tered in the form of spherical beads. Some success was achieved when using solid buttons of metal, but best results were obtained when the metal was loaded as a pile of chips or flakes. The melting was done in a water-cooled copper pot under a helium atmosphere. Prior removal of contaminating gases was accomplished by successive evacuation and flushing with helium. The intensity of the arc from the tungsten-tipped electrode was adjusted so that the sample was easily melted but without excessive superheating.

Samples of beryllium, vanadium, iron, zirconium, a 70 wt.% Ni/30 wt.% Cu solid-solution alloy, and the intermetallic compound NiAl were tried. X-ray examination showed that in all materials some of the spheres gave diffraction patterns typical of single crystals; however, no exhaustive check was made to prove the absence of coherent boundaries which could conceivably result from allotropic transitions in iron and zirconium. As might be expected, a much higher proportion of smaller spheres than larger spheres were found to be single crystals. Roughly 50% of the spheres with diameters less than 0·1 mm. were found to be single crystals, while only 5–10% of the 0·5–1·0 mm. spheres were single crystals. The largest crystal which was obtained was a beryllium sphere 1·5 mm. in diameter. In some of the larger crystals a slight flattening on one side of the sphere indicated solidification while stationary with respect to the pot. However, with the Cu/Ni alloy, which wets Cu, it is believed that solidification occurred as the beads rolled across the pot.

References

Cech, R. E. & Turnbull, D. (1956). *J. Metals*, 8, 124.

Splitstone, P. L. (1955). Doctoral Thesis, The Ohio State University, Columbus, Ohio, U.S.A.

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 direcct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333 Tay Street, Brooklyn 1, N.Y., U.S.A.) or to the Technical Editor (R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark)

Editorial Notice

Dr R. C. Evans, the Technical Editor of *Acta Crystallographica*, has asked to be relieved of his duties by 1 April 1958, and Prof. Dr R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark has agreed to succeed him.

Dr Evans is one of the founders of *Acta Crystallographica*, and indeed of the International Union of Crystallography. Even before this Union was officially established at the Harvard Assembly in 1948, Dr Evans spent a great amount of thought and time in formulating the aims and draft statutes of the Union, in preparing the way for its recognition by ICSU and for its financial support, and in negotiating for the production of *Acta Crystallographica*. The style and format of the journal were established by him in conjunction with the Cambridge University Press in a way which found general approval. Dr Evans was the sole British Co-editor for the first eight volumes and at the same time was responsible for the arrangement of the production of the entire journal. Besides, he was General Secretary of the Union from 1948 to 1954. As the work in both capacities became heavier, he dropped first the position as Secretary to the Union, and, soon after, the British Co-editorship, which went over to Prof. Lipson. Evans remained, however, as Technical Editor, handling all the accepted manuscripts and seeing them through the galley- and revision-proof stages. He set his pride in a faultless production, and eliminated numerous missettings, wrong references and omissions which had been overlooked by the editors and authors.

That *Acta Crystallographica* has developed its present prestige as a leading scientific journal is to no slight extent due to the direction which Evans gave to the journal while he was the British Co-editor and to the many hours of loving labour which he devoted to its details. His last gift is a *Decennial Index* for Vols. 1–10, which is in the final stage of production.

In thanking Robert Evans for what he has done for *Acta Crystallographica* we express the hope that the relief from this heavy duty may give him the leisure he desires for work on his own problems, including a new edition of his book *Crystal Chemistry*.

Conference on the Use of the IBM 704 Computer for Crystal-Structure Analysis

A conference on the use of the IBM 704 computer for crystal-structure analysis was held on 4 and 5 November 1957 at the National Bureau of Standards (NBS), Washington, D. C., U. S. A., sponsored by the American Crystallographic Association (ACA) and the NBS. About 60 participants were present. There were four sessions. The Conference did not deal exclusively with the IBM 704; papers concerning Maniac II and Datatron computers were also given. The Conference Chairman was S. Block (NBS); the Program Chairman was V. Vand, Pennsylvania State University (Penn State).

