Public Abstract
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Title:Anisotropic Energy Transport Properties of1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)

Safety and reliability assessments for high explosives such as 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) are often based on engineering models that depend on accurate determinations of energy transport properties. These properties have yet to be determined experimentally for single crystals of TATB and related explosives, owing in large part to brittleness and difficulties in growing large, high-quality specimens. Many crystalline explosives exhibit low symmetry and complicated packing structures, which lead to significant directionality (anisotropy) in their physical properties. TATB is an extreme case as it belongs to the lowest crystal symmetry system and exhibits a layered structure similar to graphite that is more anisotropic than most other organic materials. We use atomistic simulations (mainly molecular dynamics) to gain fundamental understanding of the effects of anisotropy in TATB on energy transport processes and to provide specific information for use in mesoscale and macroscale engineering models. Atomistic simulations also yield important information on the sensitivity and limitations of these engineering models. The thermal conductivity of TATB was determined as a function of temperature, pressure, and density and is predicted to vary by as much as 70% depending on conduction direction in the crystal. We also report several methods for atomic simulations that remove significant barriers to studies for a broad class of technologically relevant materials beyond explosives including pharmaceuticals, organic semiconductors, and low-dimensional nanostructures.