Variational Methods in Multiscale Analysis

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Workshop on Mechanics of Materials

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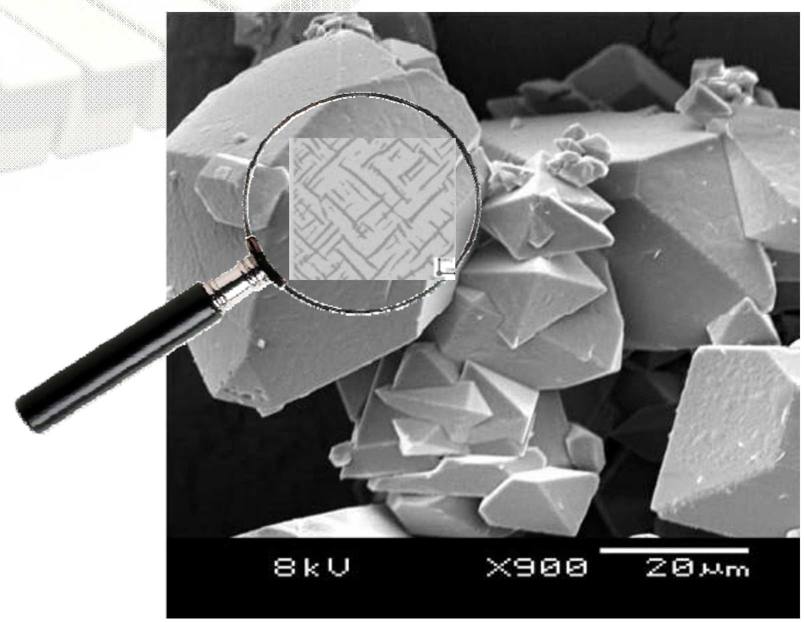
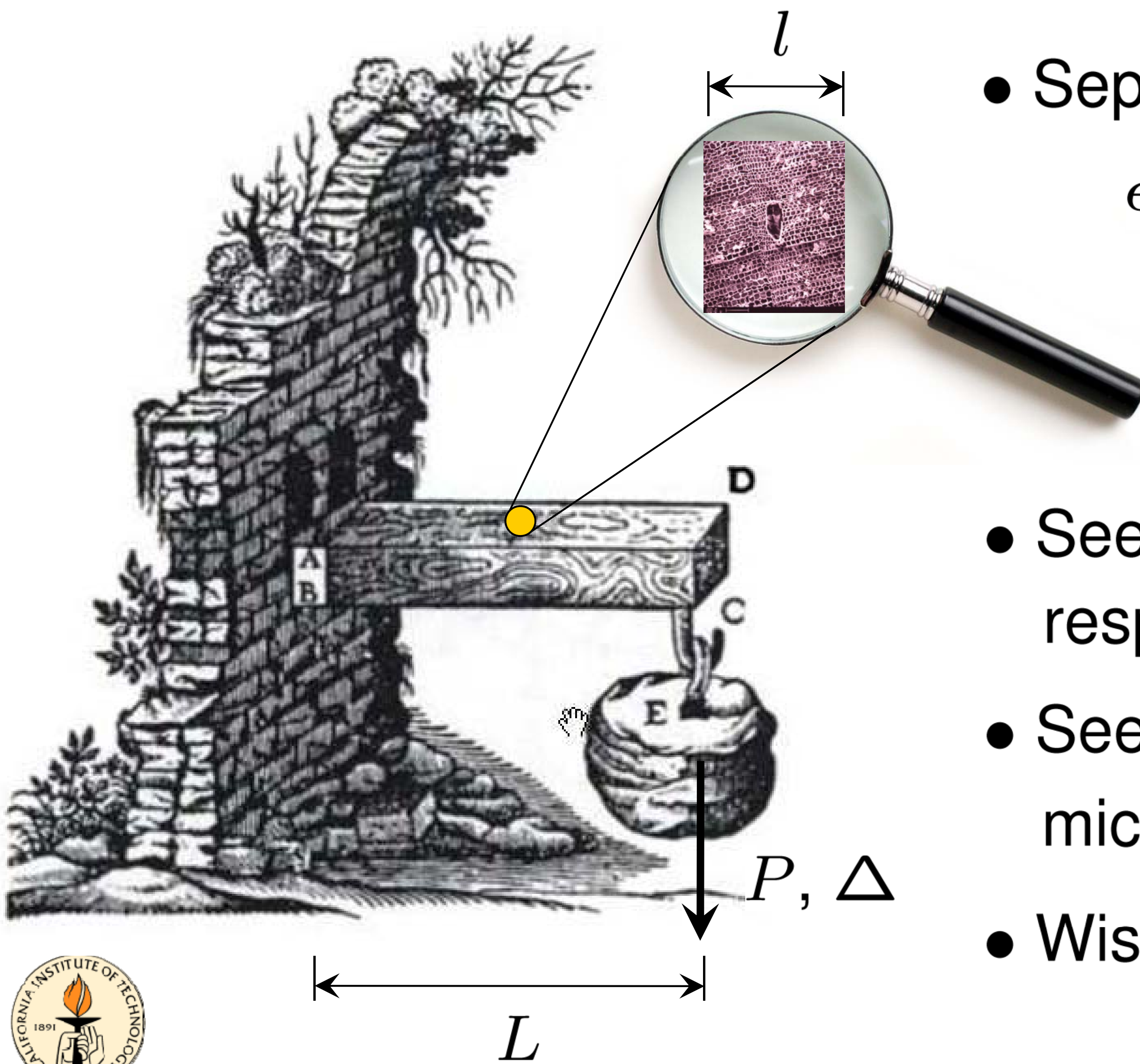
Outline

- 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?*
- Application to 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...

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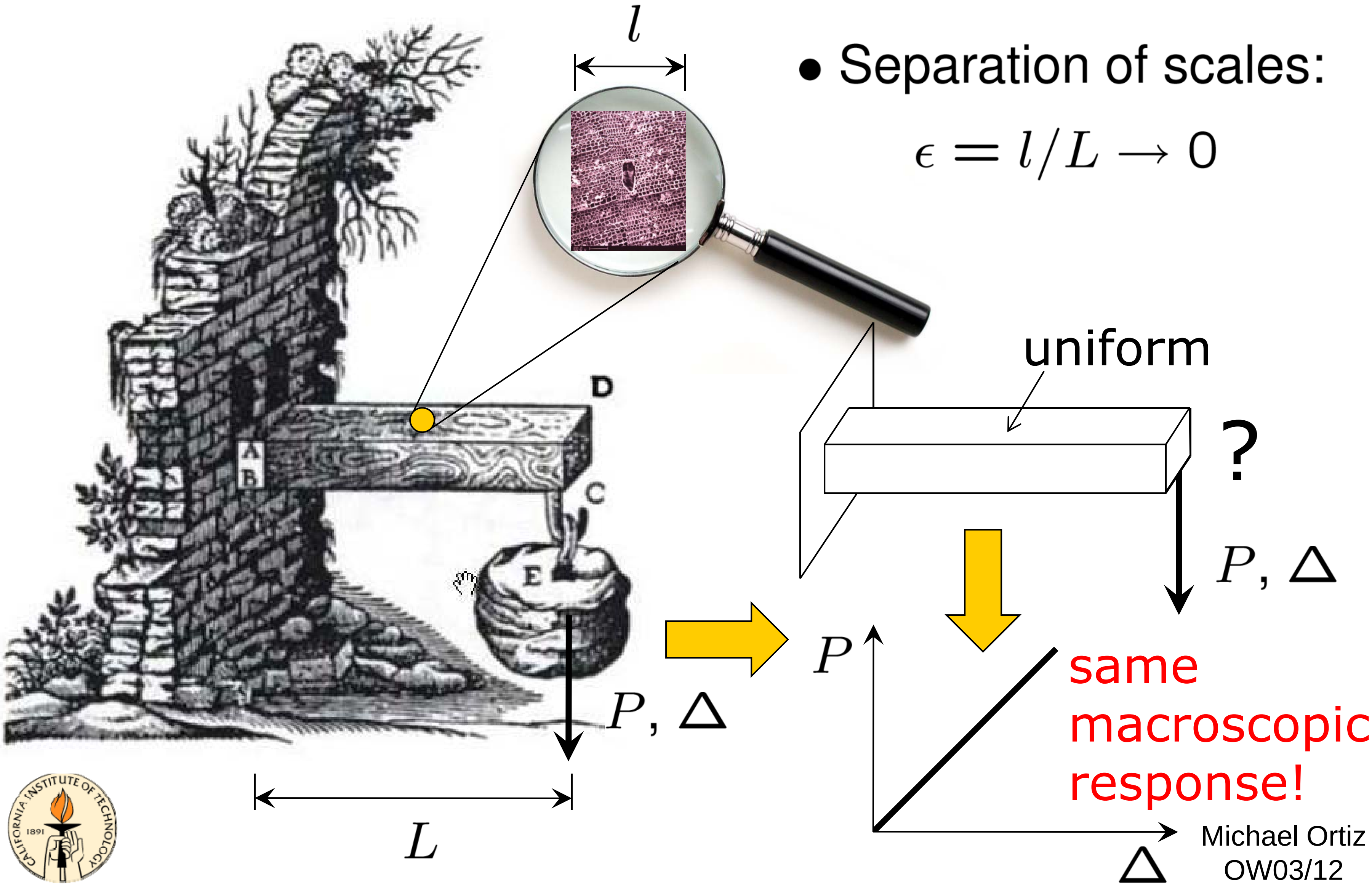
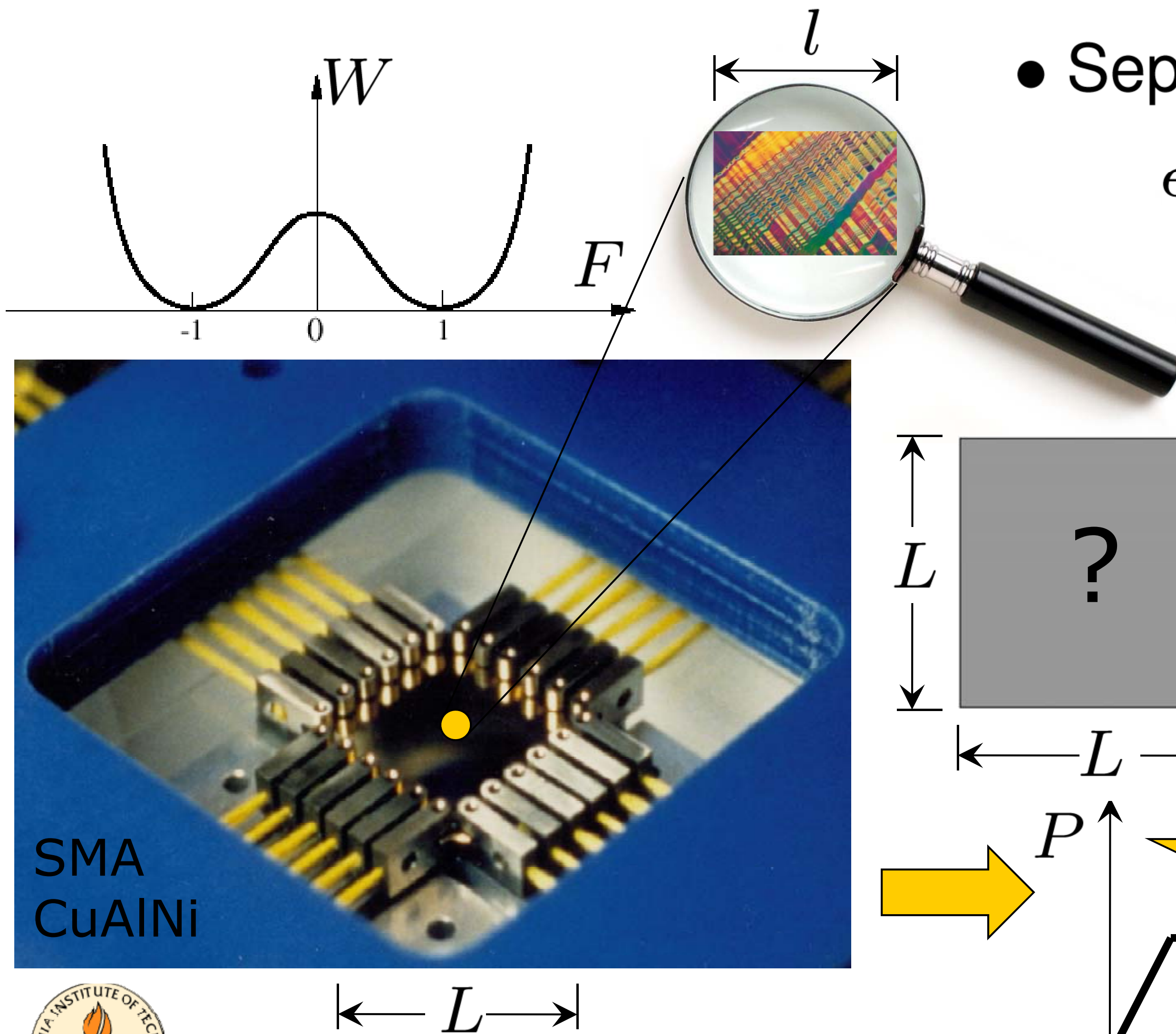
Separation of Scales - Homogeneization

