

Hydrogen in enstatite: A density functional theory study

Moe Sakurai^{1*}, Hiroshi Sakuma¹, Noriyoshi Tsujino², Eiichi Takahashi¹, Katsuyuki KAWAMURA³

¹Department of Earth and Planetary Sciences, Tokyo Institute of Technology, ²Institute for Study of the Earth's Interior, Okayama University, ³Graduate School of Environmental Science, Okayama University

Water (or more precisely, hydrogen) has a profound influence on the physical properties of mantle such as viscosity, melting temperature, transmission of seismic waves, and electrical conductivity (e.g. Hirschmann and David Kohlstedt, 2012). The hosts for water would be nominally anhydrous minerals (NAMs) such as olivine, pyroxene, and garnets, which are major minerals in mantle. In order to understand the effect of water on the physical properties of these NAMs, we have to investigate how hydrogen is incorporated in these NAMs. First-principles electronic state calculations based on density functional theory (DFT) have an advantage for understanding the positions of hydrogen in minerals. Recent first-principle study has revealed the configuration of H substitution for Mg and Si ions in forsterite (Fo; Mg_2SiO_4) (Umamoto et al., 2011). The lowest-energy structure involved four hydrogen atoms in a tetrahedral site by substituting for silicon. The calculated O-H stretching frequencies for the structure were in good agreement with experimental IR absorption spectra of Fo.

In this study, we focused on the water in orthopyroxene (Opx; $(Mg,Fe)_{2-x}Al_{2x}Si_{2-x}O_6$). The water solubility in Opx increased linearly with increasing Al_2O_3 content (Rauch and Keppler, 2002). Why does the water content of Opx increase with increasing Al_2O_3 content? The aim of this study is to understand the mechanism of hydrogen substitution in Opx.

We have calculated the electronic state in Enstatite (En; $MgSiO_3$) which is an end member of Opx using the DFT. Calculations were performed using the generalized gradient approximation (GGA-PBE) (Perdew et al., 1996). The pseudopotential method was employed. The optimized lattice constants of En without vacancies are $a = 18.4556$ Å, $b = 8.92120$ Å, and $c = 5.24794$ Å (for the *Pbca* symmetry). The $1*2*4$ k-point mesh was used for this supercell. Dynamical matrices for hydrogen atoms were computed using density functional perturbation theory (Giannozzi et al., 1991). We substituted hydrogen and/or Al^{3+} for Si^{4+} in the *T2* site and Mg^{2+} in the *M1* site. Four types of the substitution $(4H)_{Si}$, $(2H)_{Mg}$, $(Al+H)_{Si}$ and $(4H)_{Si}+(Al+H)_{Si}$ were considered. Here the ions in parenthesis refer to added ions, the subscript ions refer to removed ions. Highly reactive site in En was evaluated from the lowest unoccupied molecular orbital (LUMO) distribution around various atoms. Stable positions of hydrogen in En were estimated from the direct comparison of the vibrational frequencies obtained by experimental FT-IR method and by the first-principles methods.

The calculated O-H stretching frequencies distributed from 3800 to 3000 cm^{-1} depending on the substitution types. The frequencies for the structures of $(4H)_{Si}$, whose frequencies were dominant at high frequencies, can explain the high-intensity experimental IR absorption spectra of En. The calculated O-H stretching frequencies for the structures of $(4H)_{Si}+(Al+H)_{Si}$ were in good agreement with the experimental band which appeared only for Al_2O_3 -bearing En. In En with $(Al+H)_{Si}$ substitution, there was a remarkable change for the LUMO distribution around a Si ion in *T2* site compared to the Si ion in En without the substitution. This change of the LUMO distribution implied that the Al incorporation enhances the instability of Si ions in close *T2* site. This would be explain why the Al incorporation in En enhances its the water solubility.

