Ab initio lattice thermal conductivity of MgO using a full solution to the linearized Boltzmann transport equation

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Lattice thermal conductivity, κ_{lat}, of MgO at high pressures and temperatures, up to 150 GPa and 4000 K, are determined using lattice dynamics calculations and the linearized phonon Boltzmann transport equation (BTE) beyond the relaxation time approximation (RTA) from first principles. It is found that the complete solution of the linearized BTE substantially corrects values of κ_{lat} calculated with the RTA by ~30%, from ~39 W m^{-1} K^{-1} to ~50 W m^{-1} K^{-1} under ambient conditions. The calculated values of κ_{lat} are in good agreement with those from the existing experiments. At conditions representative of the Earth's core-mantle boundary (P = 136 GPa and T = 3800 K), κ_{lat} is predicted to be ~31 W m^{-1} K^{-1} and ~39 W m^{-1} K^{-1} by RTA and the full solution of BTE, respectively. We report a detailed comparison of our study with earlier theoretical studies.

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