Validity of the Isotropic Thermal Conductivity Assumption in Supercell Lattice Dynamics

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Superlattices [1] and nano phononic crystals [2,3] have attracted significant attention due to their low thermal conductivities and their potential application as thermoelectric materials. A widely used expression to calculate thermal conductivity, presented by Klemens [4] and expressed in terms of relaxation time models by Callaway and Holland [5,6], is derived from the Boltzmann transport equation. In its most general form, this expression involves a direct summation of the heat current contributions of individual phonons of all wavevectors and polarizations in the first Brillouin zone. In common practice, the expression is simplified by making an isotropic assumption that converts the summation over wavevector to an integral over wavevector magnitude. The isotropic expression has been applied to superlattices and phononic crystals, but its validity for different supercell sizes has not been studied. In this work, the isotropic and direct summation methods are used to calculate the thermal conductivities of bulk silicon, Si/Ge superlattices, and Si/Ge quantum dot superlattices(QDs). Group velocities for the calculations are obtained using lattice dynamics, and the calculations are validated against previous work. The results show differences between the two methods that increase substantially with supercell size. These differences arise because the vibrational modes neglected in the isotropic assumption method provide an increasingly important contribution to the thermal conductivity for larger supercells.

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