19-Crystallographic Teaching and the History of Crystallography

The idea of using optical analogues (or 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 even the 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 the relationship between 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 varied selection 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 diffaction 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 and disorder diffuse scattering in minerals; small-angle scattering in microemulsions; fluctuations of local order in liquids; quasi-crystals.

PS-19.01.13 CENET, A CRYSTALLOGRAPHIC NETWORK IN THE EUROPEAN COMMUNITY ERASMUS PROGRAM. By Henk Schenk*, Laboratory for Crystallography, University of Amsterdam, Nieuwe Achtergracht 166, 1018 WV Amsterdam

The Erasmus scheme of the European Community provides opportunities for tertiary education to exchange students and staff and to set up new teaching. Emphasis lies on the student exchanges. Students are studying in between 3 and 12 months in another country within the European Community. The most important constraint for these stays is that the full period should be recognized by the home-university for the curriculum of the student. Since a few years the Erasmus scheme is also open to the Efta countries. At present crystallography groups of 10 universities work together in the CENET Erasmus project: Amsterdam, Bologna (Lodovico Riva di Sanseverino), Bordeaux (Michel Hospital), Copenhagen (Ingrid K. Larsen), Dublin (Christine Cardin), Edinburgh (Bob Gould), Erlangen (Hans Burzlaff), Leuven (Camiel de Ranter), Lisbon (Maria Armenia Carrondo) and Thessaloniki (Panos Rentzeperis), originating from the faculties of chemistry, physics, pharmacy and geology. In CENET students of the 4th, 5th and 6th year at University are being exchanged for 3 months. This has the advantage that their stay abroad can easily be recognized as part of the research period they have to complete in nearly all curricula of the participating universities. Three students are being exchanged per group, they go to different countries and the visiting students not necessarily originate from the same countries, it rather depends on the individual research interests. To achieve this there is a complicated exchange scheme, supervised by the Amsterdam group, run via Email. The results of the student exchanges are very encouraging. The main result is an increase of mobility; it had been always possible for active students to follow courses in other countries, but mostly they lost time by doing so. In this scheme where it is obligatory for the universities involved to recognize foreign periods in the own curricula, this problem has been overcome. As a result all students may include a foreign period in their curriculum without any penalty. Individual students appreciate the possibilities very much. The teaching staff sees as major advantages the increased self-reliance of individual students and the international orientation of their groups.

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 transparant, 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 computer is to teach the student direct methods and to do the administration, while the students learn to take the essential decisions and is doing a phase extension process. With these experiences 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:
- Manual: A short explanation of the method and how to handle it.
- 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 triplets: 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 the 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 on the basis of the phases E-maps.

The program is accompanied by a programmed text, which teaches the triplet 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-NYBELEN, Département de Chimie, Faculté des Sciences, Boite Postale 825, Niamey, Niger.

