

(iBIX)", which is now constructing at Materials and Life-science Facility (MLF) of J-PARC. STARGazer has several functional components; 1) peak search from the raw data, 2) determination of the UB matrix, 3) finding the Bravais lattice, 4) refinement of the UB matrix, 5) calculate the intensities of all Bragg reflections, and 6) data visualization. The algorithms of crystallographic fundamental functions of those components referred the algorithms of program ISAW, which is a data processing software package developed on Argonne National Laboratory. In addition, STARGazer has some additional functions optimized for the measurement of protein crystals on the iBIX; real-space indexing technique to find UB matrix, refinement of the detector position simultaneously in UB matrix refinement, and finding the Bragg reflections which are overlapping with neighboring reflections. In the near future, a function to deconvolute the overlapping Bragg reflections will be added. STARGazer was developed based on a software library "Manyo-Lib", which is a framework software for data analysis at MLF developed by J. Suzuki and co-workers. Each component of STARGazer works independently as a part of Manyo-Lib, and users of other instruments in MLF and other pulsed neutron facilities can easily use the components for their data processing.

Keywords: pulsed neutron diffraction, software for crystallography, protein crystallography

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The current status of iMATERIA - Versatile neutron diffractometer at J-PARC

Toru Ishigaki¹, Akinori Hoshikawa¹, Masao Yonemura¹, Kenji Iwase¹, Dyah S Adipranoto¹, Tuerxun Wuernisha¹, Takashi Morishima², Ryoko Oishi², Takashi Kamiyama², Kazuya Aizawa³, Masatoshi Arai³, Makoto Hayashi⁴, Kazuhiro Ebata⁴, Yoshiki Takano⁴, Takuro Kasao⁴

¹Ibaraki University, Frontier Research Center for Applied Nuclear Sciences, 4-12-1 Nakanarusawa, Hitachi, Ibaraki, 316-8511, Japan, ²Neutron Science Laboratory, KEK, 2-4 Shirakata-Shirane, Tokai, Ibaraki, 319-1195, Japan, ³J-PARC Center, JAEA, 2-4 Shirakata-Shirane, Tokai, Ibaraki, 319-1195, Japan, ⁴Ibaraki Prefecture, 978-6 Kasahara, Mito, Ibaraki, 310-8555, Japan, E-mail: to_ishig@mx.ibaraki.ac.jp

Ibaraki prefecture, the local government of the area for J-PARC site in Japan, was decided to build a versatile neutron diffractometer (IBARAKI Materials Design Diffractometer, iMATERIA) to promote an industrial application for neutron beam in J-PARC. iMATERIA is planned to be a high throughput diffractometer so that materials engineers and scientists can use this diffractometer like the chemical analytical instruments in their materials development process. It covers in d range $0.18 < d (\text{\AA}) < 5$ with $\Delta d/d = 0.16\%$ at high resolution bank, and covers $5 < d (\text{\AA}) < 800$ with gradually changing resolution at three detector bank (90 degree, low angle and small angle). Typical measuring time to obtain a 'Rietveld-quality' data is several minutes with the sample size of laboratory X-ray diffractometer. To promote industrial application, a utilization system for this diffractometer is required. We will establish a support system for both academic and industrial users who are willing to use neutron but have not been familiar with neutron diffraction. The analysis software is also very important for powder diffraction, we will also prepare a software package consisting of combination of several powder-diffraction software, structural databases and visualization. The construction of iMATERIA was completed, as one of day-one instruments for J-PARC. The recent data of iMATERIA will be reported.

Keywords: neutron powder diffraction, industrial applications, materials design

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Impact of modern neutron powder diffraction instrumentation on the study of hydrogenous materials

Paul F Henry¹, Mark T Weller², Chick C Wilson³, Valeska P Ting², Marc Schmidtman³

¹Institut Laue-Langevin, 6 Rue Jules Horowitz, Grenoble, Isere, 38042, France, ²Chemistry School, University of Southampton, Highfield, Southampton, SO17 1BJ, UK, ³Department of Chemistry and WestCHEM research School, University of Glasgow, Joseph Black Building, Glasgow, G128QQ, UK, E-mail: henry@ill.fr

Traditionally, the collection of powder neutron data from hydrogenous materials has been considered largely fruitless due to its large, wavelength variable incoherent scattering contribution. This, coupled with relatively low neutron fluxes, has led to disproportionately long counting times for the quality of data collected. Practically, deuteration is often assumed to be a prerequisite for a powder neutron experiment. However, in many cases, deuteration profoundly changes the properties of the material under investigation or leads to observation of completely different structures and phase behaviour due to the role of the hydrogen bonding. Materials of technological interest in the fuel cell, hydrogen storage, mineral and fast ion-conduction areas are currently hot topics in solid-state materials research. In these materials, the position of the hydrogen and its interaction with the host lattice are of utmost importance to understand the observed physical properties. As the majority of the host materials contain heavy atoms, locating the hydrogen positions and following their evolution using X-ray diffraction techniques, even using the high fluxes of a synchrotron source, is impossible. With the advent of very-high flux, variable resolution powder neutron diffractometers such as D20 at ILL, GEM and the upgraded HRPD and POLARIS diffractometers at ISIS, WOMBAT at Opal and POWGEN at SNS as well as planned new instruments worldwide, the feasibility of studying hydrogenous materials with powder neutron diffraction needs to be revisited. The power of the currently available instruments will be illustrated using a range of example materials from our ongoing collaborative research and instrumental development programme at ILL.

Keywords: hydrogen compounds, powder diffraction techniques, *in situ* powder diffraction

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TOPAZ: A new time-of-flight laue diffractometer for new science

Christina Hoffmann¹, Robert Bau², Arthur Schultz³, Thomas Koetzle³, Paula Piccoli³

¹Oak Ridge National Laboratory, Neutron Scattering Sciences Division, P.O.Box 2008 - MS 6475, Oak Ridge, Tennessee, 37831, USA, ²University of Southern California, Los Angeles, CA, USA, ³Intense Pulsed Neutron Source, Argonne National Laboratory, Argonne, IL, USA, E-mail: hoffmanncm@ornl.gov

A next generation single crystal neutron diffractometer, TOPAZ, is currently under construction at SNS and is scheduled to be complete by early 2009. After a short commissioning period the instrument