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A Comparative Study of Ab-Initio Thermal Conductivity Approaches: The Case of Cubic Boron Nitride SAIKAT MUKHOPADHYAY, Cornell University, LUCAS LINDSAY, Naval Research Laboratory, DAVID BROIDO, Boston College, DEREK STEWART, Cornell University — Given its high strength and large thermal conductivity, cubic boron nitride (cBN) provides an important complement to diamond films for heat spreading applications. However, cBN, in contrast to diamond, is a polar material with significant LO-TO splitting in the phonon dispersion. In this talk, we examine the lattice thermal conductivity of cBN using several approaches based on first principles calculations. These approaches include: (1) an analytic modified Callaway-Debye model that relies on parameters from ab-initio harmonic force constants, (2) a fully self-consistent calculation of the thermal conductivity that links an iterative solution of the phonon Boltzmann transport equation (BTE) with harmonic and anharmonic interatomic force constants. The force constants for the BTE are calculated using two approaches: density functional perturbation theory and a real-space supercell approach. We will compare the results from these approaches, highlight the role of normal phonon-phonon scattering, and also examine the impact of optical modes and LO-TO splitting. In addition, we will discuss how isotope scattering affects thermal conductivity and compare this to other boron nitride structures (hexagonal BN, BN sheets and BN nanotubes).

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