02-Methods for Structure Determination and Analysis, Computing and Graphics

from different localized disorder in cubic insulin crystals equilibrated at different pH and salt concentrations. We have collected data on film using laborotary source, collecting 3–D data with imaging plate on synchrotron is being planned. Collecting data with good statistics is the main challenge in such studies since intensity of diffuse scattering is about 0.1 to 1 percent that of Bragg reflections and many factors contribute to scattering in background. Extraneous scattering from air, guarding slits etc. must be minimized to ensure a low and uniform background. A high order to order resolution (i.e. at least five times that of the lattice spacing), a well collimated monochromatic X–ray beam and a well characterized detector are necessary to accurately record the haloes surrounding Bragg peaks.

PS–02.05.10 EMPIRICAL AND CALCULATED THERMAL-DIFFUSE-SCATTERING CORRECTIONS FOR SINGLE-CRYSTAL DIFFRACTION DATA COLLECTED WITH A TWO-DIMENSIONAL POSITION-SENSITIVE DETECTOR. By G.J. McIntyre*, Institut Laue-Langevin, B.P. 156, 38042 Grenoble Cedex 9, France.

If the resolution of the diffractometer is assumed to be infinitely small the amount of one-phonon thermal-diffuse scattering (TDS) included in the scan through a Bragg reflection is directly proportional to the radius of the peak integration volume, the amount of two-phonon TDS to the square of the radius, and the amount of incoherent (flat) background to the cube of the radius. These differences in the dependence on the size of the integration volume can be exploited to correct for TDS and to estimate the elastic constants empirically, provided each reflection is sampled in three dimensions, as in scans made with a two-dimensional position-sensitive detector.
The TDS corrections for intensities derived by summation of counts in three dimensions are discussed in detail. The precision in the empirical method is poor for weak reflections, but, because of the slow variation of TDS with the scattering vector, the corrections for these reflections can be estimated from those of nearby strong reflections.
One advantage offered by position-sensitive detectors is optimal delineation of peak and background to minimise the estimated error in the background-corrected integrated intensity. For weak reflections this might imply integration within an envelope smaller than the instrumental resolution volume. The possible errors in the correction in this circumstance and for neighbouring reciprocal lattice points are estimated.

02.06 – Computer Graphics in Crystallography

PS–02.06.01 THE APPLICATION OF GRAPHIC DESKTOP SOFTWARE IN SINGLE CRYSTAL DIFFRACTOMETRY. By D. Abeln* and J. Kopf; Institut für Anorganische und Angewandte Chemie der Universität Hamburg, Martin-Luther-King-Pl. 6, D-20146 Hamburg, FRG.

One of the first scientific instruments to be controlled by a computer was the single crystal diffractometer (Busing, W. R. and Levy, H. A., Acta Cryst., 1967, **22**, 457). Early computer-controlled diffractometers were built at Hilger & Watts (Y290), Enraf-Nonius (CAD4), Philips (PW1000) and Siemens (AED). The programs developed for those instruments were written in assembler, mostly for a DEC PDP-8 computer. The first diffractometer software, completely written in the high-level computer-language FORTRAN IV, was the control program for the Syntex $P2_1$.

The past ten years have seen a revolution in computing and graphics hardware with the arrival of PCs and powerful graphic workstations which become increasingly faster and cheaper. New desktop systems, like GEM, WINDOWS or X/WINDOWS, allow an unexperienced user easy interaction with the computer.

In connection with the electronic rebuilding of a 22 years old, mechanically still reliable Hilger & Watts (Y290) we have developed a new graphically oriented program for the diffractometer control which uses the above mentioned advantages. A new interface (Lange, J. and Burzlaff, H., J. Appl. Cryst., 1991, **24**, 190), using a 68008-based single-board microcomputer for serving the four stepper motors of the four circles, is connected to an Atari Mega ST2 *via* the serial interface RS232. The diffractometer control software is completely written in FORTRAN77 and has the following features:

- drop-down-menus, dialog-, alert- and fileselector–boxes
- fast random peakfinding routine
- rotation- and axes-photographs
- centering routine with graphical representation of reflection profiles
- flexible indexing-, lsq- and bravais-routines
- graphical simulation of precession photographs
- ψ-scan of single reflections with transmission curve
- flexible data- and ψ-data-collection output in windows

The power of this new program Y290 is derived from a sophisticated menu-driven user interface which is much easier to use than the "classical" command-line input.

PS–02.06.02 VISUALISATION OF CRYSTALLOGRAPHIC DATA USING INTERACTIVE COLOUR GRAPHICS. K.M.Crennell*, ISIS Instrumentation Division, Rutherford Appleton Laboratory, UK

Facilities are described for the visualisation of data at the pulsed neutron source, ISIS, at the Rutherford Appleton Laboratory in the UK, where there are many instruments used to determine the molecular and crystalline structure of materials at a wide range of temperature and pressure. Programs have been written to combine data collected at a series of different operating conditions into a single multi dimensional data set, which can be visualised using image processing manipulation techniques. Examples are given of improved observation of magnetic phase changes at temperatures near absolute zero.

ISIS data collection uses a VAX cluster; most of the colour graphics is made by the UNIRAS package which can display data in 1, 2 or 3 dimensions interactively using X-terminals, or send hardcopy to PostScript printers. Examples are shown of the use of colour graphics to display data as an isometric suface and during data taking, to both monitor instrument performance and improve the quality of data collected.

Following data refinement, molecular and crystal structures need to be displayed. Examples of output made using personal computers are shown. These are becoming both cheaper and more powerful and can be a more effective display tool than a remotely connected terminal displaying graphics over a busy network.

PS–02.06.03 MOLDRAW: ADVANCED MOLECULAR GRAPHICS ON A PERSONAL COMPUTER

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