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Ultrafast Spectroscopic Studies of Vibrational Energy Transfer in Energetic Materials NEIL COLE-FILIPIAK, Sandia National Laboratories California, MICHAEL MARQUEZ, ROBERT KNEPPER, ROBERT HARMON, PAUL SCHRADER, MITCHELL WOOD, KRUPA RAMASESHA, Sandia National Laboratories — Shock-induced detonation is a key property of energetic materials (EM) that remains poorly understood. We are developing novel ultrafast laser spectroscopy techniques to test one mechanism of shock-initiation in EM, the "thermal" mechanism, where shock excitation of lattice phonon modes is hypothesized to transfer energy to intramolecular vibrations resulting in breaking of chemical bonds and reaction. Using ultrafast pump-probe spectroscopy, we are studying vibrational energy transfer from phonon modes to intramolecular vibrations (phonon up-pumping), as well as from intramolecular vibrations to phonon modes (vibrational cooling) that competes with phonon up-pumping. Through combinations of plasma-generated supercontinuum infrared (IR; 3-15 um), tunable near infrared (1.2-2.6 um), and terahertz (THz; 100-1000 um) pulses in pump-probe spectroscopy, we explore the energy transfer processes on a sub-picosecond time scale. Theoretical work is being performed in parallel using a combination of Density Functional Theory and Molecular Dynamics Simulations to elucidate vibrational energy transfer pathways and lifetimes in EM. Here we highlight the progress to date, including the spectral and temporal characteristics of the IR and THz sources as well as preliminary results on EM.

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