The 498th Geodynamics Seminar

Effects of iron on the lattice thermal conductivity of lower mantle minerals from first principles

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Determination of lattice thermal conductivity (κ_{lat}) of lower mantle (LM) minerals is a key to understanding the dynamics and evolution of the earth's deep interior. Some recent experimental studies have shown that κ_{lat} of MgO and $MgSiO_3$ are substantially reduced by Fe incorporation (Manthilake et al., 2012; Goncharov et al., 2015; Ohta et al., 2017; Hsieh et al., 2017); Okuda et al. (2017) reported very weak effects on $MgSiO_3$ at lowermost mantle pressure. So, experimental results are still largely scattered, and effects on Fe in κ_{lat} remains unclear. We recently established an *ab initio* technique to compute κ_{lat} of Fe-free systems based on the density-functional theory (DFT) combined with fully solving the phonon Boltzmann transport equation, which was successfully applied to MgO (Dekura and Tsuchiya, 2017). In this study, the technique is extended further to Fe-bearing systems, (Mg,Fe)O ferropericlase, $(Mg,Fe)SiO_3$ bridgmanite and post-perovskite combined with the internally consistent DFT+*U* technique (Wang et al., 2015). Calculations demonstrate strong solid solution effects in these phases. The effects of Fe are found to be caused by the changes in harmonic properties rather than anharmonic properties, *i.e.*, the phonon-phonon scattering.

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