Geodynamics Seminar

第295回ジオダイナミクスセミナー

Predictions of the shear response of (Mg,Fe)SiO_3 post-perovskite.

Speaker :Arnaud Metsue
(Global COE Research 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：5/13（金）午後 4時30分～
場所：総合研究棟4F　共通会議室

Abstract

Observation of seismic data put in forth evidence of a spatial anisotropy in the seismic wave velocities in the D'' layer, the lowermost part of the mantle. (Mg,Fe)SiO_3 post-perovskite (PPv) is thought to be the most abundant phase in this part of the mantle, and this mineral exhibits a strong elastic anisotropy and may contribute significantly to the seismic anisotropy in the D'' layer. However, the seismic anisotropy cannot be expressed at the rock scale if the orientations of the grains are distributed randomly. Consequently, the formation of lattice preferred orientations with an anisotropic mechanism of plasticity, such as dislocation creep, can cause the seismic anisotropy in the D'' layer. A first step to understanding the mechanisms of plasticity occurring in the deep Earth is to test the response of the PPv phase, in a geophysical relevant composition, to a plastic shear.

In this talk, we will present new results from first-principles calculations on the shear response of pure and iron-bearing $MgSiO_3$ PPv. The originality of this work is the use of internally consistent LSDA+*U* formalism to accurately describe the electronic structure of the iron-bearing systems. The response of the PPv to a plastic shear is investigated at 120 GPa through the calculations of the Generalized Stacking Faults (GSF) energy in pure and iron-bearing systems. The GSF probes the ability of the crystal to be shear homogeneously in a [uvw](hkl) slip system and gives the value of the ideal shear stress (ISS), which can be defined as the theoretical elastic limit of the crystal. We investigate ten potential <uvw>{hkl} slip systems, since these latter are not well constrained for the PPv phase. The [100](001) slip system in pure and iron-bearing phases exhibits the lowest ISS and may play an important role in the plastic deformation of the PPv phase. We show that iron decreases the GSF energy and the ISS of all slip systems. Finally, we discuss the plastic anisotropy of pure and iron-bearing phases from the values of the ISS and the orientation of applied tensile stress. Our results suggest that the incorporation of ferrous iron has a limited effect on the plastic anisotropy of the PPv phase.

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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Geodynamics Seminar

第295回ジオダイナミクスセミナー

Intermolecular interactions in deuterated hydrogen hydrate under high pressure and its implication for the stability of gas hydrates.

Speaker : Shinichi Machida
(Global COE Research 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：5/13（金）午後 4時30分～
場所：総合研究棟4F 共通会議室

EHIME UNIVERSITY GRC GEODYNAMICS RESEARCH CENTER

Abstract

Hydrogen hydrate is made of hydrogen-bonded water molecules forming cages or frameworks that include hydrogen molecules. Hydrogen hydrate is expected to exist in protostar and extrasolar planets. Then, the examination of high pressure stabilities of hydrogen hydrate is important to estimate the formation and evolution process of these bodies. High pressure experiments of hydrogen hydrate indicated that it shows remarkable stability under high pressure. This stability was considered to be produced by intermolecular interactions between the guest hydrogen molecules and the host water molecules. In order to detect the intermolecular interactions separately from the guest hydrogen molecules and the host water molecules, high-pressure experiments of deuterated hydrogen hydrate were performed. In this seminar, intermolecular interactions in deuterated hydrogen hydrate will be discussed. In addition, I developed a microscopic observation system as well as a pressure measurement system by the ruby fluorescence method. This system was set in the loading system of hydrogen gas which was developed previously. I will also show the system which was developed.

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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