menu-based character of the program. On-line help is available.

Availability: The program is available from the authors on request.

Keywords: *X-PLOR*; refinement; interactive graphics; Tcl/Tk.

The authors thank Dr T. Simonson for his interest in the work and his improvement of the manuscript.

References

Brünger, A. T. (1992) *X-PLOR. A System for X-ray Crystallography and NMR*, Version 3.1. Yale University, Connecticut, USA.

Brünger, A. T., Adams, P. D., Clore, G. M., DeLano, W. L., Gros, P., Grosse-Kunstleve, R. W., Jiang, J.-S., Kuszewski, J., Nilges, M., Pannu, N. S., Read, R. J., Rice, L. M., Simonson, T. & Warren, G. L. (1998). *Acta Cryst.* D**54**, 905–921.

Osterhout, J. K. (1993). *Tcl and Tk Toolkit.* Reading, MA: Addison-Wesley.

Urzhumtseva, L. M. & Urzhumtseva, A. G. (1996). *CCP4 Newsletter on Protein Crystallography*, **32**b, 41–43.

Urzhumtseva, L. M. & Urzhumtseva, A. G. (1997). *J. Appl. Cryst.* **30**, 402–410.

J. Appl. Cryst. (1999). **32**, 377

*TOPOS*3.1 – program package for multipurpose geometrical and topological analysis of crystal structures

V. A. Blatov,* A. P. Shevchenko and V. N. Serezhkin

Samara State University, Ac. Pavlov St. 1, 443011 Samara, Russia. E-mail: blatov@ssu.samara.ru

(*Received 17 November 1998; accepted 20 November 1998*)

The crystallographic problem: The program package *TOPOS* is intended for the automation of crystal–chemical analysis of both individual substances and a large set of crystal structures.

Method of solution: The version *TOPOS*3.1 includes the following programs.

(i) *DBMS* (database management system) allows one to edit, search and retrieve crystal structure information. All the other programs of the package (except *StatPack*) are integrated into *DBMS*.

(ii) *Dirichlet* is used for the construction of Voronoi–Dirichlet polyhedra (VDP) of atoms in crystal lattices and for the determination of geometrical and topological characteristics of atomic domains.

(iii) *AutoCN* calculates an adjacent matrix of crystal structure, including atomic coordination numbers (CN).

(iv) *ADS* (automatic description of structure) tests crystal structures for isomorphism; it determines coordination types of ligands, and the topology of complex groups and their orientations.

(v) *DiAn* performs the standard calculations of interatomic distances and bond angles.

(vi) *IsoCryst* builds, scales and rotates an image of a crystal structure and makes various standard geometrical calculations.

(vii) *StatPack* provides a statistical analysis of calculation results.

DBMS supports the unique binary *TOPOS* format of database files, which provides fast access to databases. *Dirichlet* applies a very fast 'gift wrapping' algorithm (Preparata & Shamos, 1985) to construct VDPs. *AutoCN* uses VDPs and an 'intersecting spheres' algorithm (Serezhkin *et al.*, 1997) to build an adjacent matrix of crystal structure. *ADS* takes this adjacent matrix, represents crystal structure as an infinite graph, then rolls it up into a finite graph and analyses its topology according to the algorithm of Blatov & Serezhkin (1992). All the other programs use standard geometrical and statistical analysis algorithms.

Software environment: Operating systems: MS DOS 5.0, Windows 95 or higher. Programming language: Borland Pascal with Turbo Vision library. Overlay structure: none. Subroutine libraries: Borland Pascal files for protected mode.

Hardware environment: Computers and installations: all IBM PC/AT 80386/87 (or higher) compatible computers (installation is to one directory of a hard disk). Minimum number of bits per word or byte: 16 bits per word. Minimum high-speed store required to run the program: 2 MB of RAM (4 MB or more recommended); Peripherals supported: CGA/EGA/VGA videoadaptors, Epson- or HP-compatible printers and mouse.

