Ab initio lattice thermal conductivity of (Mg,Fe)O ferropericlase at the deepest mantle

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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. (Mg, Fe)O Ferropericlase (Fp) is believed to be the second most abundant LM mineral after (Fe, Al) bearing $MgSiO_3$ bridgmanite and postpervskite (PPv). Recent experimental and theoretical studies under LM pressures showed that κ_{lat}) of MgO is substantially reduced by Fe incorporation (Ohta *et al.*, 2017; Hsieh *et al.*, 2018; Song *et al.*, 2019). However, the temperature condition is limited to a low temperature of 300 K, which is far from the actual LM condition. Therefore, the role of FP on the heat transport at the deepest mantle is still poorly understood. In this study, we determined κ_{lat} of FP at the LM pressure and temperature conditions, based on the *ab initio* anharmonic lattice dynamics techniques with fully solving the phonon Boltzmann transport equation (Dekura and Tsuchiya, 2017; 2019) combined with the internally consistent LDA+*U* technique for more precisely describing the Fe-O bond (Wang *et al.*, 2015). Calculations demonstrate strong negative solid solution effects (~-70-80% for ~13-19 mol% FeO) of low-spin Fe on κ_{lat} of MgO owing to decreases both in phonon group velocity and lifetime. An effective κ_{lat} of the lowermost mantle is then estimated for pyrolytic aggregate (FP+PPv) with pyrolytic ratio to be ~4 $Wm^{-1}K^{-1}$, which produces a net heat flow from the core to mantle ~6-7 TW. This value is more than ~50% smaller than that estimated from the core with high thermal conductivity of iron (~15 TW). This discrepancy could be reconciled by the thermally or chemically stratified layer at the top of the outer core observed seismologically (Helffrich and Kaneshima, 2010) if subadiabatic temperature gradient exists there.

Keywords: Lowermost mantle, Lattice thermal conductivity , Ferropericlase, Ab initio calculations