- Separation of scales:

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



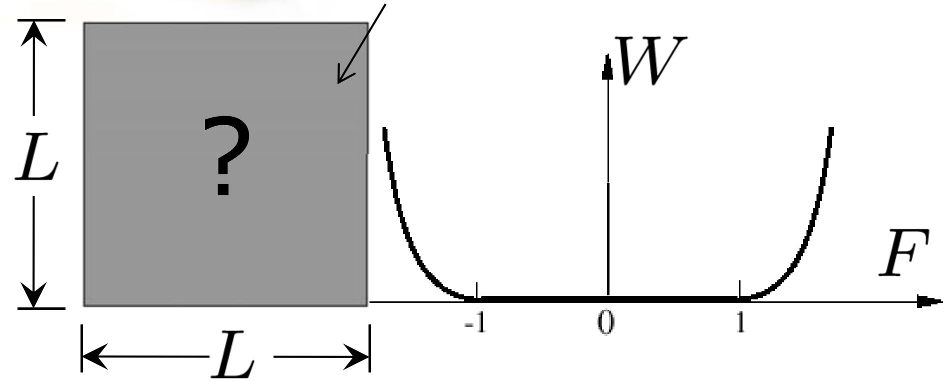
Separation of Scales - Martensite

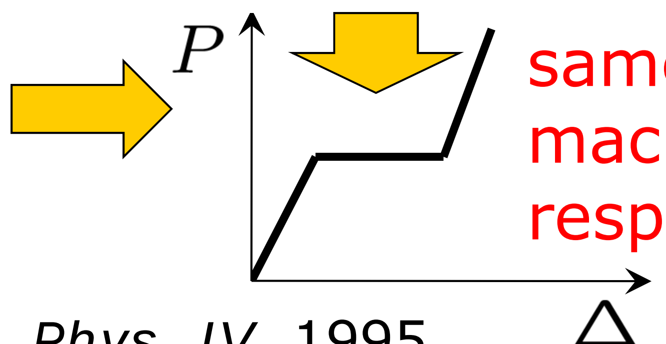


- Separation of scales:

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

no deformation microstructures!





same macroscopic response!

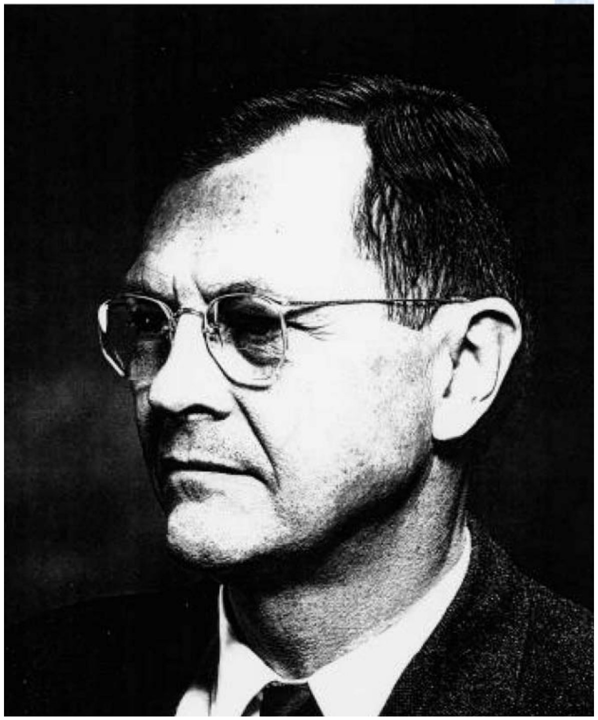
Chu, C. and James, R.D., *J. Phys. IV*, 1995

Optimal Multiscale Modeling

- We want ***effective macroscopic model*** that is homogeneous and/or ***stable with respect to microstucture*** (weak lower-semicontinuity)
- We wish the macroscopic response of the micro- and macromechanical models to give the same macroscopic response ***for all loadings*** (weak convergence under continuous perturbations)
- We wish ***return option***: It should be possible to ***reconstruct microsctructures*** from solutions of the effective macroscopic model (every minimizer of the effective macroscopic model is the weak limit of microscopic minimizers)
- Necessarily, effective macroscopic model = Weak ***Relaxation/Gamma-limit*** of micro-model!

E. De Giorgi, *Rend. Mat.*, Vol. 8 (1975) 277-294

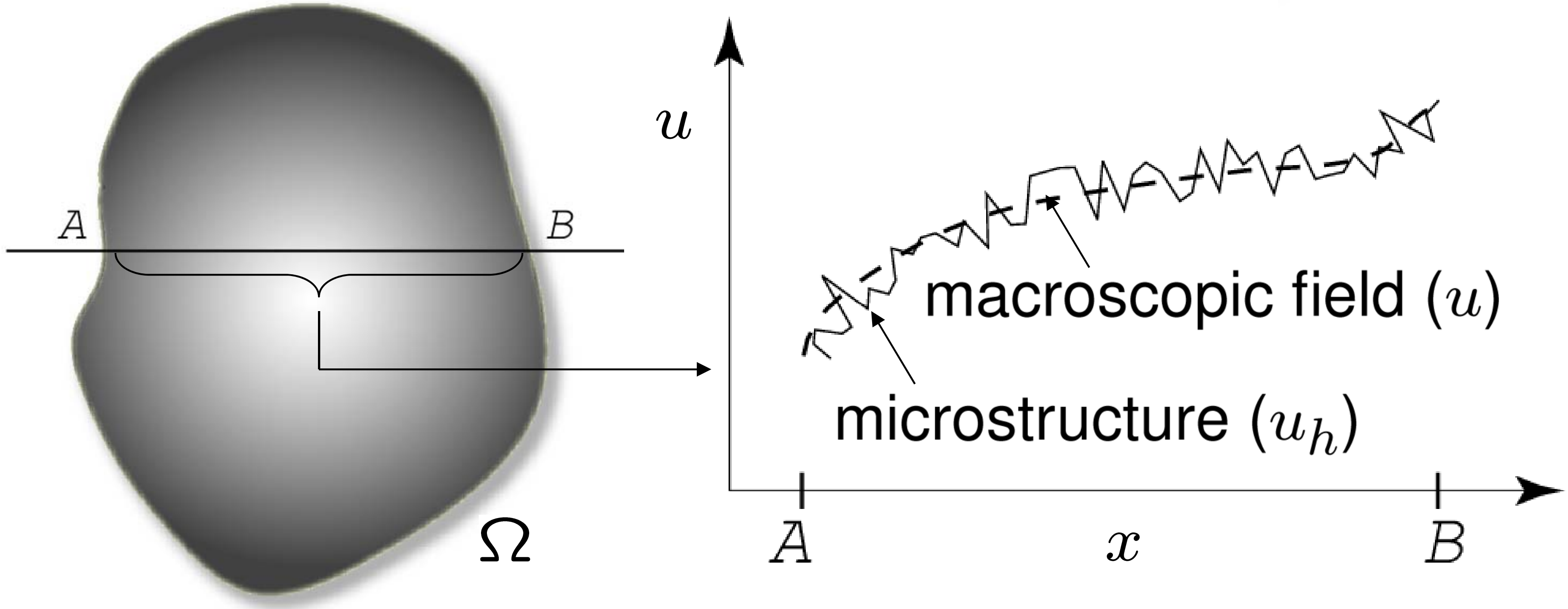
Modern Calculus of Variations



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 - Relaxation



- $F_0 =$ relaxation of F in X (w r. t. weak topology) if:

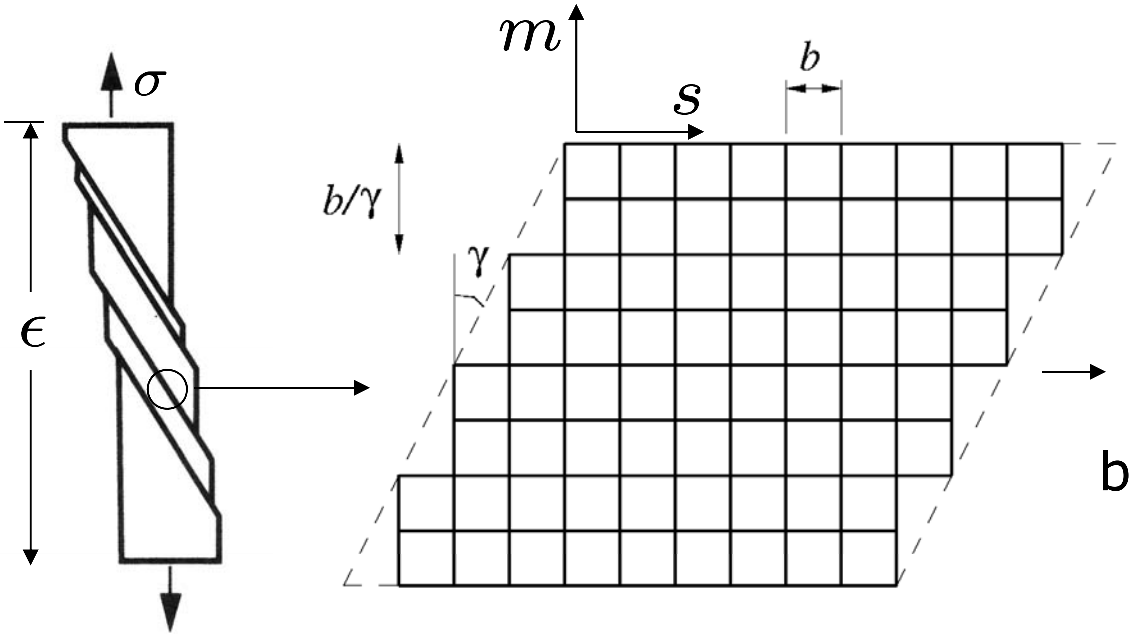
  i) $\forall u \in X$, $\exists u_h \rightharpoonup u$ s. t. $F_0(u) = \lim_{h\to\infty} F(u_h)$.

  ii) $\forall u_h \rightharpoonup u$, $\liminf_{h\to\infty} F(u_h) \geq F_0(u)$.

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!

