16.X-07 A SYNCHROTRON RADIATION CAMERA AND DATA ACQUISITION SYSTEM FOR TIME RESOLVED X-RAY SCATTERING STUDIES. J. Bordas and M.H.J. Koch, European Molecular Biology Lab., DESY, Hamburg, FRG.

Until recently,time resolved measurements of X-ray scattering have not been feasible because laboratory sources were not bright enough and suitable detectors unavailable.New developments in these fields have changed the situation. The combination of the bright X-ray beam produced by the storage ring DORIS (DESY) with suitable optics,detector and data acquisition system has enabled us to obtain time resolved diffraction patterns in the submillisecond range.

To achieve this performance the camera has to deliver a highly collimated and focused beam. The detector and data acquisition system must handle rates in excess of 10^6 photons/second. Facilities for external triggering,synchronization,time slicing and cycling have to be provided.Data reduction "in situ" is required to be able to define at any time the protocol of the next experiment.

We present and discuss the concepts behind the system and expand on some of the solutions we have chosen.The performance of the instrument will be illustrated with examples from recent experiments on biological systems.

Improvements and developments being carried out at present will also be discussed.

Hendrix J.,Koch M.H.J,Bordas J. (1979) J.Appl.Cryst. 12,467-472

Bordas J.,Koch M.H.J.,Clout P.N., Dorrington E., Boulin C. and Gabriel A. (1980) J.Phys.E:Sci. Instrum. 13,938-944

16.X-08 TWO-DIMENSIONAL POSITION-SENSITIVE DETECTORS FOR NEUTRON DIFFRACTION EXPERIMENTS USING BIOLOGICAL MATERIALS. By B.P. Schoenborn, Dept. of Biology, Brookhaven Natl. Lab., Upton, N.Y. 11973, USA.

The use of neutron scattering for biological structure analysis was made possible largely by the development of linear and two-dimensional position-sensitive counters. These detectors simultaneously collect diffraction data over a large area, have a high and uniform counting efficiency with good resolution and positional accuracy. Over the last ten years, such detectors have been developed at Brookhaven (Alberi, Fischer, Radeka, Rogers & Schoenborn, Nucl. Instrum. Methods 1975, 127: 507-523), the Institute Laue-Langevin (Allemand, Bourdel, Roudaut, Convert, Ibel, Jacobe, Cotton & Farnoux, Nucl. Instrum. Methods 1975, 126: 29-42) and Oak Ridge National Lab. (Kopp, Rev. Sci. Instrum. 1977, 48, 383-388). The instruments developed at Brookhaven use charge division with a gas mixture of He^3 and Ar at a pressure of 10 atm to provide a counting efficiency of 80% for neutrons at 1.5 A wavelength. The resolution is 2.8 mm with active areas ranging from 17 x 17 cm to 50 x 50 cm.

The use of such detectors largely overcomes the low flux that characterizes neutron experiments. In small angle scattering experiments, these two-dimensional detectors are used rather like film in X-ray work.

In neutron protein crystallography, the use of such counters controlled by a modern data acquisition system permits new approaches to data collection strategies. Instead of dealing with conventional scans like the θ-2θ scan that provides an integrated intensity as a function of a rotational parameter, the computer linked counter can be used to produce a three-dimensional reflection profile. As the crystal steps ($\Delta\omega$) through a reflection, the observed data is stored for each step in an external memory as a function of extent in 2θ and height (y) of a reflection. A typical array size for each reflection would be $20(2\theta) \times 20(\omega) \times 10(y)$. In this space the reflection will be a three-dimensional distribution with dimensions determined by the basic geometrical conditions like $\Delta\lambda$, crystal size, mosaic spread and beam collimation parameters. Knowledge of these basic parameters will allow a delineation of the reflection from the background and permit therefore an accurate intensity determination. This is particularly important in protein crystallography where high background occurs due to the large incoherent scattering of numerous hydrogen atoms.

16.2-01 CONSIDERATIONS OF EFFICIENCY AND PRECISION IN FOUR-CIRCLE DIFFRACTOMETRY. By William Clegg, Anorganisch-Chemisches Institut der Universität, Tammannstr. 4, D-3400 Göttingen, Fed. Republic of Germany.

The need to write a complete new control program for a Stoe-Siemens four-circle diffractometer has provided us with the opportunity of incorporating some novel features. Of prime importance were high data collection rates, flexibility and ease of use, without loss of precision in either unit cell geometry or intensity measurements. Key points of interest are:-

(1) A simple program command structure, extensive use of default parameters, and the possibility of queuing a sequence of commands for subsequent operation.
(2) Initial reflection search either with or without photographic information.
(3) Considerable enhancement of the Auto-indexing procedure (R.A.Sparks, Crystallographic Computing Techniques (Munksgaard, 1976), p.456) for cell determination.
(4) A choice of reflection centring procedures, with precautions to minimise systematic errors produced by instrument misalignment, backlash, etc.
(5) Matrix and cell refinement with and without symmetry constraints.
(6) Cell reduction, with output designed to assist in locating higher symmetry.
(7) Oscillation photographs about any lattice vector.
(8) Optical determination of crystal measurements and face indices (e.g. for absorption corrections).