Results are presented which compare film scanners (at 50 and 100 micron resolution), orientation matrix calculations, reflection integration and film to film scaling techniques by appropriate reference to quantities such as least squares residuals, R-factors on intensity in each case and an analysis of the agreement of the results of the different methods.

16.X-05 STATUS OF MWPC AREA DIFFRACTOMETERS. R. C. <u>Hamlin</u> and Ng.-h. Xuong, Depts of Physics, Chemistry and Biology, Univ. of Calif., San Diego, La Jolla, CA 92093 USA.

Diffraction from crystals of large biological molecules consists of many simultaneous reflections with small angular separation. To measure this radiation efficiently a photon-counting detector is required which intercepts a large solid angle and can independently count each of the diffracted beams which strike it. Ideally this detector would intercept the <u>whole</u> solid angle containing diffracted beams so that no diffracted radiation would be lost and the most possible information would be obtained from a single crystal.

Several types of detectors were proposed to meet this need. Arndt in 1966 proposed that a high-gain television detector could be used and he and others have pursued this idea but a television system has not yet been used to solve any protein structures. Georges Charpak in 1968 reported his development of the flat multiwire proportional counter (MWPC) and pointed out that this type of detector would be quite useful for detecting x-rays. In 1974 Charpak reported a more complex type of MWPC with a "spherical drift" region fitted on front which he had designed specifically for detecting x-rays. Two 50 cm \times 50 cm detectors based on this design were built at CERN. One was sent to LURE at Orsay, France and the other to MIT in the United States. The groups at these two laboratories have tested these spherical drift chambers and shown them to be suitable for large-molecule crystallographic work. The MIT group has collected a small amount of data from Ribonuclease A ($P2_1$, a=30 Å, b=30 Å, c=50 Å) a strong diffractor and reports intensity R factors in the 11-12% range. They are working on further instrument calibrations to improve this measurement accuracy.

But the original <u>flat</u> two-dimensional type of multiwire counter which Charpak had developed in 1968 (together with an x,y position readout scheme using delay lines devised by Perez-Mendez at UC Berkeley) is the basis of the MARK I detector we have been using in our lab in San Diego for 6 years. This detector has collected the data used to solve 4 new protein structures.

Two other area diffractometer systems using single, <u>flat</u> two-dimensional MWPC's are now in the beginning stages of operation. One of these is being assembled at the Univ. of Virginia. The detector has many features in common with our MARK I detector including delay line type position readout but its delay lines are faster for reduced dead time losses. Another system using a single flat multiwire counter is being assembled at the Stanford synchrotron. The detector in this system includes two very fast printed circuit delay lines needed to speed up the x,y position readout and allow counting at the high rates anticipated at the synchrotron. Both the Virginia and Stanford groups expect to collect some protein data by this summer.

In our laboratory in San Diego, a second generation area diffractometer system is now in operation. This system, called MARK II, is designed to accommodate as many as ten flat area detectors of an improved type designed especially for use in detector <u>arrays</u> and having better energy resolution and higher counting efficiency than our MARK I detector. Two of these detectors are now in operation and two more will be in operation late this year. The X-ray source for this new system is an Elliott rotating anode with monochrometer and beam intensity monitor. The crystal-todetectors can be positioned to approximate the surface of a sphere centered at the crystal. Work with 400 Å unit cells should be possible at speeds at least 200 times faster than a standard diffractometer.

16.X-06 HARDWARE AND DATA-COLLECTION SOFTWARE OF A TV AREA-DIFFRACTOMETER. By D.J. Thomas and U.W. Arndt, MRC Laboratory of Molecular Biology, Hills Road, Cambridge, CB2 2QH, England.

A strategy to collect diffraction data efficiently and accurately with an area-detector is established, and the software developed to collect such data at high speed on an area-detector diffractometer using normal beam rotation geometry is described.



The general design criteria of television detectors (U.W. Arndt & D.J. Thomas, Proc. ESF Workshop on X-ray position sensitive detectors and energy discriminating detectors (Hamburg, 1980), Nuc. Inst. & Methods: in press), our hardware (U.W. Arndt & D.J. Thomas, <u>ibid</u>.) and a method to reduce the systematic digitisation errors in collected data (D.J. Thomas, <u>ibid</u>.) have been described.

The software (D.J. Thomas, <u>ibid</u>.) used to predict at high speed the order of occurrence of diffraction spots over any part of the surface of an area-detector involves the use of unconventional lattice indices which bear a resemblance to cylindrical polar coordinates, some new algorithms in lattice theory (D.J. Thomas, Acta Cryst.: in press) and a "real-time" adaptive refinement routine to monitor the condition of the crystal and to update estimates of the spatial distortions of the detector.

It is hoped that a summary of data collected on our system can be presented.