Keywords: orthopyroxene, hydrogen position, frequency calculation, IR, density functional theory

Influence of Al incorporation on the amount of protons in MgSiO₃ perovskite

Tomoyuki Yamamoto^{1*}

¹Faculty of Science and Engineering, Waseda University

Most of the geoscientists believe that olivine-based minerals form the major constituent in the upper mantle, which extends to a depth of 660 km. Major component of the upper mantle is Mg₂SiO₄ in which there are three phases depending upon the depth, i.e., Forsterite (alpha phase), Wadsleyite (beta phase) and Ringwoodite (gamma phase). Pressure induced phase transitions occur at about 10 GPa and 15 GPa under low temperature condition from alpha to beta and from beta to gamma phases, respectively. It is widely accepted that the atmosphere and the oceans of the Earth are formed by degassing of the Earth's mantle. Most of the water may have been lost or it may still be stored in the Earth's mantle. If considerable amounts of water are present in the Earth's mantle, such water plays a key role in the geodynamics of the Earth's interior, because it affects the melting temperature and the transport properties of minerals as well as their elastic properties. Recent high pressure experiments suggested that main components of the transition zone of the mantle, wadsleyite and ringwoodite, can store significant amount of water [1-4].

On the other hand, some experiments suggested that the pure Mg-perovskite, which is one of the major component of the Earth's lower mantle, can store tiny amount of water in its structure [5,6]. However, it was reported very recently that MgSiO₃ perovskite can store more water when the Al is incorporated [7]. In the present study, the first-principles calculations were carried out to investigate the influence of Al incorporation on the amount of water in MgSiO₃ perovskite. Our preliminary results show that the solution energy of protons in MgSiO₃ decreases when the Al ions are incorporated.

References

- [1] Inoue, T., Yurimoto, H. & Kudoh, Y., *Geophys. Res. Lett.* 22, 117-120 (1995).
- [2] Kohlstedt, D.L., Keppler, H. & Rubie, D.C., *Contrib. Mineral. Petrol.* 123, 345-357 (1996).
- [3] Yusa, H., Inoue, T. & Ohishi, Y., *Geophys. Res. Lett.* 27, 413-416 (2000).
- [4] Ohtani, E., Mizobata, H. & Yurimoto, H., *Phys. Chem. Minerals.* 27, 533-544 (2000).
- [5] Murakami, M., Hirose, K., Yurimoto, H., Nakashima, S. & Takafuji, N., *Science* 295, 1885-1887 (2002).
- [6] Inoue, T., Wada, T., Sasaki, R., & Yurimoto, H., *Phys. Earth Planet. Inter.* 183, 245 (2010)
- [7] Inoue, T. & Yurimoto, H., DI13D-2451 presented at 2012 Fall Meeting AGU

Keywords: first-principles calculation, lower mantle, magnesium silicate perovskite, water storage, aluminium

Proton dynamics in ice VII

Toshiaki Iitaka^{1*}

¹RIKEN ASI

Proton dynamics in the hydrogen bond of water molecules is a basic process of physical and chemical phenomena in many chemical and life systems [1]. In the previous talk[2], we examined the proton conductivity of ice VII [3], which may exist in astronomical icy bodies, in terms of transport theory of defects and molecular dynamics simulation. In this talk, we will examine the details of defect motion by visualization as well as heat conductivity and the modulated structures[4]

[1] M. Eigen and L. de Maeyer, Proc. R. Soc. Lond. A 247, 505 (1958).

[2] T. Iitaka, Abstract of Japan Geoscience Union Meeting 2011, SMP048-01.

T. Okada et al., Abstract of Japan Geoscience Union Meeting 2011, SMP048-02.

[3] E. Sugimura et al., Phys. Rev. B 77, 214103 (2008).

[4] P. Loubeyre et al., Nature 397, 503 (1999).

