19-Crystallographic Teaching and the History of Crystallography

The idea of using optical analogues for Optical Transforms) to aid in the interpretation of X-ray diffraction patterns originated with Sir Lawrence Bragg round about 1938, and the method has developed considerably since that time. Prior to the advent of digital computers calculation of the diffraction pattern of even a fairly simple crystal structure was an enormous task, and use of optical diffraction from a model had obvious benefits, particularly for testing trial structures. With the advent of computers the task of obtaining a calculated diffraction pattern of an ordered crystal structure for comparison with observed measurements became a rather trivial exercise and use of the optical method for this purpose began to fall into disuse. On the other hand for the structural elucidation of disordered structures, amorphous materials and even liquids the transform method has continued to be used even though the diffraction pattern of eventhe most complex structural model can in principle be calculated quite readily with modern computers.

Optical Transforms are particularly useful in a teaching context where the student is able to verify for him/herself a real-space object and its diffraction pattern. In this demonstration we present examples of optical diffraction masks, the structural details of which can be inspected with the use of an ordinary micro-fiche viewer or 35mm slide projector, and whose diffraction patterns can be observed using only simple apparatus. A variety of masks will be available to demonstrate the diversity of diffraction effects which may be achieved by the technique.

In recent years we have sought to develop methods to allow the routine production of optical diffraction masks (or screens) for use as aids in the interpretation of X-ray or electron diffraction patterns. We are now able to produce, rapidly and easily, an optical diffraction mask which is a good representation of almost any real diffraction problem encountered with X-rays or electrons. Among the diverse range of problems that we have studied with the aid of such diffraction masks are: short-range order in molecular crystals; size-effect distortions in alloys; thermal disorder diffuse scattering in minerals; small-angle scattering in microemulsions; fluctuations of local order in liquids, quasi-crystals.

PS-19.01.14 SYMBAD, A CAI PROGRAM FOR TEACHING THE SYMBOLIC ADDITION METHOD. By Yuan-Fang Wang and Henk Schenk, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam, The Netherlands.

Since Direct Methods are still of growing importance as a tool of solving crystal structures from single-crystal data and most program systems for Direct Methods are not very transparent, we developed a small Computer Assisted Instruction (CAI) for the TRS80, in which the chemistry students are guided to work with the Symbolic Addition method. The main task of the course is to teach the student direct methods and to do the administration, while the students learn to take the essential decisions and to do a phase extension process. With this experience as background we wrote a CAI system in BASIC for PC's which allows more flexibility to the user. The program system is menu driven with an integrated manual. Input data for a projection of a structure are provided on disk, however, it is easy to create a local file of a suitable structure in which the overlap in projection is minimal as Direct Methods function better at atomic resolution. The program can handle projections with triclinic centrosymmetric symmetry only, and as a result in particular structures with one short axis can be used successfully.

The menu gives the following options:

- Input data: The student can choose between an input by keyboard or by disk. Keyboard data can be saved on disk for future use.
- Generation of triples: is fully automatic and generates triplets with an E3 value higher than a limit value, to be given by the student.
- Symbolic addition: In this part the computer does only the administration; the student makes the decisions, i.e. she/he chooses the sign/symbol of the three reflections in the starting set and decides whether the calculated phase of a reflection is being accepted.
- E-map: The student defines the values of the symbols and then the program calculates in the basis of the phases E-maps. The program is accompanied by a programmed text, which teaches the triple relation along the lines of chapter 1 of the proceedings of this conference and uses a similar approach to teach the principles of the symbolic addition method. The work has been sponsored in part by the Erasmus Scheme of the European Community.

PS-19.01.15 AFRICAN PATCHWORK PATTERNS AS SYMMETRY TEACHING TOOLS. By Yves Billiet and Marie-Paule Billiet-Nyelen, Département de Chimie, Faculté des Sciences, Bate Postale 832, Namur, Niger.