SOFTWARE DEVELOPMENT FOR SYNTHETIC POLYMER DIFFRACTION

Robert Rule, ICI Chemicals & Polymers, Runcorn, UK.

The aims and achievements of CCP13 have generally been perceived as being more relevant to the software needs of the Biophysics Community. However, the overall scope of the project is very much broader, and several opportunities exist for the development of software which is better suited to the requirements of diffraction or scattering from other Non-Crystalline materials. Amongst others, these include scattering from synthetic polymers, solutions, voids and liquid crystals.

In all of these areas, irrespective of the sample under investigation, the basic procedures for the reduction or correction of experimental data are identical:

- (i) normalisation by ion chamber or semi-transparent beamstop methods,
- (ii) nonuniformity (or detector response) correction,
- (iii) removal of detector artefacts (e.g removal of TACs),
- (iv) spatial distortion correction (for 2-D data).

Similarly there are several standard requirements for the manipulation or interrogation of data which are also met by the existing BSL and OTOKO programs. Thus, it is possible to redisplay the corrected data in the most appropriate form for the experiment in question (e.g. horizontal or vertical slices of 2D images, background subtraction, multiplication or division of images, exponentiation, straight line fitting and so on).

At this point, numerous approaches are taken to the treatment or analysis of the data: the integration of discrete reflections; the modelling of complete 2-D patterns; the fitting of 1-D patterns to a given theoretical form; the characterisation by inspection of kinetic phenomena such as phase changes and reactions. Naturally, much of this analysis is sample-dependent and is performed back at the home laboratory, often using software which has been developed in-house specifically for that purpose. However, it is recognised that CCP13 may be able to make a significant contribution to many of these activities, particularly through the development or collation of software that would be of general use in a particular subject area.

In the field of synthetic polymer diffraction, there are many common forms of data analysis which are not generally available (at Daresbury or elsewhere). In Wide Angle Scattering (WAXS), for example, it would be useful to have routines which provided a straightforward estimate of crystallinity, based on the fitted intensities of the amorphous and crystalline components of the diffraction pattern. Several established methods exist for this calculation [1,2] which could be applied directly to 1-D data from the INEL detector on the Daresbury SAXS/WAXS station 8-2. Further work would be required to provide similar estimates using 2-D images from, for example, the FAST detector soon to be installed on line 16-1 at Daresbury, from image plates, from multiwire area detectors or from CCD cameras.

Similarly, routines which allowed the calculation of an orientation parameter (e.g. $\langle P2 \rangle$) from 2-D WAXS patterns of oriented polymers and liquid crystal systems would also be generally useful. Furthermore, it may be helpful to investigate the packages (such as CERIUS) for simulating WAXS data. This assumes that the CCP13 suite will allow easy conversion of all 2-D datafile formats into BSL format, as described in the Newsletter of December 1992.

In small angle studies of polymers, similar generic approaches exist. A common form of analysis of SAXS data is the 1-dimensional correlation function [3,4] which is relevant to the lamellar morphology which exists in many semi-crystalline polymers and block copolymers. The correlation function is able to provide a measurement of parameters such as the crystalline and amorphous layer thicknesses and the electron density difference between the layers. The 1-D correlation function could be calculated from data produced by OTOKO using extrapolation methods combined with a Fourier transform technique. Another useful development for interpreting SAXS data from polymers (and other materials) would be the introduction of experimental uncertainty measurements. This is not a straightforward task, but would enable error-weighted fitting of experimental data to models and would improve the general appreciation of data quality.

A further improvement for SAXS analysis of polymers would be the increased use of absolute intensities (or differential scattering cross-section per unit volume) rather than using arbitrary units. The availability of absolute scattering intensities [5] enables absolute electron density values to be determined and also provides an internal consistency check when fitting data to models such as the Debye-Bucche random two-phase model or Guinier's Law.

A recent development in data manipulation and display within the CCP13 package has been the incorporation of a circular integration routine for 2-D images. This enables the azimuthal variation in intensity to be plotted for a specified range of Q values. This is particularly valuable for oriented polymer specimens in both SAXS and WAXS.

It is hoped that CCP13 may be able to incorporate more of these broad ideas into standard software packages which are generally available. Suggestions for improvements in the general capabilities of data analysis or manipulation of 1-D and 2-D diffraction patterns are very welcome. In particular, the CCP13 Workshop in May is an ideal forum for discussing the scientific achievements as well as the software needs of all 'NCD' users, regardless of the nature of the materials which they study.

REFERENCES:

[1] W. Ruland (1961) Acta Cryst. 14, 1180.
[2] A. M. Hindeleh & D. J. Johnson (1971) J. Phys. D. 4, 259.
[3] C. Vonk (1971) J. Appl. Cryst. 4, 340.
[4] G. R. Strobl & M. J. Schneider (1980) J. Pol. Sci. Pol. Phys. Ed. 18, 1343.
[5] T. P. Russell, J. S. Lin, S. Spooner & G. D. Wignall (1988) J. Appl. Cryst. 21, 581.

CHAIRMAN'S NOTE

In order to promote the development within CCP13 of software which will be generally useful in the synthetic polymer field, an application to SERC to fund a young Research Assistant in this area is currently being made by CCP13. If successful, this appointment will be made in October 1994. Those interested in details of this position should contact the Chairman.

COVER ILLUSTRATION

Fibre X-ray diffraction pattern from an oriented sample of PEN [poly(ethylene-naphthalate)] recorded on beamline 7.2 at the Daresbury Synchrotron Radiation Source by A. Mahendrasingam as part of an ICI/ Keele University collaboration.
