Anisotropic Energy Transport Properties of
1,3,5-Triamino-2,4,6-Trinitrobenzene (TATB)

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Abstract

Anisotropic energy transport properties were determined theoretically for crystals of the insensitive explosive 1,3,5-triamino-2,4,6-trinitrobenzene (TATB) using molecular dynamics simulations. Determination of these properties is necessary to predict and understand processes such as shock response and hot spot formation/relaxation and is also important for accurate parameterization of engineering models. Many properties of TATB exhibit significant anisotropy, which is thought to be due to the triclinic, graphitic-like layered packing structure. The thermal conductivity was determined as a function of temperature, pressure, and defect density; conduction within the layers is approximately 70% greater than conduction between the layers. Hot spot relaxation simulations were compared with and fit to solutions for the 1D heat equation to assess the validity of using continuum models to describe heat transport in TATB on nanometer length scales. A dissipative particle dynamics at constant energy coarse-grained model was developed for TATB and applied to micron-scale shock simulations. The predicted shock response is shown to be highly sensitive to a model parameter controlling energy transport kinetics, underscoring the need for a physics-based upscaling approach. A generalized crystal-cutting method was developed to construct 3D periodic simulation cells containing arbitrarily oriented single crystals and crystal-crystal interfaces for materials of arbitrary symmetry class. Strategies for non-uniform sampling of simulated transient phenomena were proposed that drastically reduce data storage costs.