Multiscale Modeling of High Energetic Materials under Impact Loads

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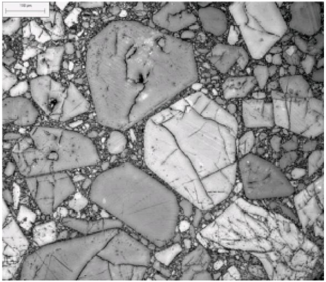
USNCCM X – July 16-19, 2009

Initiation of High Energy Materials

- HE materials initiate for an energy input much less than to heat bulk explosive
- Localized hot-spots are considered to cause detonation in HE materials
- Microscopic defects are thought to be a prime source for hot-spots
- Initiation of defect-free HE crystals are not very clear



Cracks in pressed PBX 9501, *Borne et al. [05]*

- Inhomogeneous nature of plastic deformation at sub-grain level (microstructures with localized deformation) and heterogeneity of polycrystals could cause initiation

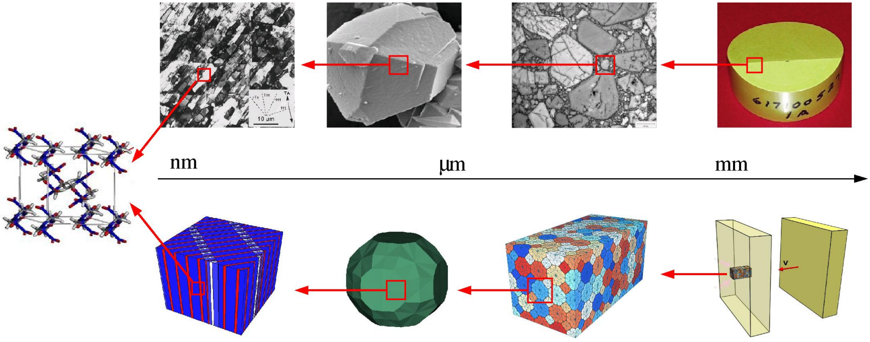
The proposed multiscale model consists of three levels

(i) Macroscale: direct resolution of 3-D polycrystalline structure with a barycentric subdivision algorithm and finite elements

(ii) Mesoscale: relaxation of a non-convex single crystal plasticity model that allows microstructure formation

(iii) Microscale: analytical construction of subgrain microstructures with localized slips and hot-spots

Multiscale Model of Initiation in HE Polycrystals



Chemical decomposition in hot-spots

Optimal subgrain microsturctures (relaxation)

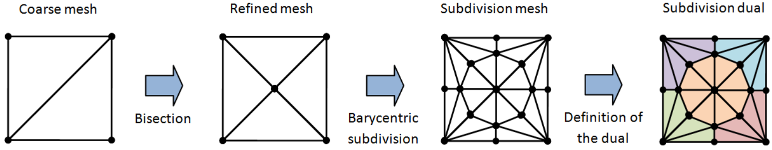
Single crystal plasticity of individual grains

Direct numerical simulation of polycrystal

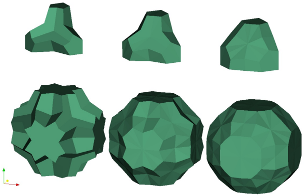
Plate impact test of explosive polycrystal

Modeling at Polycrystal Level

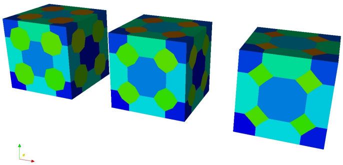
Barycentric Subdivision

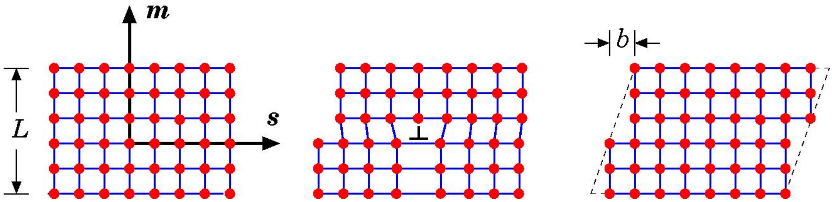


Grain Boundary Area Minimization



Polycrystal Evolution





- Additive decomposition of displacement gradient $\boldsymbol{\beta} = \nabla \boldsymbol{u}$

$$\boldsymbol{\beta} = \boldsymbol{\beta}^e + \boldsymbol{\beta}^p$$

- Due to crystallographic nature of crystals

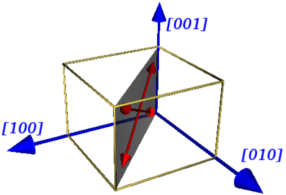
$$\boldsymbol{\beta}^p(\gamma) = \sum_{\alpha=1}^{N} \gamma^\alpha \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha \quad \text{where} \quad \gamma^\alpha = b/L$$

in terms of the slip directions $\boldsymbol{s}^\alpha$, the slip plane normals $\boldsymbol{m}^\alpha$

