

papers make fascinating reading; for many of us, though familiar with the main threads of the subject from textbooks, have never seen the original papers in which the ideas were first presented. There are extracts from the works of Haüy and Bravais, Friedel and Fedorov, in which the idea that the principal faces of crystals are those having a high reticular density of lattice points was developed. But it was realized that other influences would have to be taken into account: the detailed arrangement of atoms in complex structures, the distribution of electrical polarity, the different surface properties of the opposite faces of polar crystals. It only became possible to discuss these in the post-Bragg era, as in the extension of the Bravais principle of high reticular density by Donnay and Harker, who took into account the motif of the space group as well as the Bravais lattice, and the 'periodic bond chains' introduced by Hartman and Perdok as a rough way of estimating the relative attachment energies on different faces. Meanwhile, in the pre-Bragg era there were side-glances at other properties of crystal faces, particularly the surface energies, by Gibbs, Curie and Wulff, who developed the idea of an equilibrium form of minimum surface energy; but only in principle, for until structures were settled by X-ray diffraction there was no basis for the estimation of surface energies.

Consideration of the distribution of forces in perfect crystal structures is still not enough; imperfections, especially screw dislocations, influence the relative growth rates of different faces, and certain solvents and dissolved foreign substances may give rise to quite different crystal habits. Papers by Frank and others on dislocations are included, but although solvent and foreign solute effects are mentioned in general discussion papers by Wells and Buerger, no papers attempting explanations of these effects in terms of structure are included. In contrast to this serious omission, it is surprising to find a section *Morphology in phase space* dealing with Brillouin zones: an inclusion of questionable relevance to the theme of this collection.

Readers may differ in opinion about omissions or inclusions of papers, whether on grounds of relevance or (especially in the case of some recent papers) doubts whether the significance of contributions is great enough to entitle them to be regarded as 'benchmarks'; but on the whole this is a useful collection of papers which covers the subject fairly well, from a mineralogist's point of view. Those concerned with molecular crystals are less well served, for the relation between crystal shape and molecular shape is not considered at all. As Bernal used to say, chemists quite rightly recognize three classes of crystals – needles (flat molecules), plates (long molecules) and chunks (compact-shaped molecules). Perhaps one hardly expects to find this in a book in a geological series. But why not? Hydrocarbons are important minerals which are prominent in our thoughts at the present time.

The price is very high; this is a book for libraries, especially those concerned with the history of science, rather than for individuals.

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**Neutron scattering in chemistry.** By G. E. BACON. Pp. 186, Figs. 119, Tables 15. London, Boston: Butterworths, 1977. Price £12.50.

A review of this book, by Lynne L. Merritt Jr, has been published in the February 1978 issue of *Acta Crystallographica*, Section B, page 700.

**Crystallographic computing techniques.** Edited by F. R. AHMED, with co-editors K. HUML and B. SEDLÁČEK. Pp. 502, Figs. 134, Tables 93. Copenhagen: Munksgaard, 1976. Price Dkr 336.00.

This book contains the proceedings of the International Summer School on Crystallographic Computing, which was held in Prague, Czechoslovakia, 28 July–5 August 1975. It covers three main topics: *A*: structure solving methods; *B*: computational aspects of protein crystallography; *C*: miscellaneous crystallographic computer applications and techniques.

Papers in part *A* give chiefly an exposition of the traditionally successful symbolic addition and multisolution methods: the historical development and basic principles of direct methods, containing an interesting note on the computation of cosine invariants (J. Karle), the practical aspects of the symbolic addition procedure with many examples (I. L. Karle), the programming aspects of this procedure (Ahmed & Hall), a clear treatment of the *MULTAN* system (Woolfson) and the description of an automatic system based on the multisolution method (Andrianov & Tarnopol'skii). For the expert crystallographer it is a convenient survey of formulae, procedures and examples to have at hand.

Of the more recent developments in direct methods this book contains a remarkable contribution by Main, who introduced into *MULTAN*, as a systematization of older theories, a procedure that makes use of molecular structure. Apart from this there are some preliminaries on entirely new methods that we may expect in the near future: magic integers (Woolfson), matrix methods (Main) and a heuristic theory on the concept of neighborhoods (Hauptman).

A number of papers in both sections *A* and *B*, cover the subject of partial structure, phase refinement and phase extension in proteins. Sayre's method (Sayre), the maximal-determinant method (Tsoucaris) and the methods that modify the electron density (Gassmann, Simonov, Collins *et al.*) all seem to show a capability of improving the resolution of protein electron-density maps, starting from about 2.5 Å resolution.