Program specification: Restrictions on the complexity of the calculation: some minor facilities of the package are restricted by the number (16383) of compounds per database and of atoms per compound; however, all calculations can be made for structures of any complexity.

Unusual features: the possibility of the comprehensive crystal–chemical analysis of thousands of crystal structures in an acceptable time period.

Typical run times: one or several minutes per typical compound (up to some hundreds of atoms per unit cell). The package has been tested on databases containing more than 10 000 compounds (including peptides and polynucleotides), consisting of up to 30 000 atoms.

Number of lines of code: about 50 000 lines of the source code.

Test status: more than 25 000 crystal structures of various chemical nature (from simple compounds to peptides).

Documentation: A user manual is available.

Availability: *TOPOS* is distributed on one 1.44″ MS DOS floppy disk. A free demo version is available *via* ftp://ftp.lmcp.jussieu.fr/pub/sincris/software/structure/topdemo.zip. The *TOPOS* WWW site is located at http://www.ssu.samara.ru/Common/Structure/Chemistry/IChemistry/topos.htm.

Keywords: Crystal–chemical analysis; geometry; topology.

References

Blatov, V. A. & Serezhkin, V. N. (1992). *Kristallografiya*, **37**, 51–62.

Preparata, F. P. & Shamos, M. I. (1985). *Computational Geometry.* Berlin: Springer Verlag.

Serezhkin, V. N., Mikhailov, Yu. N. & Buslaev, Yu. A. (1997). *Russ. J. Inorg. Chem.* **42**, 1871–1910.

Crystallographers

J. Appl. Cryst. (1999). **32**, 377–378

1999 ICDD Crystallography Scholarship Recipients are Announced

The ICDD Crystallography Scholarship Committee has selected five winners for the 1999 Scholarship program. They are: Byron DeLaBarre, McMaster University, Hamilton, Ontario, Canada; Shannon Patrick Farrell, University of Western Ontario, London, Ontario, Canada; Cora Lind, Georgia Institute of Technology, Atlanta, Georgia; Oshrit Navon, Ben-Gurion University of the Negev, Beer Sheva, Israel; K. Scott Weil (also a 1998 recipient), Carnegie Mellon University, Pittsburgh, Pennsylvania.

Byron DeLaBarre's studies focus on 'Determining the Phases for a Difficult Protein Structure.' Shannon Farrell's research involves 'Sulphur *K*- and *L*-Edge XANES of 3d Transition Metal Sulphides and Silicate and Germanate Glasses.' The exploration of 'New Negative Thermal Expansion Materials Related to Cubic ZrW_2O_8', will be conducted by Cora Lind. Oshrit Navon's thesis research concerns the 'Polymorphism and the Influence of Crystal Forces on Molecular Conformation.' K. Scott Weil will continue his 'Investigation of the Formation, Structure, and Magnetic Behavior of Compounds in the Nickel–Molybdenum–Nitride System.'

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, USA). As far as practicable, books will be reviewed in a country different from that of publication.

J. Appl. Cryst. (1999). **32**, 378–379

Advanced computing in electron microscopy. By EARL J. KIRKLAND. Pp. ix + 250 (CD-ROM included). New York: Plenum Press, 1998. Price: US $72.50. ISBN 0-306-45936-1.

Because of significant improvements in instrument optics, electron sources, and detection systems, high-resolution electron microscopy has become an increasingly powerful tool for the study of microcrystalline materials. Theoretical descriptions of image production, including the transfer function of the objective lens and the multiple scattering interactions as the electron beam traverses the specimen, have been available for at least a quarter century. Why, then, should there be yet another book on high-resolution electron microscopy, a subject that has been already treated in many sophisticated monographs? The answer is implicit in the book's title.

This book, written by an expert on computer simulations in electron microscopy, shows how the greatly expanded and cheap computer power available nowadays can be used effectively for the interpretation of electron microscope experiments. It discusses how computational methods are optimally designed, a practical approach not encountered in many other texts. Several programs written by the author (*e.g.* the fast Fourier transform) are included in the text and a number of others commonly encountered in simulations are conveniently included in a compact disc to be used on a Macintosh, or PC with Windows 95 or NT. C source code is also provided for Unix-based systems. Although various possible roles of computers in modern electron microscopy are mentioned in the short introductory first chapter, the book is primarily concerned with applications to image simulation.

