

Abstract Submitted
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Mesoscale Simulations of Reaction Initiation and Growth in HE Composites using PBRB model¹ SUNIL DWIVEDI, School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA 30332, JOHN BRENNAN, U.S. Army Research Laboratory, Aberdeen Proving Ground, MD 21005, YASUYUKI HORIE, (Retired) Air Force Research Laboratory, Eglin AFB, FL 32547 — Two-dimensional (2D) finite element based mesoscale simulation results are presented to predict reaction initiation and growth in high energy (HE) composites using the physics based reactive urn (PBRB) model. The HE composites are modeled as an ensemble of grains with statistically-distributed second phase particles. Their shock response is modeled with elastic-inelastic deformation coupled with the PBRB equation-of-state model. The inter-grain response is described by the contact-cohesive model that allows grain boundary failure and creation of free surface with friction characteristics during compressive shock loading. The heat generation due to the non-linear elastic, inelastic, cohesive, and friction energy dissipation into pre-assumed statistically-distributed hot spots, surface sublimation, and gas phase reaction are described as coupled mechanisms by the PBRB model yielding the mean stress as a function of the reaction at any given time. The simulations predict the time and run to detonation with reasonable agreement with data. The relative merits of 1D hot spot idealization, embodied in the PBRB model, for generic mesoscale simulations will be discussed.

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