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Pressure, temperature, and orientation dependence of the thermal conductivity of α- and γ-RDX ROMAIN PERRIOT, MARC CAWKWELL, JOHN LAZARZ, SHAWN MCGRANE, KYLE RAMOS, Los Alamos National Laboratory — Thermal conductivity is one the important component to devise a mesoscale model of high explosives (HE) response, notably to investigate accident scenario and ignition under weak stimuli. We present results from molecular dynamics (MD) simulations in RDX (1,3,5-trinitro-1,3,5-triazinane), using the Muller-Plathe, or *reverse* non-equilibrium molecular dynamics (rNEMD), method to determine the orientation, pressure, and temperature dependence of the thermal conductivity. We find that α-RDX exhibits anisotropy between the (100) and (001) directions, and a monotonic decreasing behavior between 225 and 400 K at zero pressure. Increasing pressure also leads to a monotonic response, this case resulting in an increase of the thermal conductivity. Simulations performed in the γ-phase (above 3 GPa), show a similar response between the (100) and (001) directions, suggesting an isotropic response of γ-RDX. Results are compared to experiments performed at LANL.

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