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Thermal Conductivity of Aluminum Oxide from First Principles[1]

MOSES NTAM, JIANJUN DONG, Auburn University, BIN XU, University of Texas at Arlignton — Alumina (Al_2O_3) is a well-known ceramic material. First-principles study of lattice thermal conductivity can assist our understanding in extreme conditions that are difficult to achieve experimentally, as well as analyze the fundamental difference between other materials. We combine density functional theory and the Peierls–Boltzmann transport theory to predict the temperature and pressure dependencies of lattice thermal conductivity of the corundum phase. We use a real space super cell method to extract second force constants and third order lattice anharmonicity tensors. These are then used to directly evaluate the phonon scattering rates due to lattice anharmonicity. Our preliminary results show that at a density of 4.23 g/cm^3 Al_2O_3 has thermal conductivities of 14.8Wm^{-1}K^{-1} at 300K and 5.31Wm^{-1}K^{-1} at 1000K. Moreover, we calculated the thermodynamic properties such as thermal expansion coefficient, bulk modulus and heat capacity, which are in excellent agreement with available measurements and previous theoretical calculations.

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