a new basic life science fields as well as applied industries. To achieve the performance mentioned as above, the diffractometer will be installed on a coupled moderator which has more intense peak and integrated intensity but wider pulse shape than a decoupled moderator. It is expected that some neighbor Bragg spots will overlap partially each other along the time-axis. The overlapping of Bragg spots along the time-axis should be considered for the optimization of design parameters and It is necessary to de-convolute the overlapped spots in order to obtain a data set that has a quality good enough to identify hydrogen atoms in biological macromolecules. The three original simulation programs of TOF diffraction data with designed parameters of the diffractometer were developed to obtain information of spot-overlapping, completeness of Bragg spots and spot profiles along time-axis. The consideration of important designed parameters (divergence of incident neutron beam to a sample crystal, the distance between sample and detector surface and the best detector configuration) focused on biological macromolecular, the strategy of data collection and de-convoluting overlapped spots will be reported based on the results of simulation by using the simulation programs mentioned as above.

Keywords: J-PARC, neutron TOF diffractometer, protein crystallography

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Optics and shielding of IBARAKI Biological Crystal Diffractometer (iBIX) in J-PARC

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A novel neutron diffractometer for biologically important materials proposed by Ibaraki Prefecture Government in Japan, iBIX is currently in the construction stage at J-PARC. The optics of iBIX has been optimized by preliminary analytical estimation and the following simulation with McStas program. In this design neutrons from a coupled moderator are guided through a 17m-long and curved super mirror guide (radius of curvature = 4,300m) and a 8m-long and straight super mirror guide. The super mirror guides has tapered shape in part in vertical and horizontal directions and consist of mirrors with a variety of the critical wave number. Finally, neutrons are projected on the 1mm2 area at the sample position 40m far from the moderator with a half-angle divergence of 0.25deg. On the other hand, PHITS Monte Carlo simulator has been used to design the shielding around the guide and the detector. Using this program the estimation of background at the detector position has been also attempted to optimize slit geometry.

Keywords: J-PARC, neutron TOF diffractometer, protein crystallography

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Development of a new detector and DAQ systems for iBIX

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iBIX is a new single-crystal neutron diffractometer using the time-of-flight method (TOF) for biological and chemical crystallography, and is now being constructed at BL03 in J-PARC/MLF. This diffractometer is designed to cover the sample crystals from organic small molecules to biological macromolecules with maximum 150Å of cell dimension, therefore the Bragg peaks will be observed in high density. Detector system of iBIX is required high spatial/time resolutions to integrate these peaks accurately, and large detective region to cover the solid angle as large as possible. To realize these performances, we have been developing a new photon-counting 2D detector system and a new TOF data-acquisition (DAQ) system. The detector system is composed of two ceramic ZnS scintillator sheets, 256×2 wavelength-shifting fibers (WLSF), eight 64ch multi-anode photomultipliers (PMT), a high-speed 512ch amplifier & discriminator, and a 512ch encoder module with FPGA for time and coincidence analyses. The scintillator sheets have high detection efficiency, 30% and 45% at 1.8Å for 0.2 and 0.3 mm thickness, respectively. The WLSFs are arranged along X and Y directions with 0.02 mm gap; therefore the size of one pixel is 0.52 mm. The PMT have 17% of quantum efficiency for the light from WLSF. The detective region (133×133 mm^2) has more than 66% in the front face of the detector. The amplifier & discriminator module has 300MHz of frequency band, fixed gain (60), and 20-300 mV discrimination levels. The encoder module has many coincidence modes including various pattern-matching methods and a centroid computation method. The pulse-pair resolution is 4-5 μs. For the DAQ module, the recording rate is 5×10^5 event/s for the event mode.

Keywords: J-PARC, neutron TOF diffractometer, neutron detector

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Development of data processing software for a TOF single crystal neutron diffractometer at J-PARC

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For a single crystal diffractometer, a data processing software which extracts a HKLF list from raw data is one of the most important components. We have developed a new data processing software, named “STARGazer”, for a new TOF single crystal neutron diffractometer, “IBARAKI Biological Crystal Diffractometer

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(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