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Mechanics driven Chemical Reactions in Structural Energetic Materials. VINDHYA NARAYANAN, DEREK REDDING, Georgia Institue of Technology, SATHYA HANAGUD, Georgia Institute of Technology — Fundamental mechanisms that are responsible for shock-initiation of chemical reactions, are dominated by non-equilibrium processes including changes in reactant particle configurations caused by plastic deformation or by fracture, mixing of constituents in and around the voids, and rapid increases in temperature from mechanical work. Mechanics driven chemical reactions occur in structural energetic mixtures, during the high-pressure shock state in time scales of mechanical equilibration. These shock-induced reactions represent a unique class of chemical behavior that is not clearly understood. To understand the observed results a model is presented, in this paper, in a hybrid non-equilibrium thermodynamic framework that combines the concepts of internal variables and thermodynamic fluxes. The governing system of partial differential equations is formulated in the framework of extended irreversible thermodynamics. This represents the intimate mixing of the reactants, which is important in the reaction initiation process. The model is developed to distinguish induced or assisted chemical reactions with uniformly blended mixture theories. A yield condition that represents an increase of yield stress behind the shock front is considered. A method of determining the transition states and paths to reach the transition state due to plastic work and void collapse are also discussed. The formulated partial differential equations are integrated and results are discussed.

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