Micromechanics-Based Prediction of Thermoelastic Properties of High Energy Materials

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Outline

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  • Micromechanics Methods
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• Approach
  • Generating Microstructures
  • Generalized Method of Cells (GMC)
  • Recursive Cells Method (RCM)
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Background

Steel Container + High Energy Material Global Simulation

Microstructure of High Energy Material Micromechanics

Molecular Structure of Energetic Material Molecular Dynamics

Atomistic Simulations Quantum Chemistry
High Energy Materials

• Polymer Bonded Explosives (PBXs)
  • Particulate composites
  • High volume fraction of explosive particles
  • High modulus contrast between particles and binder

<table>
<thead>
<tr>
<th>PBX</th>
<th>Explosive (Particles)</th>
<th>Volume (%)</th>
<th>Binder</th>
<th>Volume (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PBX 9010</td>
<td>RDX</td>
<td>87</td>
<td>KEL-F-3700</td>
<td>13</td>
</tr>
<tr>
<td>PBX 9501</td>
<td>HMX</td>
<td>92</td>
<td>Estane 5703 + BDNPA/F</td>
<td>8</td>
</tr>
<tr>
<td>PBX 9502</td>
<td>TATB</td>
<td>90</td>
<td>KEL-F-800</td>
<td>10</td>
</tr>
</tbody>
</table>
PBX 9501

- Monoclinic crystals of HMX dispersed in a viscoelastic binder (Estane + BDNPA/F)

<table>
<thead>
<tr>
<th>HMX Properties</th>
<th>E (GPa)</th>
<th>v</th>
<th>α (x 10^{-5}/K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Experimental</td>
<td>15.3</td>
<td>0.32</td>
<td>11.6</td>
</tr>
<tr>
<td>Molecular Dynamics (MD)</td>
<td>17.7</td>
<td>0.21</td>
<td>7.2</td>
</tr>
</tbody>
</table>

Binder Properties

- ν = 0.49
- α = 20 x 10^{-5}/K

PBX 9501 Properties

- ν = 0.35
- α = 12 x 10^{-5}/K
Micromechanics Methods

- **Rigorous Bounds**
  - Rosen/Hashin Bounds for CTE
  - Third Order Bounds for Elastic Moduli

- **Analytical Approximations**
  - Self-Consistent Schemes
  - Differential Effective Medium Approach
  - Third Order Approximations

- **Numerical Approximations**
  - Finite Elements (FEM)
  - Boundary Integral Equations
  - Fourier Transforms
  - Method of Cells
Approximations versus Experiments

- Experimental Young’s modulus an order of magnitude higher than numerical or analytical value.

- FEM used for numerical calculations (particles do not touch in simulated microstructures).
Objective

• Predict thermoelastic properties of polymer bonded explosives.
  • Create appropriate microstructures.
  • Device computationally inexpensive numerical techniques.
Generating PBX Microstructures

Particle Size Distribution (PBX 9501)

- Random Sequential Addition of particles used to generate microstructures.
- Microstructures contain 85%-88% particles – rest “dirty” binder.
Generalized Method of Cells (GMC)

Approach: (Aboudi, 1996)
- Linear subcell displacement field
- Periodic boundary conditions
- Equilibrium and compatibility in an average sense
- Traction continuity across subcells
- Normal-shear behavior uncoupled

\[ M\sigma = D\langle \varepsilon \rangle \implies \langle \sigma \rangle = \langle M^{-1}D \rangle \langle \varepsilon \rangle \]
\[ C^* = \langle M^{-1}D \rangle \]

Problems:
- Large matrices – 6 N^2
- Poor stress bridging
- Inaccurate shear moduli

Less efficient than finite element analysis.
Recursive Cells Method (RCM)

**Approach:**
- Choose RVE.
- Discretize into $2^N \times 2^N$ subcells.
- Calculate effective properties for each block of $2 \times 2$ subcells.
- Perform recursion until the RVE is homogenized.
- Use finite differences, finite elements, boundary integrals or Fourier methods to calculate effective properties.

**Improvements:**
- Choose blocks of $k \times k$ subcells ($k>2$) as the size of the basic renormalization cluster.
- Use network approximations to calculate effective properties.

- Similar to real-space renormalization group methods that work well for percolation problems.
- Stress bridging is analogous to stress percolation.
RCM Implementation

**Element Types**

- Four and nine-noded displacement based elements for particles.
- Four-noded displacement based or nine-noded displacement/ pressure based elements for binder.

**Effective Properties**

- Calculate volume averaged element stresses and strains
- Effective stiffness matrix given by

\[
\begin{bmatrix}
\langle \sigma_{11} \rangle \\
\langle \sigma_{22} \rangle \\
\langle \tau_{12} \rangle
\end{bmatrix} =
\begin{bmatrix}
C_{11} & C_{12} & 0 \\
C_{12} & C_{22} & 0 \\
0 & 0 & C_{66}
\end{bmatrix}
\begin{bmatrix}
\langle \varepsilon_{11} \rangle \\
\langle \varepsilon_{22} \rangle \\
\langle \gamma_{12} \rangle
\end{bmatrix}
\]

- Three sets of BCs needed to solve for $C^*$ in two dimensions.
Results – FEM, 2x2 RCM, GMC

- FEM properties usually higher than experimental!
- 2x2 RCM values 2-3 times higher than FEM.
- GMC values 10 – 20 times lower than FEM.
Results – FEM, 32x32 RCM, GMC

- 32x32 RCM results are considerably closer to FEM and experimental data than 2x2 RCM results.
- However, some computational efficiency is lost because of the larger renormalization cluster.
Conclusions

• For effective CTEs use Rosen-Hashin bounds.
• For effective moduli (vol. frac. < 75%) use third-order approximation (Torquato 1998).
• For effective moduli (vol. frac. > 75%) use numerical approximations on microstructures containing circular particles (discretize using a regular grid).
• If statistics of effective properties are required, the Recursive Cell Method can be used (with an appropriate renormalization cluster size).
• The Generalized Method of Cells is inadequate for high volume fraction particulate composites.
• Modeling of particle-binder debonding is needed to predict effective properties that are closer to PBXs.
Future Work

• **Question 1.** Can the initial moduli of the components of a viscoelastic composite be used to predict the initial moduli of the composite at various strain rates/temperatures?  
  • *Mock glass/estane composites are being simulated.*

• **Question 2.** Can we quantify the amount of stress bridging in a PBX? Can we quantify the amount of initial particle-binder dewetting/debonding in a PBX?  
  • *Percolation theory approaches can be used to determine the stress percolation limit.*  
  • *Simulations of dewetting in glass/estane composites.*
Acknowledgements

• University of Utah Center for the Simulation of Accidental Fires and Explosions (C-SAFE).
• Dr. Mel Baer, Sandia National Laboratories.
• Dr. Jerry Dick, Los Alamos National Laboratories.
• Dr. Carl Cady, Los Alamos National Laboratories.
• Prof. Graeme Milton, Dept. of Mathematics, University of Utah.