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Mesoscale microstructure-explicit simulations for predicting the ignition thresholds of polymer-bonded explosives[1] YAOCHI WEI, JU HWAN SHIN, CHRISTOPHER MILLER, MIN ZHOU, Georgia Institute of Technology — Two-dimensional (2D) and three-dimensional (3D), Lagrangian, microstructure-explicit simulations are carried out to systematically assess how microstructural heterogeneities affect the ignition behaviors of polymer-bonded explosives (PBXs). The analysis provides explicit account of the heterogeneous material microstructure and captures the effects of mechanical, thermal, and chemical processes up to and around the ignition in samples at scales up to tens of millimeters. The specific mechanisms considered include viscoelasticity, viscoplasticity, fracture, post-fracture contact, frictional heating, and heat conduction. The Henson chemical decomposition model is used to track the species during reaction. Ignition behaviors are studied for piston velocities ranging between 600 m/s - 1200 m/s (shock pressures of 4 - 11 GPa). Statistically equivalent microstructure sample sets (SEMSS) are generated and used, enabling a probabilistic characterization of the ignition thresholds. The effects of microstructural attributes, including size and morphology of grains and content and size distribution of voids on ignition are delineated.

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