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Adaptation of multiscale thermal modeling methods to general crystalline solids BRENT KRACZEK, PETER CHUNG, Computational and Informational Science Directorate, US Army Research Laboratory — From the nano- to micro-scale, phonons act as the primary mechanism for energy transport and storage in most nonmetalic, crystalline materials. While phonon properties are determined by interatomic interactions on the scale of the atomistic unit cell, phenomena and microstructures of interest are often at length and time scales that are too large for atomistic simulations. The phonon Boltzmann transport equation (pBTE) enables continuum-scale calculations that capture both atomistic- and continuum-scale thermal behavior, though so far pBTE-based methods have been limited primarily to silicon [1]. We have developed a pBTE-based method for general crystaline materials with up to hundreds of atoms per unit cell. We demonstrate its applicability in silica (9-atom unit cell) and RDX (168-atom unit cell), though presently limited to one dimension in k-space. We discuss the main challenges when moving to larger unit cells, including the automated untangling of phonon dispersion data, discretization of phonon modes and the treatment of high energy modes, including the omission and/or lumping of modes and the use of reservoir modes.

[1] Chunjian Ni and J. Murthy, in *11th Intersociety Conference on Thermal and Thermomechanical Phenomena in Electronic Systems, ITHERM*, 2008, 1097

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