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Coupling Grain Scale and Bulk Mechanical Response for PBXs using Numerical Simulations of Real Microstructures SCOTT BARDENHAGEN, ANDREW BRYDON, TODD WILLIAMS, Los Alamos National Laboratory, CHRISTELLE BOUTRY, SNPE Matériaux Energétiques — PBXs are complex composites geometrically (irregularly shaped grains vary greatly in size), and constitutively (grains are anisotropic, twin and fracture). Heterogeneity at the grain scale results in localized damage and the creation of hot spots. To develop accurate, quantitative and predictive models it is imperative to develop a sound physical understanding of the grain scale material response. Numerical simulation is a useful tool to further model development. Here an inherent advantage of a particle method in discretizing geometrically complex materials is exploited to import three-dimensional material configurations from x-ray microtomography data, i.e. "real" microstructures. Numerical simulations determine representative volume element size and generate statistics on grain scale strain heterogeneity. These statistics calibrate the Stochastic Transformation Field Analysis bulk constitutive model.

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