Software Reviews

Software for review in this section should be submitted directly to the Software-Review Editor (P. S. White, Department of Chemistry, CB#3290 Venable Hall, University of North Carolina, Chapel Hill, NC 27599-3290, USA).

Lists of software presented and/or reviewed in the Journal of Applied Crystallography are available on the World Wide Web at http://www.iucr.ac.uk/journals/jac/software/, together with information about the availability of the software where this is known.

J. Appl. Cryst. (1997). **30**, 418–419

Crystallographica – a software toolkit for crystallography

Available from: Oxford Cryosystems, 3 Blenheim Office Park, Lower Road, Long Hanborough, Oxon OX8 8LN, England (e-mail: sales@cgraph.demon.co.uk; WWW: http://www.demon.co.uk/oxcryo/). Version 1.20, 1997. Price: single-user pack £595 (academic) or £1195 (industrial); additional users £95 (academic) or £350 (industrial); additional manuals £75 (academic) or £150 (industrial); student edition (no printed manual) £95.

Have you ever tried to write a program visualizing the succession of phase transitions in the powder pattern of ferroelectric $BaTiO_3$? Such a problem is not easily solved and requires advanced programming techniques, using graphing as well as crystallographic computing. A set of subroutines, dedicated to crystallographic computing, integrated with graphing and plotting routines, would surely make such a task easier. Such a system is now available: Oxford Cryosystems' *Crystallographica* is a suite of crystallographic routines, functions, predefined variables and macros, complemented by a data-graphing engine and a crystal-plotting package.* The routines are accessible either interactively through a Pascal interpreter or through a script written in Pascal. A convenient front end lets users import *SHELX* files and Crystallographic Information Files (CIFs) directly. A standard ASCII file import similar to LAZY PULVERIX format is, however, not available. The data are then stored in a crystallographic structure of variables, allowing the quick computation of properties. If any one of these variables is changed, dependent values get updated automatically. This automatic check for self-consistency is very convenient and helps to avoid error propagation. The routines and functions available in *Crystallographica* can access and modify the values in this structure, allowing for instance the calculation of the density or an angle between planes *etc.*

Running *Crystallographica* gives access to a graphical user interface. The interactive mode is easy and straightforward, working in a console window with the functions accessible *via* the command line, or partially through the menu items. The interpreter accepts Pascal commands, which takes some getting used to, but is adequate for the task. In interactive mode, *Crystallographica* operates as a convenient crystallographic desktop calculator. A powder-pattern calculation is at your fingertips, and so is a display routine that gives ball-and-stick representations of the structure. The powder-pattern routines include various profile functions and it is easy to set options for the display. Zooming in/out and pattern shifting can be accessed *via* buttons. The structure-graphing engine is also accessible *via* a button, and rotations may be done using the mouse. The structure drawing is not as sophisticated as in other programs, but the simplicity of the interface and the input makes up for these shortcomings.

The symmetry treatment in *Crystallographica* is done either through a look-up table (*via* the short Hermann–Maugin symbol) or *via* space-group generators. The latter allow for user-defined symmetries in nonstandard settings, as well as nonstandard supergroups, like *F4/mmm*. Such a treatment for symmetry is both elegant and powerful, if, for instance, one wants to explore various group/subgroup relationships and the effects on the multiplicity of the atomic positions. However, the program provides no checks (yet?) of the self-consistency of the symmetry produced. An elegant symmetry-generation program, giving generators and checking for self-consistency, is actually incorporated in *GSAS* and *NRCVAX*, and this can be used to obtain the basic generator set for all possible self-consistent space-group symbols.

A small script was written as a test program, which illustrates the oxidation/reduction of the high-T_c superconductor $YBa_2Cu_3O_{7-x}$, starting out as an orthorhombic structure with full oxygen content ($x = 0$) and going to the tetragonal oxygen-deficient structure ($x = 1$). The transition was set up, for ease of use, as being linear with the oxygen content and without internal rearrangement of the atoms. This is not quite correct but does little to the overall changes in the intensity calculation. The data for $YBa_2Cu_3O_{7-x}$ were previously entered into a CIF (Y123.cif, $a = 3.827$, $b = 3.877$, $c = 11.708$ Å, and O4 in $0,\frac{1}{2},0$), making the data available in a script. The script is given here.

```
{ procedure declaration ModifyCell }
procedure ModifyCell(n:integer);
var a,al,b,bl,c,cl,occupancy,occl:real;
var i:integer;
begin
  { first get the unit cell and }
  { occupancy parameters from the CIF }
  GetCell(a,b,c);
  GetOccupancy("O 4",occupancy);
  for i:=1 to n do
    begin
    { modify parameters in steps of 1/n }
    al:=a+(i*0.031/n);
    bl:=b-(i*0.019/n);
    cl:=c+(i*0.156/n);
    occl:=occupancy*i/n;
    { write modified parameters back }
    SetOccupancy("O 4",occl);
    SetCell(al,bl,cl);
  end;
  { reset to initial parameters }
  SetCell(a,b,c);
  SetOccupancy("O 4",occupancy);
end; { End of procedure definition }

{ Executable statements }

{ Read CIF }
ReadCif("Y123.cif");

{ Prepare powder simulation }
SetPowderRange(20,30,0.01);
AddGraph("Powder Simulation","","");
PlotPowder("Powder Simulation","Y123");

{ Continuously cycle, modify parameters }
{ in steps of 1/10 }
while true do ModifyCell(10);
```

