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ACTOR: AUTOMATED CRYSTAL TRANSPORT, ORIENTATION AND RETRIEVAL

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A high-throughput, general purpose robotic system has been developed which transports flash-cooled crystals securely and safely, automatically mounts crystals on most goniometers, optically centers them in the x-ray beam, screens for diffraction quality, collects and processes diffraction images, recovers the crystals and stores them in a liquid nitrogen dewar. The system is a refinement of the proven actor system from abbott laboratories [1].
Magnetic crystal storage and transport magazines are designed to hold up to 60 crystals in a standard dry shipper with easy access to any of the positions. The system is based on a general purpose 5-axis programmable robot that allows the system to be used in an infinite number of configurations including horizontal, vertical or virtually any other goniometer axis orientation. The unique non-magnetic end-effector securely grips standard hampton pins and places them on a ìglide goniometer magnet without the need to move cryosystream nozzles or beam stops. The ìglide goniometer translates the crystal ± 3 mm in all directions in as little as 2 micron increments for centering. All operations are controlled by director, a software tool which totally automates the high-throughput process of selection, centering, screening, collection and retrieval of crystals. The entire procedure has been optimized for high-throughput crystallography at synchrotron beamlines and in the home lab.
References

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Keywords: HIGH-THROUGHPUT CRYSTAL MOUNTING ROBOTICS

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A NEW APPLICATION OF LARGE LENS-COUPLED CCD X-RAY DETECTORS

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Bruker introduced lens-coupled CCD detectors two years ago. Since then we have reported on their use for macromolecular crystallography. However small molecule crystallographers have become interested in these devices, particularly because of their active area. At ALS, for example the large area (300 mm diameter) allows for positioning the detector at $2\theta = 0$ and collecting high resolution data most efficiently. This is despite the bending magnet source spectrum limitation of high flux at 14 KeV, or lower, i.e. longer wavelength than Mo Kα. Calibration of these detectors will be discussed and example of data collection will be given.

Keywords: **DETECTOR SYNCHROTRON LENS-COUPLED**

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THE CANADIAN LIGHT SOURCE (CLS) AND THE CANADIAN MACROMOLECULAR CRYSTALLOGRAPHY FACILITY (CMCF)

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The Canadian Light Source (CLS), a third-generation 2.9 GEV synchrotron light source, is currently under construction. The protein crystallography beamline is one of the seven beamlines to be constructed initially (of 35 beamlines at total capacity). The CMCF is planned to be a 50 m long undulator beamline to facilitate studying small crystals (approx. 50 mm) and crystals with large unit cells (approx. 1000 angstroms). Mad phasing will be one of the major applications of the beamline. Spectral range: 6.5 kev - 18 kev (1.91 - 0.69 angstroms), calculated flux at 12 kev (1.0 angstrom), approx. 1 x E14 ph/s/0.1/percent/bw and the focused spot size at the sample (horizontal x vertical) 0.15 mm x 0.05 mm (fwhm) generated from the 7th harmonic.
Advanced user interface and control software, together with fully automated robotic sample mounting and alignment will allow data collection in fedex mode and with remote observation.
The beamline is expected to be commissioned by the end of 2003 and will become available to the user community in January 2004. A proposal for a second protein crystallography beamline is going through the evaluation process. Additional beamlines are being developed for powder and small molecule crystallography.

Keywords: **SYNCHROTRON MACROMOLECULAR CRYSTALLOGRAPHY BEAMLINE**

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DOSE RATE vs. DOSE DEPENDENCY OF RADIATION DAMAGE TO PROTEIN CRYSTALS

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There is no specific “crystal-killing” property of third generation synchrotron radiation sources as has sometimes been claimed. There are however, recent reports of anecdotal evidence for dose-rate effects observed at high intensity beam lines, and some stations, including SBC 19-ID, routinely attenuate radiation.
We present the results of radiation damage experiments at 100K using crystals of HLA-A2 Class I MHC, BTB domain, US2/HLA-A2 complex and λ3. The question whether radiation damage is a function of dose rate or just of accumulated dose was assessed by exposing each of the five sample protein crystals to alternating high and low flux densities, while keeping the dose per exposure constant. The study was carried out at the SBC beamline 19-ID. The high flux density used was $1.8 – 2.5 \times 10^{15}$ photons/s/mm^2 (flux: $2.2 – 3.2 \times 10^{12}$ photons/s; beam size: 0.065 mm FWHM horizontal, 0.020 mm FWHM vertical; slit size: 0.10 mm horizontal, 0.05 mm vertical). The low flux density was 1/10th of the high flux density (by insertion of a 0.5 mm thick Al-filter). The exposure time per frame was 0.5 s for the high flux density and 5 s for the low flux density. There was significant radiation damage observed in frozen samples exposed to the intense X-ray beams. The damage observed as a function of accumulated dose did not depend on the flux density nor on the dose per frame. Damage was solely proportional to the cumulative dose absorbed by each sample.

Keywords: **RADIATION DAMAGE SYNCHROTRON RADIATION CRYOCRYSTALLOGRAPHY**