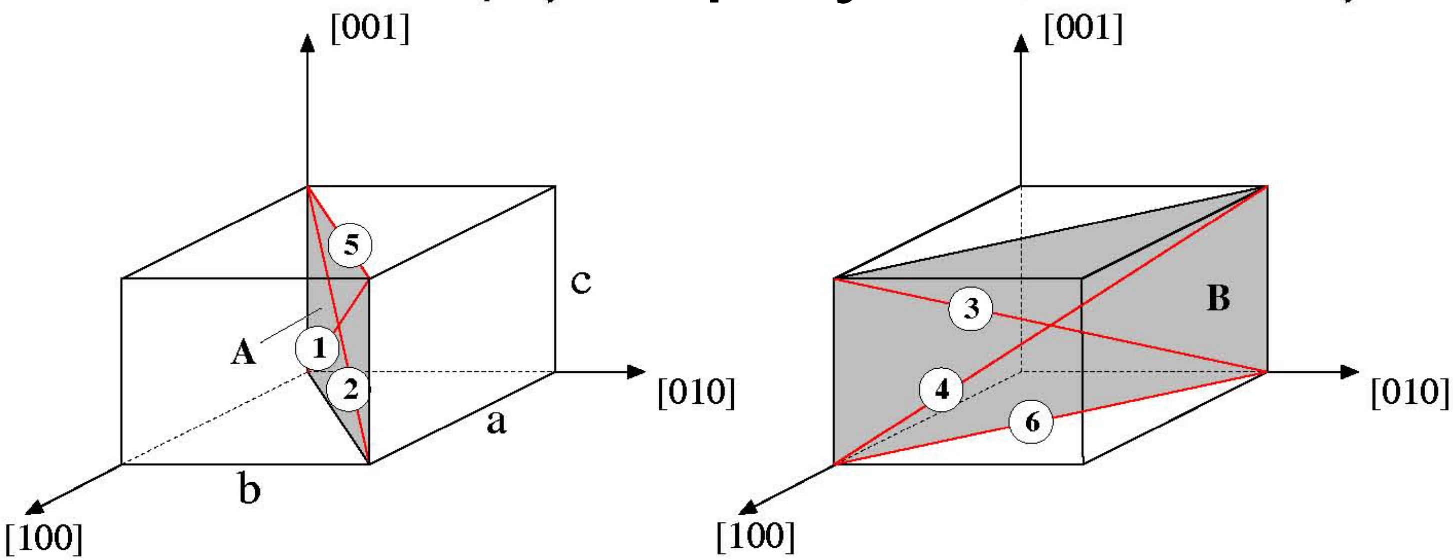
- Elastic constants assumed to decrease linearly with temperature, vanish at melting:

