The 437th Geodynamics Seminar

Technical development in *ab initio* phonon transport properties of minerals

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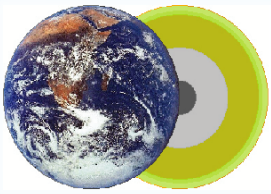

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Abstract

Determination of thermal conductivity (κ) is key to understanding dynamics and therefore evolution of the Earth's interior. *Ab initio* prediction of κ of minerals requires microscopic understanding of the lattice anharmonicity owing to the phonon-phonon interaction. The phonon lifetime (τ) is an essential physical quantity for the prediction of κ. We recently developed an efficient *ab initio* computational method for κ of silicate minerals with complex structure based on the *reciprocal-space* method. Although this method was found pretty powerful particularly for the low-thermal conducting materials such as $MgSiO_3$ Perovskite (Mg-Pv), we found that overestimation of κ might arise in our computational treatment especially when the method is applied to high-κ materials such as Mg-PPv under high-P. In addition, it was also found not easy to apply our method to strongly correlated systems such as Fe-bearing minerals. Therefore, some technical developments on τ may be highly desired for a deeper understanding of the lower mantle conductivity. We therefore recently developed a new numerical method for obtaining anharmonic phonon coupling strength and lifetimes based on the *real-space* anharmonic lattice dynamics. In this presentation, I will talk about detailed information on the computational method, and show preliminary results on κ of Mg-PPv determined by the developed real-space approach in the testing phase.

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