MOLECULAR DYNAMICS SIMULATIONS OF THE SHOCK RESPONSE OF THE ENERGETIC MATERIALS PENTAERYTHRITOL TETRANITRATE AND HEXAHYDRO-1,3,5-TRINITRO-1,3,5-S-TRIAZINE

Reilly M Eason

Dr. Thomas D. Sewell, Dissertation Supervisor

ABSTRACT

Energetic materials are the key active ingredients in explosive formulations. They possess large amounts of stored chemical energy along with the ability to rapidly release this energy. The initial chemical and physical events leading to detonation of energetic materials are difficult to study through purely experimental methods due to the small spatial and temporal scales these events occur on. Molecular dynamics is a classical mechanics based computer simulation methodology that can study these small space and time scales. This research focuses on the use of molecular dynamics to study the shock response of two energetic materials: PETN and RDX. The orientation dependent shock response of PETN was quantified by calculating changes in structural and thermal properties including: relative center-of-mass displacements, temperatures, and changes in dihedral angle distributions. Shock-induced collapse of voids as a potential source of hot spots was studied in RDX. The magnitude of energy localization resulting from void collapse was characterized by calculating temperatures and pressures.