

ML.19-B SUPERSPACE GROUPS IN CRYSTALLOGRAPHY. By A. Janner, 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 Aalst et al., *Acta Cryst.* (1976) **B32**, 47; Fouget et al., *Phys.Rev.B* (1978) **18**, 3645). 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) **15**, 643). 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 supercrystal) 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 supercrystal invariant. The diffractive 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 limiting possible reflections has been established (de Wolff et al., *Acta Cryst.* (1981)). A proposal for representing diagrams of equivalent general positions has also been made (de Wolff, *Colloque Pierre Curie*, Paris (1980)). Crystals are known requiring up to d=3 additional dimensions, but the majority of incommensurate crystals involve d=1 only. For a number of crystals superspace groups assignment has been made, permitting an explanation of structural and diffractive properties observed (*Acta Cryst.* (1980) **A36**, 399 and 408). 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 macroscopic level, superspace groups lead to the usual 32 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 Law of Rational Indices is needed, and where an extension to superspace of the Bravais-Friedel-Donnay-Harker 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, *Physica* (1971) **56**, 185 and 205). 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.C. 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 macromolecules. 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. Sternberg et al., 1979, *J. Mol. Biol.* **130**, 231-253; Frauenfelder et al., 1979, *Nature* **280**, 558-563; Artymiuk et al., 1980, *Nature* **180**, 563-568). The results are consistent with other experimental evidence and with computer simulations of the dynamic behaviour of proteins (e.g. McCammon & Karplus, 1980, *Ann. Rev. Phys. Chem.* **31**, 29-45; Northrup et al., 1980, *Nature*, **287**, 659-660).

ML.20-B THE RENAISSANCE OF POWDER DIFFRACTION: From Ugly Duckling to Beautiful Swan. By J. I. Langford, Department of Physics, University of Birmingham, Birmingham B15 2TT, England.

Many factors have contributed to the spectacular revival of interest in powder diffraction. High intensity sources of X-rays and neutrons, improved instrumentation and new forms of detector have made it possible to collect reliable and accurate data within minutes or even seconds. Powder methods have also benefited from advances in computer technology and programming procedures; more data can be processed in a given time and automatic on-line control is now a matter of routine.

It is in the field of crystal-structure refinement that there has been a marked rejuvenation of powder methods. Following the pioneering work of Rietveld (*Acta Cryst.* 1967, **22**, 151), total-pattern analysis rapidly gathered momentum in the hands of neutron diffractionists (Hewat, *NBS* 1980, Special Pub.No.567,111). Now, with further impetus from synchrotron radiation and energy-dispersive methods (Glazer & Hidaka, *Acta Cryst.* 1978, **A34**, S331), the number of structures refined from X-ray data is increasing steadily (Young, *NBS* 1980, 153).

Less spectacular, but nevertheless important advances have occurred in the indexing of powder patterns and in lattice-parameter determination (Shirley, in 'Crystallographic Computing', Delft Univ.Press, 1978). Given reliable data, a unique cell can usually be obtained for stoichiometric substances, irrespective of the crystal symmetry. One of the principal uses of powder methods is the identification of unknown phases and, with the aid of a small computer and improved data-packing procedures, on-line search-match can be carried out. Development of other traditional applications, such as line-broadening