Application to crystal plasticity

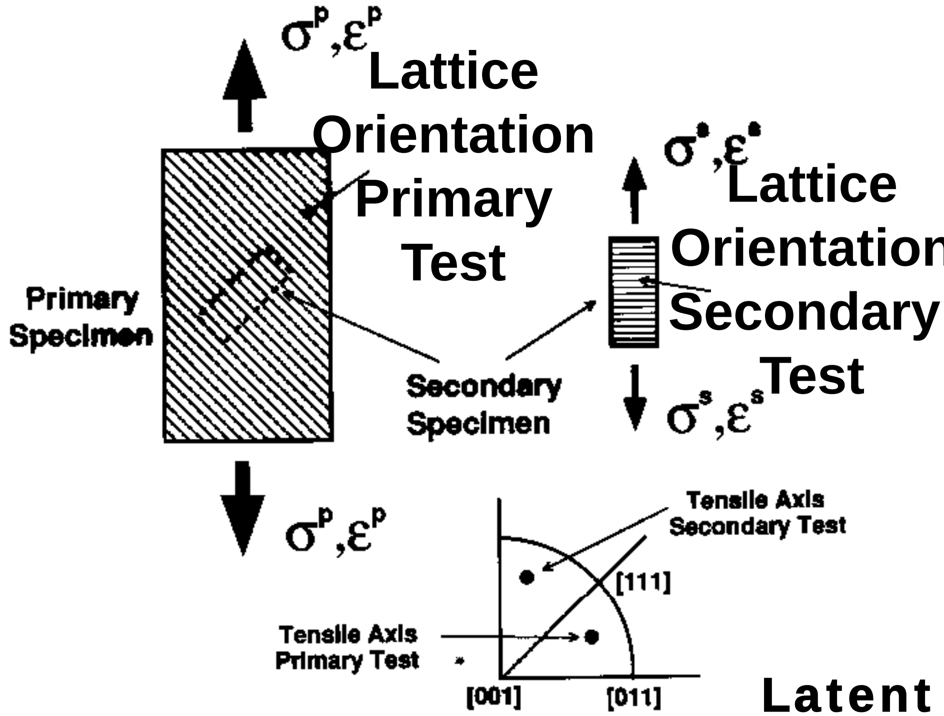


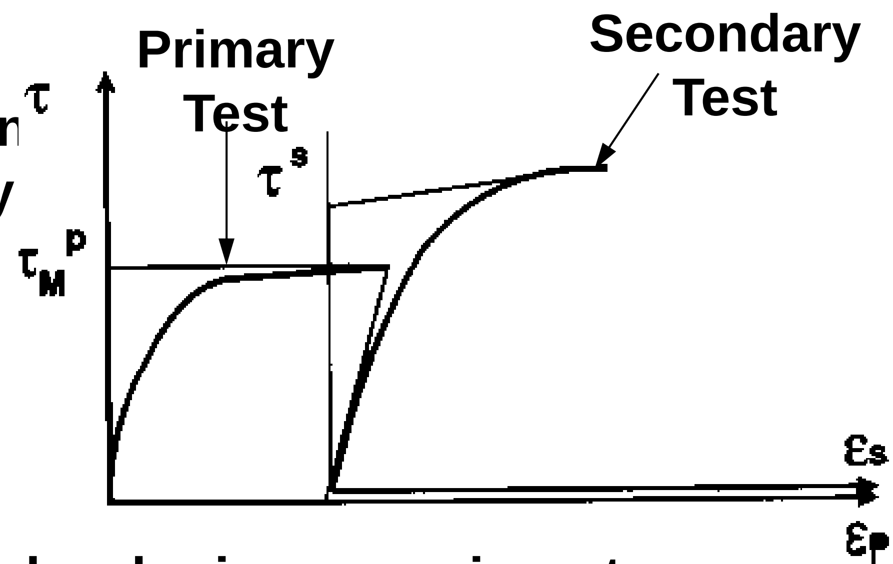
Irreversible accommodation of shear deformation by crystallographic slip

- 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! (strong latent hardening)
- Monotonicity: $\gamma(t_2) > \gamma(t_1)$, if $t_2 > t_1$

$\Rightarrow$ deformation theory of plasticity!

Strong latent hardening





Latent hardening experiments

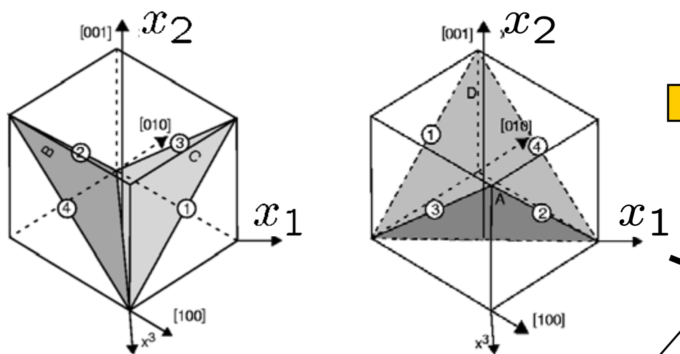
UF Kocks, *Acta Metallurgica*, **8** (1960) 345

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

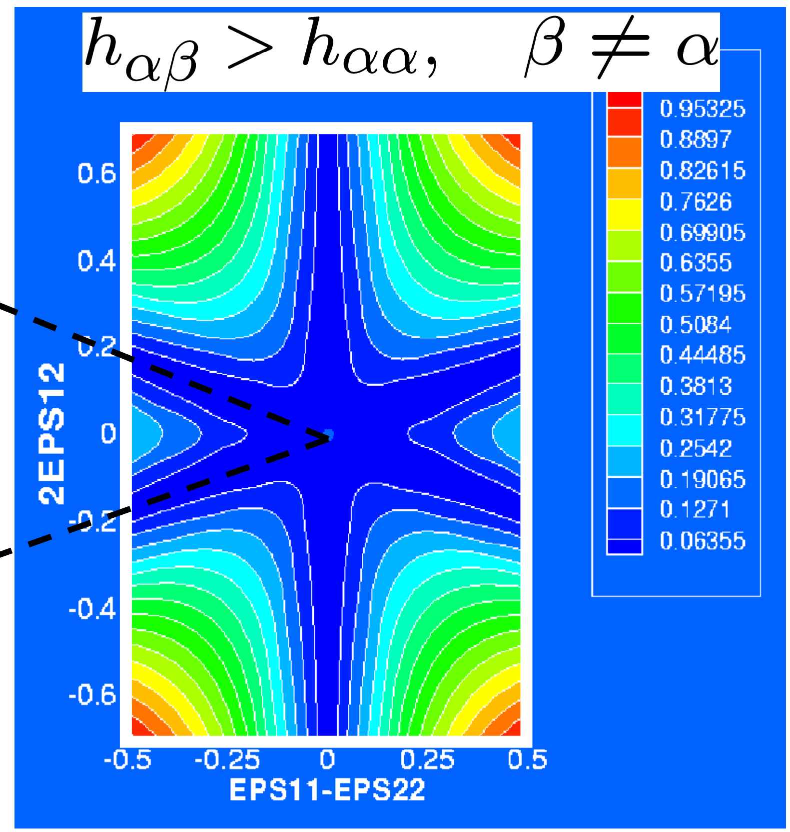


$$\beta^p \in \gamma s \otimes m + so(3)$$

(Single slip)

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

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



$W(\nabla u)$

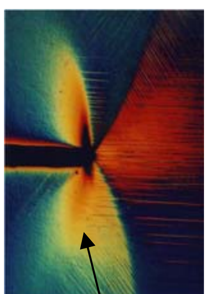
Crystal plasticity – Relaxation

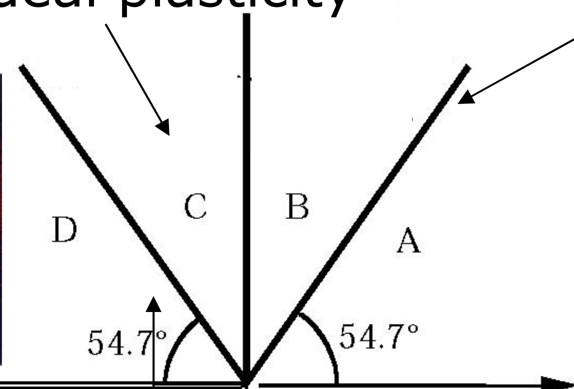
Theorem [S. Conti & MO, 2005] *On* $X = \{u \in BD(\Omega) :$ div$u \in L^2(\Omega)\}$ *with strong* L^1*-convergence:*

$$F_0(u) = \int_{\partial\Omega_d} W^\infty((u-u_0)\otimes\nu)\, d\mathcal{H}^2 + \int_\Omega \underbrace{W^{**}(\mathcal{E}u)dx}_{\text{Ideal plasticity}} + \int_\Omega \underbrace{W^\infty\left(\frac{E_s u}{|E_s u|}\right) d|E_s u|}_{\text{Slip-line energy}}$$

Ideal plasticity

Slip-line energy



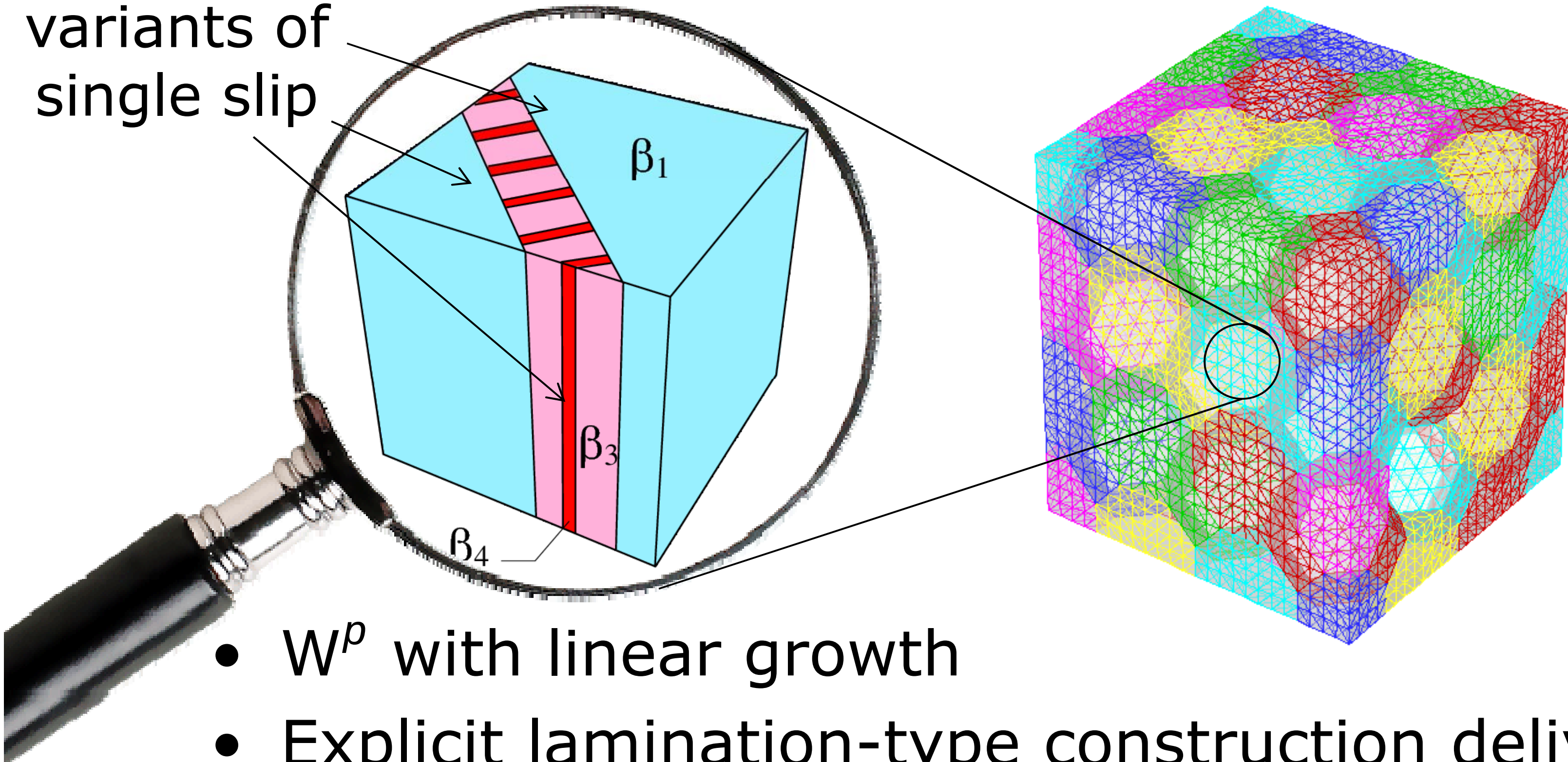


where: $W^\infty(A) = \lim_{t\to\infty} W^{**}(tA)/t$, $\epsilon(u) = \mathcal{E}u dx + E_s u$

