

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 mm²) 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 × 10⁵ 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