Keywords: ice, high pressure phase, proton dynamics, electric conductivity, heat conductivity, defect

In-situ neutron scattering experiments of ice VI under high pressure and low temperature

Kazuki Komatsu^{1*}, Kazuya Nakayama¹, Tamami Koizumi¹, Hiroyuki Kagi¹

¹Geochemical Research Center, Graduate School of Science, The University of Tokyo

In-situ neutron scattering experiments for ice VI under high pressure and low temperature were carried out in order to investigate the long-standing problem of the order-disorder transition of ice VI. We used 99.9 % D₂O as sample, in contrast with the study of Salzmann et al. (2009) who used D₂O with 0.01 mol/L DCl. We also used the newly developed P-T variable cell (Komatsu et al., in press) which allows us to explore pressure and temperature individually; it is essentially important for this study because compression under low-temperature is necessary to make fine powdered iceVI. Cup-shaped WC anvils, TiZr encapsulating gaskets and duralumin support ring were used as anvils and gaskets, respectively. Their combination of anvils and gaskets has much less attenuation for both incident and scattered neutron; the intensity is 2.6-5.2 times more than the conventional single toroidal anvils. Another run which includes Pb as a pressure maker with D₂O was also conducted to find the anomaly in P-V-T relationship, which was reported by Mishima et al. (1979).

The neutron diffraction patterns taken at any P-T conditions we explored (0.6~1.7 GPa, 100-240 K) were well explained by the disordered iceVI structure model, and no additional peaks were found in this study. The observed V-T relationships at 1.3 GPa have no clear anomaly, but seems normal, which means that no strong evidence to show the transition from disordered to ordered-state was observed.

References

- B. Kamb, A. Prakash, W. C. Hamilton, and S. J. LaPlaca, quoted by B. Kamb, in *Physics and Chemistry of Ice*, edited by E. Whalley, S. Jones, and L. Gold (Royal Society of Canada, Ottawa, 1973).
- Iizuka, R., Yagi, T., Gotou, H., Komatsu, K., and Kagi, H. (2012) *High Press. Res.*, 32, 430-441.
- Johari, G.P., and Whalley, E. (1976) *Journal of Chemical Physics*, 64, 4484-4489.
- Komatsu, K., Moriyama, M., Koizumi, T., Nakayama, K., Kagi, H., Abe, J., and Harjo, S. (2013) *High Pressure research*, in press
- Kuo, J.L., and Kuhs, W.F. (2006) *Journal of Physical Chemistry B*, 110, 3697-3703.
- Mishima, O., Mori, N., and Endo, S. (1979) *Journal of Chemical Physics*, 70, 2037-2038.
- Salzmann, C.G., Radaelli, P.G., Mayer, E., and Finney, J.L. (2009) *Physical Review Letters*, 103.

High resolution neutron powder diffraction of methane hydrate at high pressure

Takuo Okuchi^{1*}, Shigeo Sasaki², Satoshi Takeya³, Masashi Yoshida², Naotaka Tomioka¹, Narangoo Purevjav¹

¹ISEI, Okayama University, ²Faculty of Engineering, Gifu University, ³REEF, National Institute of Advanced Industrial Science and Technology

Neutron plays complementary role to x-ray in material science at high pressure, especially as the most powerful probe for structural analysis of hydrogen-bearing compounds. J-PARC (Japan Proton Accelerator Research Complex) now becomes one of the strongest pulsed neutron sources which give us such a probe. Here we present our recent high-resolution neutron powder diffraction result of fully-deuterated methane hydrate at high pressure, which was measured at TAKUMI beamline (BL19) at J-PARC MLF (Materials and Life Science Experimental Facility), using compact high-pressure anvil cells. For this purpose we have developed a new-type cell design suitable for time-of-flight neutron diffraction.

Keywords: methane hydrate, neutron diffraction, high pressure

Phase changes of hydrogen- and methane-hydrates under low temperature and high pressure

Hisako Hirai^{1*}, KAGAWA, Shingo¹, TANAKA, Takehiko¹, MATSUOKA, Takahiro², OHISHI, Yasuo³, YAGI, Takehiko¹, OHTAKE, Michika⁴, YAMAMOTO, Yoshitaka⁴

