Point Defects in Materials

F. Agullo-Lopez, C.R.A. Catlow, and P.D. Townsend

Academic Press, 1988
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This treatise on point defects in materials provides a welcome addition to the bookshelves on materials science. Although progress is covered periodically in the proceedings of conferences on subsets of this subject area, no comprehensive discussion of this important and extensive field of knowledge has been published for many years.

The book covers the general concepts of point defects, a wide range of experimental and theoretical techniques that are being applied to study point defects in materials, and points out the importance of defects for many properties of, and processes in, solids. A listing of the subject areas covered in the 14 chapters gives a flavor of the book: defects in solids; thermodynamics of point defects; energetic methods of defect production; photolytic damage to materials; point defects in halides, oxides, and semiconductors and metals; experimental techniques—general, optical, electron and nuclear; computer modeling techniques; quantum mechanical methods; statistical mechanical models; and applications. The chapters provide selected references which are reasonably up to date.

The book is intended to be suitable for final year undergraduates as well as postgraduates and other researchers. Its organization seems to reflect in part the differing needs of these audiences. The first half of the book is devoted to the basic concepts of point defects, their general thermodynamic and diffusion properties, and the nonequilibrium production of defects followed by more detailed discussions of point defects in halides and oxides, and somewhat less detailed treatments for defects in semiconductors and metals. The first half of the treatise is fairly self contained with a moderate number of references to later parts of the book; it could serve quite well for an undergraduate course on the subject. Generally, the concepts are clearly described.

The second half of the book is devoted to experimental and theoretical techniques which have been and are being applied in the study of point defects. This part should be of much value particularly to postgraduate students and researchers who consider working in this field. It gives a rather exhaustive list of techniques for investigating defects. The details given for the techniques, and their strengths and weaknesses, varies considerably, but this does not detract from the usefulness of the discussion, since in most cases appropriate references can be found to dig deeper. Frequently, examples of applications to particular questions regarding defects are provided, which complements the knowledge gained in the first part of the book.

This book, as any, has some shortcomings. More appeal to physical intuition would be helpful for the novice. Without doubt, the thoroughness of coverage of defect knowledge for the four major types of materials, highly ionic (halides), mixed conductors (oxides, variable valence states), covalently bonded (semiconductors) and metals, decreases in this order. The authors acknowledge this in the preface with a comment that "...emphasis here is on semiconducting and insulating materials, in part because these are better suited to detailed microscopic characterization." The treatment of defects in metals provides the essentials, but is not up to date. For example, the embedded atom method (see, e.g., S.M. Foiles, M.I. Baskes, and M.S. Daw, *Phys. Rev.B* **33** (1986) p. 7983), used with good success in recent years, is not mentioned in the discussion of interatomic potentials in the chapter on computer modeling techniques. The coupling between defect fluxes and solute element, which leads to radiation-induced phase instabilities, is hardly mentioned in a short discussion of radiation-enhanced diffusion in metals. It would have been desirable to provide references to recent conference proceedings on the areas covered less thoroughly in the book, e.g., for metals: "Vacancies and Interstitials in Metals and Alloys," C. Abromeit and H. Wollenberger, eds., *Materials Science Forum*, Vol. 15-18 (1987).

The applications chapter, which contains a small but interesting selection of sometimes little known applications, does not provide references for the reader who might want to learn more on the subject. Often the origins of data, presented in tables and figures, and of a number of short statements regarding observations or interpretations given in the text, are not obvious; however, they usually can be tracked down with some guessing among the references given. Flaws, such as giving reference to an edited volume instead of the individual article or providing a wrong publisher, and "typos" are more an annoyance than a detraction to the value of the book. The readability of portions of the text could have benefited from thorough editing. Also, symbols are not always clearly defined. Figure captions could have been more informative, e.g., some complex crystal structures are presented without sufficient description, in caption or text, to visualize easily their topology.

The volume is well illustrated with good quality drawings and graphs. Good selections of references are generally provided for the chapters. The overall appearance of the moderately priced book is commendable with regard to clear print, good reproduction of figures and sturdy binding.

Point Defects in Materials undoubtedly fills a significant void among the recently published comprehensive treatments of important subfields of materials science and solid state physics. It certainly will be a welcome aid for teaching an advanced undergraduate or graduate course on this pervasive subject area. The extensive review of experimental and theoretical techniques available for the investigation of point defects will be very valuable for beginning as well as established researchers in the field. Despite some shortcomings of the book, the authors must be commended highly for a valuable contribution for the materials community to draw on.

Reviewer: Hartmut Wiedersich is a senior scientist in the Materials Science Division, Argonne National Laboratory. His field of interest for many years has been defects in general, and radiation effects in metals and alloys in particular.

Solids and Surfaces: A Chemist's View of Bonding in Extended Structures

Roald Hoffmann

VCH Publishers, 1988
ISBN: 0-89573-709-4

Some 26 years ago high-vacuum systems became economical and standard in many laboratories, and this made possible a new era in surface science. Today materials scientists with a wide range of technical backgrounds in chemistry and physics are making new (and, most importantly, reproducible) discoveries in this field. The accurate structural, thermochemical, spectroscopic and kinetic data now available make the field appealing and challenging to theoretical chemists and physicists.

Roald Hoffmann is one of the theoretical chemists who has been attracted by surface science. Like many chemists he believes that the Huckel method, which has enjoyed enormous success in organizing data on the structure and properties of organic molecules (especially hydrocarbons), provides a universal language for discussing the quantum structure of any molecule or solid, organic or inorganic, metals, semiconductors, insulators, ionic crystals, and so on. His aim in this beautifully produced book is to discuss surfaces using this technique, which he has employed in collaboration with many graduate students and postdoctoral research

associates over the last decade.

