8th. World Congress on Computational Mechanics (WCCM8)
5th. European Congress on Computational Methods in Applied Sciences and Engineering (ECCOMAS 2008)
June 30 – July 5, 2008
Venice, Italy

INELASTIC DEFORMATION IN SHOCK LOADED ENERGETIC MOLECULAR CRYSTALS

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Key Words: *Shockwave Loading, Inelastic Deformation Mechanisms, Polyatomic Molecular Crystals, Energetic Materials, Molecular Dynamics.*

ABSTRACT

We have recently undertaken large-scale non-equilibrium molecular dynamics studies to aid our understanding of dynamical processes in the cyclic nitramine high explosives HMX and RDX, in particular the inelastic, anisotropic response of crystals of those materials subjected to quasi-static and shock loading [1, 2]. The same force field used by Sewell and co-workers [3] in preceding simulations of HMX equilibrium properties is employed for the present research. The overarching goal of this work is to provide information that can serve as a foundation in basic science for the formulation of improved mesoscale constitutive models for the constituent materials in selected energetic formulations. The medium-term scientific challenge that stands as a prerequisite to this larger objective is to carefully identify, characterize, and quantify the dominant mechanisms of localization and dissipation in such materials, under a variety of prescribed quasi-static and dynamic loading scenarios that lead to inelastic deformation of the crystals. The focus of the present talk will be the shock response of structurally perfect, but properly thermalized, HMX and RDX crystal; and shock localization in RDX crystals containing 20 nm defects (voids).

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