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

(W. Crone and T. Shield, *JMPS*, 2002)

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…

S. Conti & MO, *ARMA*, 2005

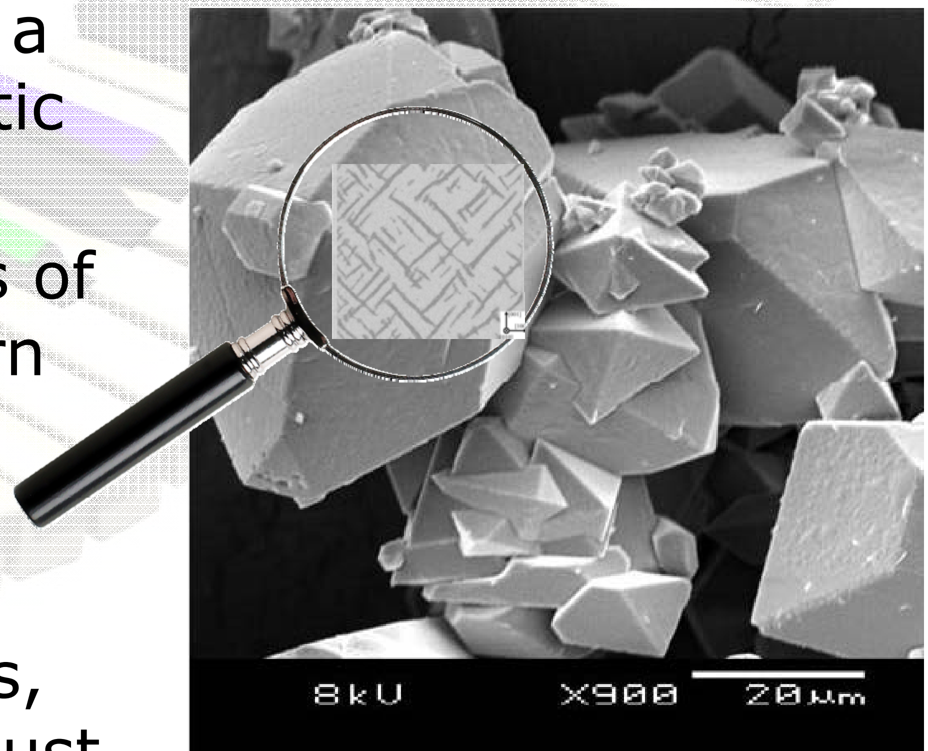
Application to High Explosives (HE)

- 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

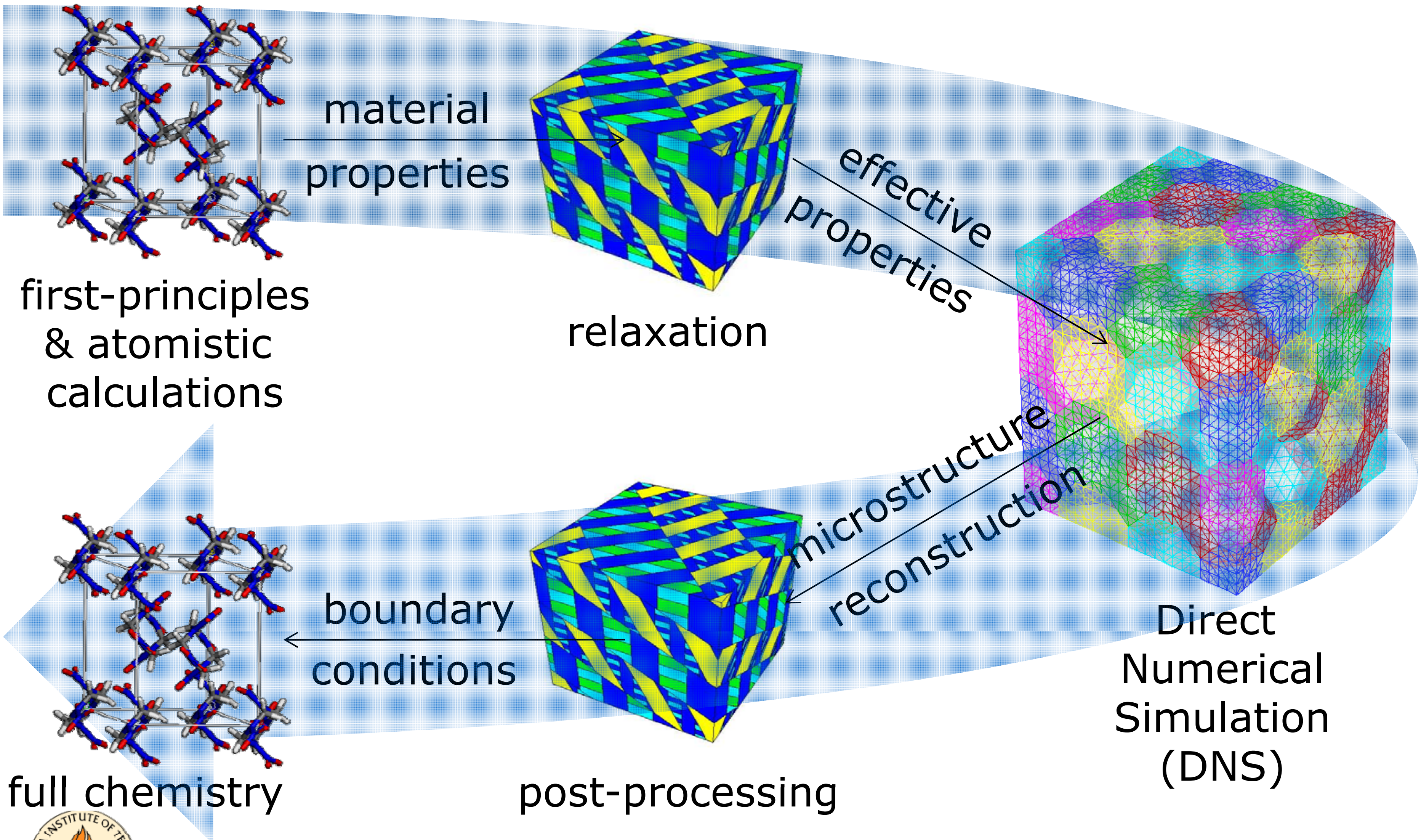
- Can hot spots arise as a result of localized plastic deformation?
- Can small-scale details of the deformation pattern (partially) explain detonation sensitivity?
- Need to predict deformation microstructures, extreme events! (not just average behavior)



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

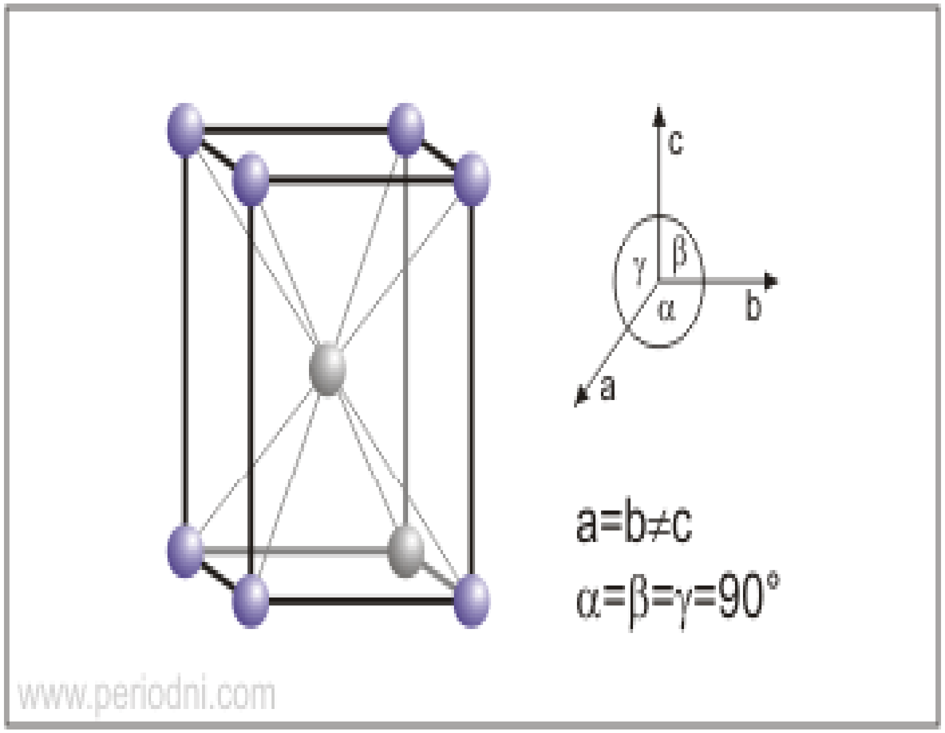
HE – The relaxation 'boomerang'



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

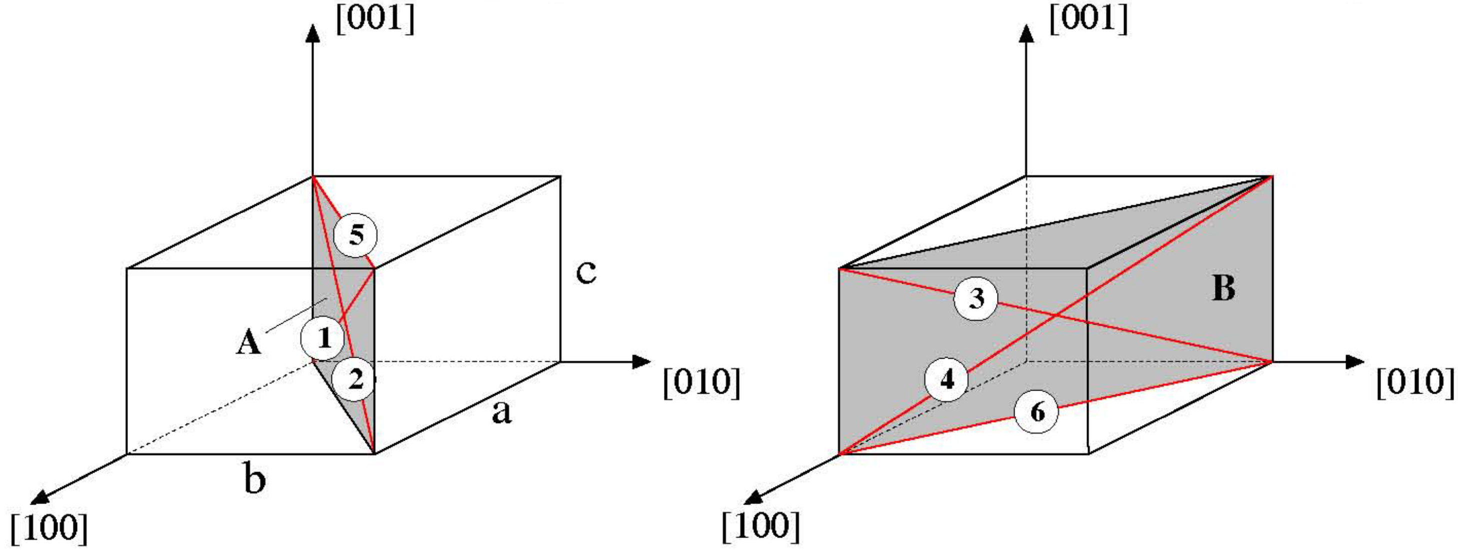
- Elastic constants assumed to decrease linearly with temperature, vanish at melting:

