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Prediction of Shock Initiation Thresholds and Ignition Probability of Polymer-Bonded Explosives using Mesoscale Simulations

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ABSTRACT

The design of new materials requires establishment of macroscopic measures of material performance as functions of microstructure. Traditionally, this process has been an empirical endeavor. An approach to computationally predict the probabilistic ignition thresholds of polymer-bonded explosives (PBXs) using mesoscale simulations is developed. The simulations explicitly account for microstructure, constituent properties, and interfacial responses and capture processes responsible for the development of hotspots and damage. The specific mechanisms tracked include viscoelasticity, viscoplasticity, fracture, post-fracture contact, frictional heating, and heat conduction. The probabilistic analysis uses sets of statistically similar microstructure samples to directly mimic relevant experiments for quantification of statistical variations of material behavior due to inherent material heterogeneities. The particular thresholds and ignition probabilities predicted are expressed in James type and Walker-Wasley type relations, leading to the establishment of explicit analytical expressions for the ignition probability as function of loading. Specifically, the ignition thresholds corresponding to any given level of ignition probability and ignition probability maps are predicted for PBX 9404 for the loading regime of U_p = 200 – 1200 m/s where U_p is the particle speed. The predicted results are in good agreement with available experimental measurements. A parametric study also shows that binder properties can significantly affect the macroscopic ignition behavior of PBXs. The capability to computationally predict the macroscopic engineering material response relations out of material microstructures and basic constituent and interfacial properties lends itself to the design of new materials as well as the analysis of existing materials.

Keywords: PBX; Energetic material; Ignition threshold; Binder properties; Energy dissipation

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