lectures and practical work given, for example, in this University, for the degree of M. Sc. (Crystallography), by specialists in each field.

To be able to run an X-ray equipment, to measure and interpret X-ray photographs, to complete a structure analysis and write a paper on it is *not* a sufficient training for a modern crystallographer, any more than to be able to carry out a complicated chemical analysis is sufficient training for a chemist. Most of us know this, but have not faced the implications, because we prefer research to pedagogy. But this is not the way in which the best research is ultimately done. Perhaps it is a pity that we call our science 'Crystallography', when it is really the study of the solid state, with all that that implies.

I am clear that while trained chemists, biochemists, physicists, geologists, engineers or mathematicians may eventually make good crystallographers, the training of a really first-class crystallographer must include something of all these sciences and does, in fact, merit much more careful planning than it has hitherto had. Crystallography could be a first-degree subject in itself, with these other subjects as necessary or desirable ancillaries, and with *branches* of crystallography as subsequent fields for specialization.

Meanwhile I maintain that the places where even a partially adequate training in crystallography can be obtained are few indeed, not more perhaps than a dozen. I should be glad to be proved wrong.

Notes and News

Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

International Union of Crystallography

The Union has received the following most generous donations as contributions towards the expenses of its publications:

From the Netherlands Organization for Pure Research (Z.W.O.) the sum of fl. 15,000 (approximately £1,500) for *Structure Reports*.

From Messrs CIBA A. G. the sum of Swiss fr. 2,000 (approximately £165) for *Acta Crystallographica*.

Commission on Crystallographic Nomenclature

The Executive Committee has accepted the recommendation of the Commission that E. W. Nuffield (Canada) should be co-opted on to the Commission.

Conference on Defects in Crystalline Solids

The H. H. Wills Physical Laboratory of the University of Bristol, England, in co-operation with the International Union of Pure and Applied Physics (particularly its Commission on the Physics of the Solid State) and with The Institute of Physics, is organizing a conference on 'Defects in Crystalline Solids' from 13 to 17 July 1954 in Bristol. While not excluding other subjects in the field the organizers propose to give particular attention to defects such as dissolved atoms, vacancies and F-centres, to microwave resonance methods of investigating their properties, and to the way in which they re-act with dislocations. Thus dislocations will be discussed in their chemical aspects, as influencing diffusion and precipitation in the solid state, rather than in relation to plastic flow.

It is hoped that a number of authors from overseas will personally present their papers, and with this in mind the Conference has been arranged to follow immediately after the General Assembly of the International Union of Pure and Applied Physics.

Board and lodging will be provided in Wills Hall (a student hall of residence) on special terms, or at hotels.

The Conference is open to any scientist interested in this field, subject to the limitations of accommodation.

Further particulars may be obtained from the Secretary, H. H. Wills Physical Laboratory, Royal Fort, Bristol 8, England, or from the Secretary, The Institute of Physics, 47, Belgrave Square, London S.W. 1, England. Those wishing to attend the Conference are asked to apply to the former, marking the envelope '1954 Conference' and stating whether they wish to be accommodated at Wills Hall or at an hotel and for what nights accommodation is required.

Photoelasticity and Photoplasticity

The International Union of Theoretical and Applied Mechanics announces that a Colloquium on the above subject will be held in Brussels, Belgium, from 29 to 31 July 1954. The Union also announces that a Colloquium on the Solid State will be held in Madrid, Spain, during 1955.

Crystallographers interested are invited to attend these meetings; further information may be obtained from the Secretary of the Union (F. H. van den Dungen, 48 avenue de l'Arbalète, Boitsfort, Brussels, Belgium).

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 2, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Computing Methods and the Phase Problem in X-ray Crystal Analysis.

Edited by RAY PEPINSKY. Pp. ix+390. Pennsylvania State College: X-ray Crystal Analysis Laboratory. 1952. Price $7·50.

The reviewer particularly valued the opportunity of re-reading this volume for the present notice, and reflection has led to an enhanced opinion of its worth. Although primarily intended as a report of contributions to a conference held at Pennsylvania State College in April 1952, the descriptions of the X-RAC and S-FAC and of the theoretical work inspired by these machines have much permanent value and are certainly worthy of record.

