Effects of iron on the lattice thermal conductivity of lower mantle minerals evaluated by *Ab initio* anharmonic lattice dynamics simulations

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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, $(Mg,Fe)SiO_3$ bridgmanite (Brg) and (Mg,Fe)O ferropericlase (FP), combined with the internally consistent DFT+U technique (Wang et al., 2015). Calculations demonstrate strong solid solution effects in both Brg and FP. The effects of Fe are found to be caused mainly by the substantial changes in harmonic properties.

Keywords: Lower mantle minerals, Lattice thermal conductivity, Solid solution effects of iron, Ab initio calculation