Hoffmann's discussion is charming and highly readable. His students have evidently found the formalism and language of energy band theory, as practiced by physicists, a serious stumbling block, and he devotes most of the book to translating band results into Huckel language. For those who share his convictions about the universal significance of the Huckel approach this book should prove highly rewarding.

But what about the results? Here Hoffmann and his collaborators have fared poorly, and their published research papers overall show very little agreement with experiment. In contrast, by now quite a number of theoretical physicists have derived results which not only agree with experiment (to within 0.1 eV on electronic energy levels, for example, which is some 10 to 20 times better accuracy than Hoffmann gets), but in many cases where the experiments were difficult, actually predicted results which were later confirmed experimentally.

Does your theoretical success in staying in contact with the cutting-edge of experiment affect your pedagogy? Evidently. Hoffmann correctly identifies CO on Ni as a prototypical example of chemisorption on surfaces. But when he comes to discuss bonding in solids, the *only* examples he selects are decidedly arcane: ternary transition metal compounds such as $ThCr_2Si_2$ or $Na_3Fe_2S_4$. Nowhere do we see anything about the most studied and best understood elemental and binary solids, such as Si, Ge, GaAs, W, transition metal silicides, and so on. Considering the pedagogical nature of this book, it is hard to justify this curious selection of subjects.

The practicing materials scientist will be disappointed by the omission from this book of any mention of empirical methods other than the Huckel method, such as Miedema's approach to intermetallic compounds, which predicts surface segregation in intermetallic alloys. In The Merry Widow we learn that "das studium der weiber ist schwer." So is materials science.

Reviewer: J.C. Phillips, a freelance theorist is a senior member of the technical staff at AT&T Bell Laboratories, Murray Hill, New Jersey. He recently wrote The Physics of High-T_c Superconductors *(Academic Press, Boston, 1989).*

Introduction to Quasicrystals

Edited by M.V. Jaric

Academic Press, 1988

ISBN: 0-12-040601-2

Introduction to Quasicrystals is the first volume in a series from Academic Press titled "Aperiodicity and Order." The book contains six chapters by authors who, for the most part, have been active in quasicrystal research since the first icosahedral phases were discovered in 1984. The articles are clearly written and provide an overview of the field useful to students and researchers alike.

The two opening articles emphasize the role that local icosahedral order plays in metallic crystals and glasses. Chapter one, by David and Clara Shoemaker, enumerates the possibilities of icosahedral ordering and icosahedral networks in complex alloys. Most of the article is devoted to a catalogue of examples drawn from the authors' long experience with the structure of intermetallic compounds. There is perhaps a bit too much detail for the casual reader, but it serves to illustrate the point of the article, namely that an understanding of the icosahedral arrangements of atoms found in complex intermetallic alloys can be a useful aid in unraveling the atomic structure of icosahedral quasicrystals.

The notion of frustration in icosahedral systems and its analysis through the study of polytopes in curved space, briefly mentioned in the first chapter, are the focus of the second chapter by Michael Widom. Widom begins with a general discussion of local icosahedral ordering in atomic clusters, liquids, and glasses. After introducing the mathematics of polytopes, he describes how glasses, icosahedrally coordinated crystals and quasicrystals may be generated by different procedures for flattening the polytopes from curved to Euclidian space. The chapter is a precis for much of the thinking on frustrated icosahedral order in condensed matter up to the time of Schectman's discovery of icosahedral AlMn.

The metallurgy of icosahedral and decagonal quasicrystals is the topic of the next chapter by Robert Schaefer and Leonid Bendersky. Emphasizing work on AlMn and AlCuLi phases, the authors do a sensible job of pulling together disparate information on the stability, formation, thermodynamics, and orientation relationships of these and other phases.

The final three chapters deal with theoretical questions of quasicrystals. The fourth chapter, by Per Bak and Alan Goldman, discusses quasicrystals and other incommensurate structures as projections of higher dimensional periodic structures. Aspects of higher dimensional crystallography are also addressed. The issue of stability is treated in the next chapter by Ofer Biham, David Mukamel and S. Shtrikman. The authors adopt a Landau theory approach, but also include results from numerical simulations. They conclude with an interesting discussion of stability in the presence of small elastic deformations and the possibility of lock-in transitions.

The last chapter, by Tom Lubensky, is a careful introduction to the elasticity and hydrodynamics (long wavelength dynamics) of quasiperiodic structures. Although rather long (it comprises one third of the book), the article is quite readable and strikes a good balance between general theoretical considerations of quasiperiodic structures and specific results for icosahedral quasicrystals. The article includes a discussion of phasons in quasicrystals (also addressed in chapter four), treating both phason dynamics and static disorder in the form of quenched phason strains.

On the whole the book provides much useful information; I recommend it for anyone seriously involved in quasicrystal research and, generally, as a worthwhile addition to research libraries serving physicists and materials scientists. A regrettable flaw of the book is the lack of an adequate introduction which could have served to tie together the separate articles, give the reader a broad sense of where the field is going and fill several gaps in the presentation. For example, a brief review of the experimental status of the field, as well as some mention of competing models, would have helped orient the newcomer to the field.

Reviewer: Peter A. Bancel is a postdoctoral laboratory employee at IBM T.J. Watson Research Center. His research is in quasicrystals.

ERRATA:

The photo published on p. 47 of the December 1989 *MRS BULLETIN* was that of Robert A. Frosch and not that of D. Allan Bromley.