Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985). 18, 189–190].

J. Appl. Cryst. (1993). **26**, 144

XTALLAB and *POWDER* – computer assisted instruction in elementary crystallographic methods.

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The crystallographic problem. Addressing a significant part of the many facets of crystallographic methodology is not feasible in the undergraduate chemistry curriculum. Though X-ray diffraction has led the way to significant structural discoveries, crystallographic techniques receive, at best, only a cursory review during the undergraduate course of study.

Method of solution: *POWDER* and *XTALLAB* and their accompanying supplements were designed to provide the undergraduate junior or senior physical-chemistry student with computational experience using basic crystallographic methods to supplement knowledge obtained through course lectures.

Unlike other crystallographic laboratory exercises (Lessinger, 1988; Loehlin & Norton, 1988), these experiments require no previous computational experience or special crystallographic software. Each experiment can be run on a PC and can be performed in one 3h laboratory period. The experiments are each broken into two parts – a description of the crystallographic theory and calculations involved and an interactive computer program. Knowledge gained from the descriptive material is applied to the solution of a practical X-ray diffraction problem. *POWDER* helps the student index a powder photograph, decide the cubic lattice to which the crystal belongs and find the crystal's lattice constant. *XTALLAB* was designed to acquaint the student with the method of crystal structure determination based upon X-ray diffraction data obtained with single crystals. To simplify calculations and viewing of the trial molecule, the structure determination is carried out on a relatively planar structure with a short cell axis which allows for two-dimensional analysis. Used in conjunction with each other, *POWDER* and *XTALLAB* combine to provide the student with an elementary understanding of crystal structure determination based upon X-ray diffraction data obtained from powder photographs and single crystals.

Hardware environment: *POWDER* and *XTALLAB* require a 286/386/486 IBM or clone PC, an EGA color monitor and a math coprocessor.

Availability: Programs and documentation are available from the authors.

This research was supported by the United States Department of Energy under contract no. W-7405-Eng-82, Office of Basic Energy Sciences, Materials Science Division.

References

Lessinger, L. (1988). *J. Chem. Educ.* **65**, 480–485.

Loehlin, J. H. & Norton, A. P. (1988). *J. Chem. Educ.* **65**, 486–490.

Crystallographers

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).

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Professor **Mary F. Richardson**, Chemistry Department, Brock University, St Catherines, Ontario, Canada, was named Canadian Professor of the Year by the Council for Advancement and Support of Education, Washington, DC, on 15 June 1992. The citation states that she has focused on getting students, especially women, interested in chemistry. She led the committee that developed the women's studies programme at Brock University and also worked extensively with colleagues to review and revise the undergraduate curriculum for chemistry students. Additionally, she played a part in the design of an adjustable-height wheelchair so handicapped students could reach normal-height research equipment and library shelves. Professor Richardson is also a national expert on the chemical composition of beer and beer making and periodically lectures on this topic.

New Commercial Products

Announcements of new commercial products are published by the Journal of Applied Crystallography *free of charge. The descriptions, up to 300 words or the equivalent if a figure is included, should give the price and the manufacturer's full address. Full or partial inclusion is subject to the Editor's approval and to the space available. All correspondence should be sent to the Editor, Dr A. M. Glazer, Editor* Journal of Applied Crystallography, *Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, England.*

The International Union of Crystallography can assume no responsibility for the accuracy of the claims made. A copy of the version sent to the printer is sent to the company concerned.

J. Appl. Cryst. (1993). **26**, 144–145

Thin-Wall Capillary Tubes: Quartz, Glass and Borosilicate

A full line of thin-wall capillary tubes made from quartz, special glass and borosilicate glass for sampling and instantly sealing liquids, crystals and fine powders is being introduced by Charles Supper Company, Inc. of Natick, Massachusetts.

Supper Capillary Tubes feature a funnel shape at one end and are 89 mm long for sampling a wide range of liquids and fine powders. Available in 15 different sizes from 0.1 to 3.5 mm with a 0.01 mm wall, they are made from quartz, special glass and borosilicate glass, depending upon the linear absorption coefficient desired.

Packaged in convenient 25-tube containers, Supper Capillary Tubes are ideal for applications where samples must be

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instantly resealed, typically using conventional wax methods, and then transported. In addition to wax, the special glass tubes can also be cut and then resealed using an ordinary match flame.

