Predicting Phonon Properties of Silicon from First Principles Calculations

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To predict the thermal conductivity of a dielectric or insulating material requires the phonon frequencies and lifetimes. Typically, empirically derived potentials (such as Stillinger-Weber) are poor at predicting phonon properties. This poor behavior can be traced to the empirically derived harmonic and anharmonic force constants, which are necessary to calculate the phonon frequencies and lifetimes. To make accurate predictions, we use *Ab-Initio* calculations (specifically density functional theory calculations) and a supercell approach to calculate the harmonic and anharmonic force constants. The finite difference method is used to calculate the harmonic and cubic force constants, which is exact in the limit of small atomic displacements. A simplified algorithm is used to calculate the force constants, which is computationally more demanding than other algorithms but is conceptually much simpler. With the force constants, phonon perturbation theory can be used to extract the phonon lifetimes and compute the thermal conductivity under the relaxation time approximation. These results are compared to the Stillinger-Weber potential and *Ab-Initio* molecular dynamics simulations, which are very computationally demanding.