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A diffraction technique for the study of crystals in conditions of instability. By H. JUDITH MILLEDGE, *University College, London, England*

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When single crystals are unstable or are maintained under conditions—e.g. of high pressure or high or low temperature—which it is not easy to keep steady, the time in which sufficient accurate diffraction data can be accumulated is limited. Equi-inclination oscillation photographs taken on modified Weissenberg equipment with $\nu=45^\circ$ are found to be an excellent method of rapidly recording three-dimensional data, especially for automatic processing.

It is advisable to arrange that the diffraction spots on any one (cylindrical) film should be resolved by about 1 mm. and there is no need for more than 1.5 mm. between layer lines. Thus if the useful area of the film is $6 \times 17 \sim 100$ cm.², it would be possible to record up to about 5000 spots on a single film. A film containing about 700 spots looks sparsely populated. For a given crystal (depending on its symmetry) the oscillation may be one of 179° about a long (non-primitive) axis, or by using successive shifts of the film-holder, interleaving and overlapping oscillation photographs about a short axis may be taken on the same film (if it is desirable, for example, to get a measure of the rate of change of intensity with time). The advantage of using $\nu=45^\circ$ is that this gives the same resolution for the rotation axis and all axes normal to it with one crystal setting, although for special purposes other equi-inclination angles may be used. Other advantages are

(a) that the spots lie along straight lines, which is convenient for intensity measurement by photometer;

(b) that the spot shapes are good and reasonably uniform over the film (much better than for a set of equi-inclination Weissenberg photographs);

(c) that for anisotropically-shaped crystals, especially if they are needles oscillated about the needle axis, the anisotropy due to absorption can be minimized and absorption corrections are relatively easy to apply;

(d) that the total exposure time for a given amount of 3-D data is far less than by other methods;

(e) that all the data may be obtained on one film-pack, or if the unit cell is a large one, on far fewer film-packs than by precession or Weissenberg techniques, with a corresponding diminution of systematic correlation errors;

(f) that one crystal mounting will cover about two-thirds of the limiting hemisphere, i.e. of the total available 3-D data, unless anomalous dispersion is involved, for oscillation angles which vary with the point-group and the symmetry of the rotation axis. Over 85% of the data may be obtained from the one mounting if the inclinations 0 to 45° are also used.

(g) By suitable interleaving of such oscillation photographs on one film, intensities at different temperatures, or different times, or of hkl , $\bar{h}k\bar{l}$ reflexions in the case of anomalous dispersion may easily be compared.

(h) For suitably chosen rotation axes the same hkl reflexions may be repeated on different layer lines on the same film, which assists intensity correlation.

The use of equi-inclination oscillation photographs is not new; Whittaker (1953) used them for work on fibres, for example. But many textbooks give the impression that oscillation photographs are not a satisfactory method of obtaining three-dimensional data. In fact they are superior to other types of photograph in every respect except ease of indexing, and now that this can be done by means of computer programmes, even this disadvantage has been removed.

An account of the modifications needed for the Weissenberg equipment, of the various intensity correction factors required (especially the layer-to-layer film factor) and of the method of indexing will be given in a more detailed publication.

Reference

WHITTAKER, E. J. W. (1953). *Acta Cryst.* **6**, 93.

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International Union of Crystallography

Commemoration Meetings in Munich, Germany, 25–31 July 1962

On the occasion of the fiftieth anniversary of Max von Laue's discovery of the diffraction of X-rays by crystals, and of the first crystal-structure determinations by X-ray diffraction by W. H. and W. L. Bragg, a Commemoration Meeting 'Fifty Years of X-ray Diffraction' was held in Munich, Germany, from 25 to 27 July 1962. The meeting was organized by the Ludwig-Maximilians-Universität München, the Bayerische Akademie der Wissenschaften and the International Union of Crystallography. It was followed by a Symposium entitled 'Recent Advances in the Experimental and Theoretical Methods of Crystal-structure Research', organized jointly by the

International Union of Crystallography and the Sektion für Kristallkunde der Deutschen Mineralogischen Gesellschaft, and held from 28 to 31 July.

A total of about 530 scientists and 120 accompanying members, from 27 countries, registered for the meetings. Generous financial support received from UNESCO through ICSU enabled the Union to offer travel grants to a relatively large number of invited speakers. Substantial financial support was further received from the Bundesministerium des Innern, the Bayerische Staatsministerium für Unterricht und Kultus, and from some twenty industrial firms; this support was used to defray

part of the organizational expenditure. The organizers of the meetings as well as the participants owe a debt of gratitude for these donations.

