6M detector is a two-dimensional hybrid pixel array detector, which operates in single-photon counting mode (Broennimann et al., 2006). It consists of 2527 x 2463 pixels with a pixel size of 0.172 mm. This detector features several advantages compared to current state-of-the-art CCD and imaging plate detectors. The main features include: no readout noise, superior signal-to-noise ratio, a point spread function of one pixel, readout time of 5 ms, framing time of 100 ms, a dynamic range of 20bit, high detective quantum efficiency (100% at 8 keV, 80% at 12 keV, 50% at 16 keV) and the possibility to suppress fluorescence by an energy threshold. The short readout and fast framing time allow to take diffraction data in fine-phi-slicing mode with continuous rotation of the sample without opening and closing the shutter for each frame. Because of the specified properties, this detector is especially suited for the study of weak diffraction phenomena, time-resolved experiments and accurate measurements of Bragg intensities. Results from various x-ray experiments are presented, including crystallographic diffraction data, as well as results from diffuse scattering and x-ray absorption experiments. All data have been collected with the PILATUS 6M detector at the X06SA and X05LA beamline of the SLS. Broennimann, Ch., Eikenberry E. F., Henrich B., Horisberger R., Huelsen G., Pohl E., Schnitt B., Schulze-Briese C., Suzuka M., Tomizaki T., Toyokawa H., Wagner A. (2006). J. Synchrotron Rad. 13, 120-130.
Kraft, P., Henrich B., Eikenberry E. F., Schlepuetz C. M., Kobas M., Graafsma H., Broennimann Ch. (2008). J. Synchrotron Rad, submitted.

Keywords: macromolecular crystallography, area detectors, detector development

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Remote access to the SSRL protein crystallography beam lines

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Protein crystallography users of the Stanford Synchrotron Radiation Laboratory (SSRL) have the option to conduct diffraction experiments from their home institutions by means of advanced software tools that enable network-based control of highly automated beam lines. Remote experimenters have access to the same tools as local users, and have the ability to mount, center, and screen pre-frozen samples, and to collect, analyze and backup diffraction data. Central to this remote access capability is the Stanford Auto Mounting (SAM) system which transports samples directly from a cassette or uni-puck storage container in a liquid nitrogen-filled dewar, to the beam line goniometer. SAM is seamlessly integrated into the Blu-Ice/DCS beam line control system. This efficient and reliable system gives researchers the ability to screen up to 288 crystals without human intervention and remount the best quality crystals for data collection. The technical details of the beam line automation and remote access developments and the impact on macromolecular crystallography experiments will be presented.

Keywords: remote access, macromlolecular crystallography, automation

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Exploiting the anisotropy of anomalous scattering boosts the phasing power of SAD/MAD experiments

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The anisotropy of anomalous scattering (AAS) in crystals of brominated nucleic acids and selenated proteins is shown to have significant effects on the diffraction data collected at an absorption edge. For conventionally collected single- or multi-wavelength anomalous diffraction data, the main manifestation of AAS is the breaking of the equivalence between symmetry-related reflections, inducing intensity differences that can be exploited to yield extra phase information. We present a new formalism for describing AAS which allows these effects to be incorporated into the general scheme of experimental phasing methods, using an extended Harker construction. This requires a paradigm shift in the data processing strategy, since the usual separation of the data merging and phasing steps is abandoned. The data are kept unmerged, down to the Harker construction where the symmetry-breaking is explicitly modelled and refined and becomes a source of supplementary phase information. These ideas have been implemented in the phasing program SHARP. Refinements on actual data show that the exploitation of anisotropy of anomalous scattering can deliver substantial extra phasing power compared to conventional approaches using the same raw data. Examples are given that show improvements in the phases which are typically of the same order of magnitude as those obtained in a conventional approach by adding a second wavelength data set to a SAD experiment. Such gains - which come without collecting new data - are highly significant, since radiation damage will frequently preclude the collection of a second wavelength data set. Finally, we outline further developments in synchrotron instrumentation and in the design of data collection strategies that could help to maximise those gains.

Keywords: anisotropy of anomalous scattering, SAD/MAD phasing, polarised dispersion

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Microcrystal manipulation with laser tweezers

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Over the last years huge investments in several structural genomics initiatives have been undertaken to automate all steps from protein expression to structure solution. Robotic systems are used in almost all steps from protein expression to sample changers on synchrotron beamlines. The last purely manual step is the transfer of the crystal from the crystallization drop onto a support for the subsequent X-ray diffraction experiment. Crystal “fishing” is relatively easy for crystals with dimensions >25 microns, however difficult for smaller crystals. As microfocus synchrotron beamlines allow data collection of crystals with dimensions of only a few microns, new approaches have to be found to facilitate and automate this last manual step. Laser tweezers which are routinely used for cell sorting offer the