

$F_D \exp(i\varphi_P)$ is $(\varphi_P - \varphi_D)$, and so the correctly weighted amplitude is $f_D \cos(\varphi_P - \varphi_D)$. Since f_D is generally small compared with F_P or F_H , it is clear from Fig. 1 that $F_D = F_H - F_P \simeq f_D \cos(\varphi_P - \varphi_D)$, and is, therefore, the correctly weighted amplitude for the phase discrepancy $(\varphi_P - \varphi_D)$.

The error in φ_P itself is accounted for by the factor m_P . The two phase errors are approximately independent, so that in the difference synthesis the figure-of-merit, m_D , for a reflection is given approximately by $m_P \cos(\varphi_P - \varphi_D)$. The mean figure-of-merit for all reflections is given by

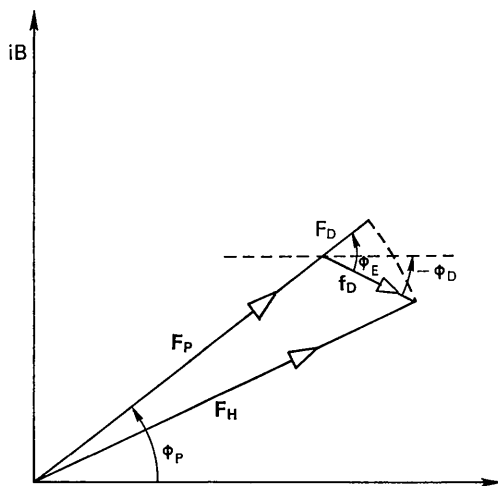


Fig. 1. $F_P = F_P \exp(i\varphi_P)$ is a structure factor for the native crystal and $F_H = F_H \exp(i\varphi_H)$ is the corresponding structure factor for this crystal slightly modified. The vectorial difference between them is $f_D = f_D \exp(i\varphi_D)$; f_D is, therefore, the correct difference coefficient. $F_D = |F_H - F_P|$ is the amplitude of the approximate difference coefficient, and $\varphi_E = \varphi_P - \varphi_D$ is the difference between the phase of the correct and approximate coefficients.

$$\langle m_D \rangle = \langle m_P \rangle \langle \cos(\varphi_P - \varphi_D) \rangle. \quad (2)$$

The phase φ_D is *random* with respect to φ_P . Taking account of the sign of $(F_H - F_P)$ the phase discrepancy is seen to be uniformly distributed in the interval $(-\pi/2, \pi/2)$. The mean value of the cosine over this interval is $2/\pi$, so that

$$\langle m_D \rangle = \langle m_P \rangle (2/\pi). \quad (3)$$

The quantity $\langle m_P \rangle$ is, of course, usually known from the structure analysis of the native material.

The root-mean-square error in an electron density function is related to the mean figure-of-merit through a formula given by Dickerson, Kendrew & Strandberg (1961). The relation depends on the assumption that errors in the coefficient amplitudes are small compared to errors in the phases, and is, therefore, of dubious validity for difference synthesis in which amplitude errors are large. A complete error analysis of the difference synthesis is, therefore, still lacking.

In summary, it has been shown that a difference Fourier synthesis calculated using $m_P(F_H - F_P) \cdot \exp(i\varphi_P)$ as coefficients has a mean figure-of-merit of $(2/\pi) \cdot \langle m_P \rangle$, and is correctly weighted in the sense of Blow and Crick.

I should like to thank Dr Max Perutz for his helpful comments.

Note added in proof: a very complete analysis of errors in the difference Fourier technique has recently been given by Henderson & Moffat (1971).

References

- BLOW, D. M. & CRICK, F. H. C. (1959). *Acta Cryst.* **12**, 794.
 DICKERSON, R. E., KENDREW, J. C. & STRANDBERG, B. E. (1961). *Acta Cryst.* **14**, 1188.
 HENDERSON, R. & MOFFAT, J. K. (1971). *Acta Cryst.* **B27**, 1414.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

An introduction to crystallography. By W. KLEBER. Pp. 366. Berlin: Veb-Verlag Technik, 1971. Price Dm 36,00.

The original *Einführung in die Kristallographie* first appeared in 1956 and its popularity is demonstrated by the fact that the German edition currently in print is the tenth; the book under review is a translation by W.A. and A. M. Wooster of this tenth German edition. It is very sad to record that Professor Kleber died in 1970 without having seen the first English edition.

The title *Introduction to Crystallography* – which incidentally has already been used by more than one author – could be interpreted in many ways; it could deal with anything from the purely formal elements of classification and symmetry to modern developments in crystal optics or in crystal chemistry. It is unusual to find a single book such

as Professor Kleber's which manages to combine successfully a considerable amount of classical theory and, at the same time, many up-to-date applications.

