s7.m0.p11 Strategies for Data Collection on a CCD-Diffracto-meter. S. Rühl, M. Bolte, E. Egert, *Institut für Organische Chemie der Goethe-Universität, Marie-Curie-Strasse 11, 60439 Frankfurt, Germany*.
Keywords: CCD-diffractometer, data collection, area detector.

Diffractometers with position sensitive counters have sped up drastically the collection of X-ray diffraction data – but the question arises how to obtain an optimum data set in spite of a shorter data collection time. This was our motivation for testing various data collection strategies using a CCD detector and for evaluating the influence of the most important parameters [1].

All investigations were carried out with three small, weakly absorbing organic light-atom structures, common in routine structure determination. In the course of our experiments the impact of the following parameters was evaluated:

- time for measuring a single image,
- scan angle increment,
- crystal-to-detector distance,
- size of the collimator,
- redundancy of the data,
- scan-mode (ω-scans or φ-scans),
- resolution of the detector,
- crystal size.

All these parameters were systematically varied in order to find optimum values for the crystal in question. The quality of the different data sets was judged from a comparison of figures of merit such as R_{int}, R_σ, R_1 and wR_2.

Although using the default parameters recommended by the manufacturer lead to good results, adjustment of the data collection parameters according to the actual problem can substantially improve the quality of the data without loss of precision.

In order to show the potential of an optimized strategy the various figures of merit were compared for two compounds, each one measured with default and optimized parameters (in addition to a data set collected on a CAD4 diffractometer in one case).

[1] S. Rühl, M. Bolte. "Strategies for Data Collection on a CCD-Diffractometer.", Z. Kristallogr., accepted for publication.

s7.m0.p12 The future powder diffraction station at the swiss synchrotron facility (SLS). F. Fauth, B. Patterson, B. Schmitt, J. Welte, *Swiss Light Source, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland.*
Keywords: powder diffraction, instrumentation, synchrotron.

The Swiss Light Source (SLS) is a 2.4 GeV synchrotron radiation facility presently under construction in Switzerland[1]. The powder diffraction (PD) station represents one part of the Materials Science beamline, which is also dedicated to computer microtomography and glancing-incidence X-ray techniques. The beamline insertion device is a 65-poles wiggler with 61.2 mm period, 7.5 mm magnetic gap and a 1.97 Tesla peak magnetic field induced by NdFeB-based permanent magnets. The beamline energy range extends from 5 to 40 keV with the critical energy at 7.5 keV. The beamline optics consist of a first vertically collimating mirror, a Si_{111} double monochromator (second crystal sagitally focusing) and a vertically focusing mirror. Depending on the vertical localization, the angular divergence is 230-130 µrad (5-40 keV) for a ~1 x 0.5 mm^2 focused spot size at the sample. Without focusing option, the residual angular divergence amounts 16 µrad. Energy resolution *ΔE/E* remains below $4 \bullet 10^{-4}$ over the entire energy range. High angular resolution data will be collected using a 5-channels Si_{111}-analyzer/NaI scintillator detection setup. The major novelty of the SLS-PD station resides in the ~15000-channels position sensitive detector (PSD) we are currently developping[2]. This detector, based on the Si-microstrip technology, will allow data acquisition at millisecond time scale over a 60° angular range (in 0.004° steps). It will be ideally suited for '*In-Situ'* and/or Time Resolved studies as well as for thermo-diffractometry and grazing incidence techniques. Both the 5-channels analyzer/scintillator and the PSD detection setups are integrated into the SLS-PD diffractometer which will consist of a three coaxial rotations system. Each detection setup is mounted on an independently rotary table, the third rotation corresponding to the sample rotation. Simultaneous collection of both high resolution and high intensity data will thus be possible in capillary geometry. First operation of the SLS is foreseen in the summer 2001.

[1] see 'http//www1.psi.ch/www_sls_hn' for further details
[2] Fauth F. "Toward microstrip detectors for synchrotron powder diffraction facilities", Nuclear Instruments and Methods in Physics Research A (2000) 438:138-146.