Microstructure Effects on PBX Mechanical Response

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The mechanical response of plastic-bonded explosives (PBXs) is of interest in a variety of munitions and industrial applications. PBXs are composed of energetic grains embedded in a polymeric binder. The heterogeneity at this material scale localizes energy during deformation, resulting in damage nucleation sites and hot spots. These local events ultimately drive bulk material response, such as fracture/failure and deflagration/detonation. To develop predictive models, it is imperative to have a sound physical understanding of grain-scale material response and represent material-state heterogeneity in the models.

A fully 3-D characterization of material microstructure morphology may be obtained using x-ray microtomography. From a series of images collected as the sample is rotated, a 3-D image of the specimen is reconstructed. X-ray microtomography has been used to image the energetic material PBX-N109 [1]; an example grain morphology is depicted in Fig. 1.

Packings of spheres are common approximations to granular composite microstructures. These packings can be generated fairly easily, but they miss a distinguishing characteristic of PBXs, namely the irregularity of the grain shapes, and in particular the presence of corners that may cause regions of high local stress. An example is depicted in Fig. 1.

At Los Alamos National Laboratory, we performed computational experiments on various microstructures, and calculated bulk properties. These results are reported in Table 1 for both tomography data microstructures and spherical grains. "As-received" tomography data is labeled "raw." Image processing techniques were used to soften features and remove pixel-scale noise in tomography data and this case is label "smoothed." All cases give remarkably similar bulk properties.

It is concluded that grain shape may have very little effect on the initial bulk properties for an elastic, perfectly bonded mixture. Certainly, packed spheres provide an excellent surrogate for determining bulk properties. The grain volume fraction is the most important parameter by far. While somewhat surprising, the result is consistent with analyses using idealized microstructures. Good estimates of bulk properties (within 5%) may be obtained with surprisingly small RVEs (containing eight or fewer spheres).

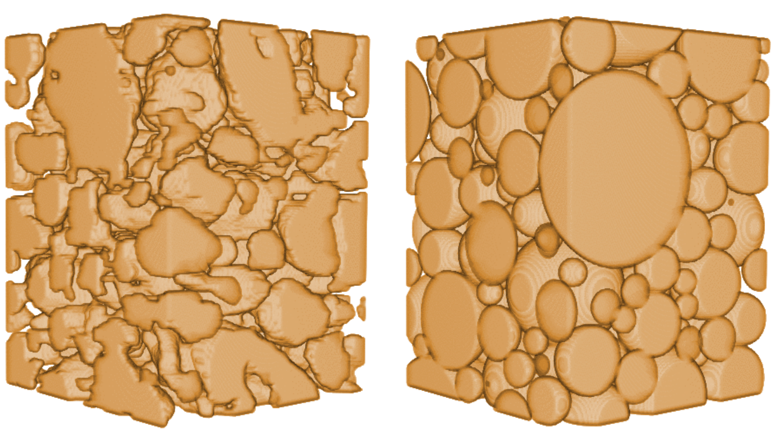

Fig. 1.
Examples of grain morphologies used in computations. On the left is x-ray microtomography data for PBX-N109, on the right a packing of spheres.

Histograms were used to compare material state for different microstructures and assess the importance of grain shape to the distribution of strain-state statistics. Histograms of strain state for the cases in Table 1 are displayed in Fig. 2.

Table 1. Comparison of Bulk Properties

Cases	Volume Fraction HMX	Bulk Modulus (GPa)	Shear Modulus (GPa)
Tomography (smoothed)	63.7%	9.61	3.79
Tomography (raw)	65.0%	9.65	3.80
Tomography (raw)	64.1%	9.61	3.79
Tomography (raw)	65.1%	9.65	3.80
Tomography (raw)	66.4%	9.66	3.80
Spheres	66.4%	9.67	3.80

These histograms are remarkably similar, again illustrating insensitivity to microstructural details for elastic, perfectly bonded mixtures. However, some differences may be seen in the main peak and the shoulder to its left. These features correspond to more compressive strain in the grains, and less in the binder, for packed-sphere microstructures. This difference is due to the microstructure. While in the tomography data each grain tends to be coated with dirty binder, in the case of the packed spheres, most spheres touch one another initially. This connected network of spheres provides an embedded load-bearing structure that carries slightly more load and shields the dirty binder.

The same data as Fig. 2 are replotted on a log scale in Fig. 3 to examine differences in the tails of the distributions. It is in the tails that the effect of irregular grain corners might be expected to become apparent, appearing as an increase in the frequency of large strains. The tails of the distributions for the packed-sphere microstructure are clearly shifted slightly toward larger strains than the tomography microstructures. This is precisely the opposite of what would be expected based on grain shape alone. The shift is again due to the connected substructure of contacting spheres, and strain concentrations associated with contact mechanics. The binder coating on the grains in the tomography data pads grain contacts and reduces strain concentrations.

These considerations suggest enhanced sensitivity of the packed-sphere microstructure as one might expect simply from contact mechanics playing a large role. Some micrographs of PBXs suggest the larger grains are well coated with dirty binder in PBX-9501 [2], which should provide a desensitizing effect.

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[1] S. Lecume, et al., "Structure of Nitramines Crystal Defects Relation with Shock Sensitivity" in *Proceedings of the 35th International Conference of ICT* (Karlsruhe, Germany, 2004) pp. 2-1–2-4.
[2] B.E. Clements and E.M. Mas, *Model. Sim. Mat. Sci. Eng.* **12**, pp. 1–15 (2004).

Funding Acknowledgements
NNSA's Advanced Simulation and Computing (ASC), Materials and Physics Program; and Campaign 2, Dynamic Materials Properties.

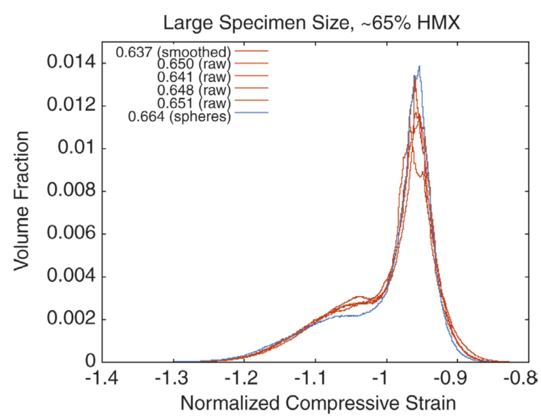

Fig. 2. *Strain-state histograms.*

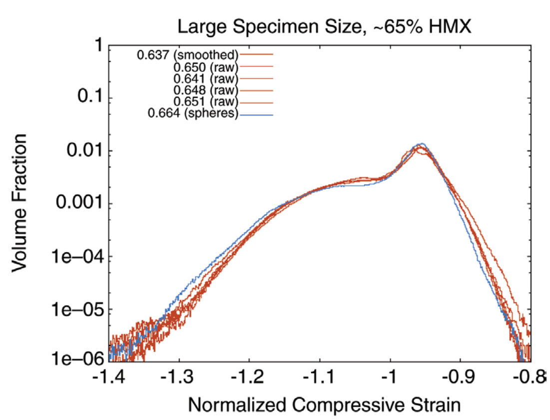

Fig. 3. *Strain-state histograms.*