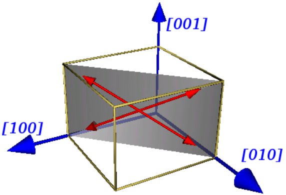
Modeling at Single Crystal Level

Slip Systems of body centered tetragonal PETN Single Crystals

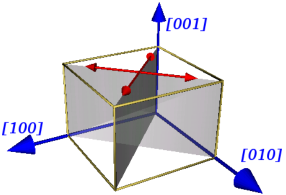
Slip System	I	II	III	IV	V	VI
Slip Direction	$\pm[1\bar{1}1]$	$\pm[1\bar{1}\bar{1}]$	$\pm[111]$	$\pm[11\bar{1}]$	$\pm[1\bar{1}0]$	$\pm[\bar{1}\bar{1}0]$
Plane Normal	(110)	(110)	$(1\bar{1}0)$	$(1\bar{1}0)$	(110)	$(1\bar{1}0)$



I–II



III–IV



V–VI

Lattice parameters: $a = b = 9.380\AA \quad c = 6.710\AA$

Variational Formulation of Single Crystal Plasticity

- The energy density has additive structure of elastic and plastic parts

$$A(\boldsymbol{\beta},\boldsymbol{\gamma}) = W^e(\boldsymbol{\beta} - \boldsymbol{\beta}^p(\boldsymbol{\gamma})) + W^p(\boldsymbol{\gamma}) \text{ with } \boldsymbol{\gamma} = \{\gamma^1, \gamma^2 \ldots \gamma^N\}$$

- Plastic parameters can be condensed out by a local minimization

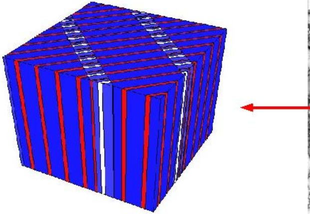
$$W(\boldsymbol{\beta}) = \min_{\boldsymbol{\gamma}\in\mathbb{R}^N} A(\boldsymbol{\beta},\boldsymbol{\gamma})$$

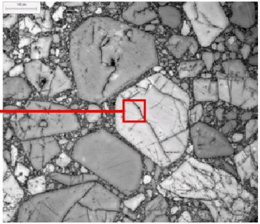
- $W(\boldsymbol{\beta})$ is non-convex and ill-posed for FEM
- Relaxation of $W(\boldsymbol{\beta})$ gives well-behaved softest average response

$$QW(\boldsymbol{\beta}) = \inf_{\boldsymbol{w}} \frac{1}{|\omega|}\int_\omega W(\boldsymbol{\beta} + \nabla \boldsymbol{w})dx$$

Relaxation and Microstructures

- Relaxation of $W(\beta)$ is not straightforward in general.
- $QW(\beta)$ is given for our problem in *Conti & Ortiz [05]*
- In addition to average response local variations of fields are important
- Heterogeneous microstructures can be generated from relaxed solution





- Microstructures allow highly localized slip lines $\Longrightarrow$ Hot-Spots

Construction of Optimal Microstructure *Conti & Ortiz [05]*

- Macroscopic deformation $\boldsymbol{\beta}$ decomposes into phases
- The first order laminates

$$\boldsymbol{\beta}_1 = \boldsymbol{\beta}^e + \sum_{\alpha=1}^{I-1} \gamma^\alpha \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha \quad \text{and} \quad \boldsymbol{\beta}_2 = \boldsymbol{\beta}_1 + \frac{1}{\epsilon} \gamma^I \boldsymbol{s}^I \otimes \boldsymbol{m}^I$$

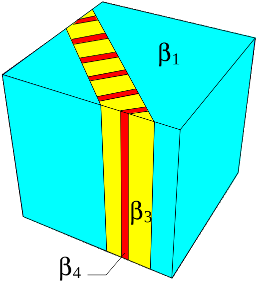
satisfying the rank one connectivity condition $(1-\epsilon)\boldsymbol{\beta}_1 + \epsilon\boldsymbol{\beta}_2 = \boldsymbol{\beta}$