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

- 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



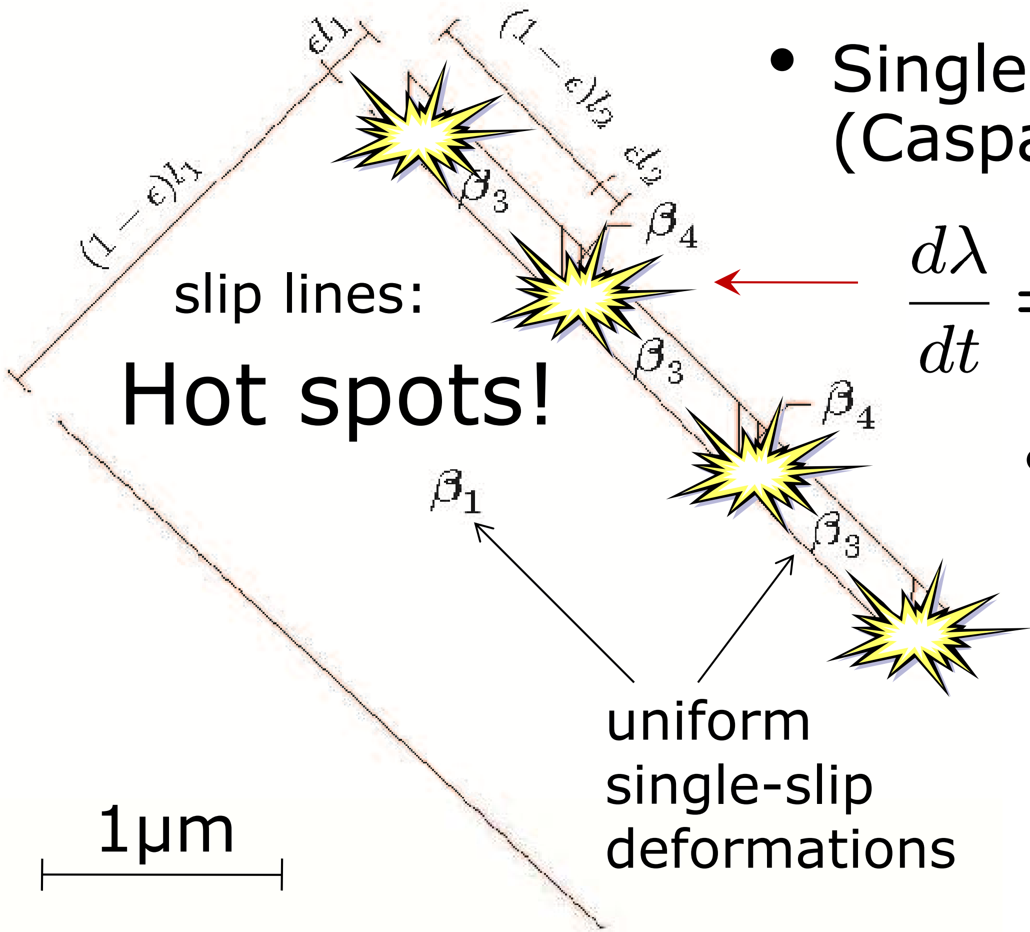
$a = b = 9.380\text{Å} \qquad c = 6.710\text{Å}$

- $\tau_c\,(\theta)$ 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):

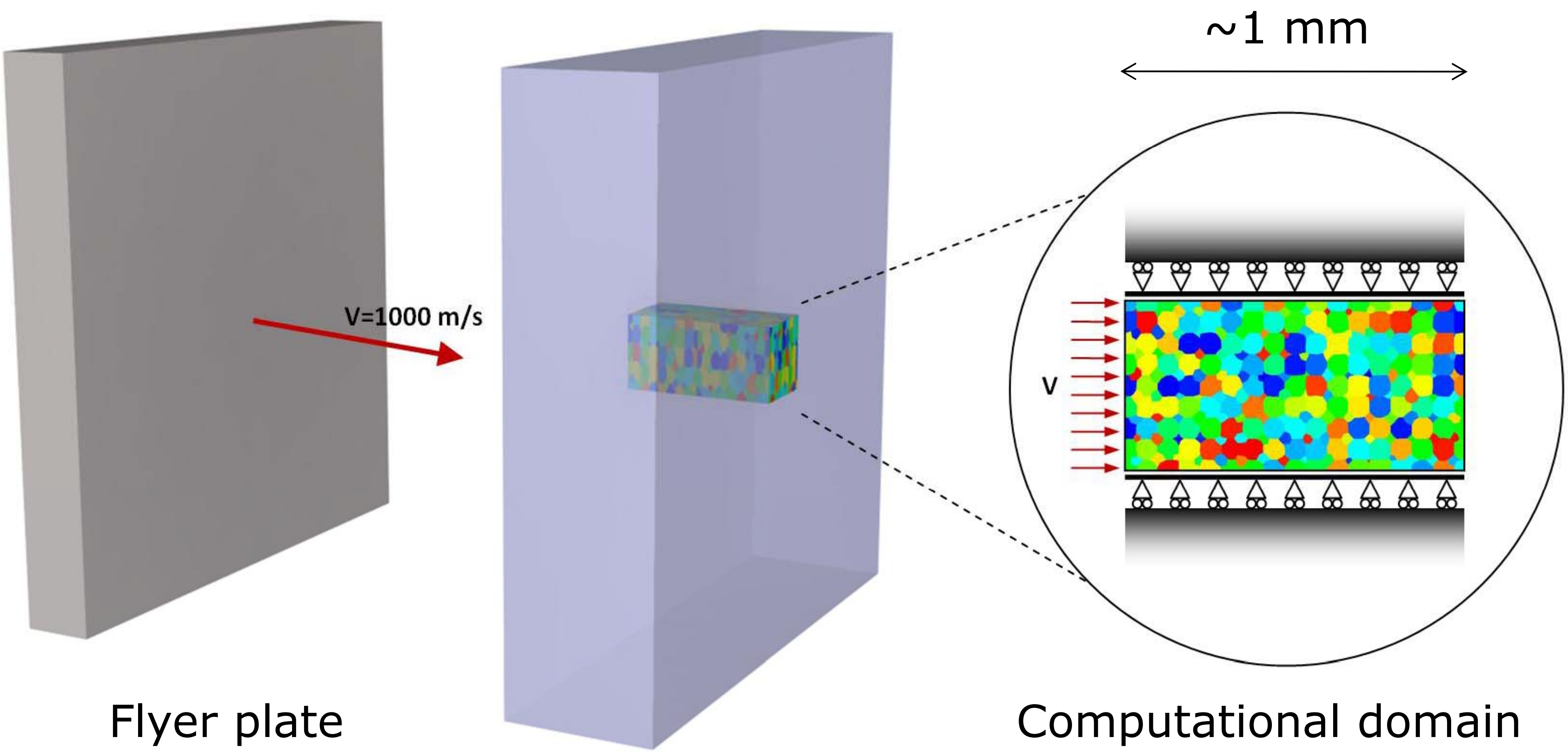
$$\frac{d\lambda}{dt} = Z(1-\lambda)\exp\left(-\frac{ER}{\theta}\right)$$