The script changes the occupancy of the oxygen position in steps of 10%, together with the lattice parameters that in a predefined parameter structure contain the information for $YBa_2Cu_3O_{7-x}$. After each change, the powder pattern is recalculated and displayed and, after each full cycle, the parameters are reset to the values for the fully oxidized system. The result is an animated powder pattern, where the orthorhombic splitting of the peaks is gradually removed, changing the peak appearance and, to some extent, the intensities. This animation is quite instructive, showing the merging of peaks and a pseudotetragonal pattern long before the last (metrically tetragonal) pattern is displayed. Various resolution/peak-shape functions may also be explored in order to investigate their effects on the powder pattern.

Developing scripts in *Crystallographica* is easy, but for people not familiar with Pascal, a debugger would be quite useful. The strictly enforced Pascal syntax can be the source of long error messages. A simple debugger examining each line of code and checking for the correctness of the syntax would be useful, so errors do not propagate. After

* Oxford Cryosystems inform us that the latest version of *Crystallographica* now incorporates VRML output for structure drawing and a new window displaying the reciprocal lattice.

some tinkering with scripts, it is straightforward to develop your own, either for teaching or research.

There are obviously other programs available that are capable of doing similar things to *Crystallographica*. For example, the freely available (DOS version) *POWDERCELL* program displays the structure as well as the powder pattern, gives distances *etc.* but does not provide access to specific functions and does not allow one to write scripts. On the other hand, systems like *CERIUS* do give superior visualization and ease of use in the user interface, but also require more powerful computers and do cost substantially more. *Crystallographica* with its seamless integration of graphing and crystallographic computing presents an extremely useful compromise. The tool set of functions as well as the display capabilities allowing one to produce 'animation sequences' lets one write scripts that can address many crystallographic problems that would otherwise require extensive programming.

Crystallographica was installed on a 486/66 processor with 16 MBytes of memory and was run under Windows 95. The performance was adequate, giving acceptable update rates of any of the animated script examples that were included in the distribution. A Pentium-processor-based system is expected to give a better performance, but even a 386 processor could be used, albeit with considerably poorer performance.

Crystallographica is definitively recommended for anybody involved in X-ray diffraction who needs to write programs dealing with nonstandard problems, integrating graphing as well as powder-pattern calculations. It is a great tool for teaching aspects of symmetry and diffraction, and it is strongly recommended.

THEO SIEGRIST

Bell Laboratories
Lucent Technologies Inc.
Murray Hill
NJ 07974
USA

Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

J. Appl. Cryst. (1997). **30**, 419

Handbook of crystal growth. Vol. 2: Bulk crystal growth. *a*: Basic techniques; *b*: Growth mechanisms and dynamics. Edited by D. T. J. HURLE. Pp. xv + 1299. Amsterdam: North-Holland Elsevier Science Publishers, 1994. Price Dfl 695, US$ 397.00. ISBN 0-444-81554-6. A review of this book, by Peter Rudolph, has been published in the May 1997 issue of *Acta Crystallographica Section A*, pages 403–404.

Handbook of crystal growth. Vol. 3: Thin films and epitaxy. *a*: Basic techniques; *b*: Growth mechanisms and dynamics. Edited by D. T. J. HURLE. Pp. xviii + 1065. Amsterdam: North-Holland Elsevier Science Publishers, 1994. Price Dfl 695. ISBN 0-444-81556-2. (Set price, 3 vols., Dfl 1450. ISBN 0-444-8993-2.) A review of this book, by Robert B. Heimann, has been published in the May 1997 issue of *Acta Crystallographica Section A*, pages 404–406.

Molecular beam epitaxy. 2nd edition. By M. A. HERMAN and H. SITTER. Pp. xiv + 453. Heidelberg: Springer-Verlag Gmbh & Co., 1996. Price DM 98.00. ISBN 3-540-60594-0. This book 'describes a technique in widespread use for the production of high-quality semiconductor devices. It discusses the most important aspects of the MBE apparatus, the physics and chemistry of the crystallization of various materials and device structures, and the characterization methods that relate the structural parameters of the grown (or growing) film to the technologically relevant procedure. In this second edition two new fields have been added: crystallization of as-grown low-dimensional heterostructures, mainly quantum wires and quantum dots, and in-growth control of the MBE crystallization process of strained-layer structures. Out-of-date material has been removed.'