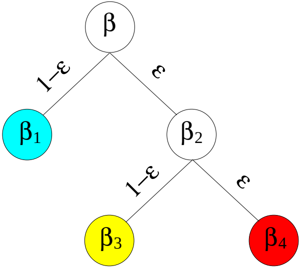
- The second order laminates

$$\boldsymbol{\beta}_3 = \boldsymbol{\beta}^e + \sum_{\alpha=2}^{I-1} \gamma^\alpha \boldsymbol{s}^\alpha \otimes \boldsymbol{m}^\alpha + \frac{1}{\epsilon} \gamma^I \boldsymbol{s}^I \otimes \boldsymbol{m}^I \quad \text{and} \quad \boldsymbol{\beta}_4 = \boldsymbol{\beta}_3 + \frac{1}{\epsilon} \gamma^1 \boldsymbol{s}^1 \otimes \boldsymbol{m}^1$$

satisfying the rank one connectivity condition $(1-\epsilon)\boldsymbol{\beta}_3 + \epsilon\boldsymbol{\beta}_4 = \boldsymbol{\beta}_2$

- Second order laminate microstructure for double slip cases $\alpha = I, II$



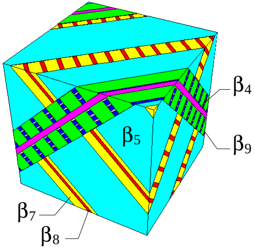


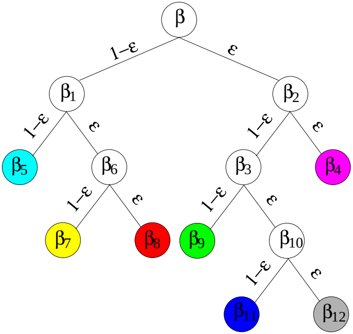
$$\boldsymbol{\beta} = (1-\epsilon)\boldsymbol{\beta}_1 + \epsilon\boldsymbol{\beta}_2 \qquad \boldsymbol{\beta}_2 = (1-\epsilon)\boldsymbol{\beta}_3 + \epsilon\boldsymbol{\beta}_4$$

$$\boldsymbol{\beta}_2 - \boldsymbol{\beta}_1 = \frac{1}{\epsilon}\gamma^{II}\boldsymbol{s}^{II}\otimes\boldsymbol{m}^{II} \qquad \boldsymbol{\beta}_4 - \boldsymbol{\beta}_3 = \frac{1}{\epsilon}\gamma^{I}\boldsymbol{s}^{I}\otimes\boldsymbol{m}^{I}$$

Modeling at Microstructure Level

- Fourth order laminate microstructure for multi-slip cases





$$\boldsymbol{\beta} = (1-\epsilon)\boldsymbol{\beta}_1 + \epsilon\boldsymbol{\beta}_2 \qquad \boldsymbol{\beta}_2 = (1-\epsilon)\boldsymbol{\beta}_3 + \epsilon\boldsymbol{\beta}_4$$

$$\boldsymbol{\beta}_1 = (1-\epsilon)\boldsymbol{\beta}_5 + \epsilon\boldsymbol{\beta}_6 \qquad \boldsymbol{\beta}_6 = (1-\epsilon)\boldsymbol{\beta}_7 + \epsilon\boldsymbol{\beta}_8 \ldots$$

Thermal Softening of Elastic Constants and CRSS

- Elastic constants $\mathbb{C}_{ij}$ are assumed to depend on temperature and vanish at melting temperature θ_{melt}

$$\mathbb{C}_{ij}(\theta) = \mathbb{C}_{ij}(\theta_0)\frac{\theta - \theta_{melt}}{\theta_0 - \theta_{melt}}$$

- CRSS values τ_c^α depend on temperature, *Stainier et al. [02]*

$$\tau_c^\alpha(\theta) = \tau_{c0}^\alpha \frac{k_B\theta}{G^\alpha} \text{asinh}\left(\xi^\alpha \exp\left(\frac{G^\alpha}{k_B\theta}\right)\right)$$

where k_B Boltzmann constant, and G^α and ξ^α additional parameters

Chemical Decomposition Model

- Temperature of hot-spot is computed assuming adiabatic heating

$$\Delta\theta_{hs} = \frac{\tau^{\alpha}\Delta\gamma^{\alpha}}{\rho c_v}$$

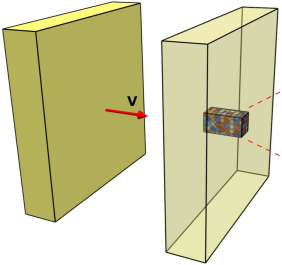
- Chemical reaction is modeled by an Arrhenius type depletion law *Caspar et al.[98]*

$$\frac{d\lambda}{dt} = Z(1-\lambda)\exp\left(-\frac{E}{R\theta_{hs}}\right)$$

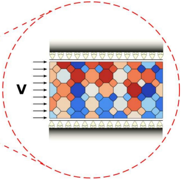
where Z, E, R are parameters and $\lambda \in [0, 1]$ reaction progress variable