For the organization of the meetings various Committees had been established. The general responsibility was with a Congress Committee headed by F. Bopp, with P. P. Ewald, F. H. Laves, G. Menzer and D. W. Smits as members. The scientific programme was arranged by a Programme Committee consisting of G. Menzer (as Chairman for the Commemoration Meeting), W. Hoppe (as Chairman for the Symposium), R. Brill, M. J. Buerger, A. Guinier, F. H. Laves and W. H. Taylor. Many of the local arrangements had been made by a Committee for Special Purposes during the Congress, which worked under the chairmanship of H. J. Meister. Members of this Committee were Miss Th. Hutzler, who headed the Congress Office, Mrs Elly Schwab, who was in charge of the ladies programme, E. Berkl, H. Dachs, A. Hermann, S. Schwarzmann, H. Weichselgartner and E. Weidemann.

The Commemoration Meeting was held in the Deutsche Theater, the Symposium took place in the Large Physics Auditorium of the University. The meetings were formally opened on Wednesday morning 28 July. After a musical introduction played by the Münchner Kammerorchester, F. BOPP, on behalf of the organizers, welcomed the participants, and in particular the official delegates. Addresses of welcome were next read by the Staatsminister ALOIS HUNDHAMMER, who spoke on behalf of the Landesregierung; by Stadtrat H. BERGSTERMANN, who represented the Oberbürgermeister of Munich; by the Rector of the University of Munich, JULIUS SPEER; and by the President of the Bavarian Academy, F. BAETHGEN. A large number of addresses had been received from Academies and other learned Societies, but as time was lacking to read them all, only the beautiful scroll received from the Science Council of Japan was shown and read. The Dean of the Faculty of Sciences of the University, R. HUISGEN, was the next speaker and announced that the Faculty had decided to renew the doctorate which the President of the Union, P. P. EWALD, had received 50 years ago. On behalf of the Union P. P. EWALD then read an address of welcome, and continued with the first lecture of the Commemoration Meeting on the events leading up to Laue's idea. The description of the actual first implementation of this idea was given in the next lecture by W. FRIEDRICH. A short film followed showing 'live Laue diagrams', i.e. such diagrams recorded cinematographically in the Westinghouse Laboratories by means of an image intensifier while the crystal was being rotated. SIR LAWRENCE BRAGG then told how the work on X-ray diffraction was taken up by his father and himself and how one discovery followed upon the other in one and a half year of hectic work. The session was concluded by some summarizing words of P. DEBYE.

In four morning and afternoon sessions on 25, 26 and 27 July, fifteen further invited lectures were given in which the history and development of the diffraction techniques were described, and the results obtained in the various fields of research for which these techniques are being used. The names of the speakers and the titles of their papers are listed in the next section of this report.

The actual Commemoration Meeting was formally closed at the end of Friday morning 27 July. It was followed by the Symposium on Saturday 28, Monday 30

and Tuesday 31 July, at which 6 invited and 57 contributed papers were read (see list below). Short abstracts of most of these papers were included in the programme booklet which was distributed to all participants. These abstracts have been republished in the *Physikalische Verhandlungen* (1962), 13, 113; they will also be republished in the *Fortschritte der Mineralogie*. On Wednesday 1 August some fifty people participated in an informal discussion on 'Problems of Thermal Diffuse Scattering by Crystals'. Another informal discussion group had met earlier during the congress period, the topic of discussion being the 'Borrmann effect'.

For the members of the meetings a most attractive programme of social events had been arranged. It started with an informal gathering at the Löwenbraukeller on Tuesday 24 July. On Wednesday evening 25 July the Oberbürgermeister of the city of Munich, represented by Bürgermeister BAYERLE, was host at a reception in the Alte Rathaussaal; and on the next evening the Bavarian Prime Minister received the participants in the Antiquarium der Residenz. Following this reception the Congress Dinner was enjoyed in the Hotel Bayerischer Hof. The main speaker at this dinner was W. GERLACH, who at the end of his speech offered the participants a booklet containing the two classic papers of Max von Laue, and his autobiography. This booklet was published as a *Festgabe* by Friedrich Vieweg & Sohn, who had generously contributed to its cost of printing. On Friday 27 July a lunch was offered by the firm of Siemens, which preceded a bus excursion to the Chiemsee, with visits to the Fraueninsel and the Herreninsel. The chamber music concert played by the Morasch-Quartett in the candle-illuminated palace on the latter island will long be remembered by all participants in this excursion. On Saturday evening 28 July the members of the meetings were offered a violin recital by the young Japanese violinist Miss Tomiko Shida, who was accompanied at the piano by Gernot Kahl; or alternately a visit to a theatre on that evening or on Sunday 29 July.

