

The 467th Geodynamics Seminar

Technical development on phonon transport property of lower mantle minerals: Theory and Application

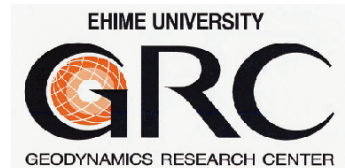
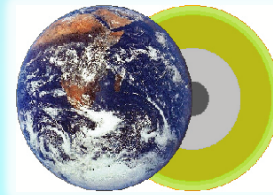
Dr. Haruhiko DEKURA (Lecturer, GRC)

Date: 14 April (Fri.) 2017, 16:30 ~

**Venue: Meeting Room #486, Science
Research Bldg. 1, Ehime Univ.**

日時: 2017年4月14日 (金) 16:30~

**場所: 愛媛大学 総合研究棟 I
4階共通会議室**



Abstract

Determination of lattice thermal conductivity (κ_{lat}) of lower mantle minerals is key to understanding the dynamics of the Earth's interior. Although it was impractical in the deep Earth pressure (P) and temperature (T) condition for a long time, recent experimental and computational developments have been extending the accessible P and T ranges. We recently succeeded in developing an *ab initio* technique to calculate κ_{lat} at any P and T condition based on the density-functional theory (DFT) combined with anharmonic lattice dynamics theory. The technique was then applied to major end-members of lower mantle minerals, MgSiO_3 bridgmanite (Dekura, Tsuchiya, Tsuchiya, 2013, PRL) and MgO periclase (Dekura, Tsuchiya, 2017, under revision). Next we extend our technique to more realistic Fe-bearing minerals in conjunction with the internally consistent DFT+ U technique (Wang, Tsuchiya, Hase, 2015, Nature geoscience) to deal with such strongly-correlated systems. In this presentation, I introduce the current situation of our technical development and research on κ_{lat} .