s8b.m1.p5 **Towards automated Laue data processing: application to the choice of the optimal X-ray spectrum.** D. Bourgeois[a,b], U. Wagner[c] & M. Wulff[a]. *a : ESRF, BP 220, 38043 Grenoble, France, b: LCCP, UPR 9015, IBS, 38027 Grenoble, France, c: Institut für Chemie, Karl-Franzens-Unversität, A-8010 Graz, Austria.*
Keywords: methods crystallography, data collection, acquisition.

The availability of third generation synchrotron sources has triggered new interest in using the Laue technique to perform time-resolved experiments on macromolecules on very fast timescales [1,2].

Wigglers have long been considered as the insertion devices (ID) of choice for Laue crystallography, because they provide a smooth and broad bandpass of X-rays. However, the strong polychromatic background generated by a wiggler is particularly detrimental to the inherently poor signal-to-noise ratio associated with ultra short exposures. It was proposed that single-line undulators could be of special interest for Laue diffraction [3].

To determine the most suitable type of ID for time-resolved Laue crystallography, we compared Laue data sets collected on photoactive yellow protein with three insertion devices: a wiggler, a wide bandpass undulator and a single-line undulator. Our results show that the use of single-line undulators will generally yield –by far– the best compromise between data quality, acquisition time, and radiation damage.

We also developed a software (based on Lauegen, Prow, Lscale and the CCP4 suite), which enables to complete reduction of the data with essentially no user intervention, making Laue processing almost as straightforward as monochromatic data processing. Interactive work is limited to the indexing of only one Laue pattern. More importantly, we show that the data quality is substantially enhanced when soft-limited predictions (SLP's) are used instead of the usual hard-limited predictions. SLP's are generated by fine-tuning the resolution limit across the available X-ray spectrum [4]. With sharply varying spectra from undulators, SLP's are essential to prevent integration of many non-measurable reflections, whose noisy intensities, if measured, would be amplified in the normalization procedure and contaminate the valid data to a considerable extent.

We show that the generation of the SLP's can be improved by incorporating additional information from a set of monochromatic structure factor amplitudes corresponding to a closely related structure (a 'resting' or a 'dark' state). This significantly enhances the ability of Laue data to detect subtle structural rearrangements.

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s8b.m1.p6 **A New Software for Fine-Slice Data Collection Method for Protein Crystallography.** N.H. Xuong[*], A. Arvai[+], C. Nielsen[+], and R. Hamlin[+], [+]*Area Detector Systems Corporation, 12550 Stowe Dr., Poway, CA 92064 USA and* [*]*Dept. of Chemistry & Biochemistry, UCSD, La Jolla, CA 92093-0359 USA.*
Keywords: fine–slice, data collection, protein crystallography.

The goal of this project is to write a new software package to process data for Protein Crystallography collected with the fine slice method. In this method, each frame of X-ray diffraction is collected with the crystal rotated by a very small angle, for example 0.1°. This is in contrast to the standard rotation method where the crystal would rotate by a larger angle in the range of 1° per frame.

We have obtained very encouraging results. First we were able to develop a preliminary, but complete, software package for fine slice data collection for protein cristallography. Using this software to process a lysozyme data set, we obtained an R_{sym} factor of 3.5% which is lower than the 4.2% R_{sym} factor obtained with a set of data collected with the standard rotation method on the same crystal. This fast and preliminary comparison means that we are on the right track. Our program is running quite fast taking an average of about 200 seconds on an Alpha computer to process data 250 frames (a 20° rotation).

Second, we have also found a method that can solve the indexing problem in an automatic way, by simply using part of our software to process about 20 fine slice data frames. The resulting crystal and detector parameters can be used to process standard rotation data or fine slice data that come after the first 20 fine slice data frames. This automatic crystal indexing method will be extremely helpful in a high-volume data collection environment such as structural genomics.

s8b.m1.p7 **Different 'ways' in multiwavelength anomalous dispersion (MAD) data collection.** G. Sainz, G. Leonard, V. Stojanoff. *European Synchrotron Radiation Facility* and A. Thompson, *EMBL Grenoble Outstation and ESRF.*
Keywords: methodology, multi-wavelength anomalous dispersion, structure determination.

The different multi-wavelength anomalous dispersion (MAD) data collection strategies and their effect on the structure determination on the selenium and the iron edge will presented.

The multiwavelength anomalous dispersion method originally proposed by Hendrickson and co-workers [1] is based on the minimisation of systematic errors in data collection by collecting Bijvoet and dispersive differences as close in time as possible. This can be achieved either by positioning the crystal to record Bijvoet pairs on the same frame or by using "inverse beam" geometry. Data is collected in either case by dispersive differences in small angular wedges at different wavelengths with rapid wavelength cycling. At the ESRF good results have also been obtained from either completely random crystal orientations by collecting highly redundant data sets or from the collection of complete data sets for each wavelength. This strategy allows to keep the wavelength constant for long periods of time thus making the MAD method accessible to non-rapidly tunable beam lines. We discuss the effect of the alternative strategies: a) mirror symmetry, Bijvoet pairs on the same image; b) inverse beam method; and c) random orientation on the quality of the electron density map and the final structure determination quality at two commonly used wavelength, 0.97 and 1.74 angstroms.

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