The secret is undoubtedly in the author's attitude to his subject. In the very first words of the introduction Professor Kleber points out that, while physics and chemistry are concerned with processes and changes, crystallography – in common with mineralogy, botany, zoology, etc. – is more concerned with the study of a specific object, in this case, a crystal. It is thus possible to include, quite logically, in a single volume, not only a very careful and precise section (about 90 pages) on the basic theory of crystal structure, starting from the laws derived from measurements of external morphology, dealing systematically with all the various symmetry operations and in considerable detail with the 32 crystal classes, but also with sections of similar length on crystal chemistry and on crystal physics and a

somewhat shorter, but extremely valuable and modern section, on crystal growth.

The crystal growth section provides a concise introduction which would be invaluable to workers in a great many borderline fields, such as metallurgy, material sciences, *etc.* Discussions are included of what the author calls 'crystal pathology', that is the various disorders and imperfections that arise when departures from precise regularity of the lattice occur. In the crystal chemistry section the author manages to compress an amazing amount of detailed discussion on bonding, structure types, resonance structures, *etc.* and includes a brief summary of the main features of molecular crystals. The final section provides an authoritative and, again, surprisingly concentrated statement of the main features of crystal physics, dealing with measurements of density, specific heat, hardness, elastic deformation, thermal, electrical and magnetic properties, crystal optics, X-ray electron and neutron scattering.

It is – as the author himself points out in his preface – not a book to be read on one's own; it is highly condensed. As a textbook for a comprehensive course in crystallography at third-year undergraduate or M.Sc. level and with adequate laboratory work and supporting lectures and seminars it would be excellent. It is also the kind of book that any experienced crystallographer would wish to have on his reference shelves because of its breadth of coverage and its concise and economical way of presenting information.

The translators have done their work well and are to be congratulated on making this very useful and scholarly work available to English readers.

C. A. TAYLOR

*Department of Physics
University College
P.O. Box 78
Cardiff CF1 1XL
Wales*

Neutron physics 2. By G. E. BACON. Pp.xi + 141. London: Wykeham Publications Ltd, 1970. Price £1:50

The author of this book is known to every specialist in neutron diffraction for his excellent, and by now classical, textbook on that subject. The present book has a much wider scope and is written for the non-specialist. Dr Bacon has, with the assistance of an experienced schoolmaster, Dr G. R. Noakes, written a very readable account of a wide subject covering neutrons, their discovery, properties, reactions and detection, neutron sources, and application of neutrons for studying static and dynamic properties of solids and liquids. Each chapter contains one or more problems with answers.

The book is written for sixth-formers or undergraduates in English schools and universities. It should, however, be of interest to everybody who is seeking a popular survey of current research and applications of neutron physics. I know of no book that is more suited for technical personnel working with or for a neutron physicist, or for specialists in other fields who want to know what neutron physics is. It is a pleasure to recommend this book.

T. RISTE

*Institutt for Atomenergi
Kjeller
Norway*

An introduction to mathematical crystallography.

By A. W. JASWON. Pp.xi + 125. London: Longmans, 1965. Price £ 1.50.

The reader of this book is introduced to the mathematical notation of crystal-symmetries in four steps: Point group symmetries, space lattices, 'Bravais' space groups (without glide planes and screw axes) and space groups including glide planes and screw axes. These four parts are subdivided into chapters, generally starting from purely geometrical considerations and followed by the corresponding mathematical treatments. At the end of the chapters problems are set, but the book does not contain the solutions.

An introduction to group theory is unfortunately not included. The author refers to numerous texts, but an introduction to the mathematics used, combined with references to relevant literature would probably increase the effectiveness of this book.

It is recommended to crystallographers who will find it a concise but comprehensive text book of geometrical crystallography and corresponding mathematical treatment.

HEINZ SCHULZ

*Institut für Kristallographie
und Petrographie | ETH
Sonneggstrasse 5
8006 Zürich
Switzerland*

Lattice vibrations. By B. DONOVAN and J. F. ANGRESS.

Pp.ix + 190. London: Chapman & Hall, 1971. Price £2.75.

Lattice dynamics is now a very mature branch of solid state physics, but it has always been difficult to find a text which, for the serious beginner, bridges the gap between brief treatments in general solid-state physics books and comprehensive accounts of various branches of the subject in Summer School publications and review articles. Professor Donovan and Dr Angress are aiming at just such a market in their short monograph on lattice dynamics.

The book confines itself to aspects of the subject explicable in terms of the adiabatic approximation, and derives the most important results one needs to understand the inelastic scattering of neutrons and X-rays, photon-phonon interactions and thermal properties of perfect crystals. There is also a chapter on vibrations of impurities, and a short but informative Bibliography.

The presentation is in general clear, and the contents sensibly chosen; so the book fulfills its primary purpose. For the experienced practitioner of lattice dynamics the collection in one small volume of many useful results may be helpful, but few fresh insights into his discipline will be revealed. A little more space, devoted to putting lattice dynamics into slightly broader perspective, to assessing more critically the current state of the art, and to providing some vision of where lattice dynamics is heading, might have been appreciated by beginner and specialist alike.

J. A. D. MATTHEW

*Department of Physics
University of York
England*