MS36 O1

Protein Crystallography with the PILATUS 6M Pixel Detector Clemens Schulze-Briese[1], Ch. Brönnimann[1,2], E.F. Eikenberry[2], H. Billich[1], J. Diez[1], B. Henrich[1], M. Kobas[1], M. Näf[1,2], E. Panepucci[1] and T. Tomizaki[1] 1. Swiss Light Source at PSI, CH-5232 Villigen PSI, Switzerland. 2. DECTRIS Ltd., CH-5232 Villigen PSI, Switzerland

Beamline X06SA at SLS was designed for the use of the PILATUS 6M pixel detector. The main features and performance of the beamline will be reviewed briefly.
The PILATUS 6M, developed at PSI, is the first large area pixel detector to be routinely operated at a protein crystallography beamline. It combines the data accuracy of counting detectors, with very high count rate capabilities on both the pixel and the detector levels. In addition it exhibits an excellent point-spread-function, and supports frame rates of up to 12.5 Hz allowing continuous shutter-free data acquisition and fine-phi slicing.
The integration of the detector into the beamline as well as the necessary changes to the computing environment and the data processing software will be discussed. Crystallographic advances made possible by the excellent performance of the detector will be presented. Future prospects for the use of the pixel detector in the collection of diffuse scattering from protein crystals will be discussed.

MS36 O2

Modern Use of Kappa Goniometry for Macromolecular Crystallography at Synchrotrons Sandor Brockhauser[a], Florent Cipriani[a], Sean McSweeney[b], Raimond Ravelli[a], and the DNA Collaboration[c] [a]*EMBL Grenoble Outstation, 6 rue Jules Horowitz, 38042 Grenoble, France.* [b]*ESRF, 6 rue Jules Horowitz, 38043 Grenoble, France.* [c]*http://www.dna.ac.uk/*
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Most of the high throughput developments are aiming to automate routine steps. Unfortunately, this gives restrictions while performing non-standard experiments. Kappa goniometres have been used in the past by an elite group of expert crystallographers. These systems had serious instrumentational design and usability limitations. As a consequence, most synchrotron MX beamlines nowadays are no longer compatible with the traditional Kappa goniometers.
However, the call for more degrees of freedom to re-orient the sample has never completely faded. The reimplementation of "old" methods of collecting truly redundant data is becoming more and more important with the increased use of very small anomalous signals for solving macromolecular structures.
The construction of a MiniKappa Goniometer Head has allowed us to reduce one of the major risks of traditional multi-axes goniometers: that of collisions. This small device offers routine crystal re-orientation and fast data collection sweeps without stability problems. We ensured it to be fully compatible with the requirements of modern High Throughput beamlines. A comprehensive software package that includes modules for calibration, 3D virtual beamline simulation, crystal re-orientation calculation, automated sample re-centring as well as smart multi-pass strategy calculation is being developed and integrated with the data collection system DNA (automateD collectioN of datA).

MS36 O3

Sulphur SAD phasing using the UK/EMBL BM14 MAD beamline at the ESRF. Hassan Belrhali[a], Mario Bumann[b], Heinz Gut[b], Ludovic Launer[b], Hugo Caserotto[b] and Martin Walsh[b], [a]*EMBL Grenoble Outstation, 6, rue Jules Horowitz, BP181 38042 Grenoble Cedex 9, France,* [b]*BM14 CRG, c/o ESRF, B.P. 220, 38043 Grenoble CEDEX 9, France***.** E-mail: belrhali@embl.fr

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The Bending Magnet 14 beamline (BM14 [1]) at the European Synchrotron Radiation Facility (ESRF) is a UK Collaborative Research Group (CRG) beamline that is funded by the UK Medical and Biological Research Councils (the MRC and BBSRC, respectively) and is run in collaboration with the European Molecular Biology Laboratory Grenoble Outstation, France (EMBL, [2]). BM14 is an energy tuneable beamline that has been designed and optimised for exploiting anomalous diffraction for macromolecular phase determination. The beamline is particularly remarkable in that it has been shown to be able to utilize extremely weak anomalous signals arising from the constituent sulphur content present in the majority of biological samples, allowing the elucidation of their 3-D structures. A pragmatic beamline design delivering a stable and high quality beam, an inherently weaker flux when compared to insertion device beamlines avoiding radiation damages of the samples, coupled with ease of beamline use has contributed to the success rate for this *de novo* sulphur SAD phasing method. BM14 is today equipped with state-of-the-art instrumentation including a micro-diffractometer, a robotic sample changer and a large area mosaic MAR CCD detector. The facility is moreover in the forefront of automation developments through collaborations on-site with the ESRF and the EMBL and through participation in the UK funded e-HTPX and the EU funded SPINE projects. Taken as a whole, these improvements have substantially increased the range of samples that are tractable at the beamline which can vary from well behaving crystals and small to medium sized proteins, to poor quality microcrystals on the 1-10 micron range and large macromolecular complexes including recently the elucidation of an 8M Daltons virus at 3Å resolution.
BM14 will continue operations as a UK/EMBL CRG beamline until December 2008. From 2009, EMBL in collaboration with the ICGEB [3] are planning (subject to funding) to continue BM14 operations and future developments as a macromolecular crystallography beamline.

[1] http://www.bm14.ac.uk/,
[2] http://www.embl.org/,
[3] http://www.icgeb.org/.