

times as they occur; the design is based on the existing design for the beam position monitor [1]. We use a Uniblitz x-ray shutter with a PtIr blade located downstream of the beam defining slits. The device is operated in air with He flowing into it from an attached scatter guard.

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[1] Alkire R. W., Rosenbaum Gerold, Evans G., *J. Synch. Rad.*, 2000, 7, 61.

Keywords: synchrotron, instrumentation, timing-shutter

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An X-ray Chopper for Time-resolved Crystallography

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A chopper has been developed for time-resolved (pump-probe) x-ray crystallography, with pulse lengths continuously adjustable from DIAMOND single bunch extraction (3µsec) to 45% of rotation time (45msec at 10Hz). Rotation frequency can be DC to 50Hz. This allows access to all time windows from hours to picoseconds. The chopper transmits 0.002% of flux at 25KeV (0.5Å), with improved blocking at lower energy. The chopper can be phase-locked to the synchrotron bunch clock, and includes an on-board digital delay (waveform) generator with 10ns resolution and 16 channels of output for triggering lasers, gating high-speed electronics, etc. The chopper is controlled via an RS232 interface to Windows PC software, with all high-speed electronic processing being performed by a Field Programmable Gate Array (FPGA).

The parameters for chopper design are presented, and the overall mechanical operation, along with the control electronics and logic. Results of initial testing at Daresbury station 9.8 are provided, as well as opening time jitter and accuracy measured to verify single bunch extraction at DIAMOND.

Keywords: time-resolved, pump-probe, synchrotron

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Modeling the IRF of Synchrotron Powder Diffractometers with focusing Optics

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We extend the theory developed by Caglioti, Paoletti, Ricci [1-3] and Sabine [4,5] that provides an analytical description of the Instrumental Resolution Function (IRF) of single crystal and powder spectrometers consisting of collimators and crystals by including the effect of collimating and refocusing mirrors. Two cases are explicitly considered: the case when both collimating and refocusing mirrors are bent to a parabolic shape and the case when the collimating mirror is bent to a parabolic shape and the refocusing mirror is flat. The effect of isotropic sample size is also considered as a possible additional contribution to the peak width.

Experimental IRFs collected at the Swiss Light Source Materials Science beamline powder diffractometer at different photon energies and in both optical configurations are modeled by our analytical expressions and the agreement found is good. All experimental tests are performed using the Na₂Ca₃Al₂F₁₄ (NAC) standard powder.

[1] Caglioti G., Paoletti A., Ricci F. P., *Nucl. Instrum.*, 1958, 3, 223.

[2] Caglioti G., Paoletti A., Ricci F. P., *Nucl. Instrum. Methods*, 1960, 9, 195.

[3] Caglioti G., Paoletti A., Ricci F. P., *Nucl. Instrum. Methods*, 1962, 15, 155.

[4] Sabine T. M., *J. Appl. Cryst.*, 1987, 20, 23. [5] Sabine T. M., *J. Appl. Cryst.*, 1987, 20, 173.

Keywords: high-resolution X-ray powder diffraction, synchrotron

X-ray instrumentation, modeling

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Microcrystal X-ray Analyses using LTV Camera at Spring-8 BL02B1 Beamline

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Single crystal X-ray analysis is conventional and powerful tool in order to explore new functional materials and understand those chemical and/or physical properties. However, the single crystal analyses are frequently encountered difficulties because of extremely small sizes of the crystal specimens.

High intense synchrotron radiation should enable us to perform the crystal structure analyses of such very small crystals with several micrometers. As the first step of developing the technique of microcrystal structure analysis, we tried to do the single crystal structure analyses for small organic compounds using the low-temperature vacuum X-ray camera installed at Spring-8 BL02B1 beamline.

Cytidine crystal with dimensions 6.7 x 5.0 x 3.3 µm³ was used for measurement. Although the crystal structure could be solved by the direct method, all the non-hydrogen atoms were refined isotropically and hydrogen atoms located geometrically.

The structure analysis of chiral C60-fullerene *cis*-3 bisadducts crystal with dimensions 100 x 75 x 2 µm³ was also carried out. The crystal structure could be solved by the direct method and all the non-hydrogen atoms were refined isotropically. The absolute configurations were first established by combination of this study and CD studies.

Keywords: single crystal, small crystals, synchrotron X-ray diffraction

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The Phase 1 Macromolecular Crystallography Beamlines on Diamond

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Diamond is the new 3rd generation synchrotron source being built in the UK just south of Oxford. Seven beamlines are funded as part of Phase 1 which includes 3 beamlines for macromolecular crystallography (MX). The beamlines will use radiation from 3 in-vacuum undulators; each will be canted to allow a second undulator to be placed in the straight to provide radiation for a side station.

The beamlines will provide radiation tunable over a wavelength range of 0.5A – 2.5A. Significant emphasis is being placed on the automation of the beamline in terms of both hardware and software. Each of the beamlines will have diagnostics to allow the beam to be monitored remotely. The experimental station will be equipped with high quality crystal viewing systems and robotic sample changers to enable automated mounting for both cryocooled and room temperature capillary mounted samples. One of the beamlines will also include facilities for biological containment at Category 3 level at the experiment. This facility will open up opportunities for carrying out exciting structural work that it is currently very difficult to carry out due to the restrictions imposed by the safety requirements associated with working with biological pathogens.

These beamlines are scheduled to be commissioned in 2006 and will come on-line for users in 2007.

Keywords: macromolecular synchrotron X-ray crystallography, crystallography instrumentation synchrotron radiation, automation