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The present talk describes novel powerful imaging for X-ray fluorescence (XRF) and X-ray diffraction (XRD). So far, the scanning-type imaging has been widely used in those techniques. Though recent progress in high-spatial-resolution imaging using synchrotrons is significant, there have been a clear limit; because of the step-scan, the imaging requires a long measuring time. In many scientific applications, X-ray imaging that are much more rapid, e.g., capable of high-speed resolution have been demanded. It is possible to do X-ray imaging without performing any scans. Here, the method uses quite a wide beam, which illuminates the whole sample surface in a low-angle-incidence arrangement (0.5~3 deg). The detector used is a CCD camera working at 30 fr./sec, equipped with a collimator inside, and the distance between the sample surface and the detector is set extremely close, in order to enhance both spatial resolution and efficiency. Note that the imaging is done with one shot. In the case of XRF imaging, distinguishing elements are required and, therefore, most of the experiments were performed with monochromatic or quasi-monochromatic X-rays. The procedure for XRD imaging uses a combination of exposure and incident X-ray energy scan (or just tuning). Since the present experiment employs a fixed small-angle incidence and also a fixed diffraction angle of around 90 deg, the diffraction plane here is inclined at about 45 deg from the surface of the specimen. By scanning the energy of the incident X-rays, one obtains a diffraction peak, which corresponds to the lattice spacing. Further instrumental details and many applications will be presented.

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Keywords: X-ray imaging, rapid X-ray measurement system, CCD detectors

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Low noise multichannel ASIC for readout of SSD used in diffraction for powder and multilayer samples

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We present 64 channel integrated circuit designed in CMOS 0.35 μm technology for readout of silicon strip detector used in X-ray diffractometry applications. This integrated circuit called DEDIX (Dual Energy Digital Imaging of X-rays) connected to silicon strip detector works in a single photon counting mode and is able to select photons from a given energy window. The main parameters of this ASIC are low noise performance (110 el. rms for Cdet=1pF), high count rate capability (up to 1 Mcps/channel) and very good channel to channel uniformity (effective threshold spread below 7 el. rms). Using the ASICs we have built several 128-channel modules with silicon strip detectors of different strip length (1 or 2 cm) and different strip pitch (50 μm, 75 μm and 100 μm). We have used these modules in diffractometry applications as a replacement of a proportional counter. The measurements were speeded up by over 100 times when using our module. These modules have been tested using different samples, where we compare: results obtained with and without photon selection in a given energy window, the influence of silicon detector strip pitch, measurement, when the module fixed on the diffractometer arm is moving in step or continuously scan mode. We also performed some measurements of multilayer structures, and due to low noise, good uniformity of channels and high rate capability, the measurement time have been significantly reduced without loosing the diffractogram quality.

Keywords: silicon strip detector, integrated circuit, DEDIX

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A new biological neutron diffractometer (iBIX) in J-PARC

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Since 2004, Ibaraki Prefectural Government in Japan has started to construct a TOF neutron diffractometer for biological macromolecules for industrial use at J-PARC, near JRR-3 in JAEA. From December in 2008, Ibaraki University will operate this machine with a support of Ibaraki Prefecture. The diffractometer is designed to cover sample crystals which have their cell edges up to around 150 Å. It is expected to measure more than 100 samples per year if they have 2mm^3 in crystal volume. The efficiency is more than 100 times larger than the present high performance diffractometers, BIX-4 in JRR-3 reactor in JAEA. To realize this performance, a coupled moderator (intense neutrons, but broad pulse in time resolution) was selected. In addition, two important and key items should be developed; a new detector with high spatial resolution (less than 1mm) and a special software to de-convolute overlapped Bragg reflections in data reduction. The detector uses ZnS:Ag/^{6}LiF scintillator with wavelength-shift-fiber (WLSF) system. The software has been designed using a complicated kind of profile-fitting method. The current status of the construction and developments will be reported.

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

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Optimization of design parameters of IBARAKI Biological Crystal Diffractometer (iBIX) in J-PARC

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IBARAKI prefecture in Japan has started to construct the TOF neutron biological diffractometer (IBARAKI Biological Crystal Diffractometer: iBIX) for industrial use at BL03, MLF in J-PARC. The diffractometer is designed to cover the samples have their cell edges up to around 150 angstrom and to achieve the efficiency which is more than 100 times larger than the present high performance diffractometer, BIX-3 (JRR-3, JAEA, Japan) in order to pioneer 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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