

Acta Cryst. (1981). A37, 445

Commission on Journals

Submission of Manuscripts Based on Powder Diffraction Profile Fitting or Refinement (Rietveld) Methods: Deposition of Data

A steadily increasing number of manuscripts that depend on the use either of powder diffraction profile fitting or refinement (Rietveld) methods are being submitted for publication. Commission policy has recently required that figures in such manuscripts that present the experimental and calculated diffraction profiles of the material studied should also contain the difference profile ($I_{\text{obs}} - I_{\text{calc}}$), as an aid to the reader. It is recognized that the primary diffraction data cannot be extracted satisfactorily from such figures. The Commission has now decided that, in addition to the figure, the authors of such manuscripts should deposit the numerical intensity of each measured point on the profile, as a function of scattering angle.

The attention of authors is also drawn to notices concerning stereofigures [*Acta Cryst.* (1978). B34, 3846], dimensions of material for deposition [*Acta Cryst.* (1979). B35, 792], estimated standard deviations, SI units and anisotropic thermal parameters [*Acta Cryst.* (1979). B35, 1302] submission of connected computer output [*Acta Cryst.* (1979). B35, 2284–2285], chemical-connectivity relationships [*Acta Cryst.* (1980). B36, 1524], and estimated

standard deviations with a zero value for varied parameters [*Acta Cryst.* (1980). B36, 2508], in addition to the information given in *Notes for Authors* [*Acta Cryst.* (1978). A34, 143–157].

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Acta Crystallographica

Appreciation of Co-editors' Service

The Co-editors of *Acta Crystallographica* and the *Journal of Applied Crystallography* serve the crystallographic community with great devotion and distinction, and it is appropriate that the Executive Committee of the Union records its sincere appreciation for the work of all present and past Co-editors from time to time. The Executive Committee particularly wishes to express its appreciation and gratitude, on behalf of the Union and the international crystallographic community, to Dr P. J. Wheatley for his 12 years of outstanding service as a Co-editor of *Acta Crystallographica*. On his retirement as a Co-editor at the end of 1980, Dr Wheatley had dealt with 3033 papers. In the last five years, he received between three and four hundred manuscripts annually. A notice concerning the redistribution of new manuscripts submitted to *Acta Crystallographica* that must inevitably accompany his retirement has been published in *Acta Cryst.* (1981), A37, 138.

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.

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Ordering in strongly fluctuating condensed matter systems. Edited by T. RISTE. Pp. xvi + 474. New York: Plenum Press, 1980. Price US \$55.00.

This book consists of a collection of papers, both invited and contributed, which were presented at a NATO Advanced Study Institute held at Geilo, Norway, 16–27 April 1979. On the whole, it represents a timely and well organized review of the present status of both the theory and supporting experimental work relating to ordering in strongly fluctuating systems and phase transitions.

The introduction to each of the specific areas covered in the book is developed in an invited, tutorial paper. These introductory treatises tend to be well written and serve both to familiarize the reader with the current status of the field and to lay the groundwork for some of the more 'state-of-the-art' papers which follow. An excellent example is the paper by Villian on *Two-dimensional solids and their interactions with substrates*. This begins with a review of existing theories of idealized two-dimensional (2D) systems, followed by comparisons with experimental data on real 2D systems, with particular emphasis on adsorbed layer systems. Further approximations to 2D solids are then considered through discussions of incommensurate solid

phases. This review concludes with discussions representing further departures from the idealized case, e.g. anisotropic substrates are considered through the Pokrovskii–Talapov model for commensurate–incommensurate transitions. Following this, the ideas are clearly demonstrated by application to rare-gas monolayers on graphite. Specific applications of other theories developed in the text are made to low-dimensional magnets, mercury chain compounds, smectics and spin glasses.

One observation that appears to have evolved at the conference is the realization that, based on theoretical considerations, there are a number of non-linear excitations, such as solitons, walls, dislocations and vortices, which can be expected to occur at or below points of lower critical dimensionality. Some of these, such as 1D magnets, have been experimentally verified, but apparently many of these theoretical predictions are still awaiting experimental support.

Since each of the thirty three papers contained in the book is separately prepared, usually by a different author (some authors have contributed more than one paper), there are the expected variances in style, notation and typescript (photo-offset printing was used). But since each paper is essentially self-contained, the development of ideas is usually coherent and intelligible. Also, although occasional typographical errors do occur, they are certainly not abundant, perhaps to

the credit of the editor. It is unlikely that this book would make a suitable graduate text, but it does provide the interested reader with an excellent review of the current status of a rapidly growing and dynamic field of phase transitions.