An opening address, by Pepinsky, in which various sponsors receive thanks, leads to generalizations on the nature of the information implicit in X-ray single-crystal diffraction data. A review paper, by Bijvoet, on mathematical and computational problems of X-ray analysis follows; this contains a large number of un-precise formulae, for example eq. (1) (p. 10), eq. (3) (p. 15), eq. (1) (p. 16), and particularly the description of least-square methods. Papers by Beevers, Patterson, and Buerger consider various aspects of implication or image theory. The contribution of Beevers is, in the reviewer's opinion, the most attractive, and forms one of the clearest expositions of the subject in print. A paper, by MacGillavry, on relations between Harker–Kasper inequalities and Buerger equalities makes the (too often forgotten) point that both methods are likely to be useless on complicated structures. Goedkoop follows with some relations between structure factors (a minor error occurs in eq. (1. 2) (p. 61), which, however, does not invalidate the subsequent discussion); the well-known Banerjee analysis is repeated for the second time (it occurred previously in Bijvoet's paper) and, assuming that the phases of F values are known, is used to derive relations between structure factors. After deriving various standard inequalities and determinantal relations, a section on the possibility of practical application concludes with the remarks that 'with growing number of atoms a point is reached beyond which no structure determination is possible, independent of the methods used'—an observation with which the reviewer heartily agrees—and that '... mathematical tools are available for an 'automatic' structure determination ...', which seems more speculative. Next follows a paper by Friedman on mathematical aspects of the phase problem in which the statement appears (p. 75) that non-negativity does not define a unique density distribution; there follows a derivation of several inequalities depending upon non-negativity, atomicity and bounded positivity. Equation (10) (p. 77) is misprinted in a way that may cause confusion. A further paper by Bijvoet deals with the isomorphous-replacement method of phase determination, and the ambiguities which result from its application to non-centrosymmetric structures; a short description of Bijvoet's elegant absorption-edge technique for eliminating this difficulty concludes the paper.

What may be called the 'phase section' concludes with a note by Ahmed on the diffuse-scattering technique of phase determination first suggested by the present reviewer. A further subgroup of papers on analogue X-ray computers follows: Robertson, Beevers & Robertson, and Ramsay & Lipson describe mechanical devices for Fourier synthesis and structure-factor calculation. The last authors give a pessimistic picture of the use of the Hägg machine at Manchester and Beevers & Robertson have produced an excellent description of classical integrator theory as applied to one-dimensional Fourier summation.

Bunn, in an exquisitely composed paper, considers the relative advantages of the Fly's Eye and X-ray microscope optical analogue calculators and Pepinsky's X-RAC and S-FAC, and this should be read by all aspiring machine designers. Hanson, Taylor & Lipson discuss their technique for introducing phase and amplitude into the X-ray microscope, and produce some excellent photographic illustrations, although it is a pity that Fig. 6(*c*) (p. 117) has not been given the same orientation as (*a*) and (*b*). One wonders why the mica-plate technique has worked so well at Manchester whereas Perutz, at Cambridge, (mentioned by Bunn) obtained only poor results.

The final sub group of this section deals with digital computing methods. A paper by Cox describes the binary and ternary punched-card methods used at Leeds, which, however, require the use of a gang punch—an item of equipment not available with all installations. Hughes, in a paper too vague to be really useful, describes the punched-card installation at the California Institute of Technology, and gives the interesting estimate of $40 for the cost of a three-dimensional synthesis on this equipment. The penultimate paper of the first section, by Ordway, deals with high-speed digital computers and, in particular, with the application of SEAC to crystal-structure analysis. An introduction to the preparation of problems for a machine of this type and a functional description of the SEAC are followed by an analysis of the calculation of d_{hkl}, F_{hkl} and f_{hkl} by the machine. It is interesting to notice that, even with this very fast machine, with 1000 terms a two-dimensional synthesis requires 1 hr. and a three-dimensional synthesis 8 hr. On the other hand the calculation of 1000 F values takes only 20 min. The cost of computing is quoted at $1 per minute. The section concludes with a note by Perutz on protein analysis, in which the use of Fourier transforms of chains is discussed.

The second section of the book consists of a description, by Pepinsky, of the history, design, construction and future of the X-RAC. The discussion is, in general, pleasantly written and it is well illustrated. An amusing piece of information (p. 171) is that the X-RAC was conceived during a carousel (roundabout) ride in a Boston amusement park. The S-FAC (structure-factor automatic calculator) and data storage facilities which are to be added to X-RAC will make the installation one of very great power, although Pepinsky's description of 'The Compleat Crystallographer' is perhaps over optimistic

(p. 272). A comment which may be made is upon the notation used for Fourier syntheses and structure factors: there appears no good reason for the introduction of such unfamiliar and inelegant expressions as that given on p. 261 (eq. (15)) when the standard and accepted symbols are available.

The final section of the book is composed of nine appendices. The first, by Pepinsky, describes the preparation of problems for the X-RAC and reproduces standard forms for use by those fortunate enough to have access to the machine. The second appendix, also by Pepinsky, deals with the extension of the range of indices available on the X-RAC. The use of a non-standard notation leads (p. 295, eq. (2)) to the remarkable result:

$$\bar{F}(\bar{R}) = \exp\left[-2\pi i \bar{R}.\bar{t}\right].\bar{F}(\bar{R}) .$$

The third appendix, by MacGillavry & Pepinsky, considers the application of conditions on $\varrho(x, y, z)$ (e.g. non-negativity) to the X-RAC and the possibility of sign determination. Appendix 4, by MacGillavry & Pepinsky, analyses the calculation of F values by sampling the continuous density distribution at points on a lattice. This technique, originally due to Beevers, is shown to be capable of accurate results so long as the lattice chosen has at least four times as many points as there are (H, K) values. A valuable point is made on p. 312, which can be condensed to 'In = Out', and should be noted by all protein crystallographers.