The first session was almost wholly devoted to the discussion of the IBM 704 computer, problem preparation, and IBM scientific activities. The second session dealt in detail with crystallographic programs now available or in preparation. The third session was chiefly concerned with evaluation of results and applications of the programs. The fourth session consisted of a one-hour FORTRAN seminar, followed by a meeting of the ACA Temporary Committee on Crystallographic Computing.

The first session was opened by Wallace R. Brode (NBS) with 'An introduction to the National Bureau of Standards', describing the NBS activities, scope and organization. This was followed by B. G. Oldfield (Service Bureau Corporation), who presented 'The IBM 704 and problem preparation', outlining the internal organization of the IBM 704 computer. The combination of great speed of execution (24 microseconds for most commands) and large capacity of rapid-access memory (4096 words of 36 binary digits each per one magnetic core) makes this computer a very powerful machine. Most of the present IBM 704's are two-core machines, but their capacity can be extended up to 8 cores. Magnetic drums and magnetic tapes extend the usefulness of the computer.

M. Abramowitz (NBS), in 'Pitfalls in computation', described the use of the one-core IBM 704 on problems in crystallography, spectroscopy, navigation, etc. T. R. Horton (IBM), in 'IBM scientific activities', gave a topical exposition on orbit computations of artificial satellites. This was followed by 'Contour mapping program', presented by H. Bedient (U.S.A.F.), a program of interest to crystallographers, although developed for weather forecasting. The output consists of printed values of the desired function at the selected grid points on an octagonal grid. Between the grid points, the last digit of the function, obtained by interpolating between the values at the grid points, is printed. If only the even digits are printed a map is obtained on which the contours can be seen easily and the maxima are clearly evident. The resolution across a sheet is limited to 120 printer wheels. This can be increased by glueing several printed sheets side by side. A 240 × 240 character map takes just over 3 minutes to print. This type of presentation will need to be further developed and may then become of real usefulness in crystallography.

In the paper 'Several programs for the Datatron computer', D. R. Petersen & J. M. Turley (Dow) discussed the listing of permitted reflections and calculation of $\sin\theta$ and d for a crystal, the reduction of the intensity measurements to values of F_o, the Fourier summation, and the computation of the interatomic distances and angles. The Datatron computer is an intermediate magnetic-drum machine, comparable to the IBM 650. A special pseudo-code was developed at Dow for coding. The data-reduction program allows reduction and scaling of data from several films, and gives estimates of standard errors from multiple observations of the same reflection. The distance program is not exhaustive, and calculates the distances and the angle for triplets of atoms, read by the program.

The first session was closed by a paper 'Trends in mathematical application' by L. Robinson (IBM), who discussed the use of the IBM 704 in business simulation, statistics and other fields.

The second session was opened by an introductory paper 'The least-squares program NY XR1', presented by D. Sayre (IBM). This program was one of the first even written for the IBM 704. It is composed of two, independent parts. The first accepts the reciprocal unit-cell constants on cards and the Miller indices, weights, and observed magnitudes of the structure factors, on magnetic tape. The output consists of a binary tape carrying these quantities and $\sin\theta$. The second part uses this tape as input during each iteration cycle. In addition, the scale, number of atoms to be included and refined, the atom types, fractional atomic co-ordinates, isotropic atomic temperature factors, scattering-factor tables and a space-group sub-program are also required. The flow of the program can be varied by setting external sense switches, which can cause, for example, the omission of temperature factors, the non-refinement of co-ordinates, or the non-refinement of temperature factors, and the writing of calculated structure factors on BCD output tape.

In the next paper, 'Modifications of Sayre's IBM 704 machine least-squares program NY XR1 for refinement of crystal structures', V. Vand & R. Pepinsky (Penn State) described modifications and extensions to D. Sayre's program. Triclinic crystals can now be processed. Input and output have been standardized to conform to SHARE specifications. Provisions for multiple-job processing and non-stop operation were introduced. Experiments are in progress with automatic convergence control to save machine time. Other improvements include simulation of anisotropic temperature factor—where permissible—by atom split, provision for atoms at special positions, calculation of standard errors in co-ordinates, and provision for refinement using the differential-synthesis method. Portions of space-group equations are coded on separate interchangeable binary cards, each of which can carry up to 22 instructions. By selecting a sequence of specific cards, a great variety of space-group equations can be composed. Recently, major effort has been directed to rendering the program operation fully automatic, so that it could be run without the presence of a crystallographer. Most of the program control has been transferred from the sense switches to special automatic control cards, read one at a time at the ends of refinement cycles. Sense switches are still used to overrule the control cards, if desired. The program has been used in the Penn State laboratory in various versions for over a year, and over 35 structures have been processed, the disagreement factor often dropping below 10%.

