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Movement of Single-Crystal Protein Samples at Synchrotron Beamlines

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Aside from normal rotational motion during collection of diffraction data from protein single crystals at synchrotron beamlines, additional movement of the nylon cryoloops holding these samples has been observed, due likely to the action of the nitrogen gas stream used to cool the samples cryogenically. A series of experiments was performed on the bending-magnet beamline (19BM) of the Structural Biology Center at Argonne's Advanced Photon Source in an attempt to characterize cryoloop movement. A baseline for the goniometer and timing shutter was established by measuring the profile of the 220 reflection from single-crystal silicon rod during data acquisition. Single-crystal silicon cubes, approximately 200 µm on a side, were mounted in 20-µm, single-fiber Nylon 66 cryoloops, and 220 reflection profiles were recorded. When compared with the silicon rod measurements, movement of the cryoloops was clearly evident. When shutter timing and synchronization among the goniometer, timing shutter and area detector are known and correct, diffraction data from low-mosaicity (less than 0.25° FWHM) lysozyme single crystals are a sensitive probe of cryoloop movement, as manifested in processing statistics resulting from both integration and scaling of the data.

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Keywords: cryocooled crystallography, protein crystallography, synchrotron radiation

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Harmonics-free Channel-cut X-ray Crystal Monochromator with focussing Effect

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X-ray crystal monochromators designed such, that the diffraction surface is machined into particular curved shape may favorably influence the properties of diffracted beam. As was shown by us earlier, a longitudinal parabolic or transversal groove may focus the diffracted beam in sagittal or meridional direction, respectively.

Another known example is a channel-cut crystal monochromator with curved diffraction surface which keeps the position of an exit beam fixed. Here, we show theoretically, that the channel-cut crystal monochromator with one diffracting surface machined into an exponential shape may reject higher harmonics in a broad wavelength range and at the same time the exit beam is convergent.

Keywords: X-ray monochromators, X-ray optics, dynamical X-ray diffraction theory

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Aberrations of Bragg-case Diffractive-refractive Optics (Sagittal focusing)

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The diffractive-refractive optical device consisting of four crystals in (+,–,–,+) setting with longitudinal parabolic grooves has a geometrical aberration which influences the achievable focus size. This aberration is discussed analytically by using the improved formula for the calculation of focusing distance, which respects the finite distance between optical elements. The calculation of the intensity distribution surrounding the focus is illustrated by a ray-tracing method based on the dynamical theory of diffraction. It demonstrates an achievable focus size. Finally we discuss that this aberration may be suppressed by the slight narrowing of the groove profile. In particular, the parameter a in the equation of parabola has to slightly grow with x. A practical application may require an ultra-precise manufacturing of the grooves.

Keywords: X-ray optics, X-ray focusing, X-ray and synchrotron radiation instrumentation

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SER-CAT: The Advanced Photon Source's Latest Protein Crystallography Facility

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SER-CAT, Sector 22 APS (www.ser-cat.org), provides both an insertion device (22ID) and a bending magnet (22BM) beamline for macromolecular crystallography. Beamline 22ID ($6x10^{11}$ photons/sec over 100 x 100 μm^2), hosts a MAR 300 CCD detector and a custom Rosenbaum kappa goniometer. Beamline 22BM ($2x10^{11}$ photons/sec over 60 x 80 μm^2), hosts a MAR 225 CCD detector and an ALS style sample auto mounter and is being developed as a fully automated beamline with remote user participation access capability. Both beamlines are MAD/SAD capable. The current operational envelopes are 0.5Å to 2Å with a ΔE/E of 5 x 10^{-5} using Si 220 for 22ID and 0.62Å to 20Å with a ΔE/E of 2 x 10^{-4} using Si 111 for 22 BM.

SER-CAT's goal is to provide its members with immediate access to one of the most modern synchrotron data collection facilities in the world. This is done by the continued integration of new technologies and methodologies, and by providing its users with outstanding user support. Since October 2003, 22ID has hosted more than 410 investigators from its 23 member institutions. Over 7000 data sets have been collected, 110 structures have been deposited in the PDB and 90 papers have been published. Beginning January 1, 2005 SER-CAT began hosting general users on 22ID.

Keywords: SER-CAT, synchrotron, remote user participation

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PETRA III: a Low Emittance High Energy Synchrotron Radiation Source

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The research center DESY in Hamburg, Germany will transform its 2304m long storage ring PETRA into a third generation synchrotron radiation source from 2007 on. A detailed description of this plan has been published in a technical design report [1]. The key parameters will be as follows: the particle energy will be 6 GeV at a current of 100mA. The horizontal emittance will be 1nmrad which will be a record low value for a high energy storage ring. In order to keep the thermal load on the storage ring as well as on beamline optics constant a top up operation mode is envisaged. In the first phase 13-15 undulator beamlines will be available. Undulators will be between 2m and 20m in length. First users are expected in 2009.

The scientific spectrum of the first beamlines to built ranges from structural biology to hard X-ray materials science. The majority of the planned beamlines will include a micro-focus option taking advantage of the extremely small source size of the storage ring.

[1] a) *PETRA III Technical Design Report*, DESY 2004-035, 2004; b) http://www-hasylab.desy.de/facility/upgrade/petra_tdr.htm

Keywords: synchrotron radiation, X-ray techniques, X-ray diffraction

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