Appendix 5, by Pepinsky, discusses the use of positive kernels in terminating a Fourier series at a small number of terms without producing diffraction effects, and gives particular attention to the form $\{(1+\cos x)/2\}^m$.

Appendix 6, by Calderon & Pepinsky, extends the non-negativity criterion of Herglotz, which is the basis of polynomial and inequality theory, and leads naturally to Appendix 7, by the same authors. In the latter, the bounded-polynomial method is discussed, and the possibility of using the X-RAC in a steepest-descent process is suggested.

Appendix 8, again by Calderon and Pepinsky, considers the uniqueness of solutions and concludes that non-negativity and finite total mass are sufficient to define a unique solution in the centrosymmetric case of a *non-periodic* structure, but not otherwise, a result which has been tacitly assumed by Bragg and Perutz in their work on haemoglobin.

Appendix 9, by Sayre, concludes the book; it forms an excellent summary of Fourier transform theory, as applied to structure analysis, and contains some account of sampling methods for structure-factor calculation. A minor blemish is the use of a non-standard notation.

Although many of the papers contained in the book have now appeared elsewhere, and despite the numerous misprints, the work can be thoroughly recommended to all research workers in X-ray structure analysis. No other complete account of Pepinsky's X-RAC is readily available, and this alone makes the book worth reading. Moreover, most of the other papers in the collection are ones which crystallographers will like to have gathered together for easy reference. Considering the style of binding (limp card) the cost of the book is high.

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Data for X-ray Analysis. Volume I. Charts for Solution of Bragg's Equation.

By W. PARRISH and B. W. IRWIN. Pp. 108. Eindhoven: Philips. 1953. Price $2.

Data for X-ray Analysis. Volume II. Tables for Computing the Lattice Constant of Cubic Crystals.

By W. PARRISH, M. G. EKSTEIN and B. W. IRWIN. Pp. 90. Eindhoven: Philips. 1953. Price $2.

These volumes are the first of a series which is intended to supplement the *International Tables* by describing methods for facilitating certain routine calculations of rather specialized interest. If the standard of these first two volumes is maintained, it seems that the complete series will be very useful indeed to those who deal chiefly with the applied side of X-ray diffraction.

The first volume is of interest to those who are concerned with identification of materials by means of their powder patterns. It consists entirely of a large number of graphs of spacing against angle (θ and 2θ) for the $K\alpha$ lines of Mo, Cu, Co, Fe and Cr radiations; where necessary, separate curves are drawn for $K\alpha_1$, $K\alpha_2$ and their weighted means. The graphs are drawn on extremely open scales, and so are not subject to the usual criticism that graphical methods are not very accurate. On the other hand, the large scales necessitate several pages for each radiation, and one would have thought that the information could have been presented more compactly in tabular form.

The second volume is more diversified, and presumably owes its existence to the difficulties sometimes met with in identifying cubic substances from the A.S.T.M. index; if a powder photograph can be recognized as that of a cubic compound, identification is often more certain if its lattice constant, a, can be accurately measured.

The tables make use of the equation $a = \sqrt{N}.\frac{1}{2}\lambda/\sin\theta$, where $N = h^2+k^2+l^2$. Values of $\sqrt{N}.\frac{1}{2}\lambda$ to six decimal places are given for the wavelengths of the α_1, α_2, and β_1 lines of the K radiations of Cu, Ni, Co, Fe and Cr, for values of N up to 378. Division of this quantity by the observed value of $\sin\theta$ for a given line gives the apparent value of a derived from that line. The results may then be plotted against $\sin^2\theta$, or $\frac{1}{2}(\cos^2\theta/\sin\theta+\cos^2\theta/\theta)$, extrapolation to $\theta = 90°$ giving the true value of a; both these functions are presented.

An extensive list of lattice constants of cubic substances is included, together with representations of typical powder patterns, in the form of lines of varying heights, drawn at appropriate positions on $\log d$ scales.

It is perhaps unfortunate that the values of wavelengths used in the computations (*J. Sci. Instrum.* (1947), **24**, 27) are not those more recently recommended (*Acta Cryst.* (1950), **3**, 400), but since the difference are only of the order of 0·001 %, and the uncertainty of the wavelengths is about 0·003 %, the difference is negligible for most work.

For books intended for considerable use, the bindings, of thin flexible card, seem rather inadequate and will probably not stand up well to the use they will receive. On the other hand, the price is low, and laboratories which make considerable use of the books should have no compunction in replacing them when they become outworn.

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