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Theoretical studies of shock-induced plastic deformation and phase transformations in RDX MARC CAWKWELL, THOMAS SEWELL, Theoretical Division, Los Alamos National Laboratory — The relationships between shock-induced plastic deformation and initiation sensitivity have been studied in RDX using MD simulations. Homogeneous defect nucleation in (100), (111) and (210) oriented single crystals has been studied under shock loading at particle velocities of 420, 630 and 840 m/s. Deformation by shear-bands was seen in shocks parallel to [100] at particle velocities $\geq$ 630 m/s. No evidence was found for homogeneous nucleation of defects such as dislocations or shear-bands in shocks normal to (111) and (210) at any particle velocity. These results are consistent with the steric hindrance model for initiation sensitivity and flyer plate studies of oriented RDX single crystals. The collapse of 20 nm diameter cylindrical voids was studied under the same conditions mentioned above. A variety of anisotropic material responses occur, along with significant increases in intramolecular temperatures, as the voids collapsed. Also, a previously unknown shock-induced phase transformation was observed during shocks normal to (210). This phase transformation occurs homogeneously for shocks parallel to [010] at particle velocities greater than 1 km/s. The Hugoniot for shock loading in this direction has been calculated for a defect free crystal, allowing for direct experimental assessment of this prediction.
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