List of Contributions

At the meeting the following papers were read; those with more than one author were presented by the author whose name is marked by an asterisk.

Commemoration Meeting

- P. P. EWALD (U.S.A.). Vorgeschichte der Entdeckung.
- W. FRIEDRICH (Germany). Die Versuche von 1912.
- SIR LAWRENCE BRAGG (U.K.). The early history of crystal-structure analysis.
- M. J. BUEGER (U.S.A.). Instrumentation.
- G. MENZER (Germany). Anorganische Strukturen.
- W. H. TAYLOR (U.K.). Silicates.
- J. S. KASPER (U.S.A.). Metal structures.
- J. M. ROBERTSON (U.K.). Organic structures.
- M. F. PERUTZ (U.K.). Biologisch wichtige Kristallstrukturen.
- J. LAVAL (France). Diffusion des rayons X par l'agitation thermique dans les cristaux.
- B. E. WARREN (U.S.A.). Background scattering due to disorder.
- P. DEBYE (U.S.A.). Flüssigkeiten, Gase, Makromoleküle.
- R. BRILL (Germany), A. GUINIER (France) & F. H. LAVES (Switzerland). Technische Anwendungen der Röntgen-

- analyse (Organische Chemie, Metallurgie, Anorganische Chemie).
- G. BORRMANN (Germany). Beugung am Idealkristall.
- Y. CAUCHOIS (France). Spectroscopie des rayons X.
- J. D. BERNAL (U.K.). Summary lecture.
- Symposium*
- W. HOPPE (Germany). Phasenbestimmung. (Invited paper.)
- L. I. HODGSON & J. S. ROLLETT* (U.K.). Automatic methods for heavy-atom phase determination.
- J. DONOHUE (U.S.A.). The Fourier method for structure determination.
- R. HUBER* & W. HOPPE (Germany). Lineare Gleichungen zwischen Strukturfaktorprodukten zur Bestimmung von zusätzlichen Vorzeichen in der Schweratomtechnik.
- T. WATANABÉ* & Y. TAKAKI (Japan). A modified Fourier technique in structure analysis.
- R. DIAMOND (U.K.). On the fourth and higher order inequalities.
- P. MAIN* & M. WOOLFSON (U.K.). The formulation and exploitation of linear equations between structure factors.
- D. F. GRANT (U.K.). Recent developments in the 'coincidence method' for the application of sign relations.
- H. HAUPTMAN (U.S.A.). The determination of phases directly from the Patterson function.
- K. ANZENHOFER* & W. HOPPE (Germany). Vorzeichenbestimmung mit Verwendung von Nullstellen der Pattersonfunktion.
- G. KARTHA (U.S.A.). Some methods for the solution of non-centrosymmetric crystal structures.
- I. KARLE* & J. KARLE (U.S.A.). The structure of hexaglycyl, an application of probability methods to space group *P1*.
- M. G. ROSSMANN* & D. M. BLOW (U.K.). Structural information derived from non-crystallographic symmetry.
- D. HODGKIN, M. M. HARDING* & E. COLLER (U.K.). Phase determination in rhombohedral zinc insulin.
- C. C. F. BLAKE, R. H. FENN, A. C. T. NORTH, D. C. PHILLIPS & R. J. POLJAK* (U.K.). A nearly automatic X-ray structure analysis of the enzyme lysozyme at 6 Å resolution.
- P. TOLLIN (U.K.). The determination of molecular orientation.
- C. SCHERINGER (Germany). Verfeinerung nach der Methode der kleinsten Quadrate bei Strukturen mit starren Atomgruppen.
- G. N. RAMACHANDRAN & R. PARTHASARATHY (India) (paper read by R. SRINIVASAN). Determination of space groups using anomalous dispersion.
- M. HART & A. R. LANG* (U.K.). Direct determination of X-ray reflection phase relationships through simultaneous reflection.