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Computing in crystallography. Edited by R. DIAMOND, S. RAMASESHAN and K. VENKATESAN. Pp. 450. Bangalore: Indian Academy of Sciences, 1980. Price US \$17.00, Rs 125/-; price for individuals US \$8.00, Rs 50/-.

Computing in Crystallography contains the text of 29 lectures which were delivered at a Winter School on Crystallographic Computing which was organized in January 1980 in Bangalore, India. The crystallographic techniques described in this volume range from data collection and processing to the refinement and display of completed structures.

The level of prior knowledge expected of the reader by each lecturer varies widely. Many chapters will not be understood unless the reader has a proper grasp of matrix notation. The beginner may be slightly bewildered by the lack of uniformity in the mathematical notation employed. At least three ways of denoting a matrix transpose are used, two of them being employed in one chapter. Many chapters are followed by exercises, sometimes with answers, which often add valuable material to the book.

The first four chapters of the book cover the topics of diffractometry, absorption and extinction corrections and microdensitometry of film data with a good balance between theory and practice. The next five chapters are concerned with the solution of the phase problem. An excellent chapter by Nordman describes automated vector search methods for solving Patterson functions including useful practical advice and illustrations of possible pitfalls. Multisolution methods of solving the phase problem are described in chapters by Main and Woolfson which provide good background reading for users of the packages *MULTAN*, *MAGIC* and *YZARC*.

Three chapters deal with the theory of errors and least squares. The introductory chapter on least squares in crystallography is one of the few disappointing chapters in the book. Poor explanation and typographical errors mean that the chapter is of limited value. Fortunately, Hendrickson & Konnert give a well presented and comprehensive account of restrained least squares, which is now an important technique in the refinement of macromolecules. A chapter on error analysis by Huml discusses the statistical theory of propagation of error and collects together much current wisdom concerning weighting schemes and analysis of weights from least-squares refinement. A chapter by Johnson gives a general survey of thermal motion analysis and two chapters describe charge density studies and the high-

precision crystal structure analysis which is required to make them possible.

Four chapters of special interest to protein crystallographers describe heavy-atom refinement, phase determination by multiple isomorphous replacement, and structure factor least squares with fast Fourier algorithms and automated map interpretation.

The last part of the book deals principally with computing. A chapter by Hall & Stewart describes the principles of design of the *XTAL* system and the use of the *RATMAC* preprocessor. Two chapters on mini- and microcomputers are interesting but clearly the information will rapidly become dated. Excellent chapters by Johnson and Diamond describe computer graphics, including methods of molecular displaying and interactive graphics.

In summary this book contains a wealth of information for practising crystallographers and excellent surveys for those wishing to keep up to date with recent developments in crystal structure analysis.

The Indian Academy of Sciences is to be congratulated in producing this volume cheaply enough for every crystallographer to have his own copy.

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Amorphous semiconductors. (Topics in Applied Physics, Vol 36.) Edited by M. H. BRODSKY. Pp. xvi + 337. Berlin: Springer, 1979. Price US \$49.50.

This book presents a clear review of the understanding of electronic phenomena in amorphous semiconductors, with the emphasis on those phenomena principally dependent upon energy levels in and near the semiconductor bandgap. Readers can understand those concepts which are novel to the *amorphous* state of semiconductor materials as well as those which are easily described by analogy with the well-established base of knowledge of *crystalline* semiconductors, as the editor has commented in the preface.

The introductory chapters (1–3) present the principal definitions, outline current and future trends, and describe the physical band theory of bandgap and defects in amorphous semiconductors. There are various theoretical approaches relating energy states to the spatial structure of amorphous systems. States in the gap and defects are discussed in three distinct groups: the tetrahedrally coordinated silicon-like materials, the chalcogenide glasses, and the amorphous arsenics.

Optical absorption, electronic transport, luminescence, spin effects, short-range order, doping and solar cells are described in turn (chapters 4–10). Optical absorption from defects in the gap, band tails, and interband transitions are interpreted with experimental observations. Band models are used to classify electrical conduction in amorphous semiconductors. The concept of hard and soft centres, as the origin of the electron spin resonance signals in pure and hydrogenated amorphous silicon, is discussed. Probes of short-