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

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.