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

- 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



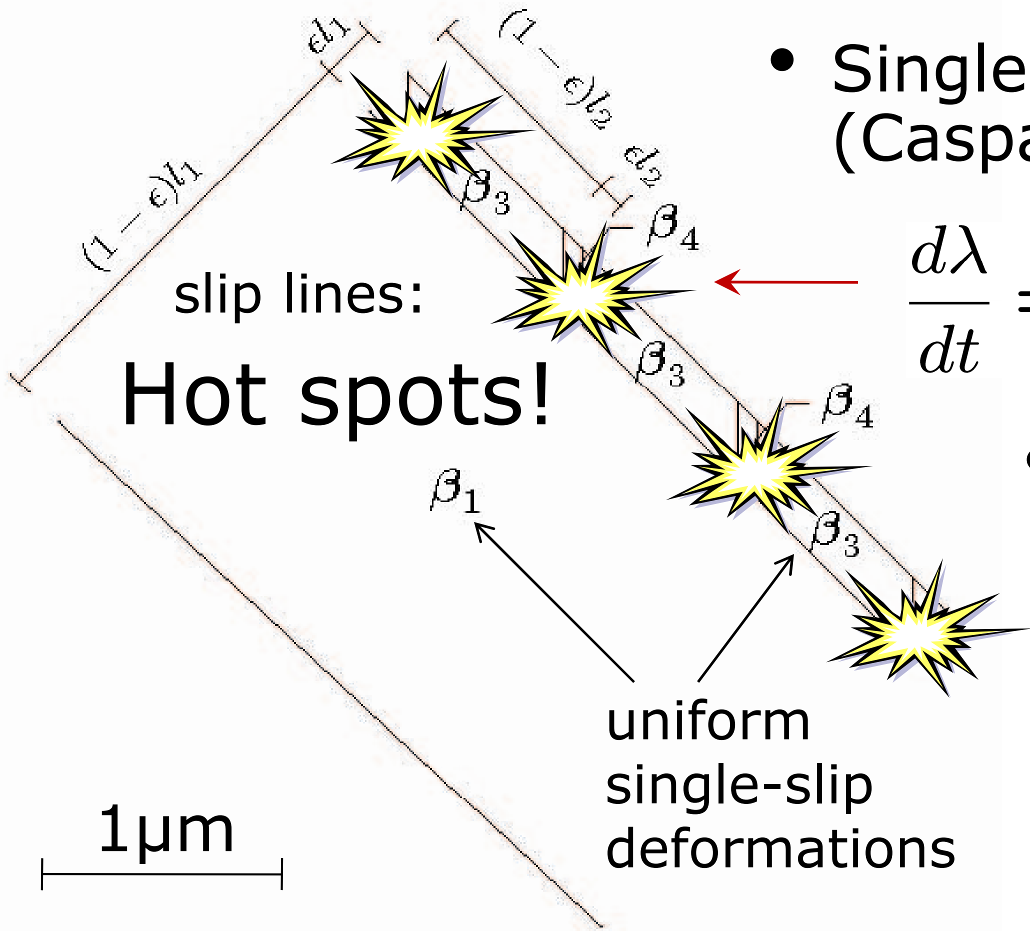
$a = b = 9.380Å \qquad c = 6.710Å$

- $\tau_c(\theta)$ 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

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

PETN – Chemistry



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

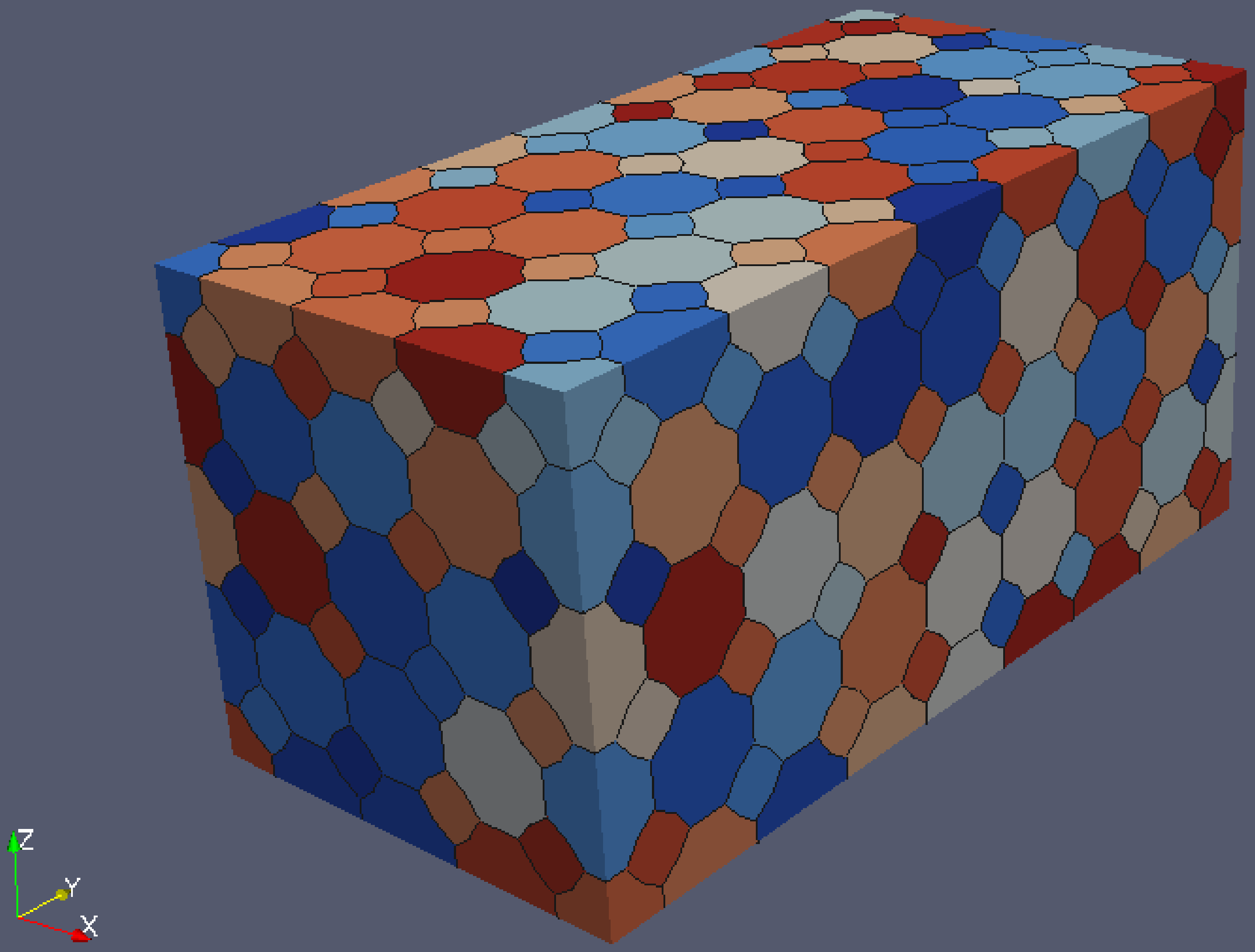
$$\frac{d\lambda}{dt} = Z(1-\lambda)\exp\left(-\frac{ER}{\theta}\right)$$

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

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

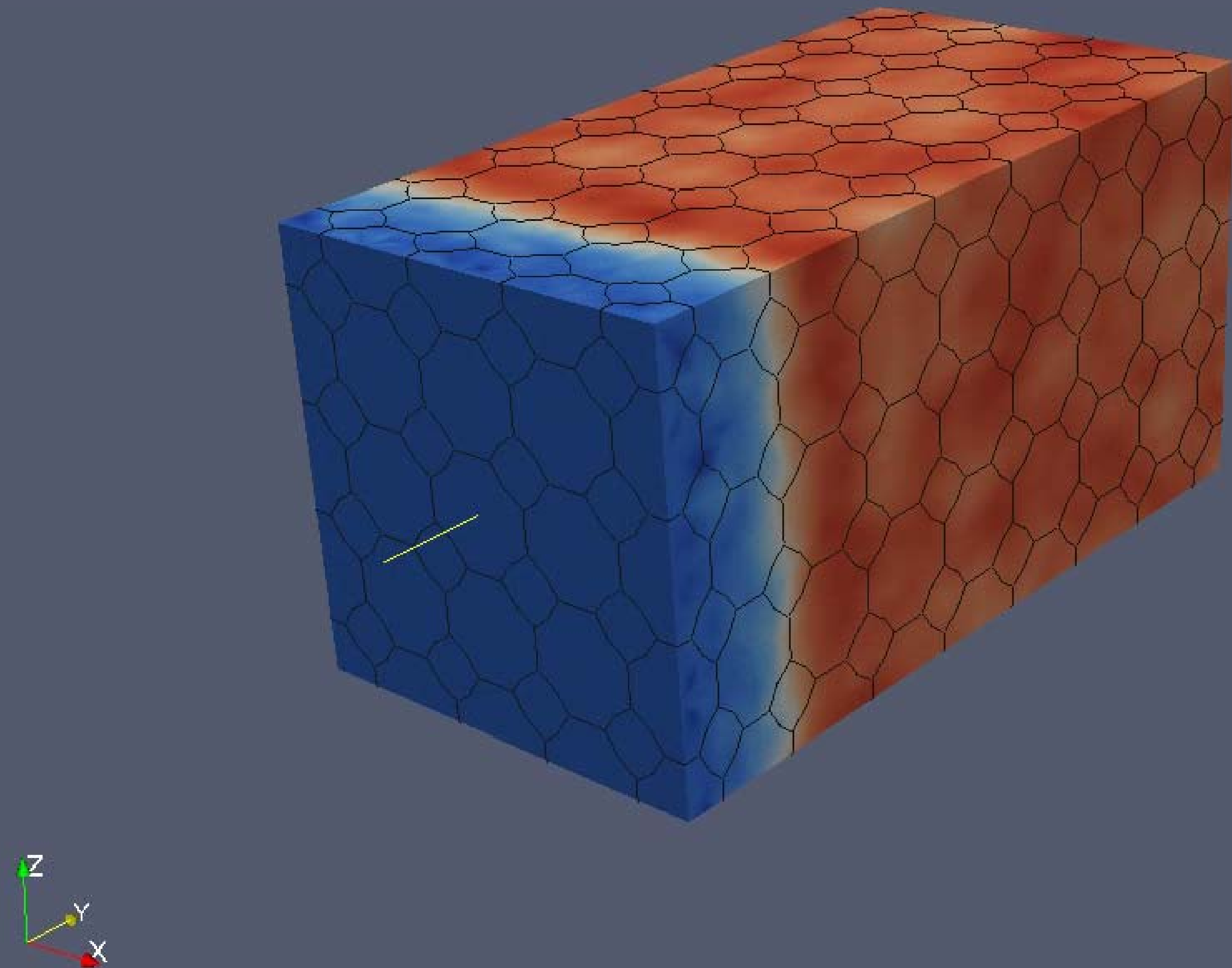
- Temperature computed assuming adiabatic heating, full conversion of plastic work to heat, heat capacity

