

Thermal conductivity of lower mantle minerals from *ab initio* anharmonic lattice dynamics*Haruhiko DEKURA¹, Taku Tsuchiya¹

1.Geodynamics Research Center, Ehime University

Determination of lattice thermal conductivity (κ) 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 .

Keywords: Earth's lower mantle, Phonon transport property, First-principles calculation