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Nanoscale Heat Conduction in Crystalline Solids JOEL CHRISTENSON, RONALD PHILLIPS, None — Heat conduction in crystalline solids occurs through the motion of molecular-scale vibrations, or phonons. In continuum scale problems, there are sufficient phonon-phonon interactions for local equilibrium to be established, and heat conduction is accurately described by Fourier's law. However, at length scales comparable to the phonon mean free path, Fourier's law becomes inaccurate, and more fundamental descriptions of heat transfer are required. We are investigating the viability of the phonon Boltzmann Transport Equation (BTE) to describe heat conduction in nanoscale simulations of the high-explosive material β-HMX. By using a combination of numerical and analytic solutions of the BTE, we demonstrate the existence of physical behavior that is not qualitatively captured by the classical Fourier's law in the nanoscale regime. The results are interpreted in terms of continuum-scale simulations of shock-induced collapse of air-filled pores in β-HMX, which is believed to be a precursory step towards complete detonation of the material.

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None

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