Thermal conductivity and isotope effect in wide bandgap semiconductors

LUCAS LINDSAY, THOMAS REINECKE, NRL, Washington, DC, ENRICO BELLOTTI, Electrical and Computer Engineering Department, Boston University, DAVID BROIDO, Department of Physics, Boston College — We have calculated the lattice thermal conductivity, $k$, of wurtzite InN, GaN, and AlN using an exact numerical solution of the phonon Boltzmann transport equation and \textit{ab initio} calculations of interatomic force constants. We find good agreement with experiment for the thermal conductivities around and above room temperature. The large frequency gap between the acoustic and the optic phonon branches in these materials limits anharmonic phonon scattering leading to large enhancements to $k$ with isotopic enrichment. We comment on the roles of various phonon scattering mechanisms on $k$ in these wide bandgap semiconductors.