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Polymorphism and Decomposition of HE Single Crystals: Insights from Static and Shock Compression Experiments

ZBIGNIEW DREGER, Washington State University

Understanding the reactive behavior of high explosive (HE) crystals at thermo-mechanical conditions generated by shock-waves is an important step toward understanding shock wave initiation of these crystals. Despite the significant differences in time scales and loading rates, static high pressure and high temperature (HP-HT) experiments can provide key results regarding structural and chemical processes in HE crystals at pressures and temperatures relevant to shock initiation. Here, we review recent progress in utilizing optical spectroscopy to understand molecular processes in HE crystals at static HP-HT conditions to gain insight into their shock initiation mechanisms. The relevant results obtained from static studies up to 20 GPa and 700 K on polymorphism, decomposition and phase diagrams will be presented for selected HE crystals: primarily for RDX and PETN, and initial results on DADNE. The significance of the stress state and the use of single crystals in these processes will be highlighted. Finally, we demonstrate that the static HP-HT results in conjunction with shock-wave experiments provide an important approach to elucidate processes related to the initiation of shocked HE crystals, including polymorphic transitions, conformational changes, identification of crystal phases at decomposition, and mechanisms governing shock induced decomposition. Work was supported by DOE/NNSA and ONR/MURI, and carried out in collaboration with Y. M. Gupta.