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Crystallographers

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This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours, etc. Items for inclusion, subject to the approval of the Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England).

Professor **N. V. Belov** died on 7 March 1982. A full obituary will be published in *Acta Crystallographica* Section A in due course.

Professor **Katharina Boll-Dornberger** (née **Schiff**), who died on 27 July 1981, aged 71, was the most prominent X-ray crystallographer in the German Democratic Republic. Drs H. and K. Fichtner write that she started her X-ray work with V. M. Goldschmidt at Göttingen in the early thirties and took her doctor's degree in the city of Vienna after her escape from Germany. After her emigration to England she had the opportunity to work with J. D. Bernal and D. Hodgkin. Returning to Germany after World War II, she established X-ray crystal structure analysis in the GDR. In 1956 she became Professor of Physics at Humboldt University in Berlin. From 1958 to 1969 she was director of the Institute of Crystal Structure Research of the Academy of Sciences of the GDR. She worked in inorganic crystal structure analysis and in protein crystallography. Her OD theory, created in the 1950's, is a geometrical approach to polytypism and stacking disorder. She introduced the concepts of partial coincidence operations and groupoids into crystallography. Crystallographers have lost a colleague of critical intelligence, deep knowledge and decisive influence on a considerable number of scientists in the GDR and in other countries.

Venkatraman Subramanian, a post-doctoral research fellow at the Crystallography Centre of the University of Western Australia, died tragically on 27 December 1981 at the age of 30 as a result of a swimming accident. Dr S. R. Hall, University of Western Australia, and Dr K. Seff, University of Hawaii, write that Subramanian was born in Bombay. He obtained a BSc in Chemistry at Madras University in 1972; an MSc at Birla Institute of Technology in 1974; and a PhD in Chemistry at the University of Hawaii in 1980. In 1974–75 he was a CSIR Research Fellow at the Indian Institute of Science in Bangalore and in 1980 was appointed as an ARGC research fellow at the University of Western Australia for the development of crystallographic computer software for the XTAL System. Subramanian was a diligent research worker with a care for detail. He was highly respected by his colleagues and admired by the many students he went out of his way to assist.

Dr U. W. Arndt, of the Medical Research Council Laboratory of Molecular Biology, Cambridge, Professor **J. D. Birchall**, Senior Research Associate at ICI, Runcorn, and Professor **M. Hart**, Wheatstone Professor of Physics, King's College, London, have been elected Fellows of The Royal Society.

Professor **Gunnar Hägg**, University of Uppsala, Sweden, has been awarded the 1982 Gregori Aminoff Gold Medal by the Royal Swedish Academy of Sciences for his pioneering applications of X-ray crystallography in inorganic chemistry. He will receive the Medal at the June session of the Academy. This is the third time that the Aminoff Prize has been awarded, the first recipient being Professor **P. P. Ewald** in 1979 and the second one Sir **Charles Frank** in 1981.

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Structure Reports

Volume 46A of *Structure Reports* has recently been published. It covers the literature for metals and inorganic compounds for 1980 (464 pages) and costs 153 Netherlands guilders for subscribers with standing orders. The full price for individual copies is 180 guilders but personal subscribers may buy a copy for their own use at 90 guilders. Orders for these publications may be placed direct with the publisher, D. Reidel Publishing Company, PO Box 17, 3300 AA Dordrecht, The Netherlands, or with any bookseller. Trade orders should be sent to Reidel.

Book Reviews

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.

J. Appl. Cryst. (1982). **15**, 359–360

Advances in X-ray analysis, Vol. 24: Proceedings of the 29th annual conference on the application of X-ray analysis, Denver, Colorado, August 1980. Edited by *D. K. Smith, C. S. Barrett, D. E. Leyden & P. K. Predecki.* Pp. xx + 428. New York: Plenum Press, 1981. Price US $ 49.50.

During the 29th Denver Conference on Applications of X-ray analysis, 74 papers were read, 56 of which are published in this volume. Following the tradition of the conferences there are reports on X-ray diffraction analysis (XRD) and X-ray spectrometry [XRS; mainly X-ray fluorescence analysis (XRF)]. It is difficult to review all the essential results and ideas contained in this volume, but a short summary will be given here.

Nowadays it is possible to obtain refined values of crystal-structure parameters from powder diffraction data by the Rietveld method, including a least-squares refinement procedure for fitting calculated and observed powder diffraction patterns. An example is given for human tooth enamel. Further, advances in the interpretation of diffraction data from amorphous materials are outlined. Qualitative and quantitative phase analysis, collection of crystallographic data, precision and reproducibility of Guinier powder patterns, and the level of XRD in Europe are discussed. The great importance of continuously scanning position-sensitive detectors in modern XRD work is demonstrated by the ten papers on this topic. Application, use and accuracy of such detectors are described; they are capable now of scanning speeds of several hundred degrees per minute, and

well resolved diagrams are obtained with their help. XRD applications from several fields of materials science like stress measurements, investigations of metallic glasses and fibrous polymers, and environmental problems are described.