High-Explosives Detonation Initiation

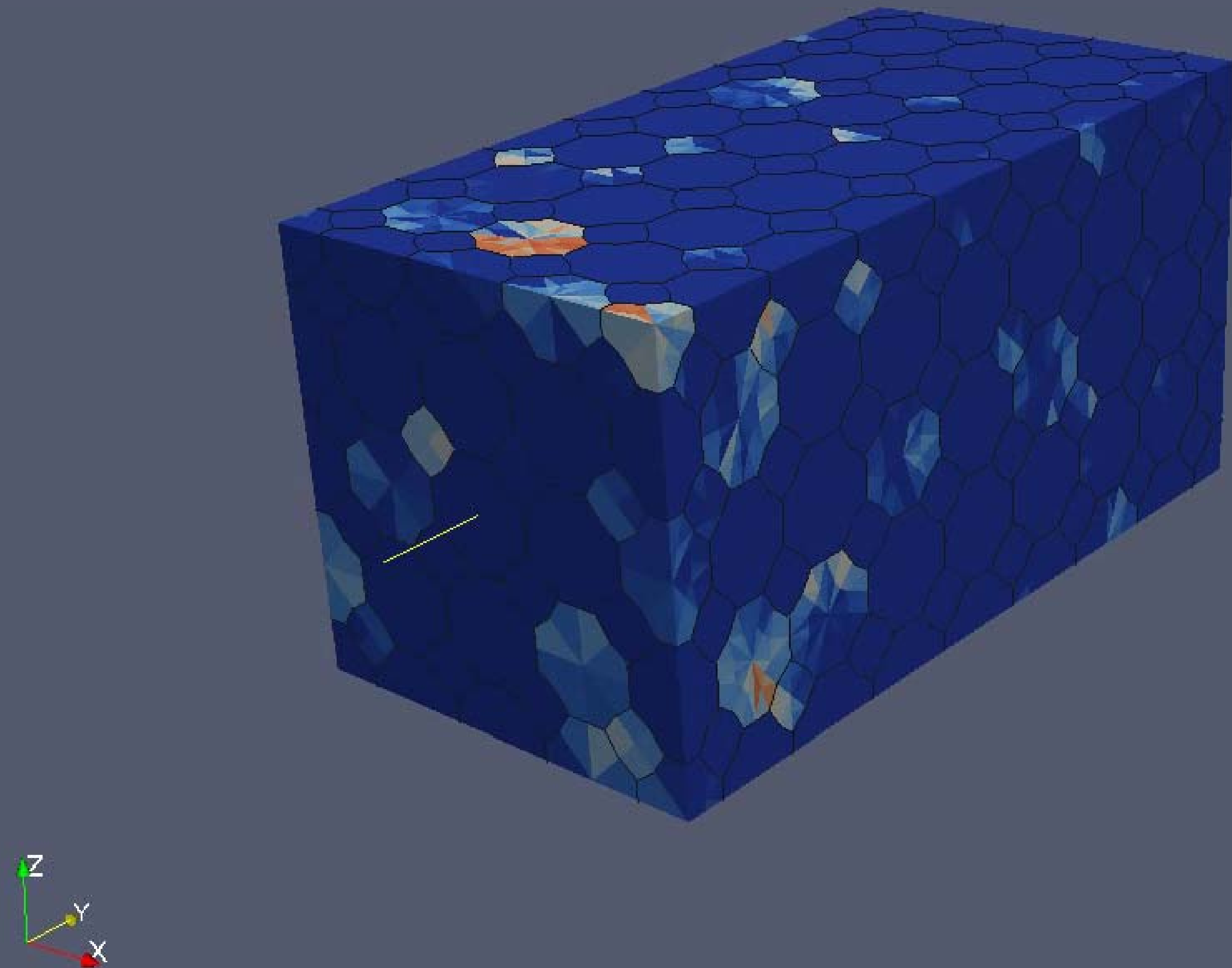


Polycrystal model and grain boundaries

PETN plate impact - Velocity



PETN plate impact - temperature



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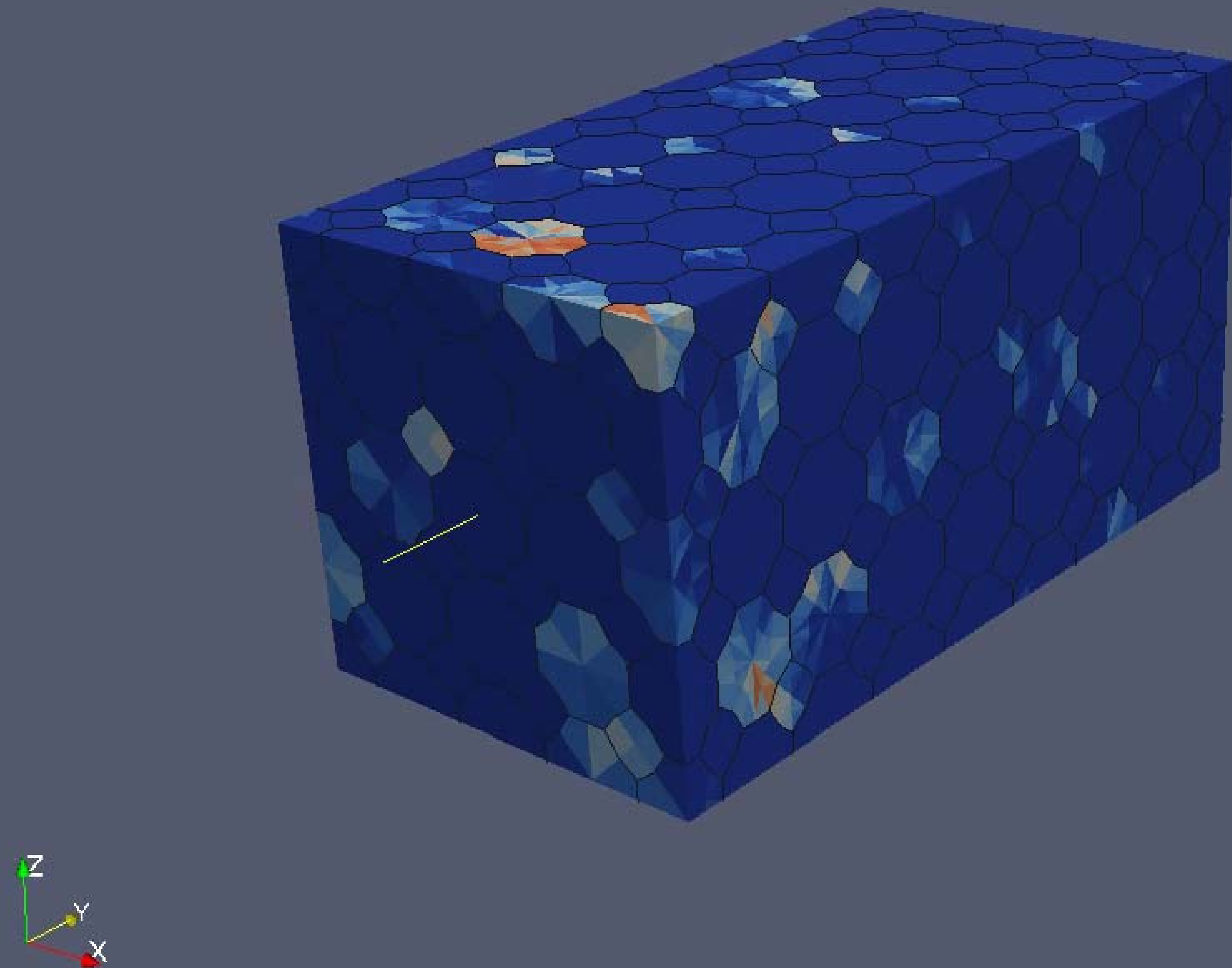

