Geodynamics Seminar

第371回ジオダイナミクスセミナー

A possible reason for forming tetragonal phase of filled ice Ic hydrogen hydrate inferred from Raman spectroscopy under low-temperature and high-pressure

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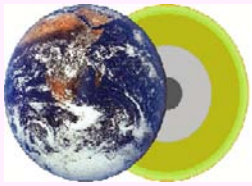
主催：愛媛大学地球深部ダイナミクス研究センター
日時：11/29（金）午後 4時30分～
場所：総合研究棟Ⅰ 4F 共通会議室



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Abstract

Hydrogen hydrate is composed of hydrogen-bonded host water molecules forming cages or frameworks that include guest hydrogen molecules. One type of hydrogen hydrates, filled-ice Ic structure (HH-C2), has been thought to have a cubic structure. An ab initio calculation predicted that the cubic structure of HH-C2 transforms to a tetragonal structure under high-pressure and low-temperature. And, an *in-situ* X-ray diffractometry (XRD) confirmed experimentally the predicted transformation of HH-C2 to the tetragonal structure. The transformation of HH-C2 was inferred to be produced by changes in the rotational or vibrational modes of the guest hydrogen molecules. In this study, Raman measurements were performed under low-temperature and high-pressure in order to examine the reasons for the transformation to the tetragonal structure. As a result, distinct split of roton $S_0(0)$ was observed at 173 K, 8 GPa. The P-T conditions at which the roton split occurred in the present Raman study were good agreement with phase boundary between the cubic and the tetragonal phase determined by the XRD study. Hydrogen molecules in the cubic HH-C2 structure are thought to be rotationally disordered at lower pressure and higher temperature. The splitting roton observed suggested that the rotational mode changed from the disordered (spherical) mode to ordered (e.g. ellipsoidal) one, which induced the deformation of the lattice, namely transformation to a tetragonal structure. In addition, XRD study for D_2-D_2O system prior to Raman study in order to investigate the relationship between the transformation and para/ortho nature of hydrogen molecules.

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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