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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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MOLDRAW [P. Uglengo, G. Borzani & D. Viterbo, J. Appl. Cryst., **21**, 75 (1988)] is a program for the graphical manipulation of molecules on personal computers, which does not require non-standard hardware. It is command driven and extremely user-friendly. It can be used to analyze the conformation of molecules resulting both from diffraction techniques or from theoretical calculations, and to study the detailed structure of crystalline materials. The main features of the program are:

-interface both to the Cambridge Structural Database and to the Inorganic Crystal Structure Database (ICSD);
-crystallographic symmetry generalized to all space groups;
-generation of the "coordination" polyhedron formed by all atoms, within a given radius, around a selected target atom;
-zooming and easy selection of any portion of the structure;
-view along any crystallographic direction or normal to any crystallographic plane;
-slabbed out portions of structures with interactive thickness selection;
-easy interface to PLUTO78 plotting program (PC version) and generation of HPLG and PostScript plotting files;
-interactive control on chemical (covalent and van der Waals radii) and graphic (graphic radius and color) atomic parameters;
-smooth rotation using the two graphic pages of the EGA board and full use of the VGA board;
-more efficient ball generation with illumination spot;
-addition, deletion, renaming, linking and unlinking of atoms;
-kit-model like representation (balls on cylindrical bonds);
-display of dotted van der Walls molecular surface;
-calculation of molecular volume;
-simulation of powder spectra;
-DOS interface and run-time setting of the program size (max. 4000 atoms);
-on-line help and user manual.

The setting up of a completely new user interface, menu and mouse oriented and still operating under standard MS-DOS is in good progress. We are also engaged in the porting of the code under MS-WINDOVS, allowing better functionality and handling of larger systems.

PS-02.06.04 A MULTIFUNCTIONAL SOFTWARE FOR CRYSTALLOGRAPHIC GRAPHICS. By Shen Jinchuan Prof. and Liang Jun Master, The Test Centre of Rocks and Minerals, China University of Geosciences(Wuhan), Wuhan 430074, P.R.China.

A multifunctional crystallographic software package has been developed by us. It can draw a lot of types of crystallographic graphs, such as crystal forms, structures and so on. All programs were written on IBM PC / AT with Turbo C++ and FORTRAN 77, and can run on PC / AT, 286, 386, 486 or other compatible microcomputers. The software includes two main parts, that is CRYSHAPE and CRYSTRUCT.

CRYSHAPE can draw any single crystal forms or combinations, the necessary input data is crystal constants, symbol of crystal class(point symmetry group) and symbols, numbers of single forms. The figures can be rotated around any axis in specified angles, that means the forms can be viewed from any direction. The figures also can be scaled.Moreover, a stereographic projection can be displayed with the figures of form. Screen display plotter output and hardcopy are in final form with no extra lines.

CRYSTRUCT is a 3-D crystal structure displaying and plotting system, which is given in polyhedrons or circles with high resolution(up to 1024× 768) and 256 colors. Hard copy also available through 24 pins dot matrix printers. Structure data such as bond length and angle can be output in standard formats in a output data file. Now this system supports TVGA and SEGA adapters.

By using this system, we have got a lot of satisfying rather complicated crystal forms and structure figures and won many favourable comments.

PS-02.06.05 CRYSTRUCT - THE CRYSTAL STRUCTURE DESIGN SUPPORTING SYSTEM. By H. Hayakawa* and E. Akiba, Department of Inorganic Materials, National Institute of Materials and Chemical Research, Japan, S. Ono, Government Industrial Development Laboratory, Hokkaido, Japan, K. Naito, M. Kawai and T. Ito, System Engineering Div. 6, Fujitsu Limited, Japan.

A new 3-dimensional crystal structure graphic system (CRYSTRUCT), which is suitable especially for inorganic crystal structures, has been developed aiming at an interfacial tool in the crystal structure design supporting system, in which various databases, calculation programs and analytical softwares should be connected with each other through the graphic system. CRYSTRUCT has been developed on FACOM S-4 series (UNIX-WS, full-compatible with Sun-4 series) in C-language using SunPHIGS. CRYSTRUCT gives the 3-dimensional structure model for the structural data: (1) Title, (2) Space group symbol, (3) Unit cell dimensions, (4) Number of atoms (L), number of atom species (M), number of bonding parameters (N), etc., (5) Atom symbol, discriminator, positional parameters, atomic radius, color number, site occupancy factor, etc. (L lines), (6) Bonding parameters which specify pairs of atoms between which bonds should be created, minimum and maximum interatomic distances limiting the region of bond formation, bond thickness, color (N lines), and (7) Others. The inorganic crystal structure database ICSD developed in Bonn University can be used as a data source. CRYSTRUCT has its own database for the space group symmetry operations which can be operated by input the space group symbol. It has also the point group symmetry operations for modeling molecules and clusters. Many possible new structures can be created by 3-dimensionally assembling the sub-structure units. CRYSTRUCT has several kinds of graphic models for representing structures : skeleton model, ball & stick model, skeleton & ball model, space-filling model and polyhedron model. In CRYSTRUCT, the graphic system is directly connected with the X-ray and neutron powder diffraction pattern fitting analysis program (Rietveld program), RIETAN.