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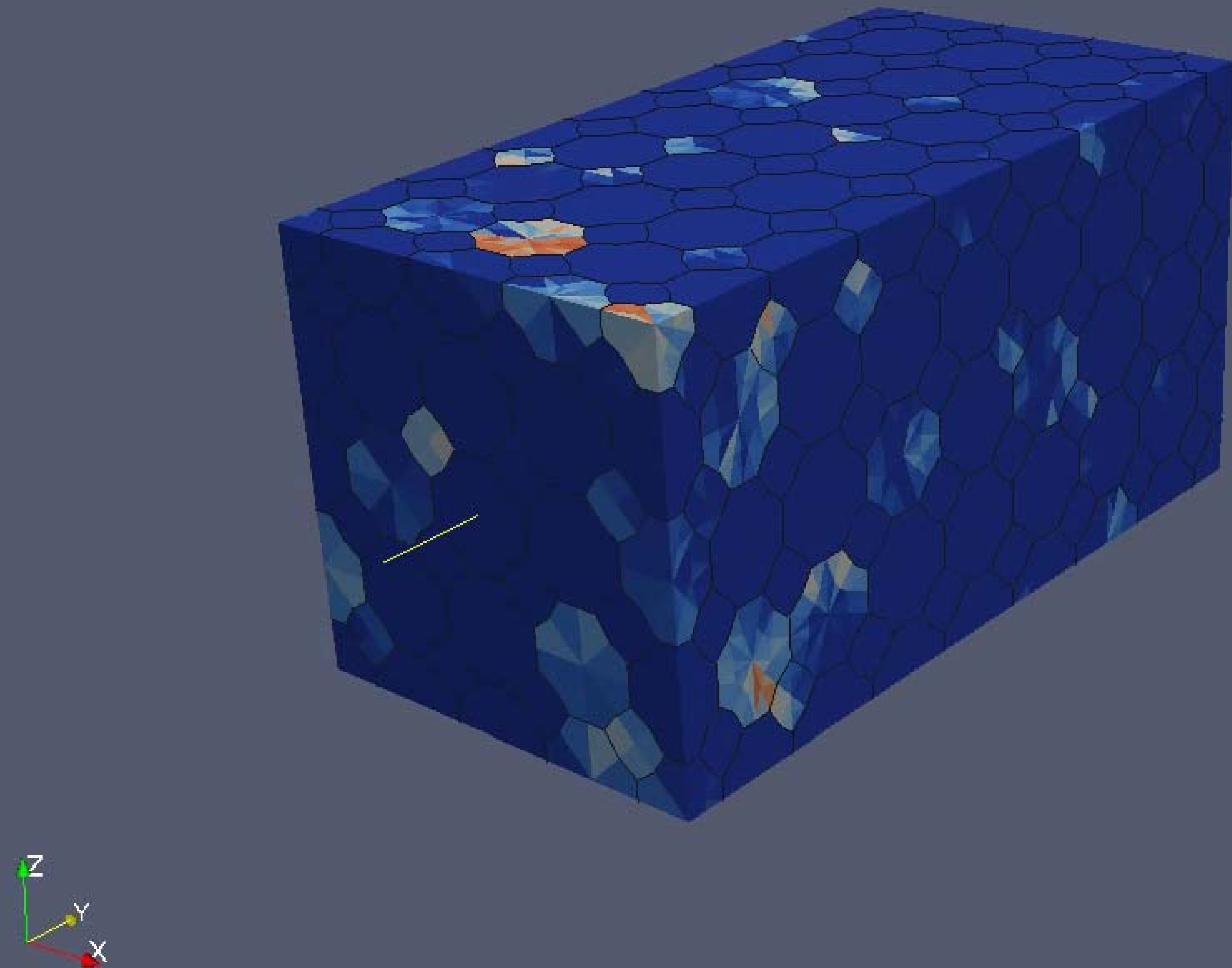

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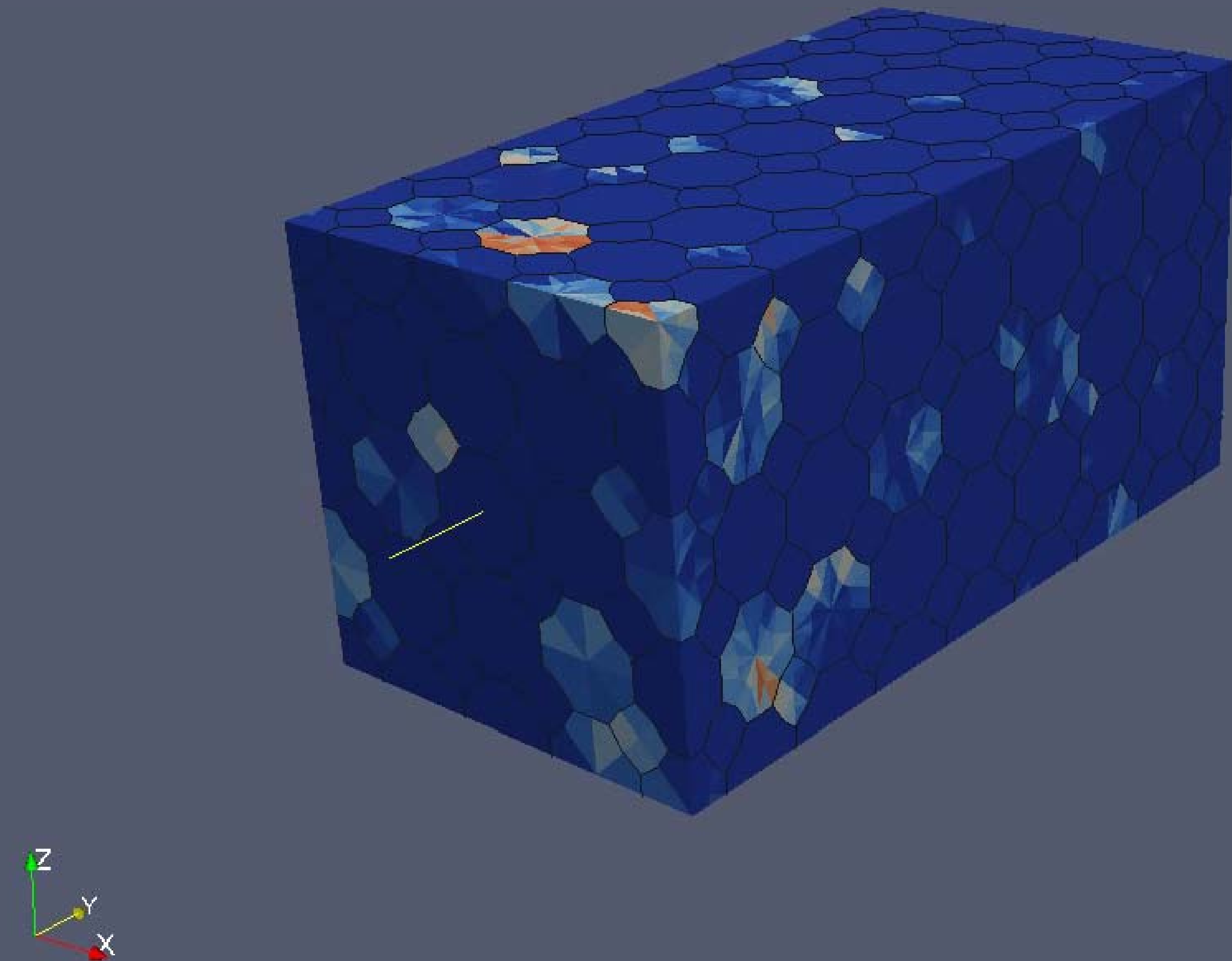
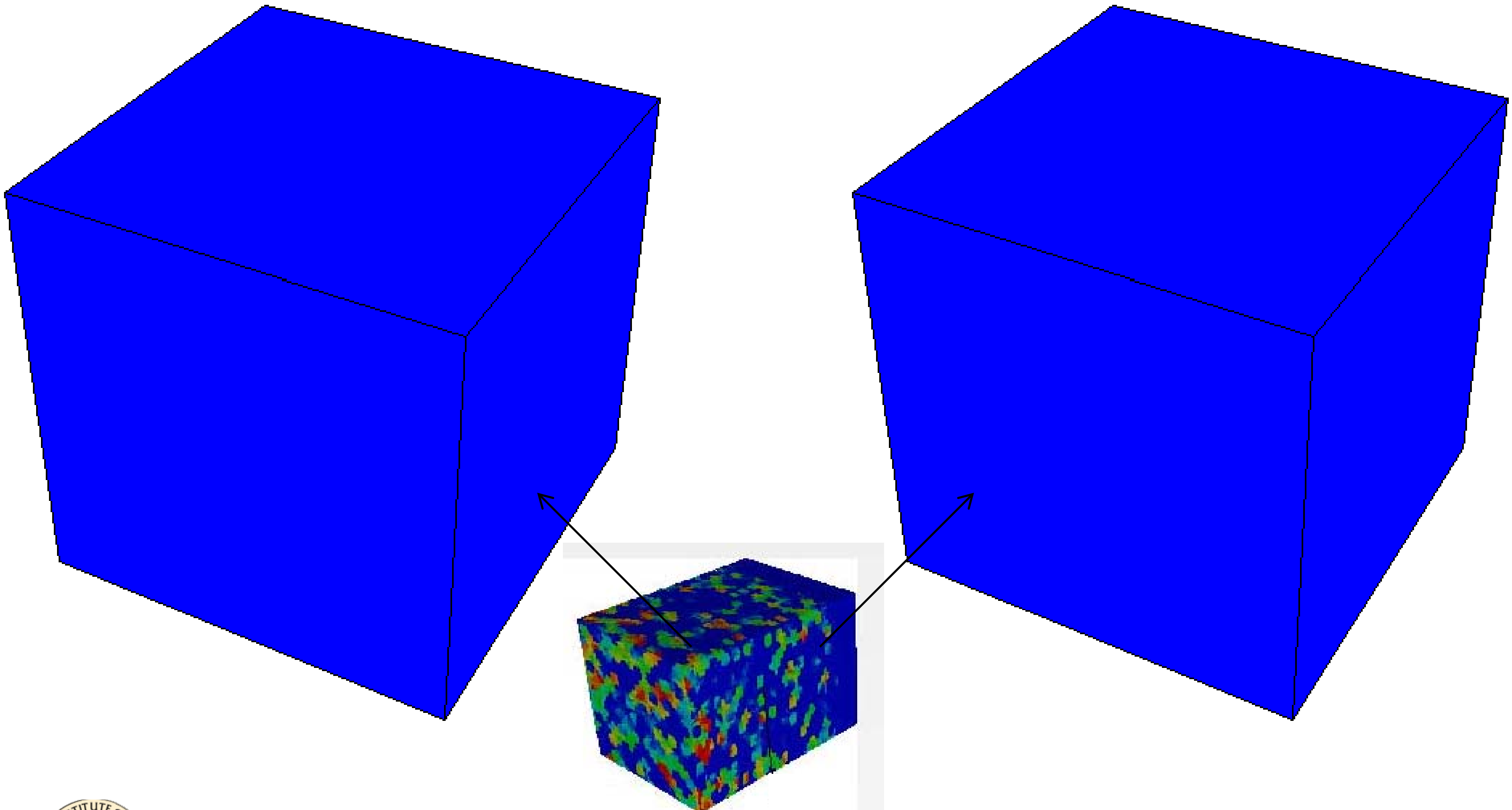


