Ab initio anharmonic lattice dynamics for Fe-bearing lower mantle minerals

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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 $MgSiO_3$ bridgmanite (Brg) are substantially reduced by Fe incorporation (Manthilake et al., 2012; Goncharov et al., 2015; Ohta et al., 2017; Hsieh et al., 2017). In contrast, Okuda et al. (2017) reported a very different result on Brg with a marginal effect of Fe. Besides, the effect of Fe on $MgSiO_3$ post-perovskite (PPv) has never been reported. Therefore, in this study, we investigate κ_{lat} of Fe-bearing LM minerals (ferropericlase (FP), Brg, and PPv) in 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) 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 of low-spin Fe on κ_{lat} of FP and high-spin Fe on κ_{lat} of Brg and PPv, as a linear decrease in log κ_{lat} of FP with increasing the Fe concentration. Our detailed analyses indicate that such strong effects occur primarily due to the substantial changes in harmonic properties and are found to be Brg > PPv >FP. The present results improve the conventional estimation of the effective LM conductivity (e.g., Stacey 1992). It is estimated to be ˜2-3 $Wm^{-1}K^{-1}$ for the pyrolytic aggregate (FP + Brg) and ˜4-5 $Wm^{-1}K^{-1}$ (FP+PPv) at 136 GPa and 4000 K, which are ˜60-80% smaller than the conventional value of 10 $Wm^{-1}K^{-1}$.

キーワード：下部マントル鉱物、格子熱伝導率、第一原理計算
Keywords: Lower mantle minerals, Lattice thermal conductivity , First-principles calculation