¹GRC Ehime University, ²KYOKUGEN, ³JASRI, ⁴AIST

One type of hydrates (referred to HH) has recently received significant interest as a clean hydrogen storage material, and methane hydrate (referred to MH), called 'fiery ice' is expected an useful natural resource. Both hydrates have been thought to be potentially ubiquitous in space objects such as icy satellites of the solar system and extrasolar planets. At lower pressures these hydrates have clathrate structures which consist of host cages formed by hydrogen-bonded water molecules with encapsulated guest species. At higher pressures, MH and HH transform to a filled ice Ih structures (MH-FIIhS) and filled ice Ic structure (HH-C2), respectively. These filled ice structures consist of a host ice framework and guest molecules contained in the voids of the host ice framework. Comprehensive studies performed under room temperature for MH and HH provided interesting properties, however, low temperature and high pressure behaviors have rarely been known except a few studies. In this study, low-temperature and high-pressure experiments were performed to clarify the phase changes of MH-FIIhS and HH-C2 in the previously unexplored region.

Clamp-type diamond anvil cells and a helium-refrigeration cryostat were used in this study. The pressure and temperature ranges for HH-C2 were 5.0 to 50.0 GPa and 30 to 300 K, and those for MH-FIIhS were 2.0 to 77 GPa and 30 to 300 K, respectively. Pressure measurements were made via a ruby fluorescence method and a diamond Raman method. Temperature measurements were made using a silicon semiconductor thermometer and chromel-alumel thermocouples. The initial samples of MH and HH were prepared by ice-gas interface method and gas-loading method, respectively. The samples were characterized via X-ray diffractometry (XRD) using synchrotron radiation at BL-10XU at SPring8 and BL-18C at the Photon Factory (KEK) and Raman spectroscopy.

In situ X-ray diffractometry revealed that the cubic HH-C2 transformed to tetragonal at low temperatures and high pressures, and that the axis ratio of the tetragonal phase changed depending on the pressure and temperature. These results were consistent with theoretical predictions performed via first principle calculations. The tetragonal phase was determined to be stable above 20 GPa at 300 K, above 15 GPa at 200 K, and above 10 GPa at 100 K. Further changes in the lattice parameters were observed from about 45 to 50 GPa throughout the temperature region examined, which suggests the transformation to another high-pressure phase above 50 GPa. Guest molecules have been known to rotate freely in both clathrate and filled ice structure under low pressure. The reasons for the transformation to the tetragonal structure can be explained as follows: the tetragonal structure might be induced due to changes in the vibrational or rotational modes of the hydrogen molecules from free-rotation state to orientational-ordered state under low temperature and high pressure.

In our previous studies of MH-FIIhS by Raman spectroscopy, orientational ordering of guest methane molecules, namely suppressing rotation, occurred at 15-20 GPa, although there was no clear change in the lattice parameters and volume by the XRD study. The present XRD study revealed clear changes in the axis ratios at 15 to 20 GPa at 300K. The Raman spectroscopy showed split of CH vibration mode of the methane molecules at the almost same pressure. These results indicated that the orientational ordering of the guest molecules resulted in deformation of the lattice. The change in rotational mode of the guest molecules is a phase change. Thus, the results demonstrate that there are guest-disordered phase and guest-ordered phase within same MH-FIIhS frame work structure. Similar changes in the axis ratios and split of CH vibration mode were observed at low temperature regions.

Keywords: hydrogen hydrate, methane hydrate, phase change, low temperature, high pressure

A neutron diffraction study of phase transition in lawsonite at high pressure

Asami Sano^{1*}, Takaya Nagai², Riko Iizuka³, Yusuke Seto⁴, Takahiro Kuribayashi⁵, Takanori Hattori¹

¹Quantum Beam Science Directorate, JAEA, ²Department of Natural History Sciences, Faculty of Science, Hokkaido Univ., ³Geochemical Laboratory, Graduate School of Science, Univ. of Tokyo, ⁴Graduate School of Science, Kobe Univ., ⁵Institute of Mineralogy, Petrology and Economic Geology, Graduate School of Science, Tohoku Univ.

Lawsonite is a hydrous mineral which is considered as a main carrier of hydrogen in the subducting slab. It has a wide stability field at the pressures from 3.5 GPa to 10 GPa, and up to 1000 C. Previous single crystal X-ray diffraction and neutron diffraction studies indicate that there exist two phase transitions at low temperature. A property of low temperature is sometimes considered to be equivalent to the behavior at high pressure, and some studies pointed out the possibility of transition at high pressure. To investigate the pressure response of hydrogen bond and phase transition in lawsonite, neutron diffraction experiment was conducted.