This paper was followed by 'Refinement of anisotropic thermal parameters on IBM 704' by W. Macintyre (University of Colorado). This program resembles portions of the Vand–Pepinsky program. The atomic scattering factors are not read in the table form, but evaluated in the first part by the Gaussian approximation of Vand, Eiland & Pepinsky. In the second part, the anisotropic thermal parameters are refined by least-squares, together with the coordinates. The scale factor is treated as a variable. The program was written fully in FORTRAN, which makes reprogramming for different space groups comparatively easy. At the end of each cycle, the average corrections to the parameters and the disagreement factors are printed in line, the detailed values and the structure factors being written on the BCD output tape. Copper tropolone was refined by this program.

W. G. Sly (M.I.T.) presented a paper 'A three-dimensional Fourier program', which uses a modified 'M-table' type of calculation on the IBM 704. The electron density can be evaluated over a 16 × 16 × 31 grid in 120ths or submultiples. Octant control is carried out by sense switches and control cards. In the ensuing discussion, doubts were raised whether the use of a M-table is more efficient than direct multiplication by F, as done by other programs. 'A FORTRAN Fourier program for IBM 704' was presented by S. Block (NBS). This program, written primarily as an exercise in FORTRAN, is for space group $P\bar{1}$. It is thus applicable to all centrosymmetric space-groups, but perhaps wasteful for some of higher symmetry. It uses about 50 FORTRAN statements. Execution time is of the order of 4 minutes per section.

'An IBM 704 program for one-dimensional Fourier summations and printing of X-RAC data sheets' was given by V. Vand, F. M. Lovell, R. Pepinsky & D. W. Smits (Penn State). This program was primarily designed for the reduction of three-dimensional Fourier or Patterson data to a form suitable for setting, section by section, on the input dials of the high-speed analogue computer X-RAC. X-RAC remains as the most efficient machine for presentation of Fourier transforms; and its present tie-in with the 704 program will eventually be extended through acceptance by X-RAC of punched-card or tape input. The program, written in FORTRAN, consists of four parts. The first part converts the decimal input data, written on a BCD tape, to binary on a tape which is then used repeatedly for each section specified by a coordinate card. The second part forms progressive totals of sines and cosines on another tape. The third part rearranges these according to space-group and X-RAC requirements, and computes a scaling constant. The fourth part scales the results and writes them on a BCD output tape, from which these can be printed out in a format directly acceptable to the X-RAC operators.

The session was closed by 'The IBM 704 program for evaluation of interatomic distances' by V. Vand & R. Pepinsky (Penn State). All the interatomic distances shorter than the arbitrarily set limit of 4 Å are evaluated. Symmetry-related atomic positions are generated by coded symmetry operations in accordance with the space-group theory. A block of 27 cells needs to be considered. The program is very fast, taking only about two minutes of 704 time for quite complex structures, and it is programmed for all space groups. The authors are presently considering incorporation of some known interatomic distances and atomic groupings as constraints in the refinement programs.

The third session opened with 'Four programs for crystal-structure analysis using the FORTRAN automatic coding system for the IBM 704' by J. L. Katz (Rensselaer Polytechnic Institute) & J. P. Jewett (Knolls Atomic Power Laboratory). One program computes two- and three-dimensional Fourier syntheses in $C2/c$ and $P2_13$. The second program calculates the peak positions and the eccentricity in peak shape for atoms from the electron-density maps. The third program calculates structure factors in the above-mentioned space groups. The fourth computes two- and three-dimensional Fourier syntheses on any general plane in the unit cell. This paper was followed by 'IBM 704 data-reduction program for X-ray intensities' by F. M. Lovell, V. Vand & R. Pepinsky (Penn State). This program has been based on the ideas of Petersen (see above). It includes the Lorentz polarization factor correction and absorption correction for cylindrical and spherical crystals.