Section *B* contains papers on protein crystallography which are also very informative to the general crystallographer: data collection (Bassi), the handling of protein data (Dodson), isomorphous replacement (Dodson, Kartha, Ashida) and anomalous scattering (Srinivasan). The increasing importance of Patterson search procedures, especially for the larger protein structures and viruses, is reflected in papers by Tollin, Blow, Bricogne, Colman *et al.* (see also, for ordinary structures, a paper by Kutschabsky and Reck on the convolution-molecule method in section *B*). The use of molecular structure and of non-crystallographic symmetry, which have always been the basic ingredients of these

methods (contrary to direct methods until recently), combined with data from isomorphous replacement, seem to be very effective in phase refinement and extension at lower resolution, especially in direct-space procedures.

Papers on coordinate refinement, with constraints, by least-squares or Fourier methods (Diamond, Steigemann *et al.*; Jensen, Freer *et al.*), on phase refinement at higher resolution by direct methods (mentioned above) and on model building (Diamond, Nagano) show the immense computational problems inherent in these methods, which have become highly important since more high-resolution data have become available.

Four major subjects can be distinguished in section C. The first is a study on electron diffraction of polycrystalline material by Imanov. Five papers give good insight into the problems and developments in the field of small-angle scattering. Special attention is given to collimation corrections (Schmidt, Walter), evaluation of scattered intensities from models of macromolecules (Šoler), and acquisition of neutron data (Klesse). Fedorov introduces large-angle scattering.

Studies on Fourier syntheses and least-squares refinements permanently hold the attention of the crystallographer. The papers on symmetry considerations (Larson), anomalous dispersion (Larson) and fast Fourier transforms will assist every programmer in getting optimum efficiency in his programs. Rollett gives remarkable conclusions on convergence in least-squares techniques.

In the last part of this chapter, developments in program design and data-handling techniques have been gathered. Owing to the rapid developments in computer design during the last decade large program systems and data systems have been set up, and are at the disposal of the modern crystallographer. A great variety of information on program design for large computers is given by Sakurai, Hall, Stewart, Sasvári, Ahmed and Morimoto. Trends in minicomputer techniques are discussed by Sparks and Gabe, and the Cambridge data base by Motherwell.

The reviewer is pleased to recommend this book to crystallographers with interest in direct methods and protein crystallography. The subjects contained in the third part are of general interest to most crystallographers. As a continuation of the proceedings of foregoing Summer Schools it is a valuable book; it provides very useful information on principles and developments in crystallographic computing.

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**Liquid crystals.** By S. CHANDRASEKHAR. Pp. x + 342, Figs. 158, Plates 16. Cambridge Univ. Press, 1977. Price £18.00.

This book is concerned with liquid crystals, the strongly anisotropic, but fluid, states which a large number of organic materials are now known to form and which possess degrees of order intermediate between those of the crystalline solid

and the amorphous liquid. Although the title is a general one, the work refers only briefly to lyotropic liquid crystals and concentrates strongly on liquid crystals formed by thermal effects on pure materials or their mixtures – the so-called thermotropic systems. Even here there is a bias, for smectic liquid crystals feature in only one of the four main chapters (additional to the brief introduction), whereas 258 pages are devoted to nematic and the related cholesteric liquid crystals.

Statistical theories of nematic order and continuum theory of the nematic state are dealt with fully in Chapters 2 and 3, respectively. These fairly complex matters are covered lucidly, and it is valuable to have these theories and their implications, on which the published work is scattered rather widely throughout the scientific literature, discussed concisely and logically between two covers. The latter part of Chapter 3 on the relationships between theory and the physical behaviour of nematics is very useful, particularly as it considers, in detail, disclinations and matters such as the twisted nematic cell, the Fréedericksz effect and electrohydrodynamics, all of which are of importance in relation to the application of nematics in electro-optical display devices.

Chapter 4 on cholesteric liquid crystals gives an account, which is again very clear, of the quite difficult optical properties of this type of mesophase. It then covers disclinations, flow properties, effects of external fields, and factors influencing the helical pitch and the relevance of these matters to the applications of cholesterics in displays and thermography.

Chapter 5 deals rather briefly with just two of the eight smectic polymorphic types (smectics A and C), and with transitions involving these phases. The account is most valuable however, expounding as it does various theories of the lamellar order of these phases and their interrelationships with the properties of these smectic states.

The book is attractively presented, and the literary style is pleasing and very readable. Diagrams are numerous and clear, and the index seems adequate. Despite the publication date of 1977 the author's preface is dated August, 1975, and it is not therefore surprising that of over 400 reference citations, the numbers decline from around 80 dated 1973, to less than 50 dated 1974 or 1975, to a handful dated 1976.

The text is surely a valuable addition to the current literature on liquid crystals and should be appreciated by anyone of graduate level and above doing research in the field of liquid crystals or concerned with their technological applications.

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**The plastic deformation of simple ionic crystals.** By M. T. SPRACKLING. Pp. ix + 242. London: Academic Press, 1976. Price £9.20.

For the majority of those who study crystals, dislocations and other imperfections are unwelcome phenomena. Nevertheless, for metals, the importance of dislocations and other structural imperfections for ductility, work-hardening