P01.08.65

Anniversary - 10 years of McStas for instrument design and science

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Since 1998, the McStas neutron ray-tracing simulation package <http://www.mcstas.org/> has been hosted at RISØ in strong collaboration with the current leading european neutron facility at ILL, Grenoble. During its lifetime, McStas has evolved to become the world leading software in the area of neutron scattering simulations for instrument design, optimisation, virtual experiments and science. This poster presents a selection of the most important achievements during the last decade, with main focus on diffractometers and crystallography.

Keywords: neutrons, instrument design, virtual experiments

P01.10.66

Development of curved position-sensitive neutron detectors for FCD at HANARO

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Four Circle Single Crystal Diffraction experiments need long scanning time for the single detector in scanning mode and it is always preferable to opt for single large area position sensitive detector covering the maximum angular scattering region and reduce the experimental duration and reactor beam utility time. In spite the fact that tube detector is accompanied with very compact and simple data acquisition setup, the experiment runs for the days and weeks at stretch. The 2-Dimensional Position-Sensitive Detector for FCD with effective window of 19x19 cm2 is initially developed and tested. The sensitive area coverage and parallax was improved by development of curved larger area 2-D PSD which covers 70 degree in horizontal direction and 45 degree in vertical one, respectively. Its preliminary result showed that the Curved structure worked as designed but the characteristic capacitance of the whole detector volume becomes larger than the designed value due to the cathodes' plane structure. Basic properties based on the plateau measurement and measuring capability from the short time diffraction measurements mentioned above on step scan and oscillation modes showed promising perspectives.

Keywords: position-sensitive detectors, neutron detectors, single-crystal diffraction

P01.10.67

Single crystal structure analysis by neutron 2D-PSD

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In the field of X-ray single crystal structure analysis, the measurement by area detector such as Imaging Plate and CCD has already prevailed. On the other hand, there is rare case using area detector by neutron. Recently, 2 dimensional position sensitive detector (2D-PSD) with a high detection efficiency and spatial resolution has been developed by Korea Atomic Energy Research Institute group. In the case of materials which has low symmetry and large unit cell, it is expected that this area detector becomes much more powerful for structure analysis comparing with a conventional method by point detector. We thus tried crystal structure analysis of several interesting samples, NaCl, MnF_2, $DyMnO_3$, β'-ET_2ICl_2, and Lupene. The neutron diffraction experiment by 2D-PSD is performed at guide-hall T2-2 port of the JRR-3M reactor at Japan Atomic Energy Agency. Wavelength was set to 1.2451Å by Ge311. Figure 1 shows the oscillation image of β'-ET_2ICl_2. We developed the program for handling the data, such as ¨peak-search¨, ¨assignment of HKL indices¨, and ¨acquisition accurate intensity¨. Details of this program and the results of structure analyses will be introduced in the conference.
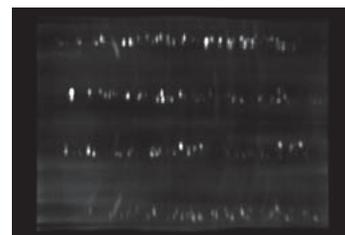
Keywords: area detector instrument, neutron diffraction techniques, neutron structure analysis

P01.10.68

Pixel array detectors for high count rate X-ray imaging

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In a pixel array detector, an efficient x-ray detection layer is coupled pixel-by-pixel to an underlying signal processing CMOS chip. By properly designing the in-pixel signal processing electronics within the CMOS chip, one can tailor the detector to a variety of x-ray imaging problems. The Cornell x-ray detector group has been developing a series of imaging devices which operate at high instantaneous count rates per pixel. Pixel architectures in the various generations of devices include multi-frame storage to record transient events on microsecond timescales, extended dynamic range imaging using combined digital and analog techniques, electronic shuttering for synchrotron bunch isolation, and high-speed, low-noise imaging from sub-picosecond x-ray pulses.

