Appendix C

ISOTROPIC DISPERSION

We reduce computational cost by taking advantage of the cubic symmetry of Si and computing an isotropic equivalent dispersion in phonon frequency ω-space. To obtain this dispersion, we start with the full dispersion in three-dimensional wavevector k-space calculated using density functional theory (DFT) by J. Carrete and N. Mingo using ShengBTE (*88*, *89*) and Phonopy(*173*) from interatomic force constants obtained with VASP.(*91–94*) Phonon frequencies $\omega_{\mathbf{k}}$, group velocities $\mathbf{v}_{\mathbf{k}}$ and relaxation times $\tau_{\mathbf{k}}$ for the three acoustic and three optical branches are functions of wavevector $\mathbf{k} = (k_x, k_y, k_z)$. We discretize the phonon frequency between its minimum and maximum values into 101 bins with equal weight $\Delta\omega$. For each polarization, the density of states for a given frequency bin ω_i is obtained by counting the number of modes N that fall into that bin, given by

$$D(\omega_i) = \frac{N}{V\Delta\omega}, \tag{C.1}$$

where V is the volume of the First Brillouin zone, calculated from the maximum wavevectors given by the data.

We obtain average group velocities using $v^2_{avg}(\omega_i) = \langle \mathbf{v}^2(\omega_i) \rangle$, or the average of the square of group velocity for phonons in a specific frequency bin. In addition, we can compute the average of the square of the speed in a particular direction, *i.e.* $v^2_x(\omega_i) = \langle v^2_{k_x}(\omega_i) \rangle$. We find that $v^2_x(\omega_i) = v^2_y(\omega_i) = v^2_z(\omega_i) = \frac{1}{3} v^2_{avg}(\omega_i)$, which confirms that the dispersion of Si is isotropic on average.

To obtain the average relaxation time, we compute $\langle \tau(\omega_i)\mathbf{v}^2(\omega_i) \rangle / v^2_{avg}(\omega_i)$. This particular averaging is chosen to maintain the spectral thermal conductivity distribution of the full dispersion.

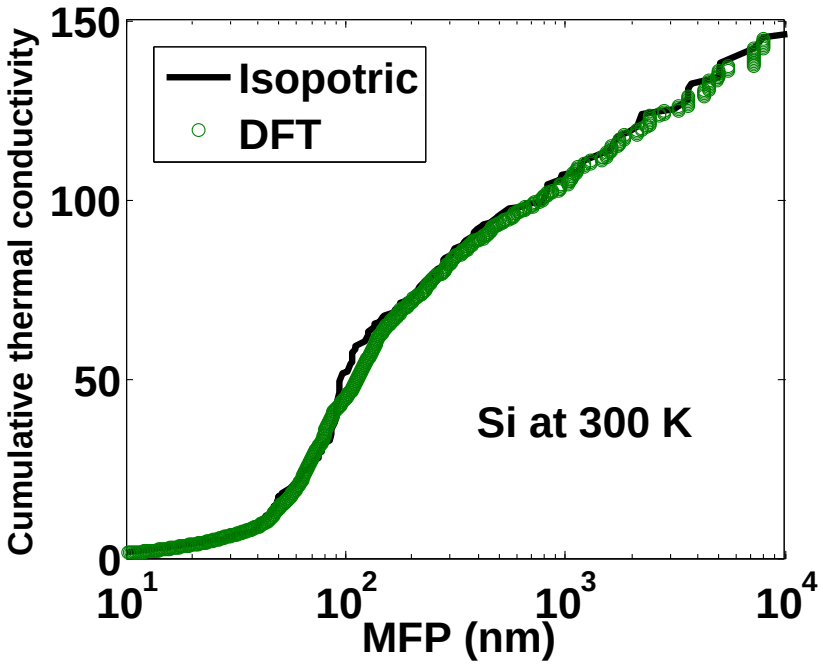

Figure C.1: Cumulative thermal conductivity as a function of phonon mean free path (MFP) for silicon at 300 K calculated by the isotropic equivalent dispersion (solid line) and the original DFT data (circles). The isotropic dispersion matches well with the ab-initio calculations as expected for a cubic crystal.

The final bulk thermal conductivity for this isotropic equivalent dispersion of silicon at 300 K is 155.0 W/m-K, very close to the original value of 155.7 W/m-K, and the cumulative thermal conductivity spectra are nearly identical, as shown in Fig. C.1.