Geodynamics Seminar

第330回ジオダイナミクスセミナー

Ab initio determination on lattice thermal conductivity of $MgSiO_3$ perovskite and post-perovskite at deep mantle conditions

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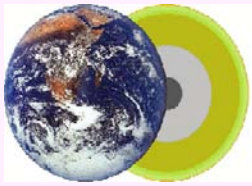
主催：愛媛大学地球深部ダイナミクス研究センター
日時：6/8（金）午後 4時30分～
場所：総合研究棟 4F 会議室



EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

Thermal transport property of Earth materials is a key to understanding the thermal evolution of the Earth, e.g., style of the mantle convection, formation of the geodynamo, and growth of the inner core. Both experimental and theoretical determinations of the thermal conductivity *k* still remain technically challenging particularly at the deep mantle and core conditions. However, *ab initio* computational method has been recently extended to transport phenomena including the thermal conduction because of some technical advances. Since the intrinsic bulk thermal conduction of insulator is caused by phonon-phonon interactions, the key parameter to predict *k* is thus the lattice anharmonicity of the materials. Earlier theoretical works calculated *k* of MgO with various approaches such as molecular dynamics simulation and finite difference method. In those approaches, large simulation cell size often should be taken account for accurate description of the long wavelength phonon scattering, and therefore the computational cost to calculate *k* tends to be expensive particularly for more complex minerals such as $MgSiO_3$. In contrast to those approaches, the anharmonic coupling strength can be determined based on the density-functional perturbation theory (DFPT). In this approach, the higher-order force tensors are calculated through a number of phonon decay channels obtained within the perturbative scheme taking care only of the primitive cell. We have been developing a technique for the calculation of the anharmonic coupling constants based on the DFPT, and applied it to $MgSiO_3$ perovskite (Mg-Pv) and post-perovskite (Mg-PPv). Here, I will show the anharmonic lattice dynamic properties and the *k* of Mg-Pv and Mg-PPv in the lower mantle conditions.

詳細は当センターホームページ: http://www.ehime-u.ac.jp/~grc/をご覧ください
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