Keywords: X-ray detectors, detector development, time-

resolved X-ray diffraction

P01.11.69

Shutter-less continuous rotation data collection from protein crystals with the X-ray CMOS detector

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The fine phi-sliced oscillation method is expected to be useful for high S/N data collection in protein crystallography. However, a small oscillation step increases total number of diffraction images and the experiment time gets longer due to the readout time of detectors. In order to enable efficient data collection with the fine phi-sliced method, we proposed shutter-less continuous data collection using an X-ray CMOS detector. In this method, diffraction images are captured by the X-ray CMOS detector with a constant frame rate, as rotating crystal in a constant speed. The shutter is kept open during data collection. The characteristic feature of the X-ray CMOS detector is rapid readout speed, and so dead time due to readout is negligible. We have been developing the X-ray CMOS detector suitable for protein crystallography in collaboration with Hamamatsu Photonics K.K. (Japan). The performance of our data collection method was examined at SPring-8 protein crystallography beamlines. Comparison with the conventional coarse oscillation method with a CCD detector demonstrated that the data processing statistics was significantly improved by this method. We also successfully determined protein structures with MAD and SAD phasing using diffraction data recorded with this method. Our results demonstrated that the shutter-less continuous rotation method with the X-ray CMOS detector has a promising potential in protein crystallography.

Keywords: protein cryocrystallography, detector development, data collection methods

P01.10.70

Novel pixel detector for in-house XRD applications

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A novel pixel detector, namely PILATUS 100K, has been developed at the Paul Scherrer Institut (PSI). It is constructed using the state-of-art semiconductor technology and demonstrates superb performance. Its single photon counting, extremely low background, very short read-out time and ultra-high count rate features are not like the other conventional area detectors. The PILATUS detector was initially designed for macromolecule study at synchrotron facilities. However, the PILATUS 100K can be used with in-house XRD system. Some of the in-house XRD application results will be shown.

Keywords: hybrid pixcel detector, XRD, SAXS

P01.10.71

Protein diffraction experiments with Atlas CCD detector

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A combination of an enhanced Cu x-ray source and of a recently acquired Atlas single chip CCD detector brings new possibilities for in-house x-ray diffraction experiments on protein samples. Introductory measurements and comparative studies regarding the performance of the CCD detector with high sensitivity, dynamic range and fast readout were performed with protein samples such as xylanase from Trichoderma reesei. Diffraction data sets of high quality were collected, including those of human CD69 receptor and other study targets. Diffraction data were processed by alternative methods. The results suggest that the Gemini Enhanced Ultra diffractometer with the Atlas CCD detector offers a viable option for in-house diffraction experiments and characterisation of protein samples before synchrotron experiments. Moreover, macromolecular diffraction data with the total Rint < 0.03 up to diffraction limit 2.0 Å can be achieved. Data processing was performed with use of the instrument software Crysalis as well as with the standard protein crystallographic software Mosflm and Scala.

Keywords: X-ray data collection, CCD detectors, protein crystallography applications

P01.11.72

The XPAD3 hybrid pixel detector applications

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The 3rd generation synchrotron sources have been a major progress in materials sciences. The hybrid pixel detectors have been developed to take a full profit of the intense monochromatic X-ray beam provided by these sources. Following the previous XPAD detectors [1] design the XPAD3 hybrid pixel detectors has been designed with a pixel size of 0.130 mm x 0.130 mm[2]. First detectors using wide Si sensors of 15 mm x 76 mm, 0.500 mm thick, are under assembly, they consist in 8 modules of 7 chips. Some others detectors have been realized using CdTe sensors and a dedicated test board allowing to connect 2 chips to the monolithic CdTe sensors [3]. This poster will report on tests carried out on single chip and single module Si detectors and CdTe detector. Using Si sensors, the XPAD3 chip can be used from low energy (4keV) up to 25 keV where the detector efficiency becomes too weak. The CdTe detector was designed to improve the efficiency at high energy and to allow 60 keV X ray to be used, but it can be still used at low energy and data have been