- 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

PETN – Plate impact test



Flyer plate

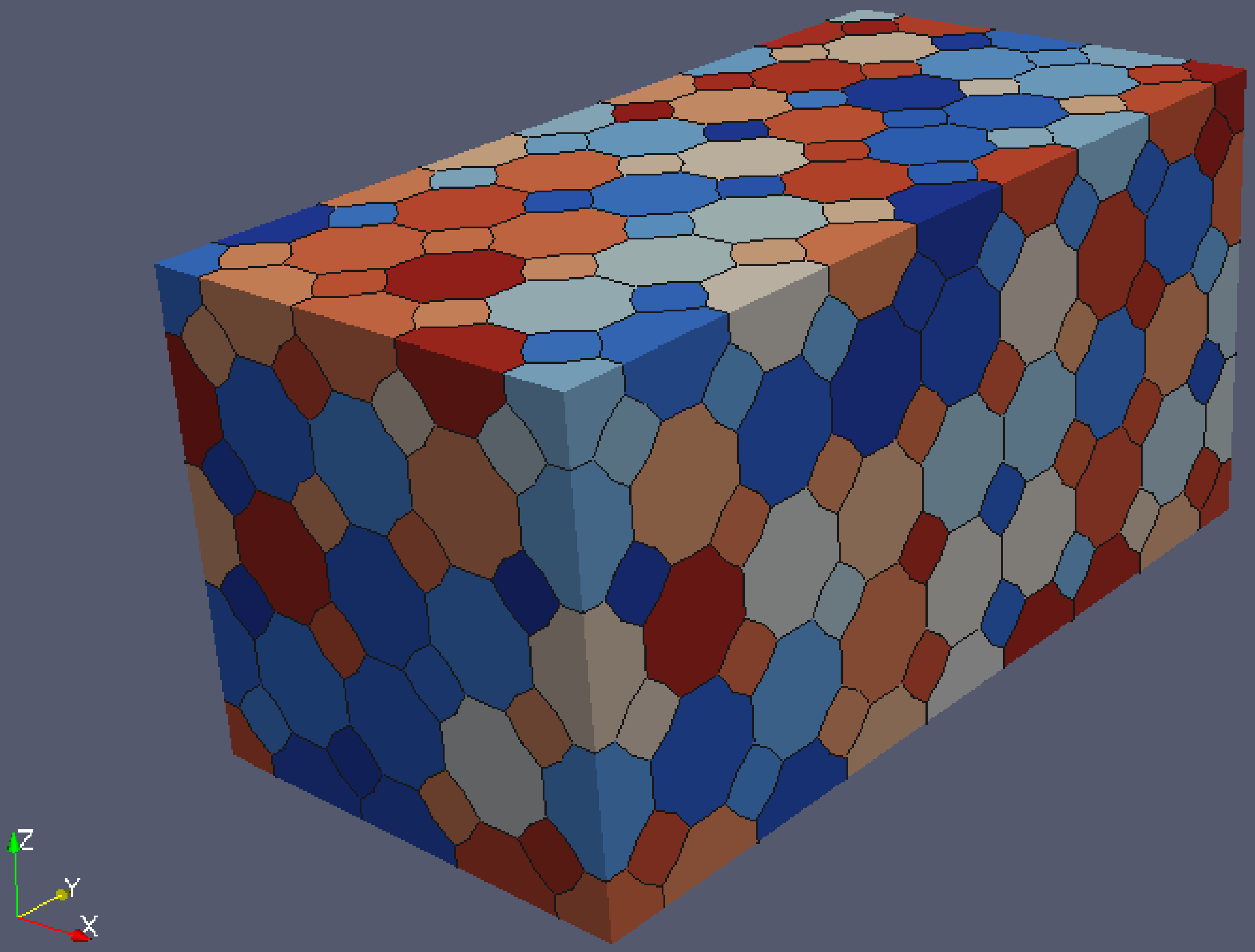
PETN target plate

Computational domain

Plate-impact configuration

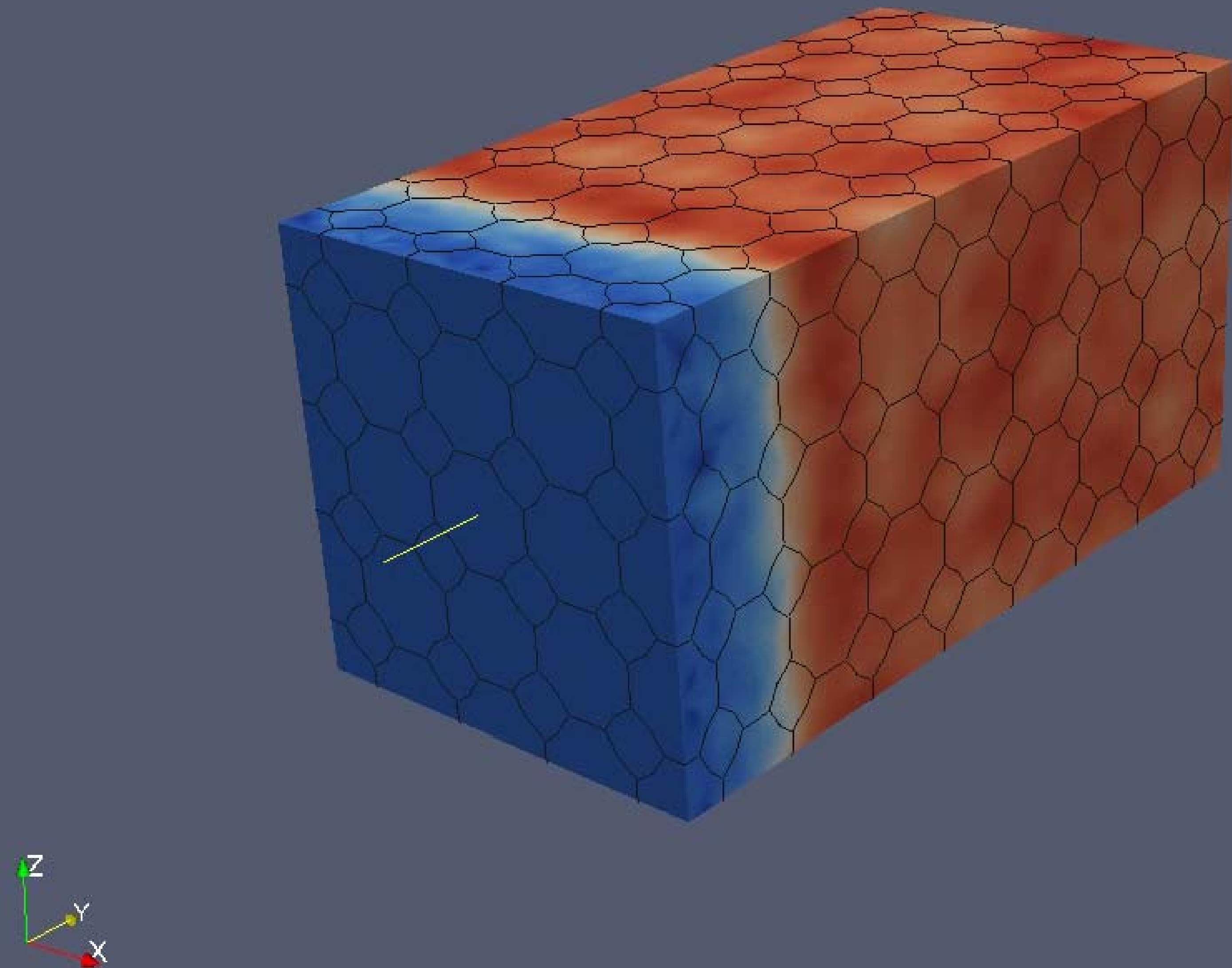
Rimoli, J.J. and MO, *Phys. Rev. E*, 2010

