(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

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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 $0.18 < d$ (Å) < 5 with $\Delta d/d = 0.16$ % at high resolution bank, and covers $5 < d$ (Å) < 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

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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-fight laue diffractometer for new science

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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 will be open for general user access. TOPAZ will be a time-of-flight Laue diffractometer using a polychromatic incident beam to collect a full data set of Bragg peaks in a matter of tens of minutes rather than hours. The instrument will be optimized for high through-put small molecule crystallography of moderately sized and complex unit cells (up to around (50 Å)^3). To achieve this goal, custom designed focusing optics are employed for incident beam transport to the sample. Highly pixilated Anger detectors have been developed, and a novel sample positioning and loading scheme will be presented. The combination of innovative development in all areas of the instrument will enable TOPAZ to measure data from standard X-ray size crystals with an order of magnitude decrease in measurement time compared to current instruments. Various sample environments will be available including cryogenic cooling, heating, and magnetic fields. The magnetic field environment coupled with the planned polarized neutron option will allow for future experiments investigating magnetic structure and phase transitions in materials. This research is supported by UT Battelle, LLC under Contract No. DE-AC05-00OR22725 for the U.S. Department of Energy, Office of Science.

Keywords: ToF Laue diffractometer, neutron single crystal diffraction, high throughput crystallography

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First results from the KOALA neutron Laue instrument

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The KOALA instrument is a single-crystal Laue diffractometer optimised for small molecule structural studies and based on a cylindrical image-plate detector. Compared to monochromatic instruments, much smaller samples (0.1 - 1 mm) can be used due to the high beam flux and the large coverage of the detector. The instrument is well suited to studies performed at multiple temperatures. The typical sample environment is a CCR with a hot-stage that provides sample temperatures from 4 to 800K. Electric-field and gas charging/discharging experiments are also possible, and a high-pressure capability will be available in the near future. The KOALA instrument has been installed and awaits the scheduled restart in May 2008 of OPAL, the new Australian research reactor. Commissioning will extend over a three month period from the reactor startup. Early results from the instrument will be presented. In particular, a comparison will be made between KOALA and the VIVALDI instrument at the ILL, on which KOALA was based. Access to KOALA is typically via a 6-monthly peer review of proposals. No access charges are made for non-proprietary research. International users are encouraged to apply.

Keywords: neutron instrumentation, single-crystal diffraction, small molecular crystallography

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Mismatch cobaltite lattices investigated by white beam neutron diffraction

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The majority of all single crystal diffraction data is collected using monochromatic sources as this eases the step from measured intensities to corrected intensities. Synchrotrons have continuously pushed the limit for what can be considered a single crystal, recently a nano-porous crystal of a few micron was investigated using a microfocused X-ray beam of 1 mu m.[1] The advances in X-ray single crystal diffraction at synchrotrons have been aided by the abundant flux and improvements of optical elements. Reactor based neutron sources have only seen minor improvements in flux compared to synchrotrons and the nature of the neutrons makes it difficult to construct optical devices. However, advances in area detectors systems and white beam diffraction methods have allow a considerable reduction of crystal size need for a neutron diffraction experiment. The size has been reduced by about two orders of magnitude from about 1 mm^3 to 0.01 mm^3. This is by no means comparable to the improvements of synchrotrons, but it allows neutron investigation of single crystals suitable for laboratory X-rays. The possibility of using relative small crystals allow exploiting the complementarities between X-rays and neutrons, without going through the effort of growing large single crystals for the neutron experiment. We present data from Laue diffraction instruments: Vivaldi, ILL and KOALA, at the new reactor source OPAL, Australia. The white beam Laue technique has been employed to elucidate the oxygen positions in layer misfit cobaltite of small single crystals V of about 0.01 mm^3. The high intensity of the white beam and the large coverage by the cylindrical area detector are crucial for reasonable data collection times.

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Keywords: Laue diffraction, neutron diffraction techniques, mixed layer compounds

P1

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Unconventional single crystal diffraction studies with hot neutrons on HEiDi at FRM II

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The instrument HEiDi at the neutron source Heinz Maier-Leibnitz (FRM II) uses hot neutrons for single crystal diffraction analysis of structural and magnetic properties of samples for which other methods are not applicable. Multiferroic compounds like $REMnO_3$ (RE=Dy, Gd) whose highly absorbing and heavy rare earth elements make it normally extremely difficult to get accurate structural and magnetic diffraction data are good examples for the unique capabilities of this instrument using both large penetration depth and large q range [1]. This contribution shows an overview of the instrument (like gain factor from hot source, see figure and [2]) and its applications in different fields of solid state physics, chemistry and crystallography concerning structural details (highly accurate atomic positions, anisotropic mean square displacements, phase transitions, local disorder, magnetism, etc.).

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