MAR12-2011-020022

Abstract for an Invited Paper
for the MAR12 Meeting of
the American Physical Society

Atomic-Scale Theoretical Studies of Energy Transfer, Inelastic Deformation, and Void Collapse in Molecular Crystals and Polymers

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Recent atomic-scale theoretical studies of shock waves in polyatomic molecular crystals and polymers will be presented, with an emphasis on the results and interpretation of molecular dynamics simulations for pentaerythritol tetranitrate (PETN), hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX), nitromethane, and poly(butadiene) (PBD). The effects of structural and mechanical anisotropy on the material response are of particular interest. Among the topics to be discussed are orientation dependent energy transfer pathways and inelastic deformation mechanisms subsequent to shock wave passage in initially defect-free nitromethane and PETN crystals, shock-induced collapse of variously shaped voids in crystalline RDX, and details of shock wave propagation and energy localization in bulk PBD and at the PBD/RDX interface.