High-Explosives Detonation Initiation

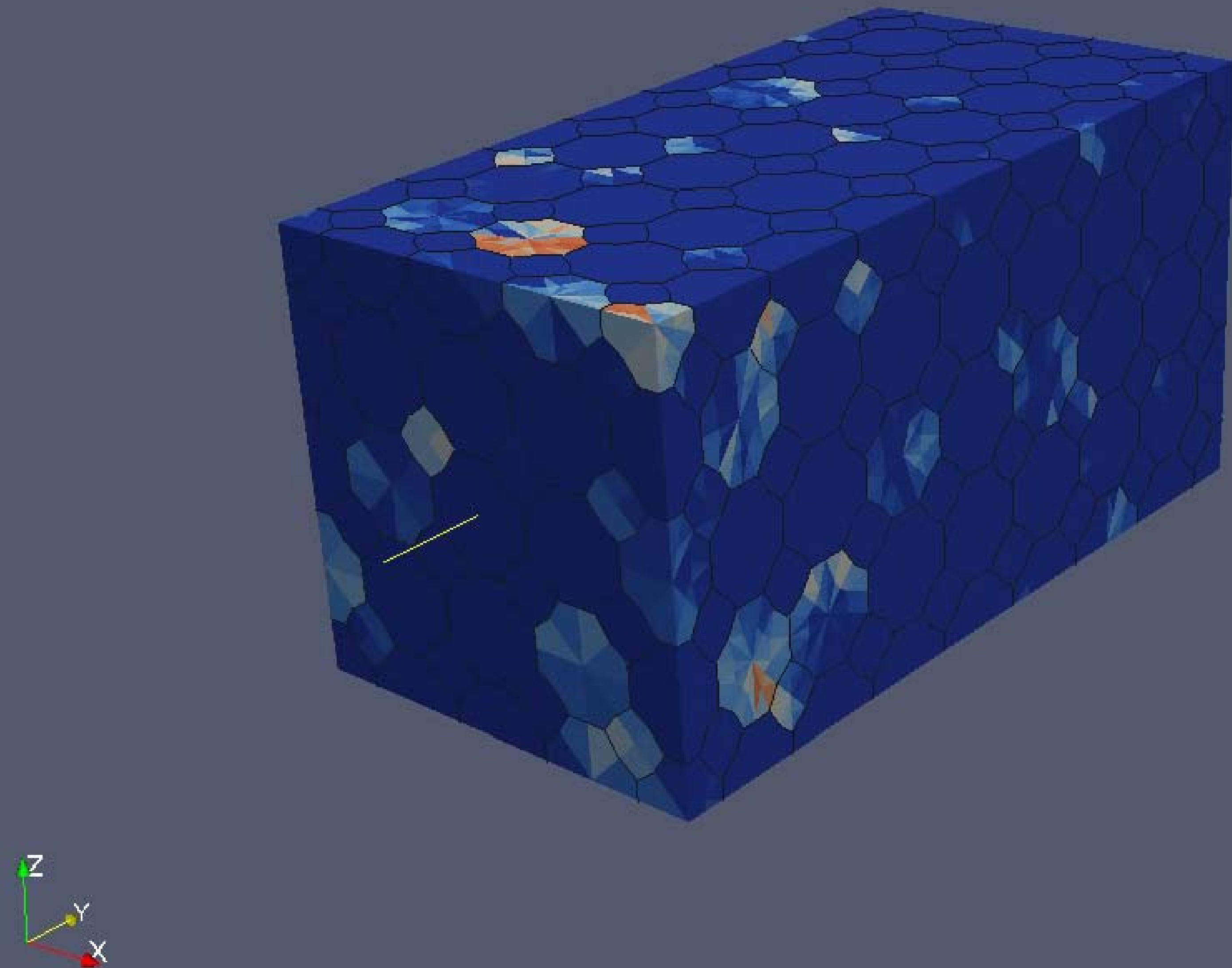


Polycrystal model and grain boundaries

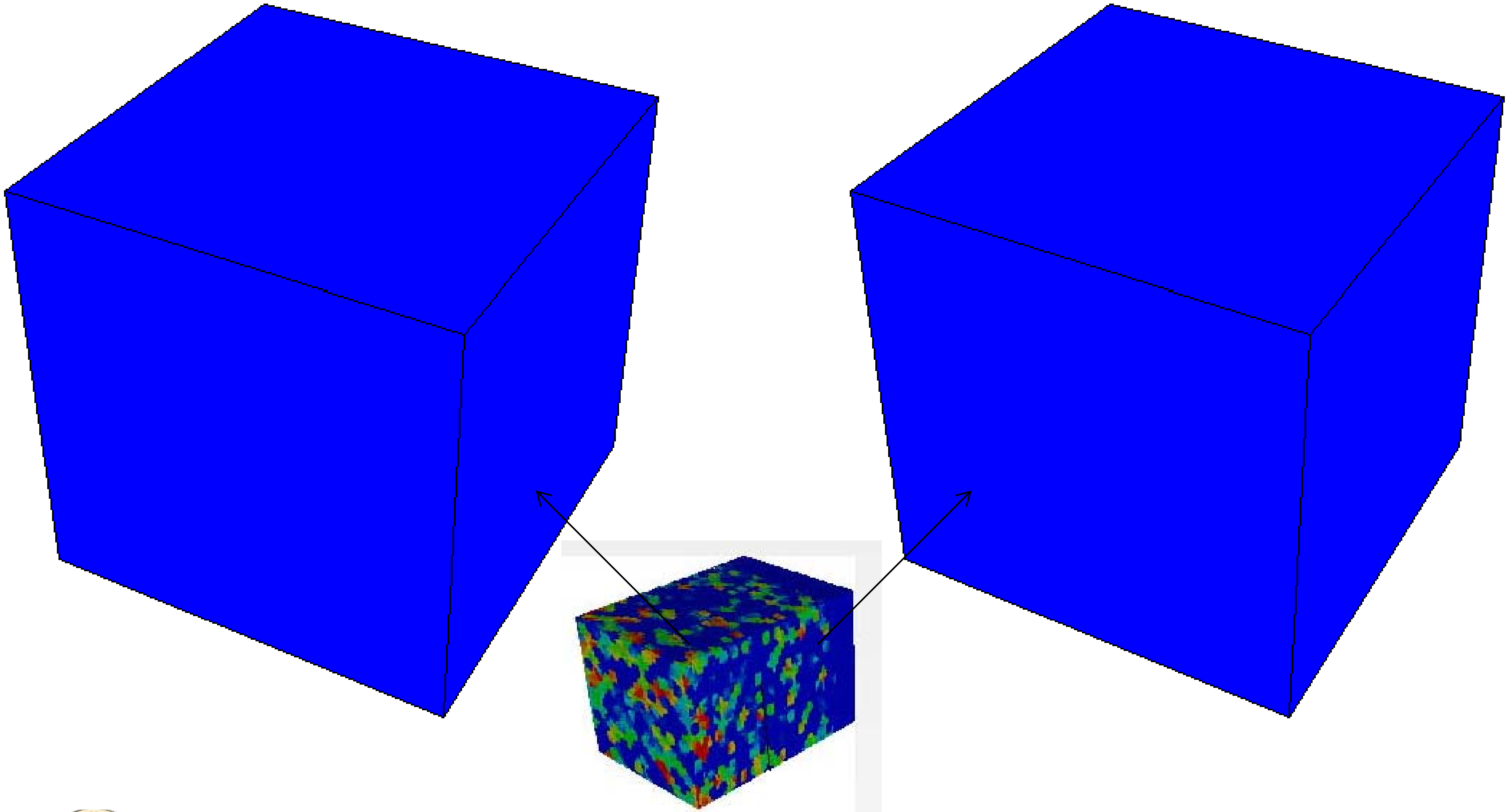
PETN plate impact - Velocity



PETN plate impact - temperature



PETN plate impact – Subgrain microstructures



Microstructure evolution at selected material points

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

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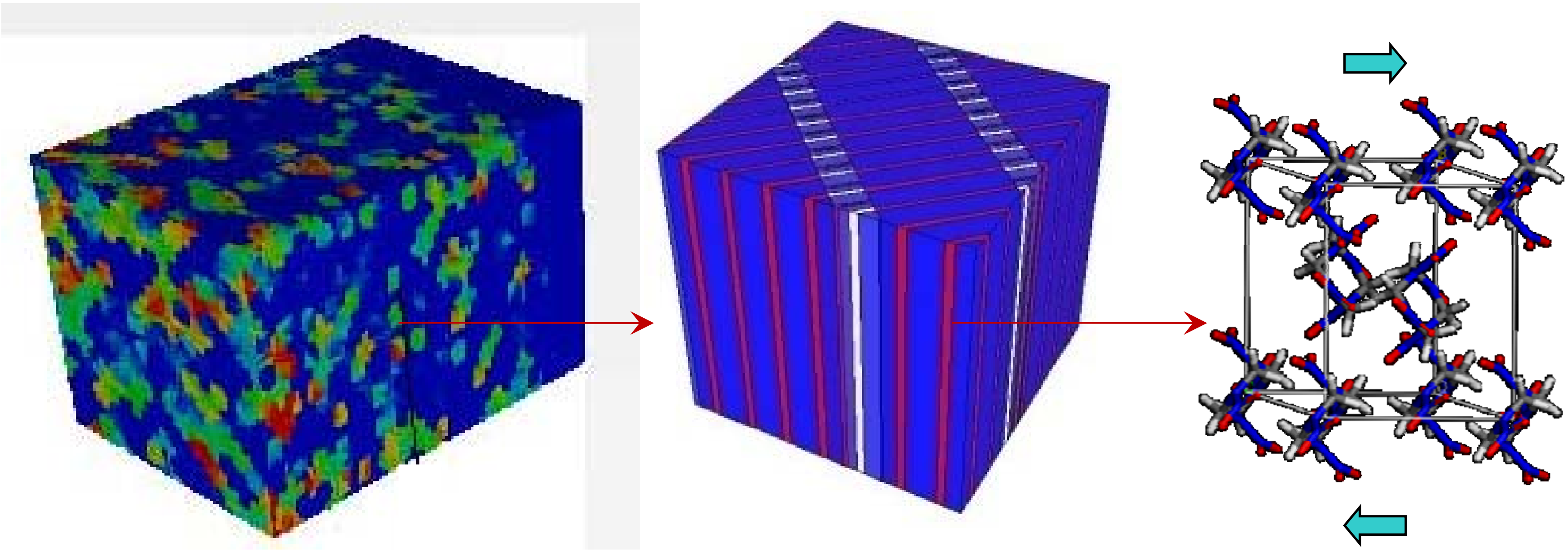
PETN plate impact – Hot-spot analysis



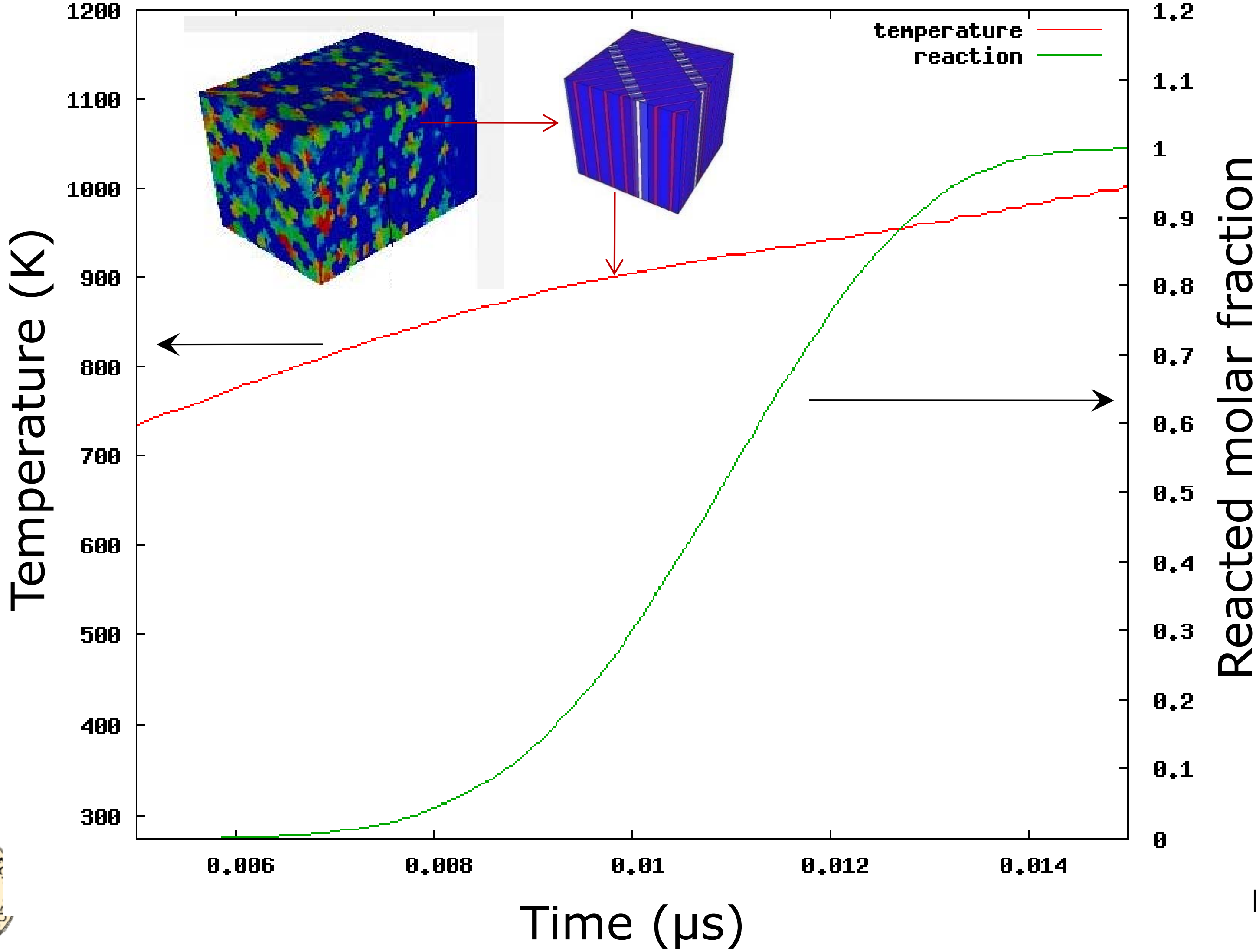
direct numerical simulation of polycrystalline PETN

reconstructed microstructure at selected material points

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

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

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



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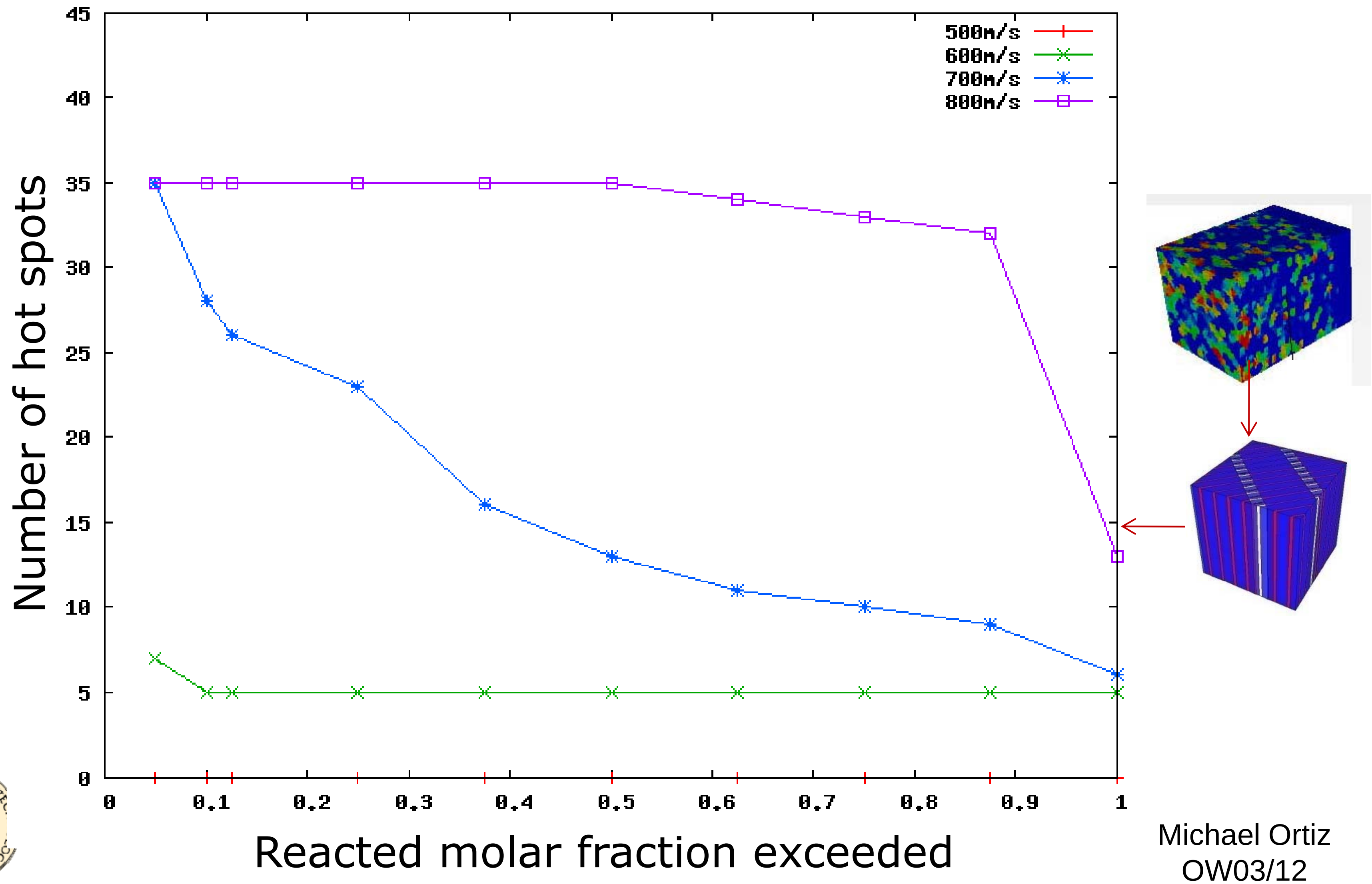
PETN plate impact - Number of hot spots



