

実験報告書様式(一般利用課題・成果公開利用)

(※本報告書は英語で記述してください。ただし、産業利用課題として採択されている方は日本語で記述していただいても結構です。)

 	承認日 Date of Approval 2017/4/10 承認者 Approver Kaoru Shibata 提出日 Date of Report 2017/4/10
課題番号 Project No. 2016B0159 実験課題名 Title of experiment Transportation of hydrogen at high temperatures in the deep Earth by quasielastic neutron scattering 実験責任者名 Name of principal investigator Takuo OKUCHI 所属 Affiliation Institute for Planetary Materials, Okayama University	装置責任者 Name of responsible person Kaoru SHIBATA 装置名 Name of Instrument/(BL No.) DNA / BL02 実施日 Date of Experiment February 15-23, 2017

試料、実験方法、利用の結果得られた主なデータ、考察、結論等を、記述して下さい。(適宜、図表添付のこと)
 Please report your samples, experimental method and results, discussion and conclusions. Please add figures and tables for better explanation.

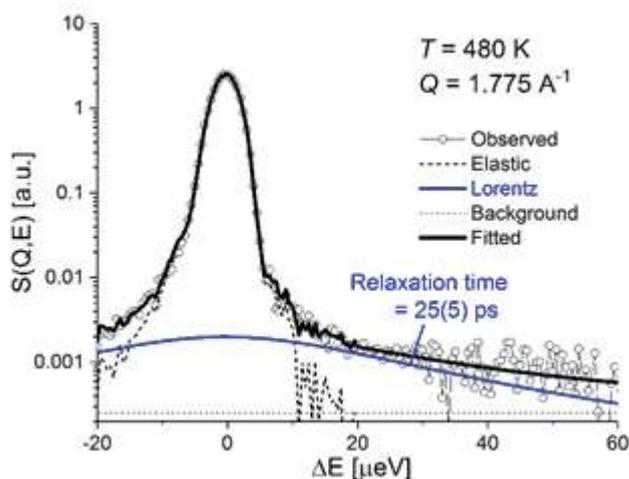
1. 試料 Name of sample(s) and chemical formula, or compositions including physical form. Dense Hydrous Magnesium Silicate Phase E [$Mg_{2+x}Si_{1+y}H_{4-2x-4y}O_6$], powder Serpentine [$(Mg,Fe)_3Si_2O_5(OH)_4$], powder
--

2. 実験方法及び結果 (実験がうまくいかなかった場合、その理由を記述してください。) Experimental method and results. If you failed to conduct experiment as planned, please describe reasons. <p>The project was technically supported by our recent progress on a mass-production scheme of hydrous deep-Earth minerals of excellent quality and quantity (Okuchi et al., Am. Mineral. 2015). A single-phase sample powder of dense hydrous magnesium silicate (DHMS) phase E was synthesized by accumulating the products of several independent synthesis runs all using this scheme. As for more details for these synthesis runs, we used a scaled-up Kawai-type cell at Okayama University along with 46 mm-sized cubic carbide anvils and a 18/10 cell assembly. Each sample made of a mixture of $Mg(OH)_2$ and SiO_2 powders in the molar ratio of 2:1 was sealed into a gold tube capsule of 5 mm outside diameter, which contained >80 mg of the mixture to be compressed to 15 GPa pressure, that corresponds to the condition where DHMS phase E exists inside the Earth. After loading this pressure, the sample was heated by applying electronic current to a cylindrical $LaCrO_3$ semiconducting furnace, which was installed inside the cell to surround the gold capsule. After the heating, the electric current was cut-off and then the synthesis product was</p>
--

2. 実験方法及び結果(つづき) Experimental method and results (continued)

recovered into ambient condition. Each product was then separately evaluated by powder x-ray diffraction to confirm whether the recovered DHMS phase E powder was single-phase, chemically homogeneous, as well as highly crystalline. Among all these recovered products, we have selected only the highest-quality ones, which were then mixed up together to prepare the sample powder for quasi-elastic neutron scattering measurements (QENS).

DNA spectrometer has the highest energy resolution among available instruments for QENS. By our previous efforts, DNA has been proved to provide sufficient energy resolution to analyze the slow dynamics of chemically-bonded hydrogen, as well as high intensity and extremely-low background to measure the mass-limited synthetic sample of deep-Earth hydrous minerals. In order to control the sample temperatures, we used a top-loading type cryo-furnace which was operated up to 480 K without problem. A representative $S(Q,E)$ of DHMS phase E obtained at DNA was shown below. The blue-colored Lorentz peak showed mobile hydrogen component.



Our specific goal in the current project was to determine hydrogen's local and translational dynamics within DHMS phase E at higher temperature conditions, which are more relevant to the physical environments of hydrous minerals in the deep Earth. We are now analyzing the results to determine relaxation times and hopping distances of local and translational motions of hydrogen at each measured temperature, as well as activation energies of these motions. We are recently demonstrating that crystal structures of prevailing deep-Earth hydrous minerals quite often involve dynamically-disordered hydrogen sites of partially-filled occupancy (Purevjav et al., *Geophys. Res. Lett.*, 2014; Okuchi et al., *High Pressure. Res.*, 2014), which are also including the structure of DHMS phase E (Tomioka et al., *Phys. Chem. Mineral.*, 2016). Such characteristics of the hydrogen sites of DHMS phase E will result in anomalously-fast transportation dynamics of hydrogen, which is suggested by the significant dynamics already emerging at 480 K as shown in the figure above.