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

02.08 - Crystallographic Computing

OCM-02.08.01 HYPERTEXT FOR CRYSTALLOGRAPHY
by R. Diamond*, Medical Research Council, Laboratory for Molecular Biology, Hills Road, Cambridge CB2 2QZ, England and A. M. McLeish, Oxford University Press, Walton Street, Oxford, OX2 6DP, UK

"Hypertext" designates a system of text and related material, prepared in machine readable form so that its presentation on a computer screen includes within it 'links' which enable the reader to invoke supporting material, references, figures etc. as he wishes, using a mouse or similar device to control the process. One such system, 'Molecular Structures in Biology', will be described both from the user's point of view and in terms of its internal construction, which is based on a 'web' which is a file defining many 'nodes' which may themselves invoke software to provide a pop-up reference, or another text, or graphics software, or a stored bit map image etc. The web itself is traversed by software known as the 'spider' which puts into execution actions specified by nodes of the web. Such techniques, coupled with the high storage capacity of CD-ROM (600 Mbytes), provide an efficient means of publishing high-volume numerically intensive data, especially data with a high degree of permanence, as in data banks, where an crystallographic application seems most likely to be fruitful MSB itself is both a textbook and a reference work, containing over 500 coordinate sets from the Protein Data Bank, plus twelve chapters of text explaining hypertext techniques, plus many references, over 1000 illustrations (bit maps), and the capability for the user to create an unlimited number of others.

OCM-02.05.02 IF WE CAN DO IT, YOU CAN DO IT: WRITING A GUI INTERFACE FOR A CRYSTALLOGRAPHIC PROGRAM
by Paul N. Snavely* and Beverly R. Vincent, Molecular Structure Corporation, 2200 Research Forest Drive Woodlands, TX 77381 USA

Many crystallographic programs are still based on card-image input. The user is required to use a text editor prepare an instruction file for program execution. While this can be a simple effective means of program control, it fails to take advantage of modern software developments. Examples will be given of graphical user interfaces (GUI) that have been developed for crystallographic programs using the MOTIF tool kit. Actual examples of source code will be shown in order to demonstrate how it is to develop a modern graphical interface.

OCM-02.08.03 PC: A CRYSTALLOGRAPHIC COMPUTING TOOL FOR EXPERTS AND NOVICES
by V. K. Pecharsky, Dept of Inorganic Chemistry, L'viv State University, L'viv, Ukraine.

The choice of type of computer(s) for daily use in the laboratory for the tasks of diffraction-data processing, crystal-structure solution, refinement and final presentation faces every crystallographer. For work on inorganic crystal structures and on small molecular structures (up to 100-150 independent atoms in the unit cell), with ca. 1000 least-squares parameters, personal computers (PCs) can be used very effectively. PCs have many advantages, viz. they are open and friendly systems, they can easily be used by students, by regular scientific staff and by experts, and their capital cost is low. With proper software and suitable user interface, success is assured for everyone. PCs are excellent tools for crystallographic computing today and probably in the future.

We will illustrate our experience with PCs by describing the software package CSD (Crystal Structure Determination) for crystallographic computing on single-crystal and powder, X-ray and neutron diffraction data developed over the past few years. It will be shown that the average time spent by a crystallographer in the solution and refinement of a crystal structure is significantly less than the time necessary to collect the diffraction data. It does not usually exceed 1-4 hours, depending on the number of free least-squares parameters. Over two thirds of this time is spent on the final stages of refinement.

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OCM-02.05.04 THE PROFILE FITTING IN SINGLE-CRYSTAL X-RAY DIFFRACTION
by Dariusz Galazka, Institute of Low Temperature and Structure Research, Polish Academy of Sciences, ul. Okólna 2, 50-950 Wroclaw, Poland.

The whole-profile fitting that plays a fundamental role in crystal-structure determination from powder samples (the Rietveld method) is rather occasionally used for processing the single-crystal intensities (Gigg 1991). Acta Cryst. A47, 22-28 and A47; Oxtoby & French (1982). Acta Cryst. A38, 837-903. Usually, the traditional background-peak-background procedure is considered to be sufficient in the latter case. The purpose of the paper is to work out a suitable method for approximating the single-crystal diffraction profiles and to test the effect of the careful data processing on the precision and reliability of the crystal-structure determination. The subjects of detailed considerations are such problems as criteria of the goodness of fit, the choice of the basic approximating function (shape function), the proper number of independent adjustable parameters, the dependence of parameters of the profile on the Bragg angle, and direction cosines of the reflections vector, and recently discussed by Schwarzenbach & Flack (Acta Cryst. 1991), A47, 134-137) and Lenstra, Geise & Van Buoltema (Acta Cryst. 1991), A47, 597-604 - treatment of the background and 'negative' reflections. The basis for the considerations is the paper mentioned above and two papers by the authors (Galazka 1993). Acta Cryst. A50, 108-115 and 116-126). Results of the present work are currently being incorporated into a computer procedure which approximates the diffraction profile and calculates the integrated net intensities. The newest results of the crystal-structure determination that includes the profile fitting, as compared with those obtained using the common approach, will be presented.

OCM-02.08.05 THE USE OF ORTHONORMAL FUNCTIONS FOR THE REPRESENTATION OF 3-DIMENSIONAL INFORMATION
by Miss L. J. Pearce*, Dr. G. E. Tranter, Mr. A. Payne, Wellcome Research Laboratories, Beckenham, Kent in collaboration with the Chemical Crystallography Laboratory, Oxford.