One main objective of the XRS part is to evaluate the advantages and/or disadvantages of the WDXRS (wavelength dispersive XRS) and EDXRS (energy dispersive XRS) methods. It is shown that in the most important industrial applications (minerals industry, metals industry) the latter is at an advantage, because it yields results of sufficient precision at lower cost and effort and because the equipment with a radioisotope source and a Si(Li) detector is portable.

The Si(Li) detector needs liquid-nitrogen cooling. As an alternative, for the analysis of high- and medium-Z elements ($Z \gtrsim 30$), a room-temperature mercury iodide (HgI_2) detector can be used. The energy resolution of this detector is poorer (optimum value 380 eV for the 5·9 keV X-rays of Fe 55) than of Si(Li), but sufficient for most of the practical applications in heavy-element analysis. A further comparison concerns the XRF and PIXE (proton-induced X-ray emission) methods; it is shown that for the analysis of samples with strongly varying matrix composition, and for $Z > 20$, PIXE is more suitable because of the smaller matrix corrections.

The papers on XRF techniques mainly deal with measures for increasing the detection limits and reproducibility of the method. This can be achieved, as is shown, by different methods of background reduction (filter, electronics for pulse handling, application of primary scatterers to polarize the radiation) and by optimizing the sample preparation techniques and excitation conditions.

As an alternative surface-sensitive analysis method to PIXE and others, the LEEIXS (low-energy-electron-induced X-ray spectroscopy) method is presented, where soft X-ray fluorescence radiation of light elements B to F excited by low-energy electrons from a cold cathode tube is detected. The method is capable of analyzing samples from such elements qualitatively and quantitatively, of measuring film thicknesses and of gaining depth profiles. The method works in primary vacuum, which is a great advantage in the investigation of industrial research problems over other surface-sensitive techniques.

Finally, computerization of XRS has great importance, as can be seen from most of the papers. In one of them a WDXRS system combined with a minicomputer is presented, which is suitable for a high-speed qualitative analysis of samples within less than half a minute. This is comparable with the speed of computerized EDXRS systems, but the resolution (precision) of the WDXRS system is much higher.

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Quantitative X-ray spectrometry.

By *Ron Jenkins*, *R. W. Gould* and *Dale Gedcke*. Pp. 586. New York and Basel: Marcel Dekker Inc., 1981. Price SFr 160.00

The authors are well known in the field of X-ray spectrometry: R. Jenkins is at Philips, Mahwah, New Jersey, R. W. Gould is at the University of Florida, Gainesville and D. Gedcke is at EG & G ORTEC, Oak Ridge, Tennessee. The book is divided into 12 chapters and seven appendices. The literature has been reviewed till 1977 and many references are given. This book is the only one of its kind to cover both wavelength- and energy-dispersive spectrometers in detail.

The first chapter is a short introduction to the subject; the second chapter explains the physics of interaction of X-rays with matter and is partly the theoretical foundation for chapters 9 and 10. Chapter 3 deals with sources for X-rays and chapter 4 is a long treatise on spectrometer instrumentation. Chapter 5 gives some necessary statistics and chapter 6 comments on general computer applications such as smoothing of spectra, background subtractions and least-squares fitting of peaks. Chapter 7 is called specimen preparation and presents brief information on this difficult subject. Chapter 8 is a well written explanation of qualitative X-ray analysis.

Chapters 9 and 10 are on quantitative analysis. This section starts with the assumption that all samples are rendered homogeneous, so that only matrix effects are to be accounted for. Next it is stated that the analyst has great difficulties in providing good standards, but nothing is said as to where such standards are got or how they are prepared. Many procedures for matrix corrections are discussed, the most sophisticated of which are the fundamental parameter methods or alpha correction procedures. The most useful – but unfortunately not always applicable – double dilution method is explained in detail. Limits of concentration ranges for different correction formulas, as well as examples of not wisely chosen ranges of standard concentrations in a series, are described.

Chapter 11 is on trace analysis and emphasizes the important role of the background for determinations near the lower limit of detection. Chapter 12 is devoted to radiation health hazards from X-rays and protection against them. Some legal aspects of US regulations are described.

This book is a valuable compendium for the practicing X-ray spectroscopist in industry and science or researchers in other fields who have to apply X-ray analysis. It seems doubtful that students could afford to buy such a comprehensive book.

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Books Received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

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Photoelastic and electrooptic properties of crystals. By *T. S. Narasimhamurty*. Pp. xxix + 514. New York: Plenum, 1981. Price US$37.50. A review of this book, by E. H. Turner, has been published in the May 1982 issue of *Acta Crystallographica*, Section A, pages 399–400.