D. T. Cromer (Los Alamos) presented 'The use of a high-speed computer (Maniac II) in indexing complex powder patterns'. This program attempts to find a unit cell of monoclinic or higher symmetry, the density of which agrees with observation. In practice, too many solutions are found which fit the data, owing to the inaccuracy of the experimental powder data. In 'The refinement of the structure of Feist's acid', D. R. Petersen (Dow) discussed results obtained by the least-squares methods. Early refinements were carried out with the IBM 604. Data from about 1000 reflections were used. Each iteration required about 30 hours and 10,000 cards on the IBM 604, and about 6 minutes on the IBM 704.

The paper 'Computer procedures in the refinement of the crystal structure of cycloserine hydrochloride' by J. W. Turley, V. Vand & R. Pepinsky (Penn State) described results obtained by using the Penn State modification of the NY XR1 program. Five different procedures were tested, starting with the same initial data: (1) refinement without hydrogens and without $F_o = 0$ data; (2) similar refinement with $F_o = 0$ added as $\frac{1}{2}(F_o)_{\text{min.}}$; (3) refinement as in (1) but with hydrogens; (4) refinement as in (2) but with hydrogens; (5) refinement as in (3) but with the shifts halved. This last gave the best results. The paper by Y. Okaya, V. Vand & R. Pepinsky (Penn State), 'Experiences in IBM 704 least-squares refinement of alums and other compounds', followed. In order to obtain a basis for understanding of ferroelectric behavior of certain alums, the structures of methylammonium, ammonium and sodium aluminum sulfate alums were re-examined, using three-dimensional X-ray data. Unexpected and very interesting structural anomalies were discovered. Other crystal structures, such as zinc and cobaltous aspartate trihydrates, $(\text{glycine})_3.H_2SO_4$, and reserpine hydrohalides, were very effectively processed. In several structures disagreement factors better than 10% were reached. The initial coordinates should be comparatively close to the true coordinates for the least-squares refinement to succeed. Wrongly-placed atoms in an otherwise correct structure manifest themselves by absurdly high temperature factors.

The fourth session was opened with a FORTRAN seminar. D. Sayre (IBM) explained the principle of FORTRAN (formula translation). It is an artificial language which closely resembles the mathematician's language, but which can be read by the IBM 704 and translated first into a symbolic assembly program (SAP) language and then into the binary machine language. It can be learned in about one or two days, whereas the SAP language requires several weeks of training. The programming effort is a fraction of that spent in ordinary programming and the resultant machine operation is about 90% as efficient.

In the discussion novices were sternly warned that the *FORTRAN Programmer's Reference Manual* must be read with extreme care. The question was raised as to whether it is possible to write programs partly in FORTRAN and partly in SAP. The present system does not have such provision included, but several ways exist by which this can be accomplished: for example, by use of dummy statements, by the use of dimension statement, or by connecting format blocks via tape.

The seminar was followed by the Meeting of the A.C.A. Temporary Committee on Crystallographic Computing, with V. Vand in the chair. Recommendations to the A.C.A. business meeting about the formation of an A.C.A. committee on computing programs were formulated as follows: the activities of this committee should cover all types of computing machines which are suitable for the solution of crystallographic problems;

information on the types of machines available should be collected and distributed; crystallographic programs should be appraised, reported, and their distribution arranged; inputs and outputs of programs should be standarized.

A tour of the NBS was arranged, and the installations of the computer SEAC and the IBM 704 were visited with demonstrations including the Fourier program of S. Block, and the contour-mapping program of H. Bedient. The newer version of the NY XR1 program was also demonstrated.

This was the third in a series of conferences on computing methods in crystal analysis, earlier ones being that at Penn State in 1950 (*Acta Cryst.* (1950), **3**, 400) and the IBM 650 conference conducted recently at the University of Pittsburgh (*Acta Cryst.* (1957), **10**, 384). Participants expressed gratitude at the success of this latest in the series.