- Extent of reaction is obtained by integrating depletion law $\frac{d\lambda}{dt}$

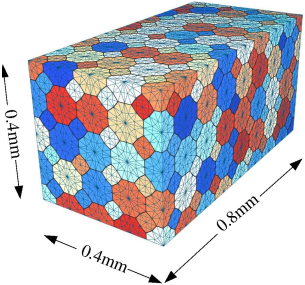
Plate Impact Test of PETN Polycrystal



Flyer and PETN Plate



Computational Model

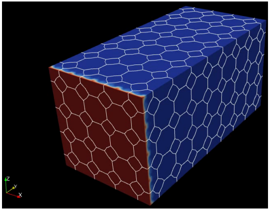


Polycrystal Model: Discretization and Grains

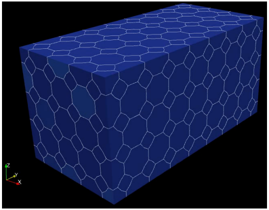
- 817 grains with maximum grain size of 0.1 mm
- Impact velocities in the range of 500 - 800 m/s
- Simulation of total 0.3μs with $\Delta t = 1 \times 10^{-4} \mu$ sec

Plate Impact Test of PETN Polycrystal

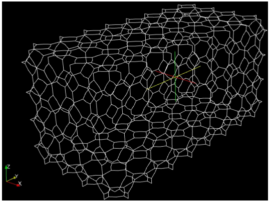
- Simulation results for v = 700m/s



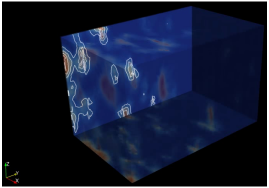
Axial Velocity



Surface Temperature



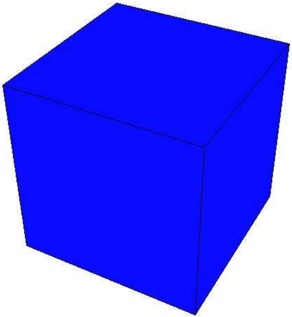
Temperature Threshold



Temperature MRI

Plate Impact Test of PETN Polycrystal

Microstructure Evolution



Temperature and Chemical Reaction in a Hot-Spot

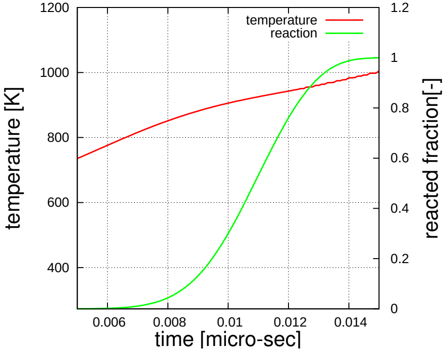
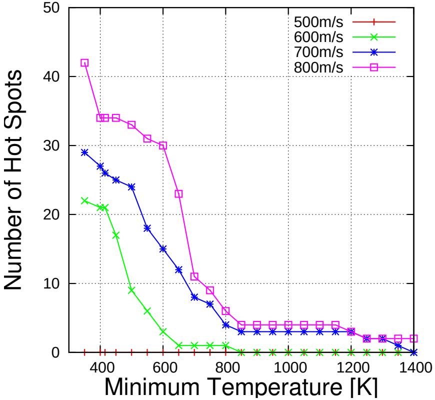
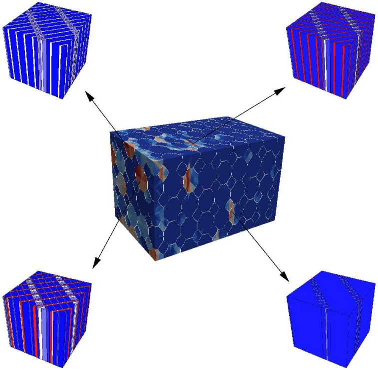


