Ab initio lattice thermal conductivity of $MgSiO_3$ post-perovskite

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Lattice thermal conductivity (κ_{lat}) of the lowermost mantle (D" layer) is one of the key properties controlling the thermal evolution of the Earth and $MgSiO_3$ post-perovskite (PPv) is believed to be the most abundant mineral in this region. Ohta et al. (2012) measured the κ_{lat} of PPv but only at 300 K, far from the mantle temperature. On the other hand, the κ_{lat} of PPv was computed under lowermost mantle *P,T* (Haigis et al., 2012; Ammann et al., 2014) but using interatomic model potentials with adjustable parameters. Reported κ_{lat} of PPv under the lowermost mantle *P,T* are inconsistent with each other. We recently established an *ab initio* technique to compute κ_{lat} 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, using this technique, κ_{lat} of PPv is calculated under the lowermost mantle condition, and it is found ~20% lower than those reported in the model potential studies. We also find that the κ_{lat} of PPv is ~50% larger than that of Brg. This indicates that the lateral variations in the core-mantle boundary heat flux would be enhanced by the Brg-PPv phase transition. Effects of anisotropy in the κ_{lat} of PPv on the heat flux will also be discussed.

Keywords: Lower mantle minerals, Lattice thermal conductivity, Ab initio calculation

