

Public Abstract

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Title:Molecular Dynamics Simulations of the Shock Response of the Energetic Materials Pentaerythritol Tetranitrate and Hexahydro-1,3,5-Trinitro-1,3,5-s-Triazine

Energetic materials are the key active ingredients in explosive formulations. Understanding the response of energetic materials is vital for the design of safe and reliable explosives. It is a challenge to experimentally study the initial events that lead to detonation in these materials. Classical mechanics based computer simulations are a useful method for the study of these initial chemical and physical events. This research focuses on the shock response of two energetic materials: pentaerythritol tetranitrate (PETN) and hexahydro-1,3,5-trinitro-1,3,5-s-triazine (RDX). Computer simulations were used to study how the shock response of single crystals of PETN varies based on the orientation of the crystal relative to the shock wave. Thermo-mechanical properties were calculated for the shocks along two different orientations to quantify the difference in response. In RDX, the potential of voids to act as nucleation sites for detonation was studied. The magnitude of energy localization from void collapse as function of shock strength was studied for three different shock strengths.