Multiscale Modeling of High Energetic Materials under Impact Loads

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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

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

Cracks in pressed PBX 9501, Borne et al. [05]
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 microstructures (relaxation)
Single crystal plasticity of individual grains
Direct numerical simulation of polycrystal
Plate impact test of explosive polycrystal
Modeling at Polycrystal Level

Barycentric Subdivision

Coarse mesh ⟷ Bisection ⟷ Refined mesh ⟷ Barycentric subdivision ⟷ Subdivision mesh ⟷ Definition of the dual ⟷ Subdivision dual

Grain Boundary Area Minimization

Polycrystal Evolution
Additive decomposition of displacement gradient $\beta = \nabla u$

$\beta = \beta^e + \beta^p$

Due to crystallographic nature of crystals

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

in terms of the slip directions $s^\alpha$, the slip plane normals $m^\alpha$
### Modeling at Single Crystal Level

#### Slip Systems of body centered tetragonal PETN Single Crystals

<table>
<thead>
<tr>
<th>Slip System</th>
<th>I</th>
<th>II</th>
<th>III</th>
<th>IV</th>
<th>V</th>
<th>VI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slip Direction</td>
<td>±[111]</td>
<td>±[111]</td>
<td>±[111]</td>
<td>±[111]</td>
<td>±[110]</td>
<td>±[110]</td>
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<tr>
<td>Plane Normal</td>
<td>(110)</td>
<td>(110)</td>
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</tbody>
</table>

Lattice parameters: \(a = b = 9.380\text{Å}\) \(c = 6.710\text{Å}\)
Variational Formulation of Single Crystal Plasticity

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

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

- Plastic parameters can be condensed out by a local minimization

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

- \( W(\beta) \) is non-convex and ill-posed for FEM

- Relaxation of \( W(\beta) \) gives well-behaved softest average response

\[ QW(\beta) = \inf_{w} \frac{1}{|\omega|} \int_{\omega} W(\beta + \nabla w) \, dx \]
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 $\Rightarrow$ Hot-Spots.
Construction of Optimal Microstructure

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

$$\beta_1 = \beta^e + \sum_{\alpha=1}^{I-1} \gamma^\alpha s^\alpha \otimes m^\alpha \quad \text{and} \quad \beta_2 = \beta_1 + \frac{1}{\epsilon} \gamma^I s^I \otimes m^I$$

satisfying the rank one connectivity condition $(1 - \epsilon)\beta_1 + \epsilon\beta_2 = \beta$
- The second order laminates

$$\beta_3 = \beta^e + \sum_{\alpha=2}^{I-1} \gamma^\alpha s^\alpha \otimes m^\alpha + \frac{1}{\epsilon} \gamma^I s^I \otimes m^I \quad \text{and} \quad \beta_4 = \beta_3 + \frac{1}{\epsilon} \gamma^1 s^1 \otimes m^1$$

satisfying the rank one connectivity condition $(1 - \epsilon)\beta_3 + \epsilon\beta_4 = \beta_2$
Second order laminate microstructure for double slip cases $\alpha = I, II$

\[
\beta = (1 - \epsilon)\beta_1 + \epsilon\beta_2 \quad \beta_2 = (1 - \epsilon)\beta_3 + \epsilon\beta_4
\]

\[
\beta_2 - \beta_1 = \frac{1}{\epsilon} \gamma^I s^I \otimes m^I \\
\beta_4 - \beta_3 = \frac{1}{\epsilon} \gamma^I s^I \otimes m^I
\]
Fourth order laminate microstructure for multi-slip cases

\[ \beta = (1 - \epsilon)\beta_1 + \epsilon\beta_2 \quad \beta_2 = (1 - \epsilon)\beta_3 + \epsilon\beta_4 \]

\[ \beta_1 = (1 - \epsilon)\beta_5 + \epsilon\beta_6 \quad \beta_6 = (1 - \epsilon)\beta_7 + \epsilon\beta_8 \ldots \]
Thermal Softening of Elastic Constants and CRSS

- Elastic constants $C_{ij}$ are assumed to depend on temperature and vanish at melting temperature $\theta_{\text{melt}}$

\[
C_{ij}(\theta) = C_{ij}(\theta_0) \frac{\theta - \theta_{\text{melt}}}{\theta_0 - \theta_{\text{melt}}}
\]

- CRSS values $\tau_c^\alpha$ depend on temperature, Stainier et al. [02]

\[
\tau_c^\alpha(\theta) = \tau_c^\alpha \frac{k_B\theta}{G^\alpha} \text{asinh} \left( \xi^\alpha \exp \left( \frac{G^\alpha}{k_B\theta} \right) \right)
\]

where $k_B$ Boltzmann constant, and $G^\alpha$ and $\xi^\alpha$ 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
  \[ \frac{d\lambda}{dt} = Z(1 - \lambda) \exp \left( - \frac{E}{R\theta_{hs}} \right) \]
  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

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

- Simulation results for $v = 700\text{m/s}$

Axial Velocity

Surface Temperature

Temperature Threshold

Temperature MRI
Plate Impact Test of PETN Polycrystal

Microstructure Evolution

Temperature and Chemical Reaction in a Hot-Spot

![Graph showing temperature and reaction fraction over time.](image)
Hot-spots based on minimum temperature criterion

Surface temperature for different impact velocities
Hot-spots based on minimum pressure
Plate Impact Test of PETN Polycrystal

- Hot-spots based on minimum chemical decomposition

![Graph showing the number of hot spots against minimum reaction fraction for different impact velocities (500m/s, 600m/s, 700m/s, 800m/s)].
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 $\mu s$

Acknowledgment: W. A. Goddard, S. Dasgupta, S. Zybin and P. Xu
Pressure Dependence of Melting Temperature

- Melting temperature $\theta_{melt}$ 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 $\theta_{melt}$