Abstract Submitted
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Theoretical study of pressure dependence of lattice thermal conductivity in MgO[1] JIANJUN DONG, Auburn University, XIAOLI TANG, UCLA — We have recently developed a computation method that combines first-principles methods and transport theories to directly calculate lattice thermal conductivities for MgO at high pressure and high temperature conditions. Within the simple single-phonon-lifetime approximation, we estimate that the blueshifts in phonon frequencies lead to an increase of conductivity at high pressure at a rate of 1.3%GPa^{-1} (300K). A further calculation using quantum scattering theory shows that the anharmonicity-induced phonon scattering rate decreases at high pressure. The estimated pressure effect related to the phonon lifetime increase is comparable to that due to the frequency blueshifts. Our final calculation results will be discussed with comparison to available experiment data and the damped-harmonic-oscillator-phonon-gas model.

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