

Micromechanical Modeling of High Energy Composites

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Abstract

High-energy polymer-binded explosives (PBXs) are composed of high-energy crystalline particles and a rubbery binder. The volume fraction of particles is approximately 92 percent. The high-energy particles have a Young's modulus that is three orders of magnitude higher than that of the binder. Efforts are currently underway to model these materials based on material property inputs from molecular dynamics simulations. Micromechanical studies using the generalized method of cells (GMC) show that the position and size of the particles have a significant effect on the homogenized mechanical properties of the composite. Stress bridging is also shown to affect the mechanical properties significantly. Micromechanical modeling is validated using experimental data for PBX-9501.

Introduction

Many high-energy composites have a very high volume fraction of high-energy particles that are consolidated using an inert binder. PBX 9501 is a composite of HMX (High Melting Explosive) crystals and a binder that is a mixture of Estane 5703 and bis-dinitropropylacetal / formal (BDNPA/F). The volume fraction of HMX in the composite is 92% (95% by weight) and that of the binder is around 7% (5% by weight). The particles have a bimodal size distribution with sizes varying from 300 microns to 10 microns. The porosity of the composite is around 1%. The HMX particles are randomly distributed in the composite. HMX crystals are linear elastic at room temperature while the binder is viscoelastic. The maximum shear modulus of HMX is around 5.8 GPa and the minimum bulk modulus is around 14.3 GPa. The binder has a Young's modulus of approximately 10 MPa. Pressing of the composite introduces microcracks in the crystals and debonds between the crystals and the binder. The HMX crystals are often in contact and thus stress bridging effects can be significant. PBX-9501 has been chosen for micromechanical investigation in this study due to the availability of experimental mechanical property data. [1,2].

The generalized method of cells (GMC) [3,4] is used to model high energy composites. This micromechanical model provides mechanical properties of the composite based on the properties of the constituent materials. Subcell continuity and equilibrium are satisfied in an average sense. This modeling method is extremely computationally efficient and yet allows the microstructure to be modeled explicitly. This paper focuses on predicting the effect of particle position and size on the effective mechanical properties of a class of high-energy composites.

Approach

To model high energy composites using the GMC approach, a representative volume element (RVE) is assumed to exist within the composite material. The known size distribution of the particles in the composite is used to generate a random distribution of particles within the RVE. Particles are approximated as circles in two dimensions (2-D) and spheres in three dimensions (3-D) as shown in Figure 1.

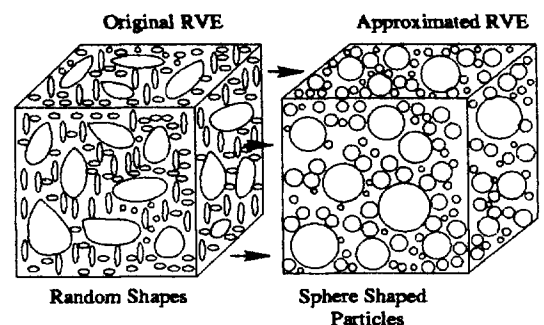


Figure 1. RVE with random particle distribution in 3-D.

A two-step homogenization scheme is used to obtain the effective mechanical properties for the high energy composite material. Using the GMC approach, a structured rectangular grid is overlaid on the RVE as shown in Figure 2, defining an array of subcells within the RVE. Note that each subcell in the RVE intersects many particles.

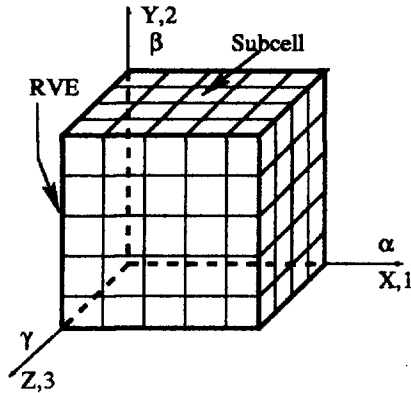


Figure 2. Discretization of RVE.

In the first homogenization step, the cumulative volume fraction of particles and fractions of particles that lie within each subcell are calculated. Next, this distribution of particles is replaced with a single, centrally located particle producing the same particle volume fraction within the subcell. A $2 \times 2 \times 2$ (8 subcell) GMC analysis is performed for this single particle subcell as illustrated in Figure 3. This GMC analysis produces the effective isotropic mechanical properties for the subcell based on the particle volume fraction.

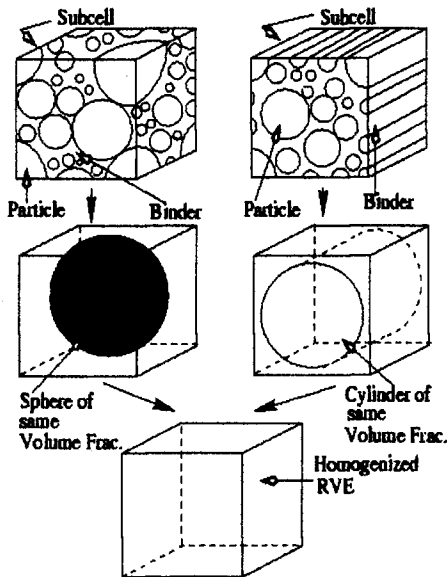


Figure 3. Subcell homogenization.