- H. BOERSCH & H. RAITH* (Germany). Modellversuche zur Phasenbestimmung im Elektronenbeugungsbild.
- G. KNESCH* & W. HOPPE (Germany). Modellversuche zur Phasenbestimmung von Elektronenbeugungsreflexen im Elektronenmikroskop.
- H. JAGODZINSKI (Germany). Fehlordnungen in Kristallen. (Invited paper.)
- A. J. C. WILSON (U.K.). General theory of the use of line-profile variance as measure of particle size, domain size, and strain.
- M. WILKENS (Germany). Zur Röntgenstreuung an Kristallen mit Versetzungen.
- U. BONSE (Germany). Zur Abbeugung interferierender Röntgenstrahlung im Deformationsfeld einer einzelnen Versetzung.
- A. MÜNSTER, K. SAGEL & P. P. WINCIERZ (Germany). Kritische Streuung von Röntgenstrahlen.
- M. KOREKAWA* & H. JAGODZINSKI (Germany). Eine allgemeine Theorie der Satellitenreflexe.
- S. TAKAGI (U.K.). A dynamical theory of diffraction for a distorted crystal.
- H. D. MEGAW (U.K.). Causes and consequences of disorder in strongly bonded structures.
- R. HOSEMANN (Germany). Zur Systematik der Parakristalle.
- G. H. SCHWUTKE (U.S.A.). Direct observation of imperfections in semiconductor crystals by X-ray diffraction microscopy.
- M. RENNIGER (Germany). Netzebenen-'Interferometrie', 'eingefrorene' und 'reversible' Gitterverzerrungen.
- J. BURGEAT*, J. DEVAUX & J. PRIMOT (France). Influence des défauts de réseaux sur la courbe de double réflexion obtenue à l'aide d'un diffractomètre à deux cristaux.
- R. BONART (Germany). Fibrillarstrukturen in verstrecktem linearen Polyäthylen.
- H. KUDIENKA (Germany). Bestimmung der Chromverteilung in $(\text{Fe,Cr})_3\text{C}$ mit Hilfe der anomalen Dispersion.
- S. SCHWARZMANN (Germany). Zur Kristallstruktur des $(\text{NH}_4)_3\text{GaF}_6$.
- K. FISCHER (Germany). Verfeinerung des atomaren Streuvermögens mit Hilfe des Verfahrens der kleinsten Quadrate.
- C. N. J. WAGNER (U.S.A.). Layer faults in *BCC* and *FCC* metals and alloys.
- K. SCHUBERT (Germany). Regelmässige Stapeländerung bei einigen Legierungsphasen.
- N. V. BELOV (U.S.S.R.). Unendliche Gruppen der Symmetrie und Antisymmetrie in einer, zwei und drei Dimensionen. (Invited paper.)
- R. PEPINSKY (U.S.A.). Automatic instrumentation. (Invited paper.)
- W. ARRINGTON, F. B. GERHARD, JR, J. A. SLITER & J. L. KATZ* (U.S.A.). A self-contained, time-sharing, computer automated single-crystal diffractometer.
- W. A. WOOSTER (U.K.). An automatic X-ray diffractometer.
- E. BERKL* & W. HOPPE (Germany). Ein- und Ausgabe mit Lochkarten an einem automatischen Zählrohereinkristalldiffraktometer.
- B. N. DELAUNAY (U.S.S.R.) (paper read by A. NIGGLI). Mathematische Beiträge zur Strukturtheorie der Kristalle. (Invited paper.)
- K. DORNBERGER-SCHIFF (Germany). Bemerkungen zur Gruppoid-Theorie von OD-Strukturen.
- G. WILL (U.S.A.). Symmetry relations in the convolution molecule method.
- D. McLACHLAN, JR (U.S.A.). The applications of information theory to crystallography.
- D. SCHWARZENBACH (Switzerland). Normierte Beschreibung von Kristallstrukturen.
- R. W. H. SMALL (U.K.). Some observations concerning the accurate measurement of single-crystal intensities using counters.

