Micromechanics Models for Plastic-Bonded High Explosives: Recent Developments

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A sound theoretical understanding must accompany experimental testing of any explosive material before one can have confidence that it will or will not detonate under a general state of dynamic mechanical loading [1]. A theoretical understanding will help ensure, for example, our ability to safely handle explosives. Our aim is to develop a theory that can aid in our prediction of the mechanical response behavior of an explosive as it is loaded over a wide range of applied stress and temperature states. Because the chemical kinetics depends on the thermal state, which is often coupled to the mechanical state, (the best known example being hot spot generation) the present investigation is also intended to be our first step to address the relationship between loading and chemical reaction in explosives.

There are many advantages to using a micromechanics analysis to model the explosive PBX-9501, and here we enumerate five of them. First, considerable information on the microstructure and thermal-mechanical properties are required for a micromechanics analysis. As a consequence, a micromechanics theory is likely to be more reliable than corresponding theories constructed from less information, for example theories that use only the results from integrated experiments. Second, local stresses and strains are determined in a micromechanics analysis. As will become clear, in our model these local stresses and strains are calculated for the coarse HMX explosive grains, the fine HMX grains, and the plastic binder. Consequently, properties such as localized heating can be calculated independently for these three constituents. Third, material properties can be tailored to the individual constituents. For example, one can develop a theory such that microcrack brittle fracture occurs in the HMX grains while the elastomeric viscoelastic properties are specific to the polymeric binder. Similarly, interfacial debonding between the HMX grains and the binder can be directly incorporated into the theory in an unambiguous way. Fourth, one would like to take advantage of the information gained from experiments done on the constituents. For example, it is expected that the plasticized Estane® binder is responsible for much of the strain rate and temperature dependence observed for PBX-9501. Experiments on the binder have been carried out over a wide range of temperatures and strain rates and this data, which can readily be used in a micromechanics theory, is difficult to use in an integrated continuum theory of the entire explosive. Fifth, having determined the constituent properties and gained confidence in the micromechanics model by comparing its predictions to experiments done on PBX-9501, one can then use our model to explore other volume concentrations of HMX and binder without the need for extensive further experimentation.

We wrote an Advanced Simulation and Computing (ASC) Program milestone report that covers the following topics: A hybrid micromechanics model is proposed for investigating the mechanical behavior of plastic bonded materials having two disparate grain sizes. In this report we discuss our hybrid model (Fig. 1) that uses the first-order Method of Cells (MOC) [2] to treat the coarse HMX grains with a Mori-Tanaka-based analysis used to treat the fine grain-binder mechanical response. The fine grains in this analysis are assumed to be spherical and uniformly distributed in the binder and have been named the dirty-binder (DB). The formal DB theory is presented in this report. While the hybrid MOC-DB model captures the average thermal-mechanical properties of PBX-9501, it is important to better understand the local fluctuations in the fields caused by the highly irregular microstructure. Direct Numerical Simulations (DNS), described in the report, attempt to model the details of the microstructure by using the finite element method (FEM) where the PBX microstructure is considered at the resolution of the fine grain-dirty binder mixture. Another approach for investigating the accuracy of the MOC-DB model is to allow for microstructural variations in conjunction with the MOC-DB analysis. This work is called statistical element sampling and has been applied to model plate impact. Methods are also described for obtaining FEM grids for the microstructure using various approaches including PBX-9501 micrographs. The HMX $\beta-\delta$ phase transition is modeled using our MOC-DB theory, appropriately generalized to include solid-solid phase transitions. The $\beta-\delta$ phase transformation in the explosive HMX has been postulated to be an important first step in the molecular decomposition of the HMX molecule [3] and is thought to be an important mechanism for the early stages of reaction. Finally, new stochastic micromechanics theories that will allow for much greater predictability are presented in the report.

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[1] P.W. Cooper, *Explosives Engineering* (Wiley-VCH, New York, 1996).
[2] J. Aboudi, "Studies in Applied Mechanics, Vol. 29," *Mechanics of Composite Materials: A Unified Micromechanical Approach* (Elsevier, Amsterdam, 1991).
[3] B.F. Henson, et al., *J. Chem. Phys.* **117**, 3780, 2002.

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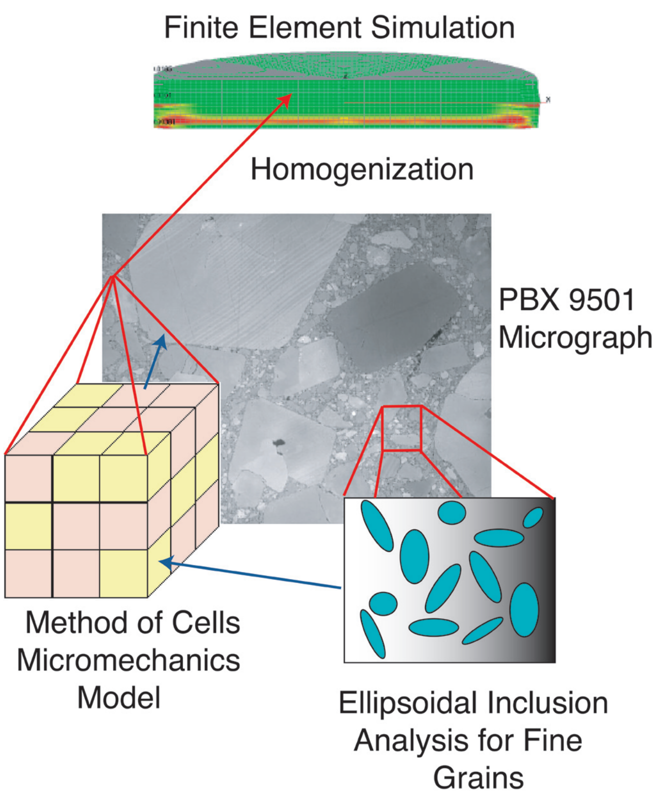

Fig. 1.
The method of cells dirty binder model.