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

Brian McMahon, Simon P. Westrip
International Union of Crystallography, 5 Abbey Square, Chester, Cheshire, CH1 2HU, UK, E-mail：bm@iucr.org

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

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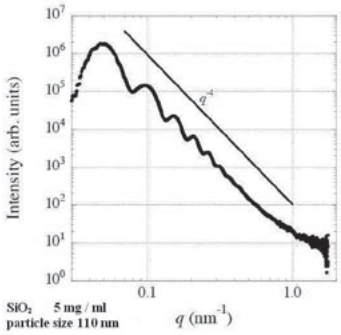
Performance of micro pixel gas chamber in small angle X-ray scattering experiments

Kaori Hattori[1], Kotaro Fujii[3], Kazuki Itoh[2], Hidetoshi Kubo[1], Kentaro Miuchi[1], Masaki Takata[2,4], Toru Tanimori[1], Ken'ichi Tsuchiya[1], Hidehiro Uekusa[3]
[1]Kyoto University, Physics, Kitashirakawa-Oiwake-Cho, Sakyo-Ku, Kyoto City, Kyoto Prefecture, 606-8502, Japan, [2]Structural Materials Science Laboratory, RIKEN Harima Institute/SPring-8 Center,1-1-1 Kouto, Sayo-gun,Hyogo 679-5148, Japan, [3]Department of Chemistry and Materials Sicence, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro, Tokyo 152-8551, Japan, [4]SPring-8/JASRI , 1-1-1 Kouto, Sayo-cho, Sayo-gun, Hyogo 679-5148, Japan, E-mail：hattori@cr.scphys.kyoto-u.ac.jp

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

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High speed readout of microgap X-ray detectors

Roger D Durst[1], Yacouba Diawara[1], Matt Benning[1], Bruce Becker[1], Vladisov Sedov[1], Greg Wachter[1], Menhard Kocsis[2], Christian Herve[2], Pablo Farajado[2]
[1]Bruker AXS Inc., 5465 E. Cheryl Parkway, Madison, WI, 53711, USA, [2]ESRF, Grenoble, France, E-mail：roger.durst@bruker-axs.com

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