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Mechanistic Modeling of Shock to Detonation Transition in High Explosives at Mesoscale[1] AHMED HAMED, MARISOL KOSLOWSKI, Purdue University — Understanding energetic materials response to different types of stimuli is of critical importance for efficient performance and safety of their applications. In this regard, developing high fidelity models for shock to detonation transition is a key challenge. Reliable prediction of this phenomenon dictates capturing the heterogeneous nature of hot-spot formation and initiation as well as the interplay between the underpinning mechanisms—spanning different time- and length-scales. We present a novel mesoscale model for the shock to detonation transition in high explosives. The model solves reactive flow equations in Lagrangian formulation with explicit consideration of the underlying mechanical, chemical, and thermal processes. Supplementary models are used to account for dissipative heating mechanisms, namely, viscoplasticity, fracture, and thermoelastic effects. For thermodynamic consistency, energy conservation equation incorporates two distinct equations of state for solid reactant and gaseous products to account for the two modes of energy transport. Statistical approach is sought for microstructure features representation. Informed by a separate investigation, hot spots critical temperature is size-dependent. All model parameters are calibrated by MD simulations.

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