Shock-induced subgrain microstructures in energetic polycrystals

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with: E. Gurses, J. Rimoli,

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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)
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

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

Polycrystalline structure: Direct Num. Simul. (DNS)

Optimal deformation microstructures (relaxation)

Atomistic models, chemistry

downscaling

upscaling
HE initiation – Multiscale modeling

Information flow for polycrystalline HE

First-principles & atomistic calculations

Boundary conditions

Post-processing

Material properties

Relaxation

Effective properties

Microstructure reconstruction

Direct Numerical Simulation (DNS)

Full chemistry
Strong latent hardening & microstructure

affine boundary conditions
\[ u_1 = \gamma x_2 \]
uniform double slip

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)

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Strong latent hardening & microstructure

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Strong latent hardening & microstructure

microstructural refinement!

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Strong latent hardening & microstructure

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Strong latent hardening & microstructure

- “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

Sir Alan H. Cottrell
ScD HonLLD FRS
Crystal plasticity – Relaxation

- Explicit microstructure construction: equilibrium deformation field compatible with macroscopic deformation, single slip in each variant!

PETN – Plate impact test

Flyer plate

PETN target plate

V=1000 m/s

Computational domain

~1 mm

Plate-impact configuration

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PETN – Elastic constants

Body Centered Tetragonal Lattice

• Elastic Constants (GPA): (Winey and Gupta, 2001)

\[ C_{11}=17.22 \quad C_{33}=12.17 \]
\[ C_{44}=5.04 \quad C_{66}=3.95 \]
\[ C_{12}=5.44 \quad C_{13}=7.99 \]

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

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

\[ \theta_{\text{melt}}(p) = \theta_{\text{melt}}(p_0) \left( 1 + \frac{a \Delta V}{V_0} \right) \]

where \( a = 2(\Gamma-1/3) \), \( \Gamma \sim 1.2 = \) Grüneisen constant

\[ a = 9.380\,\text{Å} \] and \( c = 6.710\,\text{Å} \)

• Menikoff and Sewell (2002):
PETN – Slip systems

\[ \tau_c (\theta) \text{ fitted to data of Amuzu et al. (1976)} \] and:

\[
\begin{array}{|c|c|c|c|c|c|c|}
\hline
\text{Slip System} & \text{B3} & \text{B4} & \text{A1} & \text{A2} & \text{B6} & \text{A5} \\
\text{s}^a & \pm [\overline{1}11] & \pm [\overline{1}11] & \pm [111] & \pm [111] & \pm [\overline{1}10] & \pm [\overline{1}10] \\
\text{m}^a & \begin{array}{l}(110) \end{array} & \begin{array}{l}(110) \end{array} & \begin{array}{l}(1\overline{1}0) \end{array} & \begin{array}{l}(1\overline{1}0) \end{array} & \begin{array}{l}(110) \end{array} & \begin{array}{l}(1\overline{1}0) \end{array} \\
\hline
\tau_c \text{ [GPa]} & 1.0 & 1.0 & 1.0 & 1.0 & 2.0 & 2.0 \\
\hline
\end{array}
\]

\[ a = b = 9.380\text{Å} \quad c = 6.710\text{Å} \]
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):
  
<table>
<thead>
<tr>
<th></th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R$</td>
<td>8.314 J/mol/K</td>
</tr>
<tr>
<td>$E$</td>
<td>196.742 x 10^3 J/mol</td>
</tr>
<tr>
<td>$Z$</td>
<td>6.3 x 10^{19} s^{-1}</td>
</tr>
</tbody>
</table>

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

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High-Explosives Detonation Initiation

Polycrystal model and grain boundaries
PETN plate impact - Velocity
PETN plate impact - temperature
PETN plate impact - temperature
PETN plate impact - temperature
PETN plate impact - temperature
PETN plate impact – Subgrain microstructures

Microstructure evolution at selected material points
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

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

![Graph showing temperature and reacted molar fraction over time.](image)
PETN plate impact - Number of hot spots

![Graph showing the number of hot spots versus reacted molar fraction exceeded. The graph includes lines for different impact speeds: 500 m/s (red), 600 m/s (green), 700 m/s (blue), and 800 m/s (purple). The y-axis represents the number of hot spots, and the x-axis represents the reacted molar fraction exceeded.]
PETN plate impact - Number of hot spots

Pressure exceeded (Gpa)

Number of hot spots

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PETN plate impact - Number of hot spots

Temperature exceeded (Gpa)

Number of hot spots
PETN plate impact – pop-plots

Impact velocity (m/s)

Exponent \( \sim 2.91 \)

\[ \frac{1}{\text{Number of hot-spots}} \]

Impact velocity (m/s)

Distance to detonation (mm)

Input pressure (Gpa)

Multiscale model

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

Experimental exponent \( \sim 2.01–2.58 \)

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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 → 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

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Thank you!