MS01.06.06 DATA COLLECTION STRATEGY WITH A CCD DETECTOR ON A FOUR CIRCLE GONIOMETER. Ludger Häming, George M. Sheldrick, Universität Göttingen, Germany

Most area detectors are normaly used with one or three circle goniometers. We have attached a Siemens CCD detector to our non-standard four circle goniometer (offset Huber goniometer, Stoe x-ray optics, Siemens generator and a home-made LT-device and enclosure). For diagnostic purposes the CCD system can easily be replaced by the scintillation detector within an hour. Compared with a three circle system we can vary chi, but the Eulerian cradle resticts omega to a range of about 60 degrees. We routinely collect a complete hemisphere of data. It appears to be better to collect as many equivalent reflections as possible, so we collect one structure per day rather than trying to work shifts to collect threee a day. The time for a data collection is thus independent of the unit-cell dimensions. The quality of the data is significantly improved by the higher redundancy. This enables us to obtain high-angle data for extremly weakly diffracting crystals. A semi-emphirical absorption correction can also be applied, exploiting the redundancy of the data.

MS01.06.07 CATCHING A PEAK BY THE TAIL: INTENSITY CORRECTION FOR THE FINITE SIZE OF THE "SEED-SKEWNESS" PEAK MASK Robert Bolotovsky and Philip Coppens, Chemistry Department, State University of New York at Buffalo, Buffalo, NY 14260

In [1] a novel technique for integration of peaks on imaging plates has been described. The seed-skewness method finds an optimal mask for every peak based on the statistics of the pixel intensities. Being finite in size, the optimal mask inevitably cuts the weak "tails" of the peaks, because at a certain intensity level the peak contribution to the pixel intensity vanishes and yields to the background noise. This effect causes the optimal masks for the weak peaks to be smaller than those for the strong peaks. A simple Gaussian-peak model gives an estimate of the intensity bias due to this effect. The correction can be as high as 10–20% for the very weakest observed peaks. The missing tail effect may also cause the optimal mask to split into two parts when the peak is bimodal, as happens when the α_1 and α_2 positions are sufficiently separated. A correction for this effect is based on the α_1/α_2 intensity ratio, determined either in a separate counter experiment or directly from the imaging plate data. The algorithms have been implemented in the program HIPPO [1], and applied to both synchrotron and rotating anode data. Applications to several low-temperature data sets will be presented.

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MS01.06.08 INTEGRATED BEAMLINE CONTROL FOR PROTEIN CRYSTALLOGRAPHY. Robert M. Sweet and John M. Skinner, Biology Department, Brookhaven National Laboratory, Upton, NY 11973.

We have constructed a Graphical User Interface-driven software system for control of beamline X12-C at the NSLS. The beamline is equipped with a hybrid diffractometer, consisting of an Enraf Nonius CAD4-style diffractometer, carrying a 300mm-diameter MAR Research imaging-plate detector on its I arm.

The beamline itself is equipped with fairly standard apparatus – slits, monochromator, mirror, counters, and lift table for alignment of the diffractometer to the x-ray beam. Several programs run as independent images to perform various functions: diffractometer control, MAR scanner control, image transformation, and stepping-motor and counter control. These programs are controlled by a graphical-user-interface program that integrates their functions and provides communication among them.

The system contains the full functionality expected of any diffraction system (based on Pflugrath and Messerschmidt's MADNES), and flexible control of the beamline too. One can do nearly automatic alignment of the diffractometer to the x-ray beam. A recent innovation is the automatic collection of MAD data – with a single set of instructions the system will measure multiple sweeps of data, perhaps including Bijvoet-pair data measured by the Friedel-Flip method. At each wavelength change, the absorption spectrum of the anomalous scatterer is measured automatically and analyzed to select precisely the best wavelength before the start of each sweep. A second innovation allows monitoring of the x-ray beam in the synchrotron, a pause for a refilling of the ring, and a realignment and restart after the beam has been restored and is stable

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PS01.06.09 ON EXPERIENCES WITH AN IMAGE PLATE DETECTOR COMBINED WITH A SINGLE CRYSTAL DIFFRACTOMETER. Huber. Th., Lange, J., Burzlaff, H., Institut für Angewandte Physik, Lehrstuhl für Kristallographie, Universität Erlangen-Nürnberg, Bismarckstraße 10, 91054 Erlangen, Germany, Thoms, M., Winnacker A., Institut für Werkstoffwissenschaften, Universität Erlangen-Nürnberg, Martensstraße 7, 91058 Erlangen, Germany

Most of image plate devices make use of rotation or oscillation techniques. In our system the combination of a modified three circle diffractometer originally used for Laue-techniques [1] is combined with the image plate [2]. The detector system is presented separately. The diffractometer consists of an ω-2θ-base with an additional δ-axis for the crystal. This axis is inclined by 30° against the ω-axis, thus allowing full investigation of the reciprocal lattice. Several crystal structures already determined with a normal four-circle instrument are remeasured with the new device. The results will be compared and further experiences will be reported.

[1]Lange, J. and Burzlaff, H.: Single-Crystal Data Collection with a Laue Diffractometer. Acta Cryst. A**51** (1995), 931-936.
[2]Thoms, M., Burzlaff, H., Kinne, A., Lange, J., Von Seggern, H., Spengler, R., Winnacker, A.: An improved X-ray image plate detector for diffractometry, Proc. of the EPDIC IV, Chester (1995).

PS01.06.10 A NOVEL LARGE AREA CCD DETECTOR FOR FOUR-CIRCLE DIFFRACTOMETERS. Kucharczyk, D.†, Meyer, M., Paciorek W.A. And Chapuis, G., †Kuma Diffraction, Al. Akacjowa 15b, PL-53-122 Wroclaw, Poland, Université de Lausanne, Institut de Cristallographie, BSP, CH-1015 Lausanne Switzerland

A novel CCD detector for use with a four-circle Kappa-geometry diffractometer will be presented. The large input window of >90mm diameter allows simultaneous high-resolution sampling of a diffraction pattern of >45 degrees in 2θ. The input window is shaped as a secondary beam collimator to reduce the influence of air scattering. A special CCD optics design (fully vacuum isolated) simplifies and reduces the requirements for the cooling device. Most of the vital and sensitive electronics are build into the camera head to minimise noise and interference. Low noise digitalisation electronics allow true 20-bit digitalisation of the recorded image in short time. The newly designed hardware supports various binning (electronic and/or software addition of pixels) and windowing modes (predefined regions of interest). The combination of a 4-circle goniometer and a large area detector with free selection of windows and binnings will allow the optimisation of data collection strategy for small to medium sized structures. The data processing principles and first performance results of this detector system will be presented.