the subperiodic layer and rod groups (International Tables for Crystallography, Vol. E: Subperiodic groups) and their maximal subgroups. The symmetry information has been stored in XML and provisional CIF formats. For the extension of the existing CIF-core dictionary a list of data names has been developed which refer to the specific requirements of the subgroups and supergroups of space groups [2] and subperiodic groups. The accompanying software is divided into several shells according to its complexity and proximity to the information contained in the database core. Symmetry data as generators and general positions, Wyckoff-position data and maximal subgroups of space and subperiodic groups are retrieved directly from the databases by simple tools. There are a number of online applications for problems involving group-subgroup relations between space groups: subgroups and supergroups of space groups, graphs of maximal subgroups for an arbitrary group-subgroup pair, Wyckoff-position splitting schemes for group-subgroup pairs, etc. More specialized crystallographic software is also available and is distributed according to different topics: representation theory, solid-state physics and crystal chemistry applications.

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Keywords: bilbao crystallographic server, CIF, symmetry databases

MS.96.5

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publCIF: A complete crystal structure publishing environment for authors

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The program system publCIF [1] is a fully-featured editor allowing authors to modify and add content to a Crystallographic Information File (CIF) for publication in an IUCr research journal, or in a number of other formats. The user interface offers synchronised WYSIWYG ('what you see is what you get') and raw file views of the CIF, with syntax and dictionary-based attribute validation. The editor has recently been enhanced in several ways. It allows interaction through web services with the online checkCIF validation system (including insertion, where appropriate, of a suitable validation reply form). Work is in hand to offer intelligent handling of graphics files supplied as illustrative figures to accompany an article. Most recently it has been developed to allow interactive three-dimensional visualization using the open-source application Jmol [2], including an editing toolkit to permit authors to create enhanced interactive figures and animation for online publication. Current developments are aimed at providing similar functionality to mmCIF submissions of biological macromolecular structure reports. To meet the specific requirements of the IUCr journals, the current software architecture of publCIF is largely procedural, but the development of an engine to validate dictionary attributes offers the possibility of increased methods-driven functionality with future versions of CIF. Meeting the requirements of publCIF would provide a useful development target for the new methods-based dictionary definition language DDLm.

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Keywords: CIF, publishing, software

MS.97.1

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Performance of micro pixel gas chamber in small angle X-ray scattering experiments

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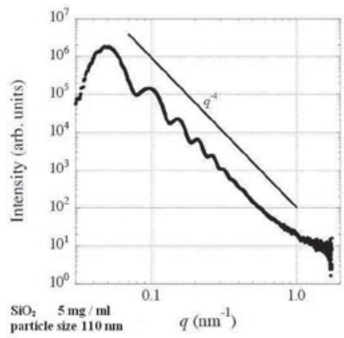
We report on the development a two-dimensional photon-counting detector based on a Micro Pixel Gas Chamber for high-resolution Small Angle X-ray Scattering (SAXS). The Micro Pixel Gas Chamber is a micro-pattern gaseous detector fabricated with printed circuit board technology. Here a 10 x 10cm Micro Pixel Gas Chamber was used, and we have demonstrated a position resolution of 120 um (RMS). Photon-counting detectors provide only statistical uncertainty as background. For this reason, photon-counting detectors are expected to achieve a higher dynamic range than CCDs and Imaging Plates. We performed SAXS experiments using nanoparticles (SiO_2) at SPring-8 and obtained a dynamic range of over 10^5. This result implies that our detector could provide high-resolution SAXS. The maximum counting rate of 5 MHz was achieved without saturation.

We performed a time-resolved experiment at the KEK photon factory. We observed the dehydration reaction of pyromellitic acid hydrate. The transition state was observed for several seconds. We also report on the performance of a large Micro Pixel Gas Chamber with a detection area of 30 x 30cm.



Keywords: gas sensors, imaging detectors, X-ray detectors

MS.97.2

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High speed readout of microgap X-ray detectors

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Since their introduction in 2004, microgap detectors have become a standard detector technology for powder diffraction and are now seeing increasing use for SAXS/WAXS and single crystal diffraction as well. Microgap detectors are true photon-counting detectors with quantum-limited sensitivity, zero noise, moderate energy resolution and zero readout deadtime. Compared to other photon-counting, imaging detector technologies, microgap detectors are significantly less expensive and also have the advantages of having no internal dead areas, not suffering from charge sharing at pixel boundaries and not requiring cooling. Because of their very high sensitivity they are ideal detectors for working with very small, weakly diffracting samples. However, to date these detectors have employed delay-line-based readout electronics which have limited their global counting rate to less than about 2 million X-rays/sec. While this is acceptable for most laboratory experiments it is clearly too slow for many beamline experiments. We have therefore undertaken a collaboration to develop a much faster readout based on the BLADE3 readout system developed at the ESRF. We report on the operating characteristics of the microgap detector and the design and characterization of the fast readout system.

