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Acta Cryst. (1980). A36, 1090

Computing in Crystallography

(Editors: R. Diamond, S. Ramaseshan and K. Venkatesan)

This book has recently been published by the Indian Academy of Sciences for the International Union of Crystallography. It contains 29 chapters incorporating the lectures presented at the International Winter School on Crystallographic Computing, which was held at the Indian Institute of Science, Bangalore, India, 4–14 January 1980 and was organized by the Union's Commission on Crystallographic Computing. The titles of the chapters are: *Diffractometer control with mini-computers; Absorption corrections for single-crystal X-ray and neutron data; The strategy of extinction corrections; Microdensitometry; Vector-space Patterson search and other stored-function sampling procedures; Automatic interpretation of the Patterson function; Symbolic addition; Multisolution methods; Other multisolution methods; Structure invariants and seminvariants; The method of least squares in crystallography; Error analysis; Incorporation of stereochemical information into crystallographic refinement; Thermal motion analysis; A systems approach to computing for charge density studies; Derivation of molecular properties by charge density integration; Heavy atom positions in macromolecules; The refinement of crystal structures by Fast-Fourier least squares; Phase evaluation and some aspects of the Fourier refinement of macromolecules; A matrix approach to the phase problem; Some problems in macromolecular map interpretation; XTAL: New concepts in program system design; Mini-computers in structure analysis; Microprocessors and microcomputers; Molecular conformation; Computer-generated illustrations; Interactive graphics; Programming methodology of artificial intelligence; A technique for overlaying common storage.*

In addition to the lectures the book includes the work sessions material of most of the lectures. This book (of about 525 pages) will be most useful to all who are engaged in crystal structure determination. Copies may be obtained from The Editor, Indian Academy of Sciences, Bangalore, 560 080, India. The price of the book is US \$17 or 125 Rupees, but individuals may purchase a copy for their personal use at the reduced price of US \$8 or 50 Rupees. These prices include postage by surface mail. Copies may be sent by airmail but at extra cost.

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.

Acta Cryst. (1980). A36, 1090–1091

Non-radiative decay of ions and molecules in solids. By R. ENGLMAN. Pp. xiii + 336, Figs. 62. Amsterdam: North-Holland, 1979. Price US \$58.50, Dfl 120.00.

This book deals with radiation absorption processes in solid-state impurity systems. In discussing these processes,

attention is focused on the conversion of the excitation energy into atomic motion of the lattice, a phenomenon commonly known as non-radiative decay. The book is divided into three parts and 22 chapters. The first chapter is devoted to a historical review of the concepts of non-radiative decay. In part I, which comprises chapters 2 to 10, an outline of the different approaches to non-radiative decay is first presented. On the basis of the reported results it is

shown that two laws, the exponential-energy-gap law and the activation-energy law, appropriately represent rate processes in solid-state impurity systems. Consideration of various possibilities of the combined decay of electronic and vibrational modes is followed by a discussion on purely vibrational relaxation within an unchanging electronic state. The vibrational relaxation rate constants have been calculated using several microscopic models. The effect of promoting (vibrational) modes on the decay rates has been examined and the results obtained from theoretical models are presented. Finally, the experimentally obtained rules governing the relaxation behaviour in several systems are given and their relationships to the theoretical framework are considered.

Part II, chapters 11 to 16, begins with a discussion on the irreversible aspect of non-radiative decay processes in solid-state impurity systems. The time evolution of the excitation and the role of the exciting light is examined and accounts are given of methods that supplement or contradict the standard approach to non-radiative decay. It is shown that the information, with which the excited system starts, is lost during de-excitation and that the saddle-point method of interpreting the theory of non-radiative decay has several weaknesses.

Chapters 17 to 22 in part III are devoted to non-radiative decay processes in various systems categorized under five broad headings: (i) transition-metal ions, (ii) rare-earth ions, (iii) *s,p*-state defects and others, (iv) organic molecules, and (v) biological systems. Each of these chapters is appended with a sizeable selection of data on non-radiative decay rates.

This book has achieved its objective of providing coherent and comprehensive information on radiationless processes in solid-state impurity systems. Chapters on various topics are specific and exhaustive. It should serve a most useful purpose in studies of subjects in which radiationless processes play a part.

The suitable biblical quotations given at the beginning of each chapter aptly justify the impression that besides being deeply devoted to the pursuit of knowledge, the author is devoutly religious – both of which are laudable virtues.

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Elektronen im Kristall. Von R. HERMANN & U. PREPPERNAU. Pp. xiv + 417. Berlin: Akademie-Verlag and Wien, New York: Springer-Verlag, 1979. Price DM 98.00, US \$57.90.

Designed for the use of advanced undergraduate students, this textbook is a valuable tool for acquiring a solid basic knowledge of the electronic properties of crystalline solids. Furthermore, it is very useful for the graduate scientist, who wants to be introduced to the field of wave propagation and high-frequency properties of crystals. A fundamental knowledge of mathematics and quantum physics is

necessary. The treatment is as far as possible understandable from the point of view of the experimentalist without losing the necessary close connection with theory. The main electronic properties are covered at a uniform intellectual level in such a way that studies can start at almost any chapter.

The book consists of ten chapters, the first five of which are concerned with the necessary basic knowledge. Chapter 1 gives a statistical treatment of the model of quasi-free carriers. It is followed by a description of lattice vibrations and phonons (chapter 2) and crystal-lattice geometry including the reciprocal lattice and Brillouin zones (chapter 3). The behaviour of electrons in the periodic three-dimensional structure under the influence of lattice potential (chapter 4) and the dynamic properties – treated by a quasi-classical model – (chapter 5) conclude the first part of the book.

Based on this foundation, the second part gives a treatment of more specialized phenomena such as electrical conductivity and the Hall effect (chapter 6), behaviour of charge carriers in a homogeneous magnetic field including Landau quantization and the resulting oscillations of the density of states (chapter 7), high-frequency electromagnetic waves in solids (chapter 8), resonance phenomena (chapter 9) and questions of propagation of electromagnetic waves in a solid-state plasma.

In accordance with its character as a textbook the references show an emphasis on books for further studies.

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Photoferroelectrics. By V. M. FRIDKIN. Pp. x + 174. Figs. 63. Berlin, Heidelberg, New York: Springer, 1979. Price DM 59.00, US \$32.50.

Ferroelectricity is now one of the matured branches of solid-state physics; however, no monograph concerning photoferroelectric phenomena has been available and the publication of Professor Fridkin's book at this time is particularly opportune. The book is a review of work on the subject as investigated by Soviet physicists, and the author of the book has himself been actively engaged in this field. Perhaps there is a need for a brief explanation of the term 'photoferroelectrics'. Most ferroelectric materials are good electrical insulators; however, some are semiconducting: the SbSI family and impurity-doped oxide-type ferroelectrics are examples. When electrons and holes are photo-excited in ferroelectrics, the charge carriers may exert some influence upon the dielectric properties. Thus, photoferroelectric phenomena such as shift of the Curie point, change of spontaneous polarization, and variation of the refractive indices take place.