V. Vand

Self-binders for *Acta Crystallographica*

Readers are reminded that arrangements have been made with Messrs Easibind Ltd. 84 Newman Street, London W.1, England, for the provision of self-binders for *Acta Crystallographica*. The binder for Vols. 1–2 is designed to carry the twelve parts of the two volumes, which are held without damage by steel wires; it is lettered with title, volume numbers and years (e.g. Vols. 1 and 2, 1948–9).

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The price of the binder is 14*s*.6*d*. post paid throughout the world. Orders should be placed with Messrs Easibind Ltd, stating clearly which style is required.

The structure of calcium ferrite

The authors wish to thank Dr Benjamin Post for pointing out an error in this paper (B. F. Decker & J. S. Kasper, *Acta Cryst.* (1957), **10**, 332). In Table 1 the *hkl* indicet for the powder pattern of $CaFe_2O_4$ are based on a unit cell in which the *a* and *c* axes have been interchanged with respect to the cell used to describe the structure.

Books Received

The undermentioned works have been received by the Editors. Mention here does not preclude review at a later date.

Tabellen zur Röntgenstrukturanalyse. By K. Sagel. Pp. viii+204. Berlin; Göttingen; Heidelberg: Springer-Verlag. 1958. Price DM. 28.

Structure Reports for 1951. Edited by A. J. C. Wilson, N. C. Baenziger, J. Wyart and J. M. Robertson. Pp. viii+588 with many figs. Published for the International Union of Crystallography. Utrecht: N. V. A. Oosthoek's Uitgevers Mij. 1957. Price 110 Dutch florins; $29·00; £10.10.0.

Experimental Crystal Physics. By W. A. Wooster. Pp. viii+115 with 47 figs. Oxford: Clarendon Press. 1957. Price 18*s*.

Mineralogische Tabellen. By H. Strunz. Pp. viii +448. with 70 figs. and 2 tables. Leipzig: Akademische Verlag. 3rd ed. 1957. Price DM. 34·00

Solid State Physics. Advances in Research and Applications. Volume 4. Edited by F. Seitz and D. Turnbull. Pp. xiv+540 with many figs. New York: Academic Press; London: Academic Books. 1957. Price $12·00; £4.16.0

Ferroelectricity in Crystals. By Helen D. Megaw. Pp. xi+220 with many figs. and tables. London: Methuen. 1957. Price 27*s*.6*d*.

Microwave Measurements. By E. L. Ginzton. Pp. xviii+515 with many figs. New York; Toronto; London: McGraw-Hill. 1957. Price $12·00; 90 *s*.

Crystal Structures. By Ralph W. G. Wyckoff. Volume II. Chapter XI, Miscellaneous Inorganic Compounds; Chapter XII, Silicates. New York; London: Interscience Publishers. 1957. Price $7·00

Crystal Structures By R. W. G. Wyckoff. Supplement III. Chapters I-VIII. (Approximately 450 loose leaves for binders.) New York; London: Interscience Publishers. 1958. Price $20·00

Tables et Abaques Par A. J. Rose. Tables permettant le dépouillement des diagrammes de rayons X et Abaques de réglage des monochromateurs à lame courbée Pp. 238. Paris: Centre National de la Recherche Scientifique. 1957. Price 1,500 French francs

Teoria Strukturnavo Analisa. By A. I. Kitaigorodskii. [Теория Структурното Анализа А. И. Китайгородский.] Pp. 284. Moscow: Publications of the Academy of Science of the SSSR. 1957. Price 10·65 rubles.

Fundamentals of Optics. By F. A. Jenkins and H. E. White. Pp. vii+637 with many figs. New York; Toronto; London: McGraw-Hill. 3rd ed. 1957. Price $8·50; 64*s*.

Dislocations and Mechanical Properties of Crystals. By J. C. Fisher, W. G. Johnston, R. Thomsen and T. Vreeland, Jr. Pp. xiv+634 with many figs. New York: Wiley; London: Chapman and Hall. 1957. Price £6.