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Shock and Laser Induced Non-Equilibrium Chemistry in Molecular Energetics MITCHELL WOOD, MATHEW CHERUKARA, Materials Engineering, Purdue University, EDWARD KOBER, Theoretical Division, Los Alamos National Lab, ALEJANDRO STRACHAN, Materials Engineering, Purdue University — In this study, we have used large scale reactive molecular dynamics (MD) simulations to study how contrasting initiation mechanisms from either shock or electromagnetic insults compare to traditional thermal initiation. We will show how insults of equal strength but different character can yield vastly different reaction profiles and thus the evolution of hot-spots. For shocked RDX (U_p = 2km/s), we find that the collapse of a cylindrical 40 nm diameter pore leads to a significant amount of non-equilibrium reactions followed by the formation of a sustained deflagration wave. In contrast, a hot spot that is seeded into a statically compressed crystal with matching size and temperature will quench over the same timescale, highlighting the importance of insult type. Furthermore, MD simulations of electromagnetic insults coupled to intramolecular vibrations have shown, in some cases, mode specific initial chemistry and altered kinetics of the subsequent decomposition. By leveraging spectroscopic and chemical information gathered in our MD simulations, we have been able to identify and track non-equilibrium vibrational states of these materials and correlate them to these observed changes. Implications of insult dependent reactivity and non-equilibrium chemistry will be discussed.

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