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Shock Compression Calculation of RDX and PETN Molecular Crystals Using the Hugoniostat Method[1] ALEXANDER SELEZENEV, ALEXEY ALEYNIKOV, NIKOLAY GANCHUK, PAVEL ERMAKOV, SERGEY GANCHUK, Sarov Laboratories, JOHN AIDUN, AIDAN THOMPSON, Sandia National Laboratories — Parameters of uniaxial shock compression were calculated for RDX molecular crystal in crystallographic direction [100] and for PETN in directions [100], [110], [001] by Hugoniostat method using the non-reactive interatomic force field [G. D. Smith and co-workers, J. Phys. Chem. B 112 734 (2008)]. P-V, D-Up, T-P and T-Up dependences have been obtained for each crystallographic direction on the Hugoniot curve. Pressure and degree of compression were obtained for which the transformation of the molecular crystal lattice takes place at MD simulation of uniaxial shock compression. The structural transformation of the RDX crystal lattice was identified at 25 GPa pressure and 0.66 compression ratio for simulation of uniaxial shock compression in [100] direction. The structural transformation of the PETN crystal lattice was identified at 8-12 GPa and compression ratio of 0.80-0.73 for MD simulation of uniaxial shock compression in [110] direction.

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