

(※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。)

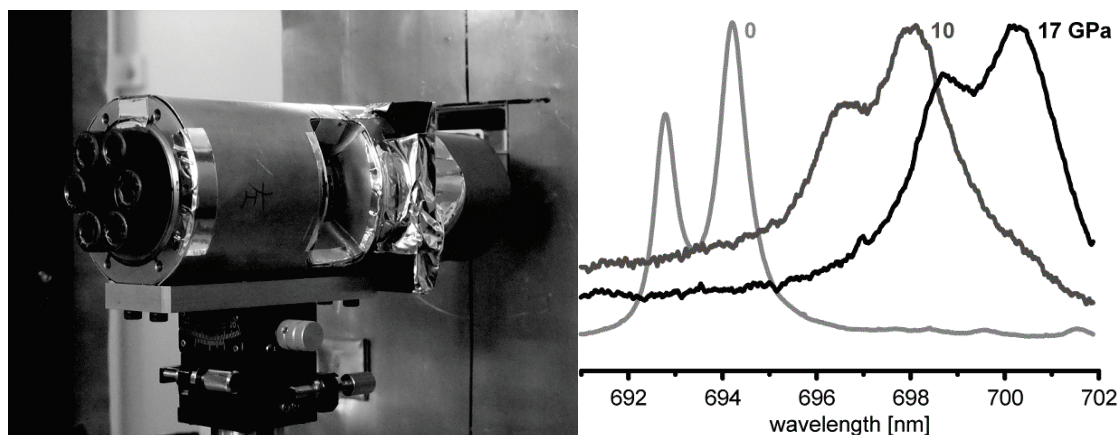
 MLF Experimental Report	提出日 Date of Report 2013.5.16
課題番号 Project No. 2012B0016 実験課題名 Title of experiment Transformation of bonding and dynamics of magnesium hydroxide at high pressures 実験責任者名 Name of principal investigator Takuo Okuchi 所属 Affiliation Okayama University	装置責任者 Name of responsible person Kazuya Aizawa 装置名 Name of Instrument/(BL No.) TAKUMI (BL 19) 実施日 Date of Experiment 2013.1.15-17 2013.3.10-13

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.

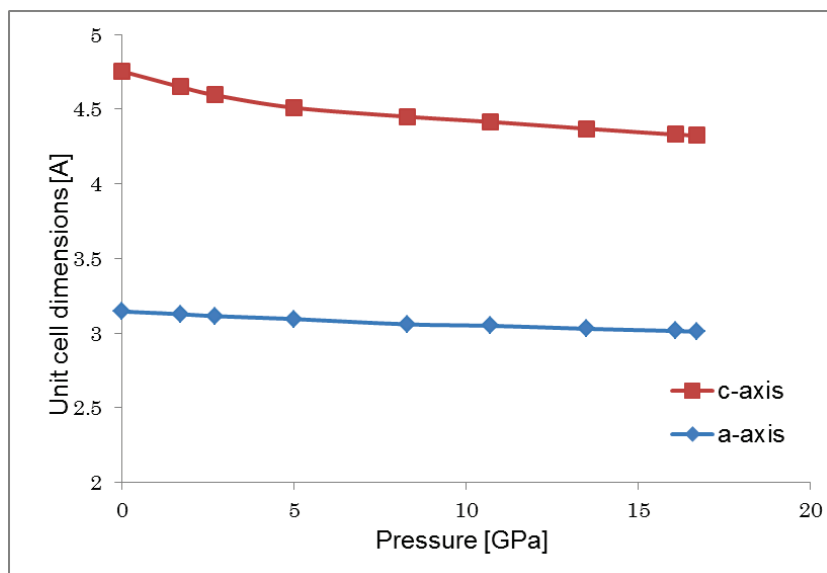
1. 試料 Name of sample(s) and chemical formula, or compositions including physical form. magnesium deuterioxide ($Mg(OD)_2$) deuterated magnesium-iron silicate ($(Mg,Fe)_2SiO_4 \cdot xD_2O$) glycerine-d8 ($C_3D_5OD_3$)

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>Powder $Mg(OD)_2$ sample of appropriate grain size for neutron powder diffraction (ca. 5~10 μm) was synthesized from MgO powder and D_2O liquid in an autoclave kept at 240°C and 40 MPa for five days. The sample was evaluated by powder x-ray diffraction and Raman spectroscopy prior to the use for high pressure experiments. No contamination of additional phase and no OH stretching peak were observed from the synthesized $Mg(OD)_2$ powder.</p> <p>We prepared several different types of compressed samples in compact opposed anvil cells, those are with different volume and pressure. To compress these samples into desired pressures, we used combinations of single crystal diamond, nano-polycrystalline diamond, and/or sintered polycrystalline diamond as two opposed anvils. We also prepared TiZr “null” alloy gaskets which is not only very strong but also nearly transparent for neutron, so that is ideal material for opposed anvil cell compression experiments. Its heat-treatment procedure was optimized to accept extensive deformation between these superhard anvils.</p>

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



A photograph of typical opposed anvil cell used for the neutron diffraction measurement and representative ruby fluorescence spectra indicating the pressure of the sample chamber are shown in the above figures. We have successfully obtained moderate-quality neutron diffraction patterns up to 8 GPa pressures for $\sim 4 \text{ mm}^3$ volume of the sample and up to 17 GPa pressures for $\sim 2 \text{ mm}^3$ volume of the sample. In most case, the sample powder was mixed with small amount of deuterated glycerin to improve the hydrostacity before compression.



Above figure shows lattice parameter change of the $\text{Mg}(\text{OD})_2$ sample with increasing pressure, preliminarily determined from the obtained neutron diffraction patterns. We are now analyzing these patterns by Rietveld refinement method to find the structure parameters related to the chemical bonding state of hydrogen, and to discuss the transportation of bonding and dynamics of hydrogen at high pressures.

以下は、MLFで内部資料として使用します。(日本語可)

The following sheet is for internal use only. Description in Japanese is acceptable.

○論文等による成果発表の予定 (Your publication plan)

a) 発表形式 ^(*1) Publication style ^(*1)	b) 発表先(誌名、講演先) ^(*2) Publication/Meeting information ^(*2) (Name of journal/book or meeting)	c) 投稿/発表時期 ^(*3) Date of paper submission or presentation ^(*3)
原著論文 その他口頭発表	Physics and Chemistry of Minerals 鉱物科学会	6ヶ月以内 2013年9月

【記入要領】(Instructions)

- (*1) 原著論文、総説、プロシーディングス、単行本、特許、招待講演(国際会議)、その他口頭発表等、具体的な発表方法を示して下さい。
Please describe planned publication and/or presentation style; *ex.* refereed journal, review article, conference proceedings, book, patent, invited talk, oral presentation *etc.*
- (*2) 成果を発表する誌名、講演先を示して下さい。
Please describe the name of journal or book you are planning to submit, or name of meeting you will make a presentation.
- (*3) およその発表予定時期を示して下さい。(3月以内、6月以内、1年以内、2年以内、2年以上先、等)
Please describe the estimated date of paper submission or presentation; *ex.* within 3 months, within 6 months, within 1 year, within 2 years, beyond 2 years, *etc.*

○成果になる予定が立たない場合の理由と今後の計画を記述してください。

In case you can not publish your results, please describe reasons and future plan.

(例:「論文になる十分な結果が得られなかった」、「複数回の実験が必要で次回の課題終了後に発表予定」、等)