Phonon lifetime of MgO by inelastic x-scattering and ab initio calculations: Implications for thermal conductivity

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Abstract

Thermal conductivity is a fundamental physical parameter that largely controls the heat transfer in Earth's interior. Despite its importance, the thermal conductivity of mantle minerals is one of the least constrained properties at high pressure (P) and high temperature (T) as direct measurements at pertinent P-T conditions remains a technical challenge. Current geophysical models rely on the extrapolations of low P data and, increasingly so, on results from ab initio calculations. However, the validity and versatility of the various theoretical approaches used in literature remain to be tested again experiments. The direct measurements of vibrational and anharmonic properties such as phonon energy and linewidth as a function of P and T provide the most straightforward benchmark for the theoretical calculations as these are the key parameters entering the Boltzmann transport equation used to calculate lattice thermal conductivity.

Here we present the determination of phonon energies and phonon widths of single crystalline MgO at room temperature and 1220K by inelastic x-ray scattering and by density functional theory. The comparison of experimental and computational results allows assessing the theoretical phonon-phonon scattering coefficients and to estimate the relative weight of intrinsic and extrinsic phonon scattering mechanisms.

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