PS23.01.09 TEACHING DIFFRACTION PHYSICS BY COMPUTER SIMULATIONS [1]Neder, R.B. & [2]Proffen, Th., [1]Institut für Kristallographie und Mineralogie, Universität München, Theresienstr.41, 80333 München, Germany, [2]Research School of Chemistry, Australian National University, Canberra, ACT 0200, Australia

A high degree of motivation and very effective learning can be achieved by combining multimedia presentations with computer simulations of structures and their corresponding Fourier transform. Computer simulations of structures [1] offer the unique advantage that the students will see both, the structure and the resulting Fourier transform. Furthermore, since any type of structure can be simulated, a systematic approach to diffraction can be taught with maximum efficiency. The students can simulate their own structures, modify these and observe the corresponding changes in reciprocal space.

In the course reported here, we guide the students through a series of simulations covering: diffraction by individual atoms and small aggregates, reciprocal space geometry, convolution, modification of a structure, crystallographic phase problem, inverse Fourier transform, anomalous scattering, powder diffraction and disordered crystals. The course is supplemented by WWW pages [2], that guide a self study and prompt the students to try out their own simulations and observe the effect in reciprocal space.

[1] Neder, R.B., (1994): DISCUS, a program to simulate defect structures and diffuse scattering. Z.Kristallogr. Suppl. **7**, 744. see: WWW: http://www.kri.physik.uni-muenchen.de /geo/crystal/discus/discus.html
[2]Neder, R.B., (1995): Teaching Guide X-ray Diffraction. see:WWW:http://www.kri.physik.uni-muenchen.de /geo/crystal/teaching/teaching.html

PS23.01.10 TEACHING CRYSTALLOGRAPHY BY COMPUTER AID. G.Polidori(*), G.Cascarano(+), C.Giacovazzo(+), A.Pifferi(#). (*)Dipartimento di Scienze della Terra, Universita', 06100 Perugia, Italy; (+)Istituto di Ricerca per lo Sviluppo di Metodologie Cristallografiche - CNR c/o Dipartimento Geomineralogico - Campus Universitario Via E. Orabona, 4 - 70125 Bari, Italy; (#)Istituto di Strutturistica Chimica 'G.Giacomello', CNR, CP 10, 00016 Monterotondo Stazione, Roma, Italy

Several books on general crystallography have been recently published which provide clear description of the fundamentals of Crystallography. However the intrinsic nature of the subject requires non-negligible efforts from the students, who have to mentally reconstruct in threee dimensions what a book can only show in two dimensions. Symmetry operations and their effects in the space, three-dimensional lattices, crystal structures etc., can hardly be dominated unless mental exercise has been made. Even in three dimensions graphic aids can help students to understand the effects of mathematical operations like Fourier transform, convolution, etc.

We started to create a computer based tool to help students to learn and teachers to be more efficient in teaching Crystallography. The guidelines of our work are those described in the recent book "Fundamentals of Crystallography", edited by C.Giacovazzo,Oxford University Press, 1992.

In our intentions this software will be a useful tool for any Department in which Crystallography plays a role.

PS23.01.11 INTRODUCING CRYSTAL STRUCTURE DETERMINATION USING SPREADSHEETS. Max R Taylor, Department of Chemistry, The Flinders University of South Australia, GPO Box 2100, Adelaide SA 5001, Australia.

A package which allows structure factor calculation and 2-D Fourier summation has been developed in EXCEL 5.0 for hands-on undergraduate use. The package may be used to illustrate structure solution on a PC by the heavy-atom method using Patterson and electron density maps and refinement by using difference maps. The maps are calculated (as you watch) on the worksheet grid and can be adjusted to scale for orthogonal projections. The maps may, of course, be printed if contouring is required. Using the "what if" feature of spreadsheets is particularly instructive, because one can immediately see the effect on the R-factor and the relevant part of the difference map, of shifting an atomic position.

After 2 or 3 lectures on principles, students are able to follow the process of structure solution from observed structure factors to atomic coordinates provided that they have a rudimentary knowledge of the use of spreadsheets. The structure of potassium bicarbonate is an ideal example to use as it has the required heavy atom and a small number of other atoms, including a hydrogen atom that can be located. A projection down the short **a** axis shows most of the structural features. If x coordinates are provided then bond lengths and angles can be calculated. Structural features such as metal ion stereochemistry, bicarbonate ion geometry and hydrogen bonding can be studied. The package is easily adapted to use other examples.

PS23.01.12 USING teXsan TO STUDY CRYSTALLOGRAPHY Beverly R. Vincent, Molecular Structure Corporation, The Woodlands, TX

Automated instrument control and crystal structure analysis software have made the determination of a crystal structure faster and easier than ever before. However, such software has allowed users to perform crystallographic analyses without requiring them to understand the fundamentals involved. With our small-molecule structure analysis package, **teXsan**, we have incorporated utilities which may be used to learn more about the diffraction experiment and to see it in terms of classical techniques.

Interactive graphical displays make use of the measured intensities to simulate Weissenberg, rotation and precession film experiments. The final coordinates are used to simulate the results of a powder diffraction experiment. Other graphical programs are provided to allow the user to see the results of the analysis in terms of space group symmetry. The user is able to generate packing diagrams which include the symmetry elements as designated in International Tables. These drawings, combined with a simulated precession or Weissenberg photograph, may be used to investigate the effects of space group symmetry on the diffracted intensities, including systematic absences.

Each automated procedure in **teXsan** is accompanied by extensive output which shows how and why a certain decision was made, as in the space group selection routine. An automatic structure solution and refinement routine is accompanied by a descriptive discussion of each step of the procedure, serving as a potential model for the less automatic procedures required for difficult structure analyses. Utilities are provided for analyzing and understanding the finished crystal structure.