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resolved X-ray diffraction

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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

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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-ofart 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

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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.

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

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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