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Mirrored continuum and molecular scale simulations of the ignition of gamma phase RDX[1] D. SCOTT STEWART, SANTANU CHAUDHURI, KAUSHIK JOSHI, KIABEK LEE, University of Illinois, Urbana, IL — We consider the ignition of a high-pressure gamma-phase of an explosive crystal of RDX which forms during overdriven shock initiation. Molecular dynamics (MD), with first-principles based or reactive force field based molecular potentials, provides a description of the chemistry as an extremely complex reaction network. The results of the molecular simulation is analyzed by sorting molecular product fragments into high and low molecular groups, to represent identifiable components that can be interpreted by a continuum model. A continuum model based on a Gibbs formulation, that has a single temperature and stress state for the mixture is used to represent the same RDX material and its chemistry. Each component in the continuum model has a corresponding Gibbs continuum potential, that are in turn inferred from molecular MD informed equation of state libraries such as CHEETAH, or are directly simulated by Monte Carlo MD simulations. Information about transport, kinetic rates and diffusion are derived from the MD simulation and the growth of a reactive hot spot in the RDX is studied with both simulations that mirror the other results to provide an essential, continuum/atomistic link.

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