Si Crystal Thermal Conductance in the TerraHertz Frequency Range by Molecular Dynamics

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The thermal conductivity of crystals submitted to AC temperature perturbations is commonly considered as independent from frequency as predicted by Fourier's Law. When the excitation frequency ω exceeds the reverse of the phonon mean relaxation time (10-100 GHz), the Boltzmann Equation including a first order approximation for the collision term leads to a ω^{-1} law for the frequency dependence of the thermal conductance. But no simple theoretical approach is able to provide the thermal behavior at heat carriers frequencies neighboring $\omega=2\pi x1.6xk_BT/h$ since mainly ω phonons are excited. We propose to use the Molecular Dynamics technique to directly compute the thermal conductance in Si crystals submitted to such perturbations. To perform this analysis, a thermal admittance is derived from the time autocorrelation of the equilibrium heat flux fluctuations. Results show that individual phonon eigen-modes are excited but the corresponding thermal conductance remains two orders of magnitude smaller compared to the one observed at lower frequencies.