

# Geodynamics Seminar

## 第297回ジオダイナミクスセミナー

### Lattice thermal conductivity of deep mantle minerals

**Speaker :** Haruhiko Dekura

(Senior Research Fellow Center, Postdoctoral Fellow, GRC)

主催：愛媛大学地球深部ダイナミクス研究センター

日時：7/1（金）午後 4時30分～

場所：総合研究棟4F 共通会議室



#### Abstract

Thermal transport property of materials under pressure and temperature is of importance for understanding the dynamics of the solid Earth and the thermal history. However, both experimental and theoretical determinations of the thermal conductivity still remain technically challenging particularly at the deep mantle condition. Recent progress in ab initio computational method based on the density functional theory (DFT) is making it possible to examine the transport phenomena including the lattice thermal conduction. The intrinsic bulk thermal conduction of insulator is essentially caused by lattice anharmonicity owing to phonon-phonon interaction. Determination of the anharmonic coupling constant is therefore the key to predicting the thermal transport property. Earlier theoretical works calculated the lattice thermal conductivity of MgO with ab initio molecular dynamics (MD) simulation or direct evaluation of the anharmonic force constants (Nico de Koker, Phys. Rev. Lett. 103, 125902, 2009; X. Tang and J. Dong, Proc. Natl. Acad. Sci. U.S.A. 107, 4539, 2010). However, in these approaches, the simulation cell size could often be insufficient for accurate description of the long wavelength phonon scattering. As an alternative approach, the anharmonic coupling strength between phonon modes can be evaluated within the density functional perturbation theory (DFPT). In this approach, the higher-order force tensors are calculated based on the perturbative scheme taking care only of the primitive cell. We have been developing a technique for calculation of the phonon linewidth to obtain the phonon lifetime. Then the lattice thermal conductivity is evaluated combining with additional harmonic-level properties. In this presentation, I show the decay process of phonons and the lattice thermal conductivity of MgO as a test for the applicability of our technique.

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## 第297回ジオダイナミクスセミナー

### Si-Al interdiffusion rate in garnet and implication for metastable mineral proportion of pyrolite

**Speaker** : Masayuki Nishi  
(JSPS Postdoctoral Fellow, GRC)

主催 : 愛媛大学地球深部ダイナミクス研究センター

日時 : 7/1 (金) 午後 4時30分～

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#### Abstract

Seismic tomography has revealed that some subducting slabs stagnate near the mantle transition region before falling into the lower mantle. It has been suggested that presence of untransformed metastable minerals might act against the subduction of a slab into the lower mantle because it could produce positive buoyancy force. Recent experimental studies and seismic observations indicate that metastable olivine survives to the transition region in the coldest center core of a slab. Pyroxene also potentially survives as a metastable phase in the transition region because the pyroxene-garnet transformation is likely much more kinetically inhibited than the transformation of olivine. However, the size of metastable regions and their effects on slab dynamics have not been constrained because there is no quantitative kinetic data on the pyroxene-garnet transformation. Here we report new experimental results on the  $\text{Si}^{4+} + \text{M}^{2+} \leftrightarrow 2\text{Al}^{3+}$  interdiffusion rate of majoritic garnet, which controls the kinetics of the pyroxene-garnet transformation. We found that the diffusion rate is slow compared to the Si diffusion rate of the other silicate minerals in the deep mantle. Kinetics of the pyroxene-garnet transformation estimated based on this slow diffusion rate indicate that a significant amount of low-density metastable regions exist in the all flow field downgoing through the transition region including the subducting slab. This leads to a positive buoyancy force of the subducting slab, resulting in slab stagnation around the transition region. Furthermore, behaviors of the falling slab into the lower mantle might be triggered by the occurrence of the pyroxene-garnet transformation after a long stagnation over 108 years because it leads to a density crossover.