- A. TAYLOR* & G. W. GOETZE (U.S.A.). Laue cinematography with the 'Fluorex Astracon'.
- W. PARRISH (U.S.A.). Effects of diffractometer symmetrical broadening factors on line profiles.
- E. A. JUMPERTZ (Germany). Ein Dreh-Präzessions-Retigraph für Kristalle kleiner 100 μm .
- P. PAULITSCH (Germany). Die Laue-Methode für Reihenuntersuchungen.
- J. C. M. BRENTANO (U.S.A.) (paper read by B. E. WARREN). Schwankungserscheinungen bei Kristallpulveraufnahmen.
- K. L. WEINER (Germany). Röntgenbeugung an dünnen Schichten.
- O. KRATKY (Austria). Ein Verfahren zur Absolutmessung von Röntgeninterferenzen.
- H. SMITH (U.K.). Use of polaroid film in neutron and X-ray diffraction.
- H. ÜBERALL (U.S.A.). Interferenzen in der Bremsstrahlung von einem Einkristall.
- C. S. BARRETT (U.S.A.). Low-temperature structure analysis. (Invited paper.)
- G. KLIPPING (Germany). Strukturanalyse bei Heliumtemperaturen.
- S. C. WALLWORK* & D. S. BROWN (U.K.). A low-temperature equi-inclination Weissenberg technique.
- A. MCL. MATHIESON (Australia). Combined use of low temperatures and a high-intensity X-ray source in the analysis of moderately complex organic compounds.
- E. NEIRA & M. CANUT* (Spain). X-ray low-temperature studies of some dicarboxylic acids.
- N. KATO (Japan). Differences between X-ray and electron waves dynamically diffracted by crystals. (Paper actually read at the informal sessions on the Borrmann effect.)

Meetings of Commissions

Immediately before and during the period of the commemoration meetings, five Commissions of the Union, i.e. those on *Acta Crystallographica*, on *Structure Reports*, on *International Tables*, on Crystallographic Apparatus and on Crystallographic Data, held business meetings in Munich. The meetings of the three publishing Commissions mainly dealt with editorial questions; that of the Commission on *International Tables* was arranged as an open meeting on Wednesday 25 July. At the meetings of the two non-publishing Commissions their current and future programmes of activities were discussed.

Meeting of Executive Committee

The Executive Committee held its statutory intermediate meeting in Munich on 23, 24 and 26 July. The following is a summary of the more important items of business transacted.

1. The application for membership in Group I received from the Hungarian Academy of Sciences was discussed and considered to be in good order for presentation to the Sixth General Assembly.

2. It was agreed to propose to the Sixth General Assembly to include in the By-Laws the procedure followed at the Fifth General Assembly in 1960 with respect to the determination of the size of the individual Commissions of the Union for the period until the next General Assembly, i.e. that these sizes be determined by the General Assembly before the nominations for members of the Commissions are made.

3. A general statement of principles regarding the organization and the operations of the Commissions of the Union, which had been drafted by a Sub-committee set up for this purpose in 1959 (see *Acta Cryst.* (1959), **12**, 955), was approved.

4. To the great regret of the Commission on *Acta Crystallographica* and of the Executive Committee, the Technical Editor of the journal, Prof. R. W. Asmussen, had requested to be released from his task before the end of 1962. Since the large and growing volume of *Acta* would make it extremely difficult, if not impossible, to find a scientist willing to continue Prof. Asmussen's task, it was agreed, at the proposal of the Commission, to appoint a full-time technical editor for the publications of the Union, with responsibility in the first instance for *Acta Crystallographica*.

5. Although the 1961 *Acta Crystallographica* account had shown a small deficit, and higher deficits could be expected for 1962 and 1963, partly as a consequence of the appointment of a full-time technical editor, the accumulated balance in the account was considered sufficiently large to meet any such deficits, and it was decided that any increases in the subscription prices should be postponed until 1964.

6. The appointment of Dr J. Trotter as additional Co-editor for the Inorganic section, and of Dr L. D. Calvert as additional Co-editor for the Metals section of *Structure Reports* were approved.

7. It was agreed that a new (third) edition of the *World Directory of Crystallographers* be postponed until the end of 1963 or early 1964.

8. It was agreed that the Union should publish a selected set of two-dimensionally periodic drawings of Mr M. C. Escher, as recommended by the Commission on Crystallographic Teaching.

9. A Sub-committee was set up to consider a more coordinated and possibly extended publication policy of the Union, with special reference to a proposal that the Union should undertake the publication of Monographs on subjects of general importance.

10. A separate Sub-committee was set up to consider the question whether or not the Union should start the publication of a journal of industrial (or applied) crystallography.

11. The proposals and recommendations from the Programme Committee for the Sixth International Congress and subsequent Symposia were discussed with the Chairman of this Committee, and approved.

12. The time-table for meetings after the Rome Congress in 1963 was considered.