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Molecular dynamics simulation of shock-induced chemical, mechanical and thermal processes in nanostructured metastable composites[1]
SHIJIN ZHAO, TIMOTHY GERMANN, ALEJANDRO STRACHAN, Los Alamos National Laboratory — Nanostructured metastable intermolecular composites (MICs) are a new class of energetic materials with a wide range of applications. MICs can be made to react to form a more stable compound while releasing a large amount of energy and exhibit several unique properties, for example, extremely fast propagation of the chemical reactions when the initial components are intermixed at the nanometer scales. The fundamental molecular-level mechanisms that govern the unique properties of these materials are to a large extent unknown. We use molecular dynamics to characterize the chemical and mechanical response of MICs induced by shock and thermal loading. We use detailed analysis methods such as the short-range topological analysis to characterize the atomic level processes responsible for the initiation and propagation of the chemical reactions. Our simulations are designed to characterize the role of composition and nanostructure on the initiation and subsequent ultra-fast propagation of chemical reactions in nanostructured MICs as well as their mechanical and thermal properties.

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