

the observation of a wealth of detail within the confines of what were formerly merely nebulous outlines. Incidentally, it has set the microscopist a pretty problem in interpretation. Electronic timing devices have made the pendulum appear a slow and cumbrous thing. The modern spectrograph, a most important industrial tool, has the lines of a gun turret rather than of a delicate scientific instrument. Any exhibition of modern scientific instruments provides both a survey of the growth of scientific knowledge and an indication of the extent to which science has intruded into every sphere of human activity.

The final word on the exhibition of scientific instruments at Copenhagen should be one of congratulation to British scientific instrument manufacturers, who in the short period of three years, after a long period of complete preoccupation with the production of instruments for military purposes, have most successfully reverted to their normal and natural activities. They have done this so completely, and in spite of the abnormal difficulties of the post-war years, that they are now able to meet the scientific, civil and industrial demands for instruments more abundantly than ever before in their history.

## INTERNATIONAL UNION OF CRYSTALLOGRAPHY

THE first meeting of the International Union of Crystallography, which was held at Harvard University during July 28–August 3, provided an opportunity for the presentation of papers on many research projects that are being carried out in different parts of the world. More than seventy such papers were read, and there were many detailed discussions.

Some of the sessions—for example, those on “Alloy Phase Structures” and “Proteins and Related Structures”—were held at the same time, and it was therefore not possible for a single observer to attend all of them and so to present an account of the whole conference. Since, in addition, the collection of abstracts alone would occupy more space than could be allowed for this article, it has been decided to describe the work relating to a few topics only. This, unfortunately, means that many papers will not be mentioned at all; but it should be understood that the papers chosen for mention are not necessarily the most important, but are those that the present writer feels competent to knit into a coherent scheme.

It is inevitable that comparison should be made between the states of progress in the various countries represented at the Congress. In the thirty-six years since X-ray diffraction was discovered, many subdivisions of the subject have arisen, and it is interesting to see how these have differently attracted different nationalities. It is, of course, undesirable that some branches of the subject should be ignored in any one country, and, by and large, this has not happened in the countries of major scientific importance; only at such international conferences does any unevenness become apparent. Conversely, contacts made at these conferences should encourage people, perhaps subconsciously, to fill up any gaps that may exist.

These observations were well illustrated by the papers presented at the conference; but unfortunately

the comparison can be made only between the United States and Great Britain; the latter had by far the largest foreign delegation and provided about one third of the papers read at the conference, while other countries—India, Canada, Sweden, Holland and Germany—provided only one tenth between them.

### Instruments and Instrumentation

The session on instruments was almost entirely American, and this preponderance was evident also in the apparatus that was exhibited. It may be argued that this was naturally so since the conference was held in the United States, but to the writer it did not seem that American superiority was too strongly emphasized; there was some British apparatus on view, and the only important omission was that of demountable X-ray tubes—otherwise all the recent developments were American.

For example, probably the most important recent advance in X-ray analysis is the introduction of Geiger counters for measuring intensities; this may ultimately release X-ray workers from the tyranny of the photographic film. Geiger-counter spectrometers are being made both by Philips Laboratories and the General Electric X-ray Corporation in America, whereas in Great Britain the author is aware of their existence only in more primitive form in certain laboratories. On the other hand, the American apparatus is directed toward the measurement of powder patterns, and, important as this measurement may be for industrial use, it has less theoretical importance than the study of single crystals. It is probable that this latter aspect is as far advanced in Great Britain as in America, but, in general, Geiger-counter apparatus is far more widely used in the United States.

As another example, Great Britain has produced nothing to compare with Buerger's precession goniometer. This instrument gives an undistorted reproduction of a section of the reciprocal lattice and is proving invaluable in the study of crystals with large unit cells. It is true that the indexing of photographs is not a limiting factor in the determination of crystal structures, but any aid to the shortening of this rather laborious operation must be welcomed and may even make practicable certain researches that are at present just outside the bounds of possibility.

In methods of Fourier synthesis, practice in the two countries is at present more or less the same; punched-card machines are greatly used by laboratories that have access to them, and printed strips, with calculating machines, are used by the less fortunate. But this balance is likely to be altered when the electronic machine at the Alabama Polytechnic Institute is completed; this machine should enable a complete two-dimensional Fourier synthesis to be presented instantaneously as an image on a fluorescent screen. With this instrument the major part of the operation will be the setting up of the coefficients; but, once these are set, changes in sign of certain coefficients can easily be introduced. It is possible that this instrument will make practicable the trial-and-error Fourier methods that have so often been suggested but never used.

Two other lines of progress must also be mentioned although they are not concerned with X-rays, namely, electron microscopy and neutron diffraction. Dr. R. W. G. Wyckoff showed electron micrographs of crystals in which individual molecules appeared

stacked together in orderly array. No intra-molecular detail appeared, of course, and it is likely that even the general appearance of the molecule is deceptive; but the fact that single molecules can now be observed is a striking testimony to recent progress with the instrument.

