Thermal conductivity of lower mantle minerals from ab initio anharmonic lattice dynamics

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Determination of lattice thermal conductivity () of lower mantle minerals is a key to understanding the dynamics of the Earth's interior. Although determination of κ was impractical in the deep Earth *P*, *T* condition for a long time, recent experimental and computational developments have been extending the accessible *P* and *T* ranges (e.g. H. Dekura, T. Tsuchiya and J. Tsuchiya, Phys. Rev. Lett. 110, 025904, 2013). *Ab initio* prediction of κ requires understanding of the phonon-phonon interaction associated with the lattice anharmonicity. We recently succeeded in developing an efficient method to calculate it based on the density-functional perturbation theory combined with anharmonic lattice dynamics theory, and applying to MgSiO₃ perovskite in the whole lower mantle *P*, *T* range for the first time. Next we extend our techniques to other lower mantle minerals such as MgSiO₃ post-perovskite, and now calculations of more realistic Fe-bearing systems are also started. In this presentation, we introduce the current situation of our research on κ .

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