PETN plate impact – Subgrain microstructures



Microstructure evolution at selected material points

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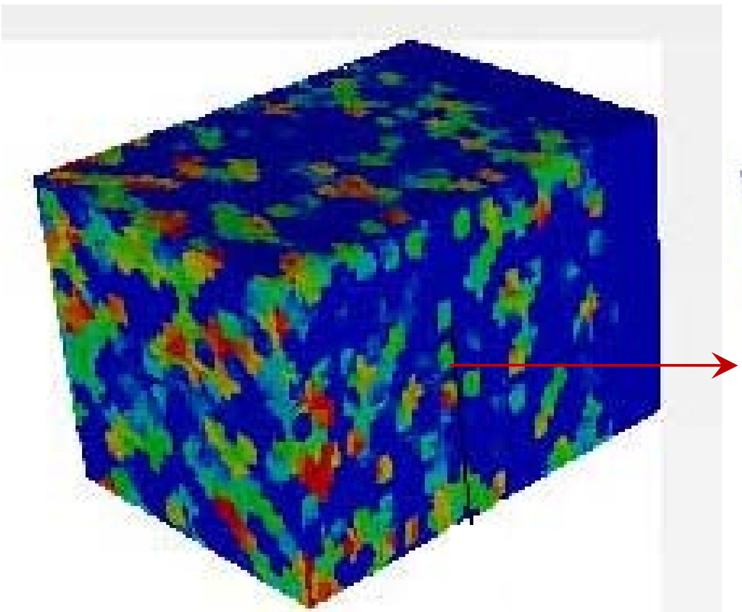
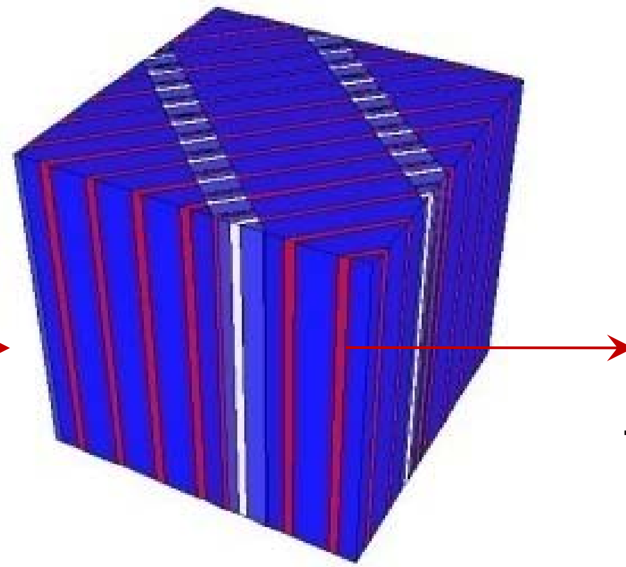
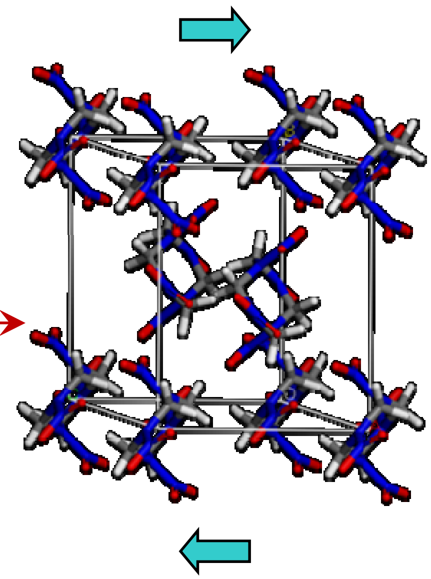
PETN plate impact – Hot-spot analysis



