

Abstract Submitted
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Reactive MD simulations of anisotropic response of PETN under high-rate shear deformation¹ XU PENG, SERGEY ZYBIN, California Institute of Technology, AIDAN P. THOMPSON, Sandia National Lab, WILLIAM A. GODDARD, California Institute of Technology — Several experiments have indicated that the shock sensitivity of single crystal energetic materials can depend on the crystallographic direction. We develop a compress-and-shear modeling approach to study the mechanisms of anisotropic shock sensitivity using the ReaxFF reactive molecular dynamics. ReaxFF is a first-principles based force field capable to reproduce the quantum chemical energies of the reactants, products, intermediates and transition states with functional forms suitable for large-scale molecular dynamics simulations of chemical reactions under extreme conditions. In this presentation we will discuss the results of high-rate shear simulations of uniaxially compressed PETN. We found noticeable differences in the physical and chemical responses of PETN for different combinations of the slip system and compression direction. The simulation results agree well with the experimental shock-initiation sensitivity data and Dick's steric hindrance theory.

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