Lawsonite was deuterated by D-H exchange reaction in the furnace under deuterated nitrogen atmosphere. High pressure and high temperature neutron diffraction experiment was conducted by 6-ram press at J-PARC MLF. Using 6-6 type anvil with TEL size of 10 mm, neutron diffraction pattern was corrected up to 6 GPa and 800 C. In addition, hydrostatic experiment at ambient pressure was conducted using Paris-Edinburgh press. New peak was observed at 1.83 Angstrom that indicates phase transition at high pressure. Detail of the result will be presented at the talk.

Keywords: Lawsonite, neutron diffraction, hydrous mineral, subducting slab

In-situ neutron diffraction observation of hydrogen positions in portlandite under high pressure and temperature

Riko Iizuka^{1*}, Takaya Nagai³, Asami Sano², Yusuke Seto⁴, Takahiro Kuribayashi⁵, Takanori Hattori², Hiroyuki Kagi¹

¹GCRC, The University of Tokyo, ²Japan Atomic Energy Agency, ³Hokkaido University, ⁴Kobe University, ⁵Tohoku University

Ca(OH)₂, portlandite, belongs to brucite-type layered hydroxides, which is considered to be a model structure of hydrous minerals. This has hydrogen bonds within the interlayer of CaO₆ octahedral sheets. Among the other isostructural hydroxides, Ca ion in portlandite has the largest cation size, which might cause unique pressure-induced phase transitions. Previous high-pressure studies reported that portlandite undergoes a phase transition to a high-pressure (high-P) phase at 6-8 GPa and room temperature [1-3], and it transforms into another high-pressure and high-temperature (high-PT) phase at >6 GPa, >200C [4,5]. The crystal structures of these unquenchable high-P and -PT phases have been determined to be different monoclinic phases by X-ray and/or neutron diffraction measurements. According to previous neutron diffraction studies of Ca(OD)₂, repulsive D...D interaction and hydrogen bonds in portlandite becomes much stronger under high pressure up to 4.5 GPa. However, there was no in-situ neutron observation on portlandite under much higher pressure and temperature conditions, where the high-P and -PT phases are stable. Therefore, hydrogen positions in the crystal structures of portlandite under corresponding such high-PT conditions are still unknown. In the present study, in-situ neutron diffraction studies under high-PT conditions were performed in order to clarify the hydrogen positions in these portlandite polymorphs.

An initial sample of powder Ca(OD)₂ was synthesized from a mixture of CaO powder and stoichiometrically excess D₂O in an autoclave at 220C for 4 days. High-PT experiments were conducted using a 6-ram press called "Atsuhime" at a new high-PT beamline "PLANET" combined with a pulsed-neutron source at MLF, J-PARC. The neutron diffraction patterns were measured at 8.3 GPa and 400C, 200C, RT during decreasing temperature. The obtained diffraction peaks were originated from only the high-PT phase of portlandite. The crystal structure parameters and atomic positions were refined by Rietveld analytical method using GSAS software. For a model structure of the high-PT phase, the parameters, of which structure was determined by neutron diffraction data at 10 K, 0.1 MPa by Leineweber et al., 1997 [5], were used.

The structure of the high-PT phase obtained at 8.3 GPa, 400C was $a = 5.076(1)\text{Å}$, $b = 5.985(1)\text{Å}$, $c = 5.763(1)\text{Å}$, and $\beta = 100.37(7)$. Each lattice parameter of a , b , c was larger than that of [5] by 6, 2, and 4%, respectively. The β angle was smaller by 3%. In contrast, among the current results, the lattice parameters and atomic positions including hydrogen was not largely fluctuated by temperature (400C, 200C, and RT) at 8.3 GPa. The isotropic temperature factor (U_{iso}) gradually increased with increasing temperature. Based on the obtained structure of the high-P phase accompanying the displacements of CaO₆ layers and Ca atoms from the original structure of portlandite. Comparing the structure of the high-PT phase to that of the high-P phase, the phase transition mechanism can be inferred. There might be at least two positions for hydrogen in the high-P phase, one of which changed from the original position to keep stable even after the formation of new Ca-O bondings. These results agree well with those from our previous Raman and IR absorption spectroscopy measurements of OH-bonds. Therefore, it is suggested that the hydrogen bonds in portlandite are strongly affected by the phase transitions, for which the role of hydrogen bonds might be a driving force.