direct numerical simulation of polycrystalline PETN

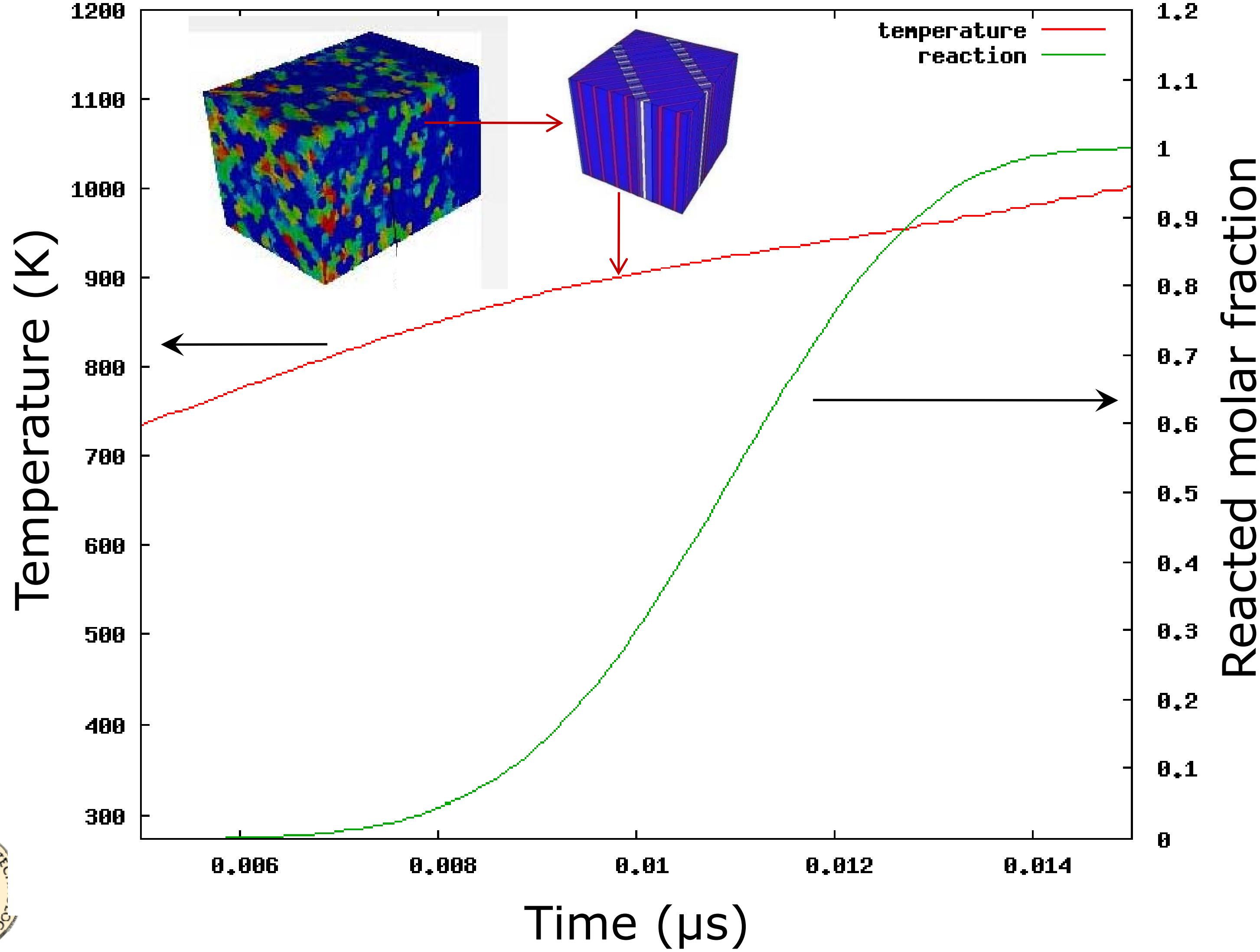


reconstructed microstructure at selected material points



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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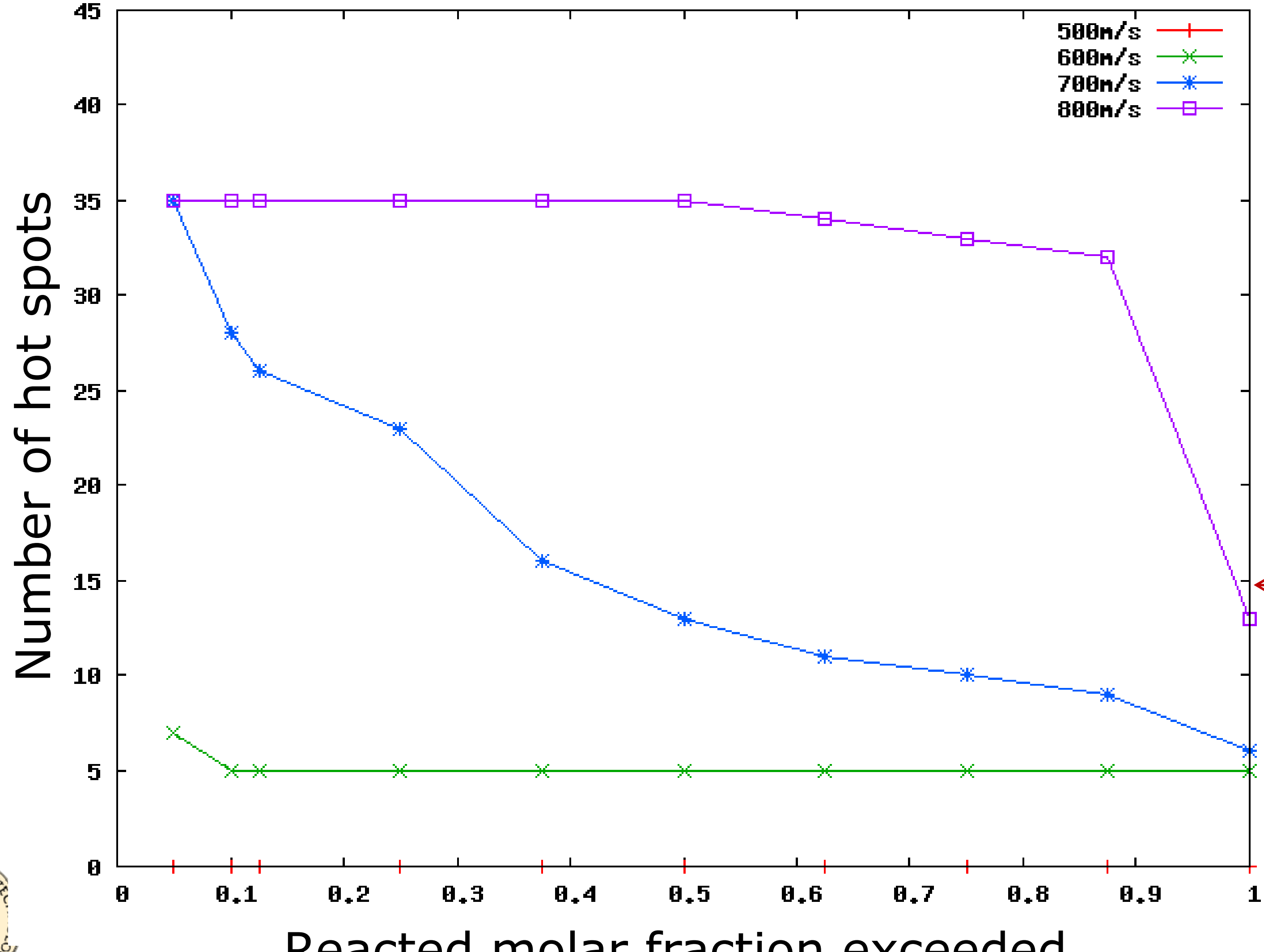
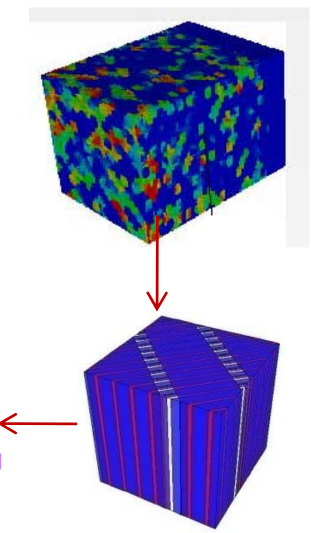
PETN plate impact - Number of hot spots