Plate Impact Test of PETN Polycrystal

- Hot-spots based on minimum temperature criterion

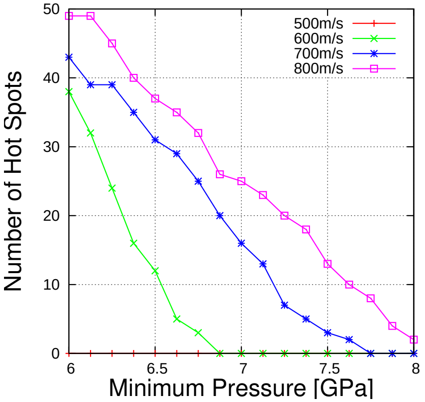


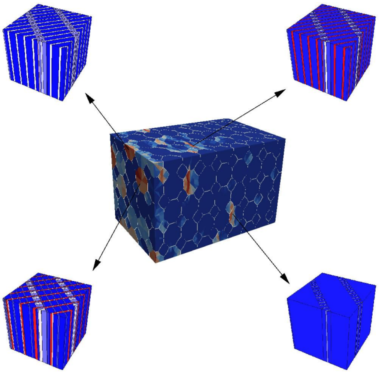


Surface temperature for different impact velocities

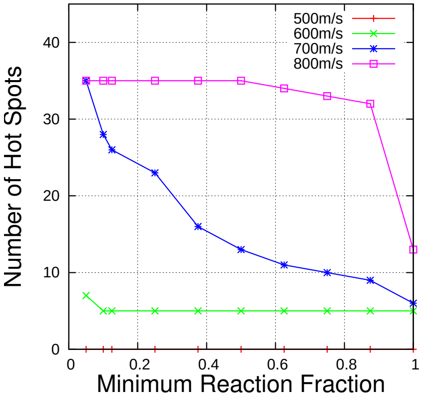
Plate Impact Test of PETN Polycrystal

- Hot-spots based on minimum pressure





- Hot-spots based on minimum chemical decomposition



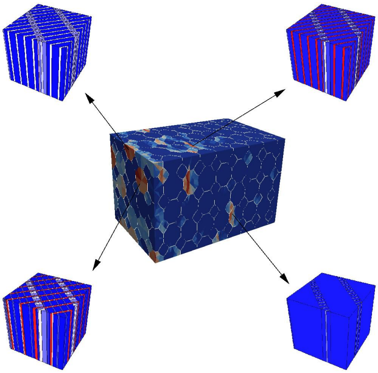
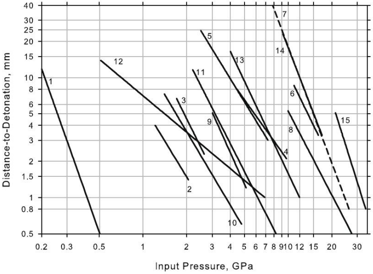
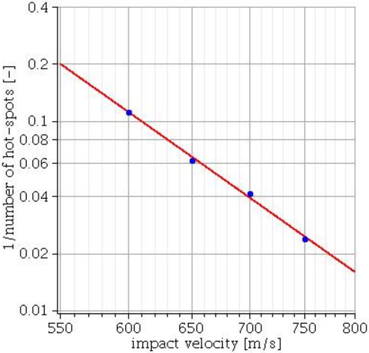


Plate Impact Test of PETN Polycrystal

- Comparison with experiments, impact pressure vs. distance to detonation



Pop-plots for several HE materials, *Sheffield and Engelke [09]*



Number of hot-spots vs impact velocity

Conclusion

- Multiscale framework bridges
  - Polycrystal structure at macroscale
  - Single crystal structure at mesoscale
  - Subgrain microstructures with localized plastic slip at microscale
- No need to introduce a priori defects for the generation of hot-spots
  Defective crystals can be generated easily as well

  (i) Voids (ii) Temperature (iii) Temperature Contour

- Heterogeneous nature of plastic deformation (microstructure formation) allows nucleation of hot-spots
- Proposed method allows to study hot-spot statistic, e.g. number, spatial distribution of hot-spots
- Macroscopic scale applications can be simulated for μs

Acknowledgment: W. A. Goddard, S. Dasgupta, S. Zybin and P. Xu

Pressure Dependence of Melting Temperature

- Melting temperature θ_{melt} depends on pressure (volume)
- The form proposed by *Menikoff and Sewell [02]* is assumed

$$\theta_{melt}(P) = \theta_{melt}(P_0)(1 + a\frac{\Delta V}{V_0})$$

where $a = 2(\Gamma - 1/3)$ and $\Gamma \approx 1.2$ is Grüneisen coefficient

- Volumetric compression of 20% gives $\sim$ 35% increase in θ_{melt}