References

- [1] Ekbundit et al., J. Solid State Chem., 126, 300-307 (1996)
- [2] Catalli et al., Geophys. Res. Lett., 35, L05312 (2008)
- [3] Iizuka et al., Phys. Chem. Minerals, 38, 777 (2011)
- [4] Kunz et al., High Press Res., 14, 311-319 (1996)
- [5] Leinenweber et al., J Solid State Chem., 132, 267-273 (1997)
- [6] Xu et al., Phys. Chem. Miner., 34, 223-232 (2007)
- [7] Xu et al., J. Solid State Chem., 180, 1519-1525 (2007)

Keywords: portlandite, hydrogen bond, phase transition, neutron diffraction, PLANET, high pressure

Hydrogen in portlandite -Neutron diffraction measurements at high pressure and high temperature-

Takaya Nagai^{1*}, Asami Sano², Riko Iizuka³, Hiroyuki Kagi³, Yusuke Seto⁴, Takahiro Kuribayashi⁵, Takanori Hattori²

¹Faculty of Science, Hokkaido Univ., ²JAEA, ³Univ. of Tokyo, ⁴Kobe Univ., ⁵Tohoku Univ.

Ca(OH)₂ is one of the simplest hydrous minerals. Because this type of structure is a component unit in complex hydrous phases such as chondrodite, it is important to understand structural behaviors at high pressure and high temperature. However, only a few previous researches can be found on crystallography of Ca(OH)₂ in the conditions of simultaneously high pressure and high temperature, although there were quite a few studies on EOS, phase relation, melting and so on, which were performed by using X-ray diffraction technique. Last year a brand-new TOF neutron beamline (PLANET) dedicated for high pressure and high temperature measurements started to operate in J-PARC, Japan. Ca(OH)₂ was selected as one of the first targeted materials measured at the PLANET.

Deuterated samples were prepared via hydrothermal treatment with CaO fine powders and excess D₂O water in a Teflon lined stainless steel autoclave at 493 K for 4 days. After the hydrothermal treatment was completed, precipitates were filtered out, washed with D₂O water, and then dried at 383 K under vacuum for 3 hours. The products were confirmed to have the CdI₂-type structure by conventional powder X-ray diffraction measurements and were checked to be deuterated by IR absorption spectra. TOF neutron powder diffraction measurements of Ca(OH)₂ were carried out from 300 to 773 K at about 3 GPa at the PLANET beamline in J-PARC, Japan. At first, temperature was increased to 773 K at about 3 GPa for annealing and then data acquisition was carried out at each temperature condition to lower temperature. The measurement time at each targeted P-T conditions was about 8 hour after the temperature reached equilibrium. Generation of high pressure and high temperature can be performed by using the 6-ram big press (Atsuhime) installed at PLANET.

Quality of diffraction patterns is surprisingly superior and only diffraction peaks from Ca(OH)₂ could be observed owing to radial collimators equipped with Atsuhime, although powder sample of Ca(OH)₂ was loaded into a cylindrical graphite furnace in ZrO₂ pressure medium cube. The detailed structure parameters such as lattice parameters and atomic coordinates were refined by the Rietveld method by using a program GSAS.