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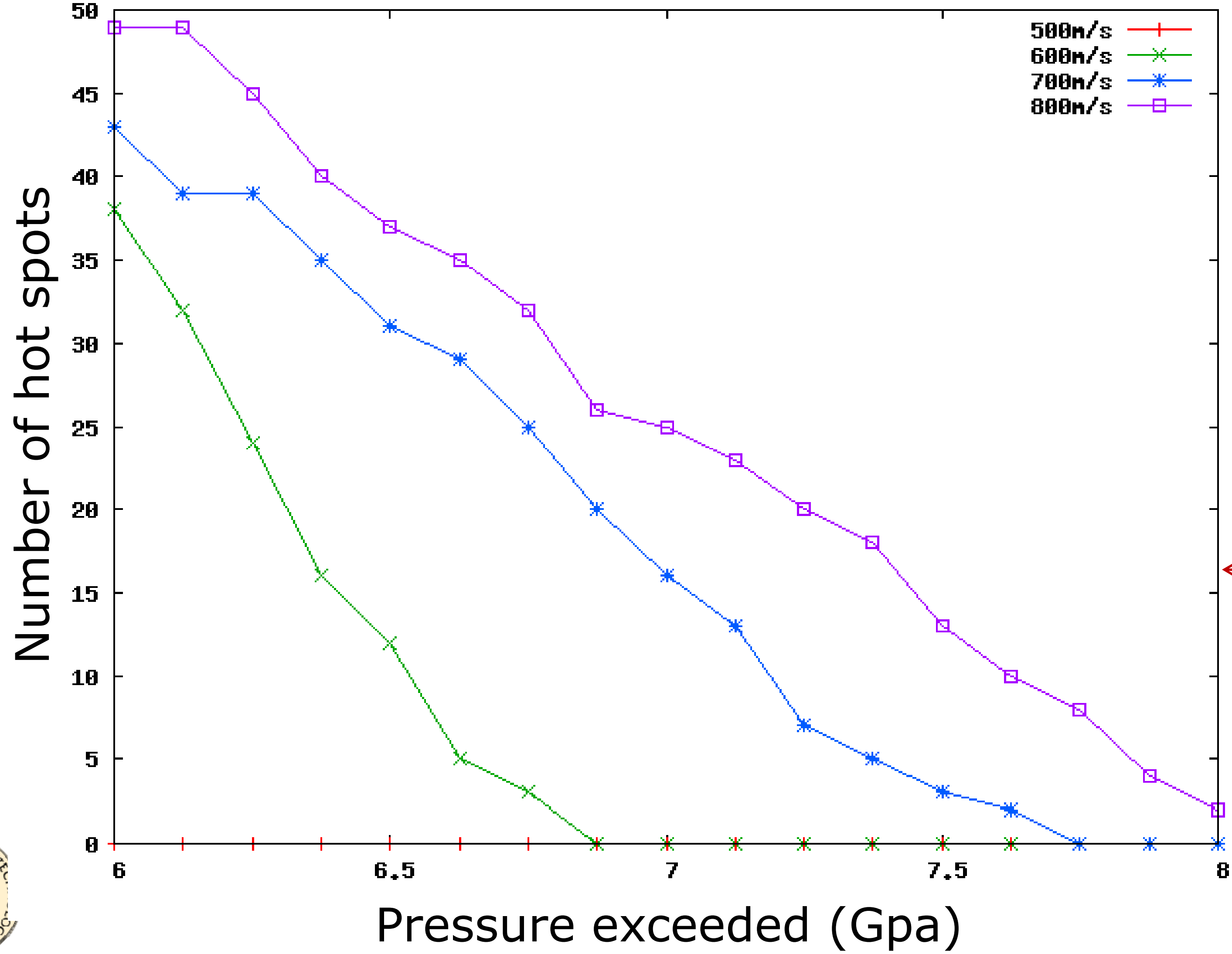

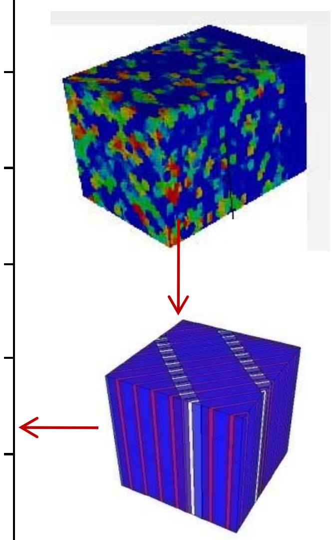

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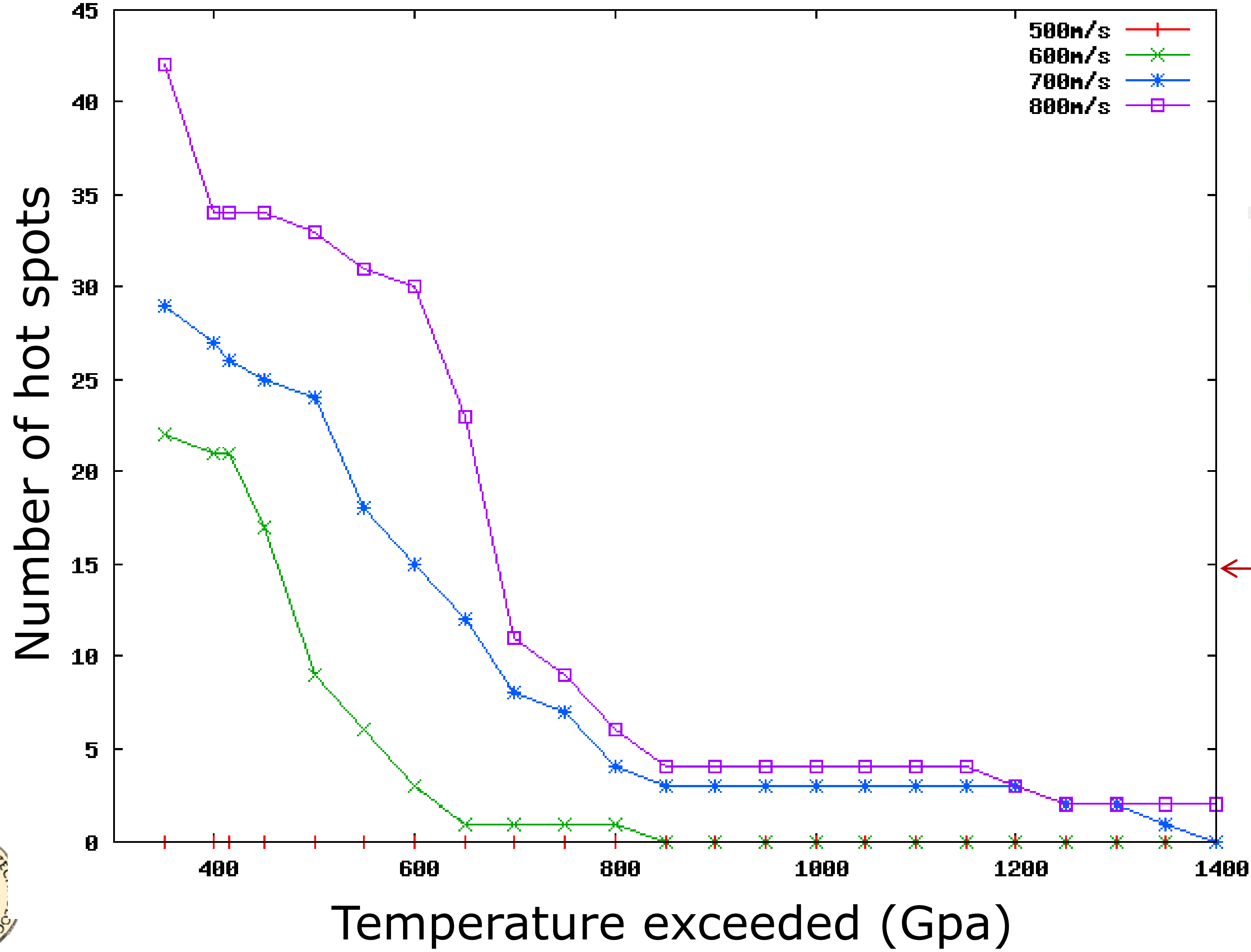

