01.1-06 THE MARK II AREA X-RAY DIFFRACTOMETER SYSTEM. By R. Hamlin, A. Howard, C. Nielsen, W. Vernon and Ng.-h Xuong, Dept of Physics, Univ. of Calif., San Diego, La Jolla, CA 92093, USA.

A new second generation area X-ray diffractometer system is now in operation in our laboratory. This diffractometer system called the MARK II system is based on the multiwire proportional counter (as was the MARK I system which has already been used to solve 3 new protein structures).

The MARK II system uses an improved type of thin, flat multiwire counter with better energy resolution (to help reject background) and higher quantum detection efficiency than the detector in the MARK I system. The MARK II system is designed to accommodate 4 area detectors (not just one as in MARK I) each with an active area of 30 cm × 30 cm. In many cases 4 detectors will allow data to be collected four times faster with no increase in crystal damage. The first two of these detectors are now in operation and the remaining two are scheduled to be in operation late this year. The detectors are mounted so that they can be positioned from 30 cm up to 2 meters away from the crystal and can be tilted to face the crystal so that they approximate a section of the surface of a sphere centered at the crystal.

In addition to the area detectors the MARK II area diffractometer system incorporates an Elliott GX6 rotating anode X-ray generator with a Supper graphite monochromator. The monochromator has now been adjusted well enough to give slightly higher CuK_α intensity than is obtained using a Ni foil filter and the elimination of unwanted white radiation is expected to result in considerable reduction of crystal X-ray damage.

The X-ray beam intensity is being monitored with a gas ionization cell mounted in the collimator. The current from this cell (proportional to the beam intensity) is digitized and fed into the on-line data collection computer for use in data scaling.

A special goniostat has been built for the rotating anode generator using the omega, phi and chi angles from a SYNTEX P1 diffractometer mounted on a track so that the crystal-to-source distance can be adjusted in the range from 30 cm to 60 cm. The larger crystal-to-source distances will be used when necessary to help separate neighboring diffracted beams from crystals with large unit cells (up to about 400 Å).

The MARK II system was first tested by collecting data from Elastase, a known protein structure, in a moderate sized unit cell ($P2_12_12_1$, a=51 Å, b=58 Å, c=75 Å) but it is designed for work with considerably larger unit cells, too. Some preliminary work has been done with crystals of glutamine synthetase (C2, a=235 Å, b=135 Å, c=200 Å, β=103°). The single area detector used was set 1.25 meters from the crystal and at this crystal-to-detector distance it was not found necessary to move the crystal any farther than 30 cm from the X-ray source to resolve neighboring diffracted beams.

The MARK II system with four area detectors and a 3 to 4 times more intense X-ray beam will be at least a factor of 10 faster than the MARK I system and at least a factor of 200 faster than a conventional diffractometer system allowing whole sets of high resolution data to be collected from single crystals barely good enough to use at all with conventional data collection methods.

01.1-07 SOFTWARE FOR A MULTIWIRE AREA DETECTOR DIFFRACTOMETER. By A. J. Howard, R. C. Hamlin, C. P. Nielsen and Ng.-h. Xuong, Depts of Physics, Chemistry and Biology, Univ. of Calif., San Diego, La Jolla, CA 92093 USA.

Software for a complex data-collection system for macromolecular crystallography must be both algorithmically sound and convenient for the user. The software package developed at the University of California, San Diego for the Multiwire Area Detector diffractometer contains algorithms which successfully obtain measurements of intensities of Bragg reflections from macromolecular crystals; in addition, users can obtain results with a minimum of training in use of the machine. The Electronic Stationary Picture method for data collection (Xuong et al. (1978) Acta Cryst. A34, 289) has recently been improved to increase the accuracy of the intensity measurements obtained from the multiwire detector. Among the improvements are a step-scanning technique which does not "miss" the reflection maxima due to coarseness in the scanning angle step, a correction for dead-time loss, a dynamic scanning-angle recentering technique, and more sophisticated criteria for on-line rejection of reflection measurements. The algorithms for obtaining predicted reflection locations (in spatial position and scanning angle) and for refining crystal orientation parameters and cell dimensions have been improved, and an algorithm for refining the detector's position in space and an automatic alignment routine have been added. Programs are available off-line for shape-fitting of reflection profiles, scaling, removing faulty observations and absorption correction. In addition, conscious attention has been paid to providing a system on which a crystallographer can proceed logically from one operation to another, entering only the input necessary to effect the new operation. Two editable, interactive "data tablets" provide most of the input to the crystallographic programs. The driving software for these tablets includes enough knowledge of crystallography and of past data runs that the number of input required from the user at any time is small. All of the crystallographic programs are linked together in what amounts to a crystallographic "operating system"; it allows for straightforward control flow and protects the user from the obscure features of the computer's own operating system. Complete documentation for the programs used on-line and off-line permit the user to become proficient in using the multiwire diffractometer in a few days.