This homogenization process is repeated for each subcell within the RVE, effectively producing an array of subcells with different isotropic properties. Thus, this first homogenization step transforms an irregular distribution of particles with the same material properties into a regular distribution of subcells with different properties.

A second GMC homogenization step is performed for the entire RVE. This homogenization produces the desired set of material properties that can be used in a structural simulation. This two-step homogenization approach has been validated using finite element modeling.

Approach

This GMC based micromechanics approach was used to determine the high-energy composite modulus ratio (E_2/E_{binder}) versus the volume fraction of particles for a particle to binder modulus ratio of 100. Results of these predictions are shown in Figure 4. A rapid increase in the composite modulus occurs beyond 70% volume fraction. It can be seen that the 2×2 GMC underestimates the composite modulus.

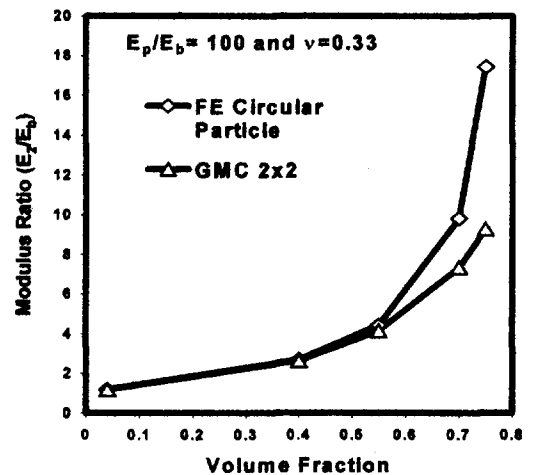


Figure 4. Comparison between 2×2 GMC and finite element analysis.

To investigate the effects of particle distributions, seven different distributions were modeled using 2-D finite element analysis and 2-D GMC analysis. A sample particle distribution is shown in Figure 5. All seven distributions had a 90% particle volume fraction. Of particular interest was the predicted modulus of elasticity for the seven particle distributions as predicted by the two methods. Results of this investigation are

shown in Figure 6. The GMC modeling approach is found to accurately produce the moduli values obtained using finite element analysis for all distributions modeled.

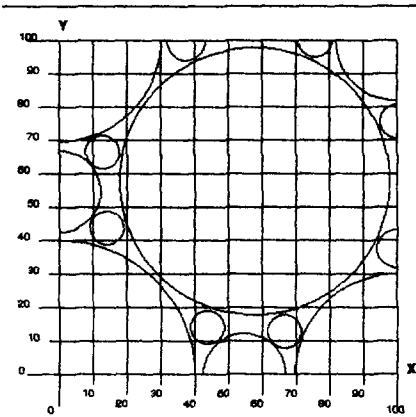


Figure 5. Representative particle distribution investigated.

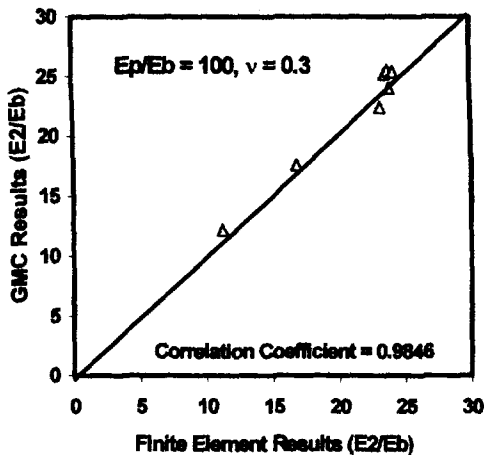


Figure 6. Correlation between GMC and finite element analysis.

Of particular interest are the differences in moduli predicted for the seven particle distributions investigated. Further investigation has shown that these differences increase as the modulus difference between the particles E_p and the binder E_b increases. Additionally, stress bridging (particle-to-particle contact) has been shown to increase the composite modulus to almost 70% of the particle modulus using finite element modeling. Current research is focusing on an improved

homogenization scheme to be used in the first step of the GMC homogenization approach to account for stress bridging within a particular subcell.

Conclusions

A two-step homogenization approach was developed for use in a Generalized Method of Cells (GMC) micromechanics modeling approach for high energy composites. This GMC-based homogenization approach was used to predict the moduli of high volume fraction particulate composites with extreme modulus differences between the particles and binder. Comparisons with finite element analysis indicate that this GMC approach is well suited for determining the effective elastic properties of the composite. This modeling approach is currently being extended to include temperature dependency, the effects of stress bridging, micromechanical damage, and a viscoelastic binder.

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