

Crystallography was created. With the publication of this new journal the Commission on *Acta Crystallographica* was replaced by the Commission on Journals, under the chairmanship of Professor Wilson. Under his leadership, *Acta* continued to attract the very best papers on crystallography and has consolidated its standing as the leading international crystallographic journal, with the result that the size of the journal has grown steadily. Efforts to contain the size of the journal have been made by strict refereeing procedures, concerted efforts by Co-editors to persuade authors to shorten their papers, the introduction of the supplementary deposition scheme for material such as tables of structure factors and, more recently, of thermal parameters, and the introduction in Section B of Short Structural Papers as a means of reporting crystal structure determinations concisely and in a standard format. In spite of all these efforts the size of the journal in 1976 was 1038 pages in Section A and 3360 for Section B. In 1976 *Acta* contained 1011 full-length articles, short structural papers or short communications as compared with 213 in 1960.

The Executive Committee of the Union would like to take this opportunity to express its deepest gratitude and appreciation, on behalf of the Union and the international crystallographic community, to Professor Wilson for 18 years of devoted service to the Union as Editor of *Acta Crystallographica*. It is confident that Dr Abrahams will continue to maintain the high standards set by his predecessors and is most grateful to him for agreeing to undertake the Editorship of the journal.

Professor Wyart has been a Co-editor of the journal since it was first published, in 1948. His contribution to the development of the journal and to crystallography in general has been immense. His thesis in 1930, on the structure of zeolites, described some of the first structure

determinations made in France using X-rays. His subsequent interest in hydrothermal synthesis led to the synthesis of granite. He prepared many of the symmetry group drawings for the 1935 edition of *International Tables*. From 1928 he worked under Professor C. Mauguin; in 1948 he succeeded Professor Mauguin and was Director of the Laboratoire de Minéralogie-Cristallographie of the University of Paris until his retirement in 1973. He created and for a long time directed the Centre de Documentation of the Centre National de la Recherche Scientifique. He was a member of the Commission on *Structure Reports* from 1948 to 1951 and from 1954 to 1963, and was a Section Editor for several years. He was a member of the Executive Committee of the Union from 1948 to 1951, a Vice-President from 1951 to 1954 and President from 1957 to 1960. The Executive Committee is greatly indebted to Professor Wyart for the many ways he has served the Union since its creation.

Professor H. Lipson, who recently retired as Professor of Physics at the University of Manchester Institute of Science and Technology (UMIST), has been a Co-editor of *Acta Crystallographica* since 1956. A notice concerning Professor Lipson's retirement from UMIST has been published in *Journal of Applied Crystallography* [(1977), **10**, 430]. After working at the University of Manchester, the National Physical Laboratory and the University of Cambridge, Professor Lipson was appointed Head of the Physics Department at UMIST in 1945. He was elected a Fellow of the Royal Society in 1957 and made a Companion of the Order of the British Empire in 1976. With the exception of Professor Wyart, Professor Lipson is the longest serving Co-editor of the journal and the Union is most indebted to him for his many years of service in this capacity. During this period he has dealt with over 4000 papers submitted for publication in the journal.

International Union of Crystallography

Polarization ratio for X-rays – A survey by the Commission on Crystallographic Apparatus

The Commission on Crystallographic Apparatus is conducting a survey of measured values of the polarization ratio for crystal-monochromated X-ray beams. This note summarizes the definition of this ratio, mentions techniques for its measurement, emphasizes that the objective of the survey is to establish the range of values observed in practice, and is an invitation to all interested people to participate.

The polarization factor in a typical X-ray diffraction experiment is

$$P = (1 + K \cos^2 2\theta)/(1 + K),$$

where K is the polarization ratio, the ratio of the beam power with π polarization to that with σ polarization. A fractional error in P will be directly reflected as a fractional error in the results. Thus it is important that P (or, equivalently, K) be accurately determined. For example, in an experiment using unmonochromated characteristic radiation, K is very nearly unity.

In the case of crystal monochromated radiation, the situation is more complicated. Consider for concreteness the case where the planes of diffraction for the monochromator and for the sample are parallel. There is apparently a common, tacit 'argument' which goes like this. 'The highest possible integrated intensities are achieved with a crystal in mosaic form. Since monochromators are chosen to give the highest possible beam power, it is probable that the polarization ratio will be very close to that given by an ideally mosaic monochromator, $\cos^2 2\theta_M$ in this geometry. In any case, the limits on K are probably $\cos^2 2\theta_M$ and the value for an ideally perfect monochromator, $\cos 2\theta_M$ '.

