ML.19-B  SUPERSPACE GROUPS IN CRYSTALLOGRAPHY. By A. Janex, Institute of Theoretical Physics, Cath. University, Nijmegen, The Netherlands.

Properties of modulated and of composite crystal structures lead to the concept of an incommensurate crystal-line phase (e.g. van Anst et al., Acta Cryst. (1976) B32, 47; Pouget et al., Phys.Rev.B (1978) 18, 3049). This structural phenomenon is very subtle but quite general in nature. It requires a revised definition of ideal crystal and of crystallographic symmetry (de Wolff, Acta Cryst. (1974) A30, 777; Janssen & the author, Phys.Rev.B (1977) 16, 653). Looking at the diffraction patterns of incommensurate crystals as a projection in the physical space arising from the Fourier transformation of a periodic function (the superspace) in a (3+d)-dimensional Euclidean space (the superspace), leads to superspace groups. Such a group is a (3+d)-dimensional space group (having some additional properties) with elements leaving the superspace invariant. The diffractional and structural properties of incommensurate crystals expressed by these symmetries can be made explicit by a suitable parametrization or by extending the crystal as a supercrystal in the superspace. This approach allows a complete classification of crystallographic symmetries which includes the usual ones (for d=0). A full list of inequivalent superspace groups for d>1, together with the conditions leading to visible reflections has been established (de Wolff et al., Acta Cryst. (1981)). A proposal for representing diagrams of inequivalent general positions has also been made (de Wolff, Colloque Pierre Curie, Paris (1980)). Crystals are known requiring up to 3 d additional dimensions, but the majority of incommensurate crystals involve d=1 only. For a number of crystals superspace group assignment has been made, permitting an explanation of structural and diffractional properties observed (Acta Cryst. (1980) A36, 399 and 409). The structure factor of an incommensurate crystal can be expressed in a symmetry adapted form by explicitly using superspace coordinates and superspace group symmetry elements (Yamamoto, Phys.Rev. B (1980) 22, 373).

On the microscopic level, superspace groups lead to the usual 23 crystallographic crystal classes in 3 dimensions. These classes, therefore, also represent a valid classification scheme for incommensurate crystals. Nevertheless, superspace symmetry does have macroscopic implications. Evidence of this has already been found in crystal growth forms, where a generalization of the Lifshitz-Kosevich law to superspace (Ravaioli-Friedel-Donnay-Jarker rule seems to hold (Phys.Rev.Lett. (1980) 45, 1700). For tensor properties the situation is analogous. The possible non-vanishing coefficients are restricted according to one of the usual crystal classes, but a superspace symmetry adapted tensorial form is possible. This allows a deeper insight into the relationship between microscopic structure and physical properties. As illustration the Lorentz tensor is considered. It is used to describe local electric field gradients and dipole fields in ionic crystals in terms of structural parameters (Colpa, Phys.(1971) 25, 105 and 209). This microscopic tensorial field normally has the same superspace group symmetry as the crystal. Once the local polarizability tensor is given, in addition, one can derive expressions for the (macroscopic) dielectric tensor (a basic quantity in crystal optics) which are structure and symmetry dependent.

Finally, the possible relevance of superspace symmetries even for commensurate crystals is briefly discussed. All these results allow one to draw the conclusion that crystal symmetry is still a wide-open field for future investigations reaching down to the foundations of crystallography.

ML.20-A  FLEXIBILITY AND DYNAMICS OF PROTEIN STRUCTURE. By D.D. Phillips, Laboratory of Molecular Biophysics, University of Oxford, South Parks Road, Oxford OX1 3PS, U.K.

From the earliest analyses of protein structures at high resolution (Kendrew et al., 1960, Nature 185, 422-427) the electron-density maps contained indications of differential flexibility and motion within these molecules. In the crystallographic refinement of such structures, as in the corresponding studies of smaller molecules, the effects of systematic errors in the data must be carefully eliminated and there is a fundamental difficulty in distinguishing between the real motion of a molecule in a single conformation and the effects of static disorder that arise when the images of molecules in different orientations and conformations are superimposed.

Crystallographic evidence shows that some proteins adopt widely different conformations under different circumstances and that this variability is related to biological activity (e.g. Huber, 1979, TIBS, Dec. 1979, 271-276). Smaller variations in conformation and the effects of complex intramolecular vibrations are observed in all proteins and recent developments in methods of refinement and experimental techniques, including data collection at moderately low temperatures, are making it possible to define them in detail (e.g. Gubern & Hidaka, Acta Cryst.l978, A34, 777; Frauenfelder et al., 1979, Nature 280, 558-563; Artymiuk et al., 1980, Nature 280, 563-564). Results are consistent with other experimental evidence and with computer simulations of the dynamic behaviour of proteins (e.g. England & Karplus, 1980, Annu. Rev. Phys. Chem. 31, 29-45; Norworth et al., 1980, Nature 285, 659-660).
A consequence of the introduction of high intensity sources and position-sensitive detectors is the possibility of time-resolved diffraction. The potential of this technique has yet to be fully realised and it is a field in which important advances of the future may well occur, particularly in the study of phase transitions involving order-disorder phenomena. For many years, until the late 1960s, work with single crystals held sway; powder diffraction was almost a fringe interest pursued by a small group of devotees in a handful of laboratories. Now the situation has changed. Single-crystal methods are largely a matter of routine and have been eclipsed by the renaissance of powder diffraction.

ML.22-A INTERACTIVE COMPUTER GRAPHICS IN STRUCTURE ANALYSIS. By W.Y. Wright, IBM United Kingdom Ltd., UK Scientific Centre, Winchester, Hampshire, UK.

Molecular graphics, the application of interactive computer graphics to molecular studies, is established as a useful tool for studying the structure of biological molecules. Scientific results being obtained with these systems are rapidly repaying the investments made for their development. For research which involves the iterative refinement of Fourier synthesis maps, molecular graphics is indispensable.

Mechanical models have always played a central role in the study of molecular structure. The substitution of computer graphics for these began when Levinthal (Scientific American 1966) built a system for folding proteins. This goal proved too difficult, but several members of his group continued the work and developed successful systems for other phases of molecular research.

In 1972 Barry and North (Cold Springs Harbor Symposium on Quantitative Biology, 36, 577) identified the requirements for a system to build molecular models into electron density maps. Successful systems for this application began to emerge about three years later. These systems have also proved useful for molecular refinement, for comparing structures, and for packing studies. Experience indicates that the greatest power of molecular graphics lies in the user's freedom to move easily between the thinking and computational phases of his work.

The development of molecular graphics systems continues, and the area of application is expanding. One emerging use is in the study of the geometry and dynamics of enzyme-substrate interactions.

ML.24-A CRYSTALLOGRAPHIC ENGINEERING, By Robert E. Nemanich, Materials Research Laboratory, Pennsylvania State University, University Park, Pennsylvania, U.S.A.

Crystallographic engineering—the design and construction of non-equilibrium crystal structures—is now a reality. Ion implantation, micro-machining, molecular beam epitaxy, and a host of other techniques developed by the semiconductor industry make it possible to devise miniaturized multifunctional composites with a wide variety of connectivity patterns. Some examples of controlled structure-property relations involving the manipulation of conduction paths, mesoscopic stress configurations, and electric field distributions will be discussed, along with applications to acoustics, electronics, optics and medicine. Scaling down leads to new quantum phenomena and surprisingly large physical effects such as hot electron behavior and composite product-properties. Biological systems often serve as models for devices incorporating self-repair, memory, and membrane effects. Present and future goals for crystallographic engineers will be described.