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Charles Supper Company, Inc., Lee Supper, Marketing Director, 15 Tech Circle, Natick, MA 01760, *USA*

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (R. F. Bryan, Department of Chemistry, University of Virginia, McCormick Road, Charlottesville, Virginia 22901, *USA). As far as practicable, books will be reviewed in a country different from that of publication.*

J. Appl. Cryst. (1993). **26**, 145

Structural and chemical analysis of materials. X-ray, electron, and neutron diffraction; X-ray, electron, and ion spectrometry; electron microscopy. By *J. P. Eberhart*. Pp. xxx + 545. Chichester (UK): John Wiley & Sons, 1991. Price £95.00. ISBN 0-471-92977-8.

This book gives a comprehensive treatment of the principles governing the use of electromagnetic and particle radiation in materials research. By identifying the concepts that are common to X-ray, electron, neutron and ion radiation, it succeeds in providing a coherent overview of interactions between matter and radiation.

The material is divided into five parts: (i) interactions of X-rays and particle beams with materials; (ii) radiation generation and measurement; (iii) the application of diffraction techniques to materials analysis; (iv) the application of X-ray, electron and secondary-ion spectrometry to materials analysis; (v) techniques of electron microscopy. Helpful cross references between chapters are given.

The first of these parts deals chiefly with the elastic scattering of X-rays, electrons and neutrons, with the development proceeding from generalized scattering objects, through discrete and continuous distributions of scattering matter, to diffraction by a crystal. The limitations of the kinetic approximation for electron diffraction are highlighted in a separate chapter, where the essential features of the dynamic theory are introduced. Consideration is also given to secondary emissions and the absorption of radiation. Thus photo-, secondary and Auger electrons are discussed, as are the generation of *Bremsstrahlung* and characteristic X-rays.

The second part gives a readable account of the essentials of radiation generation, focusing and filtering. The treatment of thermal neutrons is cursory, as this is considered to be too specialized a topic. The principles of the design of X-ray detectors (gas ionization and solid-state) are given, together with the essentials of WDX and EDX spectrometers. Brief consideration is also given to the detection of electrons and ions.

The third part of the book is divided into two long chapters, the first dealing with X-ray and neutron diffraction and the second with electron diffraction. The treatment is necessarily selective, with the emphasis on experimental considerations rather than on methods of solving structures. Although there are sections on the indexing of Laue patterns, rotation photographs and X-ray powder diffraction patterns, they provide more of an overview than a didactic treatment. The chapter on electron diffraction gives an adequate treatment of the indexing of single-crystal diffraction patterns and the merging of Laue zones in diffraction patterns. The principles of Kikuchi lines, CBD and LEED are also covered.

The fourth part is helpful in unravelling the acronyms that abound in spectroscopy, *e.g.* EXELFS, EPMA, with a glossary of these terms at the end of the book. Useful guidance in quantitative analysis is given for each of the techniques. The treatment covers elemental (XRF/EPMA) and surface (ESCA/XPS/AES/SAM) analysis, together with X-ray and electron-absorption techniques such as EXAFS and EELS. Surface analysis by SIMS is covered in a separate chapter.

The final part, dedicated to techniques in electron microscopy, provides an interesting overview. Factors limiting resolution are discussed, as are the principles of bright- and dark-field imaging in TEM. A section on HREM presents the possibilities and limitations of structural imaging and summarizes the objectives of computerized image modelling. A chapter on SEM highlights the differences in forming images with secondary and back-scattered electrons. This is followed by a brief consideration of STEM, with the final chapter describing the contemporary interest in scanning tunnelling microscopy (STM).

The general standard of presentation is high, although there are a few blemishes and typographical errors. The book has been translated by the author from the original French version, published in 1989. The translation is generally excellent, apart from a very occasional unusual choice of word.

The book focuses on the principles of the physical techniques themselves, rather than on the structure of materials. Thus it will be of value to research workers in materials science, condensed-matter physics and solid-state chemistry. The book provides the essential background information on contemporary techniques and brings out their interrelationships most effectively. Bibliographies for each chapter, together with a list of primary references at the end of the book, give the reader helpful points of entry into the relevant literature.

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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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Introductory solid state physics. By *H. P. Myers*. Pp. xi + 546. London: Taylor and Francis, 1990. Price £18.00 (paper back). ISBN 0-85066-761-5. A review of this book, by B. J. Hickey, has been published in the January 1993 issue of *Acta Crystallographica* Section A, page 215.