It was realized independently by a number of workers that the above argument is specious (Jennings, 1968; de Wolff, 1968; Olekhovich, 1969). The correct reasoning is more like this: Although appropriate monochromating materials are those which could give a large integrated intensity, it is usually advantageous to arrange the geometry so that desired rays of *both* polarizations are almost totally reflected. Under these conditions, which can be considered an extreme case of secondary extinction, initially unpolarized radiation will be monochromated to a high-power beam with polarization ratio approaching unity. On the basis of this

reasoning and measurements on typical setups, one can estimate that K would differ from $\cos^2 2\theta_M$ by about 40% for LiF at Cu $K\alpha$, 12% for graphite at Cu $K\alpha$, 8% for LiF at Mo $K\alpha$ and 3% for graphite at Mo $K\alpha$. Such errors would be intolerable in many modern experiments.

Unfortunately the polarization ratio depends on the physical state of the monochromator, beam divergences, and other geometrical factors. In the case of a diffracted-beam monochromator the size of the receiving slit and focusing conditions at the sample would also come into play, making precision measurements difficult with this configuration. In the case that the sample intercepts only a portion of the beam, it may be necessary to study this limited portion of the beam. In any case, accurate results require that the K value be measured for the actual apparatus used; the above values are only typical. Fortunately it is quite simple to achieve $\frac{1}{2}\%$ accuracy in the measurement of K ($\frac{1}{4}\%$ in P). One merely determines the center of gravity of the beam in the axial and equatorial planes (so that the average solid angle intercepted by the detector is well defined) and measures amorphous scattering at 90° in the two planes. Higher accuracies can be achieved, but only with much greater difficulty.

In spite of all these considerations, many workers do not measure the polarization ratio for their apparatus but instead assume the value $\cos^2 2\theta_M$. Some workers also do not consider the above values to be typical. This situation perhaps arises because measured values of K are not conspicuously published; they do, after all, apply only to a single apparatus. But it appears that it would be useful for it to be generally known what the range of expected values

might be. With this end in mind, the Commission on Crystallographic Apparatus of the IUCr has authorized a survey of measured values of polarization ratios obtained for crystal monochromated characteristic radiation. The Commission would be interested in collating both values which have been obtained in connection with experiments which have already been carried out and values which are newly measured. Since the primary objective of this survey is to show the range of polarization ratios which may be encountered in practice, a project with instructions to the participants is not visualized. Rather the submission of measured values along with any concomitant information will be welcomed. However, as assistance to interested workers, appendices to this note can be supplied which (1) expand on the rationale for expecting polarization ratios near unity, (2) give more detail about the simple experimental method for determining K , and (3) suggest some of the types of information which would be useful to the Commission as measured values of K are collated. *Please send your values or requests for information to Dr L. D. Jennings, Army Materials and Mechanics Research Center, Materials Sciences Division, Watertown, Massachusetts 02172, USA.*

References

- JENNINGS, L. D. (1968). *Acta Cryst.* A24, 472–474.
 OLEKHOVICH, N. M. (1969). *Sov. Phys. Crystallogr.* 14, 203–206.
 WOLFF, P. M. DE (1968). Private communication to L. D. Jennings.

Book Review

Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.

Point defects in crystals. By R. K. WATTS. Pp. xi + 312. Chichester: John Wiley, 1977. Price £16.50 (US \$27.90).

First impressions of this book are that accumulated knowledge on point defects in crystals is no longer merely quantitative but is very detailed, precise and of enormous amount. This impression will be common for most readers.

The book consists of ten chapters, the first three of which are concerned with theories on defects with tightly and loosely bound electrons and on vibrational properties of defects respectively. They are well summarized and include up-to-date references. This part is a useful and easy-to-read textbook for researchers in this area. Actually, it must be an advantage that the theories of the three topics mentioned above are collected in one volume.

The next three short chapters are titled *Defect Chemistry*, *Experimental Methods* and *Electrons in Covalent and Ionic Crystals* respectively. This part is an intermezzo to the massive descriptions that follow. The maps of valence-

electron charge density for Ge, GaAs and ZnSe should be attractive to readers.

In the last four chapters, a survey of defects in elemental crystals (silicon, germanium and diamond), III-V compounds, II-VI compounds and alkali halides is given. The structure deduced mainly from results of EPR and optical experiments is presented for individual defects. In the case of silicon, for example, a description is given for Group V donors, lithium and magnesium, sulphur, Group III acceptors, boron associates, carbon, vacancy, vacancy-germanium associate, vacancy-Group V donor associate, aluminium centres, interstitial oxygen, etc. These chapters are a sort of handbook of defects in these crystals; readers will understand the state of present knowledge as well and realise how strong is the driving force of investigations in this field.

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