The second chapter is a brief introduction to the electron microscope as an optical instrument. While much of the discussion treats the conventional transmission electron microscope (CTEM), the author demonstrates quite effectively how the optics of bright-field and dark-field scanning transmission electron microscopes (STEM) are closely related to the CTEM *via* a principle known as reciprocity. Obviously, a major component of the microscope is its objective lens. After a discussion of the relativistic electron wavelength and its dependence on electron accelerating voltage, the spherical aberration of the objective lens and its partial correction by focal changes are encountered. In the third chapter, idealized electron scattering by a weak phase object is introduced to expand the discussion of the objective lens transfer function. Various optimized lens defocus conditions that allow the maximum bandpass of information at the same contrast sign are discussed, including the well known Scherzer focus. The effects of partial coherence or total incoherence of the electron source on the imaging experiment are then introduced in terms of this transfer function.

The very interesting fourth chapter deals with image simulation, particularly the pixel detail needed to visualize various specimen details but also the optimal sampling of the image for transformation to its diffraction pattern or *vice versa*. The concept of the Nyquist limit is introduced, but not specifically in the context of the Shannon sampling theorem. Practical aspects of carrying out discrete Fourier transforms, avoiding artifacts due to image wrap-around, are mentioned, as is the most efficient way to display diffraction patterns as their power spectra. Thin specimen images are then simulated in Chapter 5, again in terms of the weak phase object. The derivation of accurate electron scattering factors is then presented in great detail, including the need for an imaginary form factor for heavier atoms. Steps in the computation of bright-field phase-contrast images are then given with examples for single atoms and a thin crystalline object (silicon). Coherence effects on these images are then reintroduced.

Chapter 6 was of particular value to this reviewer since it discusses multiple-beam dynamical scattering and its influence on images. There are two approaches to modeling multiple beam scattering, the Bloch wave solution (usually in matrix form) and the multislice calculation. Although these methods are physically equivalent, the former is shown to be computationally much more costly than the latter so that the multislice method is most often employed nowadays. Various aspects of these calculations that can lead to error are introduced including the (noncommutative) properties of some operators. Advice for slicing the crystalline specimen into optimal thin layers is given as are tests for validity of the calculation (repeat of slightly different boundary conditions for consistency) and its convergence. The problem of aliasing and bandwith on convolution operations is mentioned. Experimental design for simulating defect-containing crystals is given (the notion of periodic continuation as a superlattice). The next chapter examines a number of crystalline examples. Not only are image simulations shown here but also the production of convergent-beam electron-diffraction patterns, the most reliable way of determining space-group symmetry in crystallography (although that aspect is not mentioned). Finally the problem of quantitative matching of simulated images to experiment is discussed, with several figures of merit recommended.

The final chapter is a user's guide to the programs included in the CD-ROM. One can carry out multislice calculations of dynamical scattering and then simulate images at various degrees of beam coherence. STEM simulations are also included as is the possibility for computing convergent-beam diffraction patterns. Appendices discuss the 'shareware' included on the CD for plotting various functions such as the lens transfer function, a list of files on the CD-ROM, a nice demonstration of the central section theorem in diffraction, available sources of electron scattering factors and their parameterization for programs on the CD-ROM, bilinear interpolation and a program giving a perspective view of three dimensions.

In general, I have a very favorable impression of this book. Most of the material is presented reasonably well for someone who is already familiar with the field. (Indeed the preface suggests that the reader might have some previous familiarity with quantum mechanics, Fourier transforms and diffraction.) Again, the major recommendation for the volume is its very practical approach to computational problems, with a voice of experience pointing out where one can easily go astray. I do, however, have a few minor criticisms, even though the scientific presentation is generally first-rate. First,