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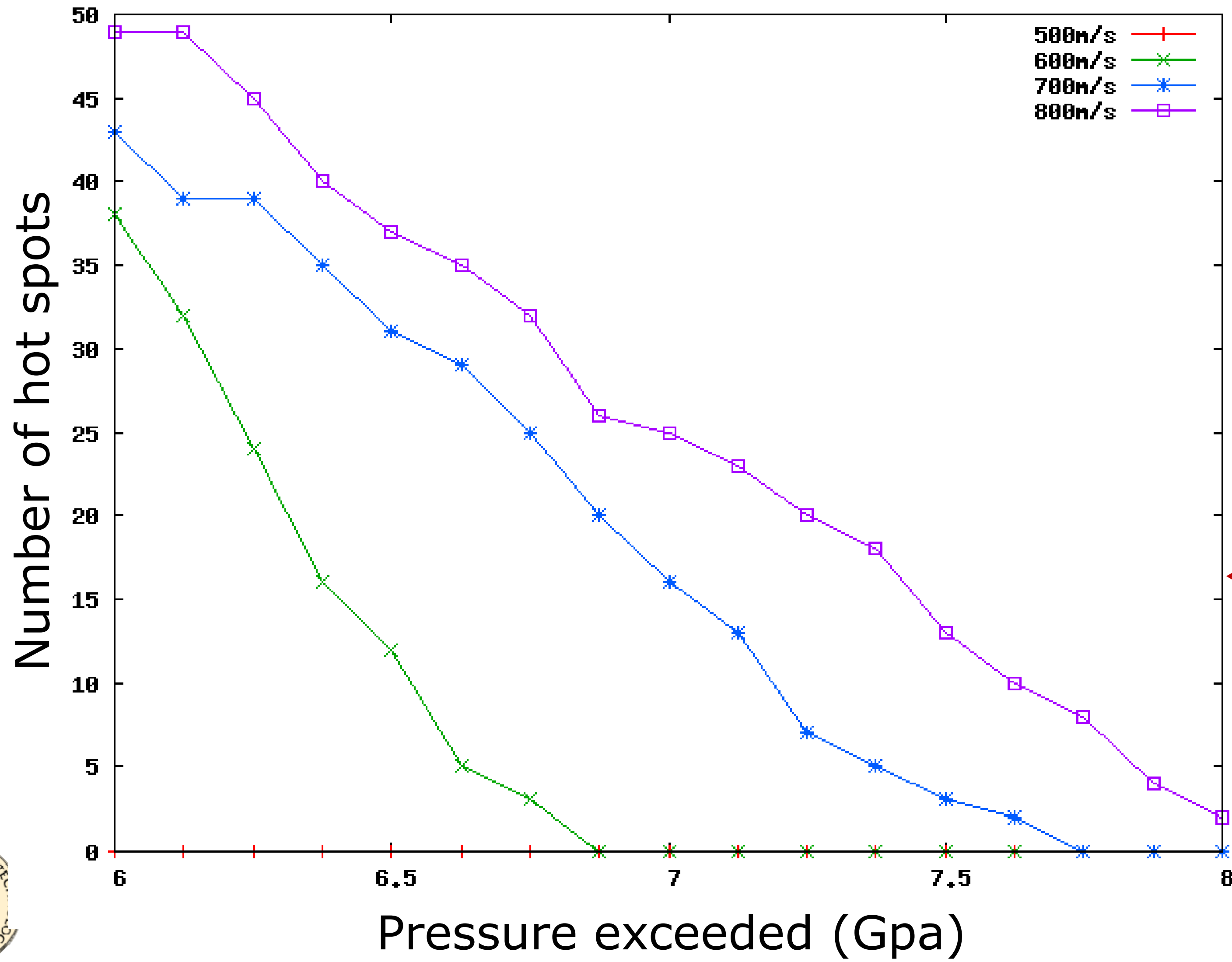

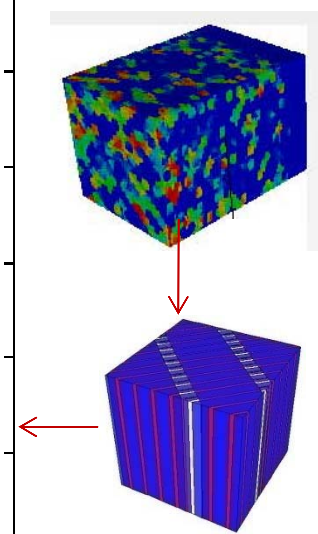

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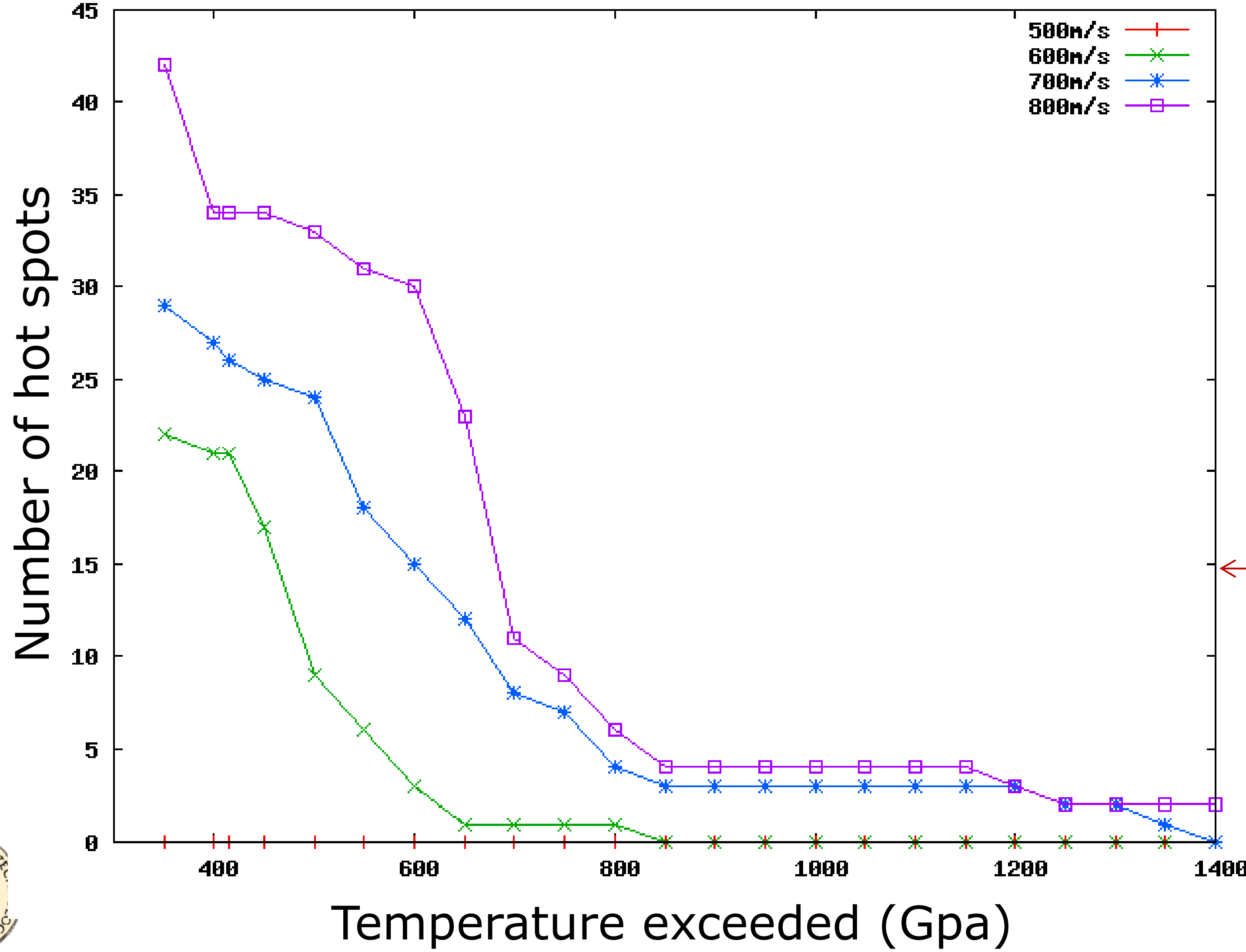

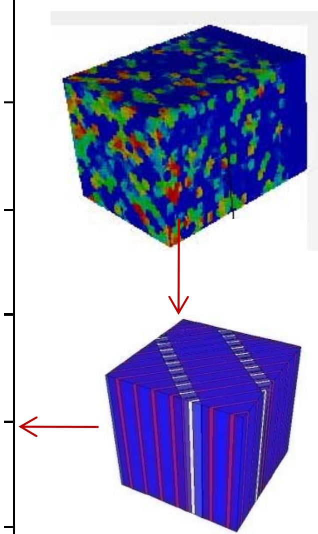

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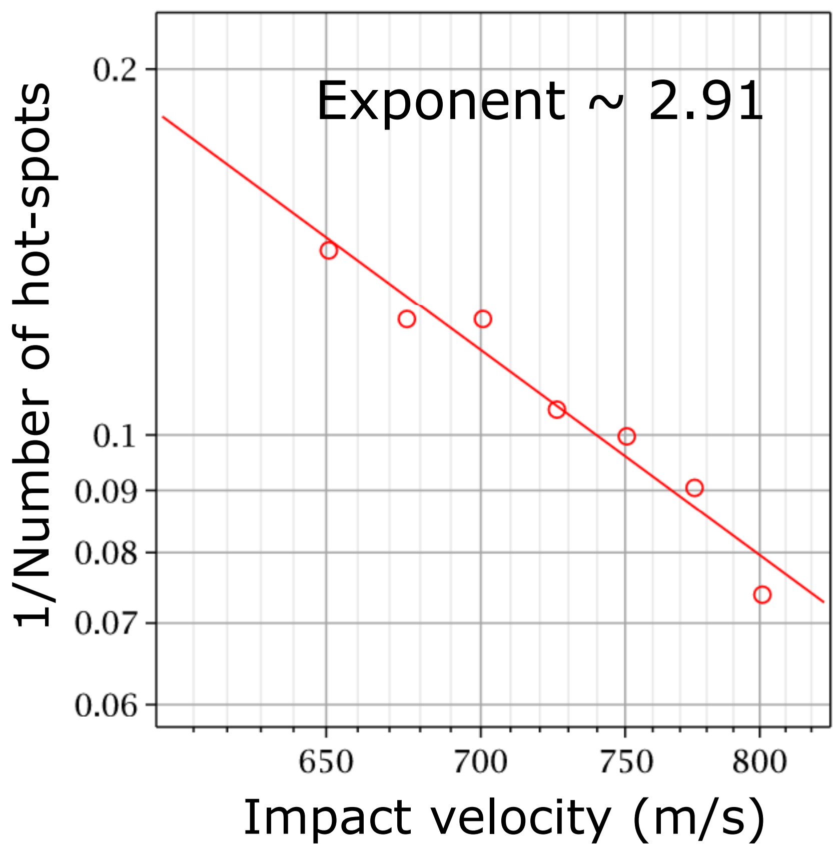
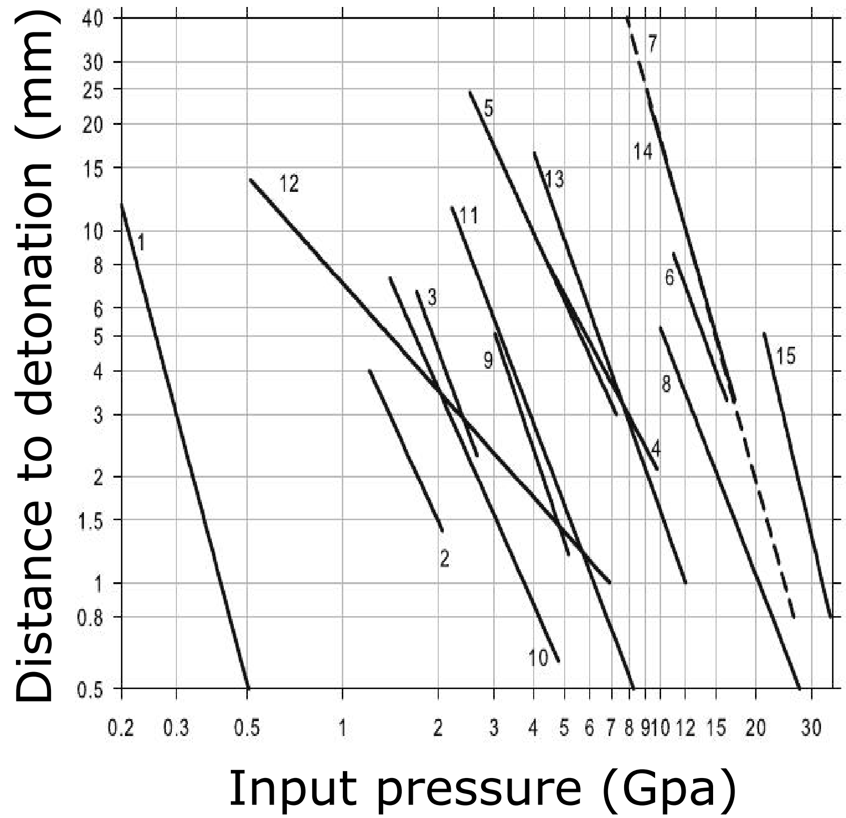
PETN plate impact – pop-plots

Impact velocity (m/s)





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

Experimental exponent ~ 2.01–2.58

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

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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)