Japan Geoscience Union Meeting 2012
(May 20-25 2012 at Makuhari, Chiba, Japan)

SIT41-07 Room:302 Time:May 20 10:45-11:00

Efficient and accurate ab initio calculations on the lattice thermal conductivity: Applications to $MgSiO_3$ Pv and PPv

DEKURA, Haruhiko[1*], TSUCHIYA, Taku[2], TSUCHIYA, Jun[1]

[1]SRFC, Ehime Univ., [2]GRC, Ehime Univ.

Although thermal transport property of materials under pressure and temperature is of importance for understanding thermal structure and its thermal history of the Earth, both experimental and theoretical determinations of the thermal conductivity still remain technically challenging particularly at the deep mantle and core conditions. However, ab initio computational method has been recently extended to transport phenomena due to some technical advances. The intrinsic bulk thermal conduction of insulator is caused by lattice anharmonicty owing to phonon-phonon interactions. The key parameter to predict the lattice thermal conductivity, k, is thus the anharmonic coupling strength. Earlier theoretical works calculated k of MgO with various approaches such as molecular dynamics simulation and finite difference method. In those approaches, the sufficient simulation cell size 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 $MgSiO_3$. Actually, to the best of our knowledge, the k of $MgSiO_3$ perovskite (Mg-Pv) or post-perovskite (Mg-PPv) at high-pressure and high- temperature still not established by ab initio calculation. In contrast to those approaches, we evaluate the anharmonic coupling strength based on the density-functional perturbation theory. 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 phonon damping function necessary to obtain the phonon relaxation time. Then k is calculated with additional harmonic-level of calculations.

In this presentation, we show that the k of Mg-Pv and Mg-PPv as a function of pressure and temperature. The k of Mg-Pv calculated at ambient condition is found to be in excellent agreement with the experiment (M. Osako and E. Ito, Geophys. Res. Lett. 18, 239, 1991). The current results are applied to evaluate the effective k and the total heat flow at the core-mantle boundary (CMB) with a composite averaging between MgO and $MgSiO_3$. This provides better constraints for the thermal evolution of the Earth.

Research supported by Senior Research Fellow Center, Ehime University.

Keywords: ab initio calculations, lattice thermal conductivity, phonon-phonon interaction, deep mantle minerals