Keywords: X-ray detector technology, area detectors, photon-counting detectors

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The PILATUS detectors: Hybrid pixel detectors for synchrotron and industrial applications

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The PILATUS detectors are large area, single photon counting hybrid pixel detectors. PILATUS detectors were developed at the Paul Scherrer Institut (PSI) in Switzerland for the Swiss Light Source. ron light sources as well as for in The detector technology was commercialized by DECTRIS Ltd., a spin off company of Paul Scherrer Institute. The detectors are based on the CMOS hybrid pixel technology, where silicon pn-diode arrays are coupled to CMOS pixel chips. This technology has major advantages: 1) Direct detection of the X-rays in the silicon leading to excellent quantum efficiency and a point spread function of one pixel, 2) single photon counting processing of the X-rays leading to noise-free data. The PILATUS modules are assemblies of 16 CMOS chips bump-bonded to one silicon sensor, with 487 x 195 pixels of 0.172 x 0.172 mm^2 leading to an area of 8.4 x 3.4 cm^2 . With more than 6 million pixels covering an area of 43.1 x 44.8 cm^2 the Pilatus 6M detector is the largest such device constructed to date. The detector is comprised of 60 modules, which are mounted on a precision frame. The main feature of the detector is its dynamic range of 20 bits, i.e. more than 1 million X-rays can be stored in each pixel. A massive parallel readout of the detector results in a readout time of 3.6 ms and a frame rate of 12 Hz is achieved. Other important features are the narrow point spread function, the absence of electronic noise, an electronic shutter and the possibility to suppress fluorescent background from the sample. The Pilatus 6M is in operation since spring 2007 at the protein crystallography beamline X06SA of the SLS. The detector is an order of magnitude faster than comparable CCDs and produces data of unprecedented quality.

Keywords: pixel detectors, protein crystallography, single photon counting

MS.97.4

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Monolithic active-matrix silicon X-ray detectors

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Two types of X-ray Active Matrix Pixel Sensor (XAMPS) were designed and fabricated: one, based on J-FET technology, has a pixel size of 90um, is 400um-thick and was fabricated at Brookhaven National Laboratory (BNL); the other, based on PMOS technology, has a pixel size of 60um, is 725-um thick and was fabricated at IBM's T. J. Watson Research Center. The prototypes are square matrices with n rows and n columns with n=16, 32, 64, 128, 256, 512 for the BNL production and n=32, 64, 128, 256, 512, 1024 for the IBM one. The XAMPS is a position sensitive ionization detector made on high resistivity silicon. It consists of a pixel array detector with integrated switches. Pixels are isolated from each other by a potential barrier and the device is fully depleted by applying a high voltage bias to the junction on the entrance window of the sensor. When the photon is absorbed, the generated electron charge drifts to the exit side of the device and is stored on a capacitor which occupies most of the pixel area. The switches are opened during this phase (data accumulation) and then closed (data readout) to allow the charge to flow to the drain, connected to readout lines. This sensor is highly efficient at the typical range of energy of interest for protein crystallography. It has ~100% fill factor, low noise, millisecond readout, single photon sensitivity and a dynamic range of more than 104 photons per frame. It can be tiled to form bigger area detectors. Future developments could include on-pixel amplifier or small 3T (three-transistors) design.

Keywords: active pixel detectors, protein crystallography, position sensitive

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The 2D X-ray detector development program for the European XFEL

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The European X-Ray Free Laser Facility (XFEL) poses extreme challenges to the design of the 2D imaging detectors, their readout electronics and the data acquisition architecture. Up to 30,000 photon pulses per second, each offering unprecedented intensities in the order of 10^{12} photons per pulse with quasi instantaneous energy deposition require the adoption of novel detector and readout schemes. The large variability in the pulse patterns and the relatively large pulse to pulse variations inherent in the FEL pulse generation process need to be coped with. The requirements from the scientific instruments for the detectors focus on size, granularity, signal to noise and dynamic range. The high intensity environment poses new challenges with respect to radiation hardness, detection speed and frame rate capabilities. One 2D X-Ray detector with 1k by 1k pixels and a readout frame rate of 5000 per second will generate approximately 10Gbyte of data per second, requiring complex architectures to direct the data flow to storage. In this contribution, the development program for the different 2D X-Ray imaging detectors for the European XFEL and the related data acquisition and control architecture will be described.

Keywords: detector development, imaging, flat panel