12 01-Instrumentation and Experimental Techniques (X-rays, Neutrons, Electrons)

MS-01.02.02 DATA ACQUISITION AND PROCESSING FACILITIES AVAILABLE AT SERC DARESBURY LABORATORY.

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Synchrotron radiation provides a source of high intensity, highly collimated, wavelength tunable X-radiation which is becoming increasingly important in studies of structure-function relationships in biological macromolecules. At a fixed wavelength, the high intensity and low beam divergence enable diffraction patterns from crystals with large unit cells to be resolved. The use of shorter wavelengths can lead to a reduction in radiation damage as well as minimising systematic errors due to absorption. Weakly diffracting samples and/or small crystals often give useful data not obtainable from conventional sources. The wavelength tunability can also be used to optimise anomalous dispersion effects and lead to phase determination through multi-wavelength methods. Alternatively, the high intensity of the radiation over a large part of the X-ray spectrum is well-suited to the Laue technique. The Laue technique can be applied not only to protein crystals where the interest is in rapid data collection, but also to extremely small crystals of the order of tens of microns long.

At the Synchrotron Radiation Source, SERC Daresbury Laboratory, two stations provide "state of the art" facilities for protein crystallography. Both stations derive their radiation from a 3-pole wiggler magnet operating at 5 tesla. Station 9.5 is a dual purpose station designed for focussed Laue experiments and rapidly tunable monochromatic applications including multi-wavelength anomalous dispersion measurements. The principal optical components are a platinum coated fused quartz toroidal mirror and water cooled channel cut Si(111) double crystal monochromator. The mirror has an acceptance aperture of 1.2 mrad. horizontally and 0.1 mrad. vertically giving a white beam focal spot size of 1.3 x 0.4 mm some 32 m from the source. The monochromator can be interposed at about 30 m from the source for monochromatic work and gives a band pass $\Delta\lambda/\lambda = 0.00015$. The station is equipped with a Mar-Research image plate detector with the option of an Arndt-Wonacott camera and X-ray film for Laue work if appropriate.

Station 9.6 is mainly used as a fixed wavelength station. The optical components are a platinum coated fused cylindrically curved quartz mirror which provides 1:1 vertical focussing and a bent triangular Si(111) monochromator giving an 8:1 horizontal defocussing at 0.895 Å with a band pass, $\Delta\lambda/\lambda = 0.0004$. The size of the focal spot at the specimen is 0.5 x 0.3 mm in the horizontal and vertical directions respectively. The station can be equipped with an Enraf-Nonius Fast TV detector system or an image plate device.

Most data processing mainly involves MOSFLM as modified by Dr. A. Leslie (Cambridge) and the CCP4 suite of programmes.

MS-01.02.03 IMAGE PLATE DATA COLLECTION IN HAMBURG

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After a relatively long shut-down, when the DORIS storage ring was rebuilt, it has come back into operation as a dedicated source of synchrotron light. At present there are three active protein crystallography beam-lines, two belonging to EMBL and one owned by the Max Planck Institute. All of them are equipped with Image Plate scanners, either originally developed at EMBL or commercial MAR devices.

The scanners used in Hamburg have a fixed image plate, which after every exposure is read-out on-line in a spiral manner and the diffraction pattern stored on computer disk after appropriate corrections and transformation to cartesian pixels. The images are then ready to be processed by any of the existing data processing packages (Mosflm, Denzo, Xds). The read-out and erasure cycle takes about 2 min. for the 180 mm plate and 5 min. for the larger, 300 mm plate.

The quality of X-ray data produced by the scanners will be illustrated by a few examples. On one side, the image plate proved to be very useful for virus data collection, where its sensitivity at short, below 1 Å, wavelengths, makes it possible to obtain more data from one crystal and achieve higher completeness. On the other hand, using the data collected with Mo Kα radiation, the structure of the very small molecule, potassium tartrate, refined to an R value of 1.35 %, favourably competing with the quality achievable on a diffractometer. Moreover, in many cases the accuracy of the anomalous signal recorded by the system allowed the solution of the protein structures with only one heavy atom derivative.

MS-01.02.04 WEISSENBERG CAMERA FOR MACRO-MOLECULES WITH IMAGING PLATE DATA COLLECTION SYSTEM AT PF, PRESENT STATUS AND FUTURE PLAN

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The Photon Factory is operating at 2.5Gev and 300mA. There are two data collection systems for macromolecular crystallography at BL6A2 and BL18B, consisting of Weissenberg camera, imaging plate, image reader (BA100 & BAS2000), data reduction program "WEIS" and autoindexing program.

The optical system of BL6A2 is equipped with bent plane fused quartz mirror and triangular bent asymmetric cut Si(111) monochrometer and that of BL18B is equipped with 1m long fused quartz bent cylindrical Pt coated mirror with 1:1 focusing and a double-crystal monochromator which can be changed either using Si(111) or GE(111) without opening the mirror house.

The main basic ideas of Weissenberg camera for macromolecular crystallography are: 1) Film cassette should be designed cylindrical to get higher resolution data nicely, 2) The radius(r) of film cassette must be the larger the better because back ground noise will decrease approximately proportional to $1/r^2$; on the other hand, Bragg reflections do not