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from different localized disorder in cubic insulin crystals. Equilibrium at different pH and salt concentrations. We have collected data on film using laboratory source, collecting 3-D data with imaging plate on synchronisation being planned. Collecting data with good statistics is the main challenge in such studies since intensity of diffuse scattering is about 0.1 to 0.5 percent of that of Bragg reflections and many factors contribute to scattering in background. Even worse scattering from air, guiding axis etc must be minimized to ensure a low and uniform background. A high order in order resolution (i.e. at least five times that of the lattice spacing), a well collimated monochromatic X-ray beam, and a well-chosen detector are necessary to accurately record the lattice 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 photon 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-photon 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 is done 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. A significant advantage of this detection is optimal delineation of peak and background to minimise the estimated error in the background-correction procedure. In experiments with the TDS-Ce-3T, the peak integration error is within an envelope of 0.5%.

02.06 - Computer Graphics in Crystallography

PS-02.05.01 THE APPLICATION OF GRAPHIC DESKTOP SOFTWARE IN SINGLE CRYSTAL DIFFRACTOMETRY. By D. Abadie and J. Köpf, Institut für Anorganische und Angewandte Chemie der Universität Hamburg, Martin-Luther-King-Pl. 5, D-20146 Hamburg, FRG.

One of the first scientific instruments to be controlled by a computer was the single crystal diffractometer (Buising, W. B. and Levy, H. A., Acta Cryst., 1997, 53, 657). Early computer-controlled diffractometers were built at Bilger & Watts (1970), Enraf-Nonius (CAD-4), Philips (PW1000) and Siemens (AED). The programs developed for those instruments were written in assembly code, mostly for DEC DP-8 computers. The first diffractometer software, completely written in the high-level computer-language FORTRAN IV, was the control program for the Syntax FC.

The past ten years have seen a revolution in computing and graphics hardware with the arrival of PCs and powerful graphic workstations which became increasingly faster and cheaper. New desktop systems, like GEM, WINDOWS or X-WINDOWS, allow an inexperienced user easy interaction with the computer. In connection with the electronic rebuilding of a 22 years old, mechanically still reliable Hilger & Watts (1970) we have developed a new graphically oriented program for the diffractometer control which uses the above mentioned advantages. A new interface (Image, 3. and Burzstadt, H. J. Appl. Cryst., 1997, 24, 180) using a X-Window based single-heart computer for serving the four upper most of the four circles, is connected to an Atari Mega ST2 via the serial interface RS232. The diffractometer control software is completely written in FORTRAN IV and has the following features:
- drop-down menus, on-line, alert- and feedback-boxes
- fast random peakfinding routine
- rotation- and axes-photographs
- containing routines with graphical representation of reflection profiles
- flexible indexing- and background-routines
- graphical simulation of precession photographs
- p- and o-scans of single reflections with transmission curve
- flexible data- and p-data-collection output in windows

The power of the new program Y299 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 crystaline structure of materials at a wide range of temperature and pressure. Programs have been written to combine data collected as 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.

The 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 isotropic surface 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 controlled terminal displaying graphics over a busy network.

PS-02.06.03 GOLDRAG: ADVANCED MOLECULAR GRAPHICS ON A PERSONAL COMPUTER. E. Ugliano*, G. Chiari* and D. Viterbo.*

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Moldram [P. Olgren, G. Forzani & D. Viteber, 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 forced 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;
- labelled out portions of structures with interactive thickness selection;
- easy interface to PLUTO/S plotting program (PC version) and generation of Metcost and Postscript plotting files;
- interactive control on chemical (covalent and van der Waals radii) and crystallographic radius and color) atomic parameters;
- smooth rotation using the two graphic pages of theEGA board and full use of the VCA board;
- more efficient ball generation with illumination spot;
- addition, deletion, renaming, linking and unlinking of atoms;
- kit-model like representation (balls on cylinders: bonds);
- display of Gotted van der Waals 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-WINDOWS, allowing better functionality and handling of larger systems.

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 stereo-graphic projection can be displayed with the figures of form. Screen display better output and hardcopy are in final form with no extra lines.

CRYSTRUCT is a 3-D crystal atlas displaying and plotting system, which is given in polyhedrons or circles with high resolution (up to 1024 x 768) and 256 colors. Hard copy also available through 24 Pias dots matrix printers. Structure data such as bond length and angle can be output in standard format in a output data file. Now this system supports TVQA and SEGAL adapters.

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

PS-02.06.05 CRYSTRACT - THE CRYSTAL STRUCTURE DESIGN SUPPORTING SYSTEM. By S. Nagasaka and S. Akiwa, Department of Inorganic Materials, National Institute of Materials and Chemical Research, Japan. (In English, with Japanese.)

PS-02.06.04 A MULTIFUNCTIONAL SOFTWARE FOR CRYSTALLOGRAPHIC GRAPHICS. By Shao Jinshun 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 crystallographic structures, and so on. All programs were written on IBM PC/AT with Turbo C++ and FORTRAN 77, and...