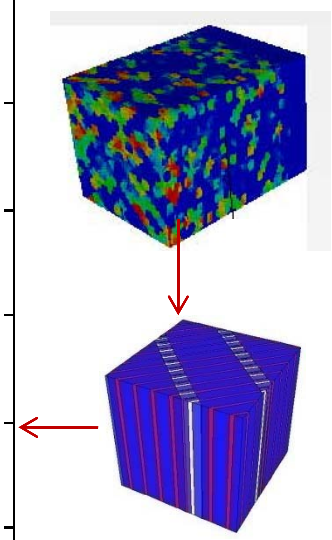

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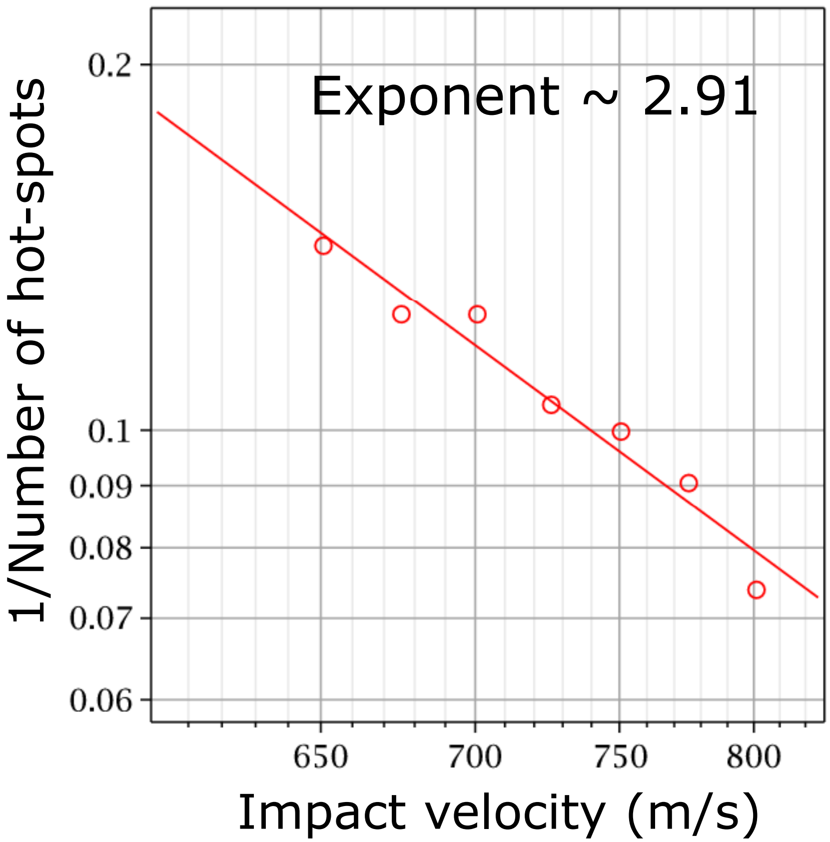
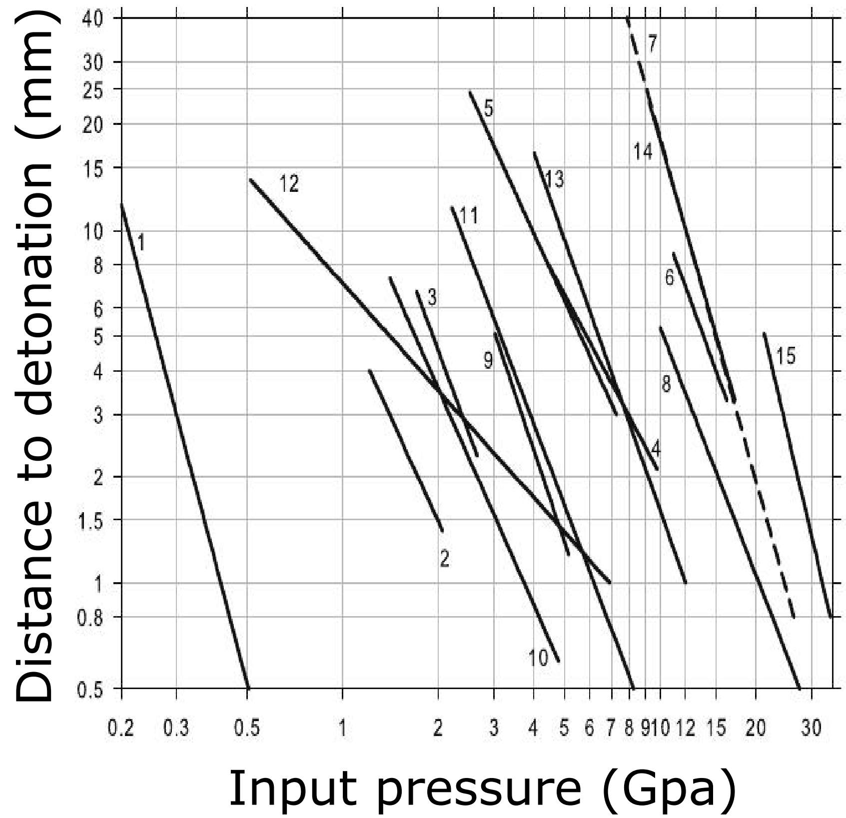
PETN plate impact – pop-plots

Impact velocity (m/s)





Multiscale model

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

Experimental exponent ~ 2.01–2.58

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Concluding remarks

- Multiscale scheme bridges:
  - *Macroscopic (device) scale*
  - *Polycrystalline structure*
  - *Subgrain heterogeneous slip*
- Calculations can simulate large samples over long times, make contact with test data
- Subgrain deformation microstructures reconstructed explicitly $\rightarrow$ B.C. for detailed atomistic calculations including chemistry
- Mechanism appears feasible, predictive
- Main predictive bottlenecks:
  - *Fundamental understanding of the plasticity of molecular crystals at dislocation level*
  - *Complex chemistry calculations over long times*

Concluding remarks

- Acknowledgement: Army Research Office through the MURI on *The Fundamental Chemistry and Physics of Munitions Under Extreme Conditions,* Grant No. W911NF-05-1-0345.
- Further reading: J. J. Rimoli, E. Gürses, and M. Ortiz, “Shock-induced subgrain microstructures as possible homogenous sources of hot spots and initiation sites in energetic polycrystals”, *PHYSICAL REVIEW B* **81, 014112 2010.**

Thank you!