Keywords: hydrogen, portlandite, high pressure and high temperature, neutron diffraction, Atsuhime, PLANET

High pressure neutron diffraction of anhydrous and hydrous albite glasses and preliminary neutron imaging in PLANET

Toru Inoue^{1*}, Akihiro Yamada¹, Satoru Urakawa², Akio Suzuki³, Hiroshi Arima⁴, Hidenori Terasaki⁵, Osamu Ohtaka⁵, Takanori Hattori⁶, Asami Sano⁶

¹Geodynamics Research Center, Ehime University, ²Department of Earth Sciences, Okayama University, ³Department of Earth and Planetary Materials Science, Faculty of Science, Tohoku University, ⁴Institute for Materials Research, Tohoku University, ⁵Graduate School of Science, Osaka University, ⁶Japan Atomic Energy Agency

We, magma group, have conducted neutron diffraction experiment under high pressure first time on February 15-21, 2012. Samples were anhydrous and deuterated-hydrous albite glasses. We used semi-sintered ZrO₂ with a dimension of 17 mm cubic as pressure medium, and enclosed the samples which diameter were 4.6 mm in the center of the cell. The anvil truncation was 10 mm. We used Ni-doped WC anvil, and adopted 6-6 type compression system. The diffraction data were collected at 2.3 and 5.5 GPa in both anhydrous and deuterated-hydrous albite glasses, respectively. The measurement times at 2.3 and 5.5 GPa were 14 and 22 hours at the live times, respectively. In this experimental period, the beam intensity was about 290 kW; this intensity was about 1/3 of the expected intensity in J-PARC in the future. Moreover, the empty and the vanadium cells under each condition were also measured, and the sample diffraction pattern were corrected by those data. Details of the results will be presented.

Moreover, the exploratory experiment of neutron imaging was also conducted. Details of the results will be also presented.

Keywords: J-PARC, PLANET, neutron diffraction, amorphous material, neutron imaging, high pressure

Measurements of silica glass and water using a high-pressure diffractometer in J-PARC/MLF

Yoshinori Katayama^{1*}, HATTORI, Takanori¹, YAGAFAROV, Oscar¹, SAITOH, Hiroyuki¹, SANO, Asami¹, SUZUYA, Kentaro¹, CHIBA, Ayano²

¹JAEA, ²Keio Univ.

Neutron diffraction measurements at ambient conditions and at pressures of 2.3 GPa and 5.5 GPa at room temperature were carried out using a high-pressure neutron diffractometer, PLANET, installed in J-PARC/MLF. We compressed a sample in a ZrO₂ cube using a six-axis press by a 6-6 method. The size of the sample was 4.6mm in diameter and 6.7mm in height. The size of the incident beam was 2.5mm in width and 4.5mm in height. The pressure was estimated from the applied load. Clean diffraction patterns without diffraction lines from surrounding materials were obtained. Measurements on heavy water at ambient conditions were also carried out. We will try to measure heavy water at high pressures. The results will be also reported.

Keywords: neutron diffraction, glass, water, high pressure

Performance and the Current Status of the High-Pressure Neutron Diffractometer PLANET

Takanori Hattori^{1*}, Asami Sano¹, Hiroshi Arima⁵, Kazuki Komatsu⁴, Akihiro Yamada³, Takaya Nagai², Yoshinori Katayama¹, Toru Inoue³, Wataru Utsumi¹, Hiroyuki Kagi⁴, Takehiko Yagi³

¹JAEA, ²Hokkaido Univ., ³Ehime Univ., ⁴Univ. of Tokyo, ⁵Tohoku Univ.

The PLANET is the world's first neutron beamline specialized for high-pressure and high-temperature experiments. The most characteristic feature is the capability to investigate the state of the matter at high-pressure and high-temperatures up to 20GPa and 2000K with the multi-anvil high-pressure apparatus. The construction was started in 2008. The beamline was commissioned in the first half year of JFY 2012 and the new data is being taken by project members. This year, the beamline is reborn to a public beamline of J-PARC. In this talk, the performance of the PLANET and the typical results are introduced.

The resolution of the diffraction pattern ($\Delta d/d=0.6\%$) was found to be almost equal to the designed value(0.5%). The elimination of the background from the sample surrounding materials, which is the most important feature of the high-pressure experiments, was found to be accomplished with the use of the severe incident collimator and radial receiving collimator system. The beamline is opened for general users since the last half year of JFY2013 (from Feb.).

Keywords: high pressure, neutron

