

even greater frame rates if hardware binning is used.

With this new mode of operation we are able to obtain ultra-fine sliced data (0.002°) on reasonable time scale ($3^\circ/\text{min}$). This means that rocking curve evolution can be mapped with high resolution while cooling through a phase transition. Fine slicing also offers a novel method for wavelength calibration by measuring many Friedel pairs from a standard granular powder material, such as NIST LaB₆.

At the price of smearing some reflections during the frame transfer, single crystal data are also available much more quickly than before. Intensity errors due to frame transfer depend on the rocking width of the crystal compared to the angular widths of the integration and transfer steps. Very sharp reflections that arrive during transfer may be completely corrupted so that these should be identified and removed during integration and scaling. For broader rocking curves, particularly where reflections are present on several frames, the main concern is that weak peaks could be contaminated by smearing from strong peaks. In practice these problems are not serious, as demonstrated by the commissioning studies that will be presented.

[1] J. C. Labiche et al, *Rev. Sci. Instrum.* **2007**, *78*, 091301.

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Automation and remote control at GM/CA CAT at the APS

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GM/CA CAT, sector 23 at the APS, encompasses two insertion device beamlines and one bend magnet beamline. The X-ray sources for the insertion device beamlines are a pair of canted undulators. All of the beamlines are controlled via a Graphical User Interface (GUI) based on the tab-style organization and presentation of SSRL's BluIce. The GM/CA-CAT implementation (JBluIce-EPICS), which communicates with the hardware through lower level EPICS control software, has evolved to include a variety of features that exploit the small beam size and divergence properties of this 3rd generation source.

In terms of automation, experimenters operate the beamlines with the same GUI whether they are using local control (sitting at the beamline) or remote control (anywhere with a valid IP). Remote access is directed through NX or Teamviewer servers to the beamline computers. This has allowed the users to gain experience in person then smoothly transition to remote control. The system has grown to include the necessary indicators for the synchrotron ring status and controls for the shutters, automounter and mini-beam. The automounters are modified versions of the Berkeley/ALS robots. These are pneumatically controlled systems coupled to motor-controlled Dewars that efficiently deliver samples from the Dewar to the goniostat. Hardware improvements to the pin base sensors and collets improved robot reliability and led to increasing user demand. All of the necessary coordination of commands to control the selection, mounting, loop and crystal centering, washing and annealing are housed in the Screening Tab or a Tools sub-Tab of the Sample Tab of JBluIce-EPICS. Future developments in the automation include the commissioning of a new Cartesian Robot in collaboration with T. Earnest and C. Cork, Lawrence Berkeley National Lab.

Two features in the automation of the data collection, the Raster Tab

and vector collect feature, are continually improving in the JBluIce-EPICS system and take advantage of the micron-sized mini-beams (5, 10, and 20 μm). At present the mini-beams are produced by accurate placement of the appropriate sized pinhole to restrict a larger focused beam. The system has evolved from the use of a single collimator to a single-button selection from a uni-body quad collimator. The tool has spawned the development of automated 2D rastering techniques (Raster Tab) to locate small or hidden crystals or better diffracting regions in larger crystals. For data collection, a feature to move the sample along a 3D vector has been incorporated into the Collect Tab. Improvements for a seamless transition from regions of interest identified in the Raster Tab and the expansion of options in the vector collect mode are currently underway. Here we will present a status report on automation and remote control applications available at the GM/CA CAT beamlines.

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Keywords: automation, macromolecular, synchrotron

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Automated *in-situ* diffraction screening at beamline X06DA at the swiss light source

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X06DA is the third macromolecular crystallography beamline at the Swiss Light Source. It has been designed to fulfill the requirements of both academic and industrial users. To achieve maximum efficiency, high degree of automation was implemented from the optics to the experimental environment. A Bartels dual channel cut monochromator (DCCM) ensures rapid energy changes (6 – 18 keV) with a true fixed exit. The obtained X-ray beam has a focal spot size of 80 x 45 microns at the sample position and a total photon flux of 51011 photons/sec at 12.4 keV. The mini-hutch end-station allows both rapid manual mounting and robotic sample exchange.

In addition, a crystallization facility, directly adjacent to the X06DA mini-hutch, has been implemented. Crystallization experiments are performed using nano-dispensing robots and drops inspection is done via an automated imaging system. The unique feature of this facility is the possibility to test the crystals for diffraction directly in the crystallization plates (in situ screening) by transferring them from the crystal hotel to the mini-hutch in an automated manner. Without any manipulation to the crystals, this gives users a rapid feedback on important parameters such as diffraction limit, anisotropy, cell parameters or mosaicity, and aids to prioritize subsequent optimization steps. Moreover, users are welcome to bring any kind of SBS standard crystallization containers, including microfluidic chips and the CrystalHarp™ which yield a particularly low background in the diffraction image.

First results obtained at the crystallization facility and future improvements will be presented. Other methodological developments such as a new type of multi-axis goniometer and phasing with weak anomalous scatterers will be described as well.

Keyword: Beamline automation, *in-situ* Diffraction Screening, crystallization