Dr. C. G. Shull gave an account of work on neutron diffraction. In this subject we pass from the orderly world of X-ray diffraction, where the intensity of scattering by an atom depends upon its atomic number, to one in which the intensity of scattering seems to be purely accidental; scattering factors have to be found by experiment and, as an extra complication, certain atoms scatter  $180^\circ$  out of phase with the others. Hydrogen is by far the best scatterer of neutrons, and thus neutron diffraction may settle certain arguments about the positions of hydrogen atoms in some organic crystals.

### Crystal Structure Determination

As a contrast to American preponderance in the session on instrumentation, the session on crystal structure determination was largely British; W. L. Bragg and his Manchester school seem to have set a fashion that still persists. This fashion is to treat the problem as a puzzle in which the clues have to be searched for before the analysis can begin. Clues can be of quite different types, but ultimately the evidence they provide must all fit together to give the final answer—the crystal structure.

The work of Mrs. D. Hodgkin and C. W. Bunn on penicillin provides the best example so far of the co-ordination of a number of separate methods. At the conference Mrs. Hodgkin described similar work by J. D. Dunitz on the structure of calciferol (see also *Nature*, Oct. 16, p. 608). The compound used was  $C_{35}H_{46}O_4NI$ , and 123 parameters were involved. Since the general form of the molecule was known, the problem was not so difficult as the penicillin one, despite the larger number of parameters; nevertheless, the work must be regarded as an outstanding example of the use of heavy atoms in crystal structure determination.

This 'sporting' approach may be contrasted with the more severely logical American approach, which manifests itself in several different ways. For example, there is Buerger's systematization of the methods of interpretation of Patterson sections—the so-called 'implication' method; most workers in Great Britain have been content to derive the information in a rather casual way, which is adequate for simpler structures but may not give all the information that is contained in the sections.

A completely new approach to the general problem has recently been suggested in the form of the 'Harker-Kasper inequalities'. To most people in Britain the method seemed to be of limited utility, but it has been completely justified by its use in the determination of the structure of  $B_{16}H_{14}$ . Since the method is of greatest use for compounds in which all the atoms are approximately the same weight, it appears to fill a gap left by the development of the 'heavy-atom' methods.

The main recent British contribution to the 'logical' approach is A. D. Booth's use of 'steepest descents', which gives the variation in parameters necessary to improve the agreement between calculated and observed intensities. The method promises to be very useful for refining parameters in known structures, but it has yet to prove its worth in determining an unknown structure.

The 'fly's eye', described by de Vos, Clews and Cochran, provides a more typical example of the British approach. No new principle is involved—merely an appreciation of the relationship between the scattering of light and X-rays—but the apparatus enables the tedious process of calculating structure factors to be eliminated and so enables more structures to be tested than if the calculations had to be done separately for each.

To summarize, it will be seen that rapid progress is still being made in the field of crystal structure determination; still more complicated structures are being brought within the scope of existing methods, and completely new methods are being discovered and brought into use. Structures are being solved that would have been considered quite impossible of solution ten years ago.

### Imperfect Structures

Important as the structures of perfect crystals may be, it must be realized that the most important materials, such as biological tissue, are highly imperfect and so their structures do not yield to standard methods of analysis. To these problems there are two methods of approach—the direct, typified by the Astbury school at Leeds, and the indirect, consisting of the study of slight imperfections first, and building on this foundation until the diffraction effects of the more complicated imperfections can be understood. Since the metals provide the simplest structures, it may ultimately appear that the biological problems are settled from an original study of metallic structures.

In this field progress seems to be about the same in both Great Britain and America. Dr. A. J. C. Wilson outlined the theory of diffraction by a one-dimensional imperfection, that for which the layers are perfect but are incorrectly stacked on each other. Examples of such imperfections were cited by Prof. W. Zachariasen, who dealt with the structure of uranyl fluoride, and by Dr. W. F. Bradley, who dealt with clays consisting of two different species of minerals. Imperfections in metals were dealt with by Dr. H. Lipson, who outlined some recent work on single crystals of  $AuCu_3$ ; this crystal gives sharp main reflexions and diffuse superlattice reflexions. In addition, Dr. J. W. Fitzwilliam dealt with the effects of local order in some binary alloys such as  $AuCu_3$ ,  $AuCu$  and  $AgAu$ .

As a contrast to these investigations, which are capable of theoretical treatment, Dr. H. M. Powell showed a remarkable set of Weissenberg photographs of the various layer lines from an organic crystal; the even layer lines showed sharp spots; but the odd layer lines showed continuous streaks along reciprocal-lattice lines. These effects can be accounted for qualitatively, but quantitatively their treatment is complicated by the complexity of the molecular structure; such photographs provide a striking challenge to the theoretician, and a complete solution of the problem should point the way to treatment of still more complicated imperfections.

The author would like to put on record his thanks to the Council of the Royal Society for enabling him to attend the conference, and to the organisers of the conference for enabling him to extend his stay in order to visit a number of laboratories where the work described in this article is being carried on.

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