

of this broad coverage, derivations of equations are generally not given, and experimental or computational approaches are not described in detail. As a result, this is not a book that could easily be used as the basis for an advanced course on the subject, but it summarizes a wealth of pertinent information, and therefore will be of considerable value as a resource for those working in the field.

After an introduction, in which the importance of the electron density for understanding chemical bonding is emphasized, the book continues with a treatment of quantum-mechanical methods (Chapter 2), followed by a discussion of experimental X-ray techniques (Chapter 3). Complementary methods, including the use of synchrotron radiation, electron diffraction and  $\gamma$ -ray diffractometry, are discussed in Chapter 4, and magnetization and spin densities in Chapter 5. Chapter 6, which carries the title 'Electron density and the chemical bond', includes an enticing description of the history of bonding concepts; it starts with Lucretius Titius Carus, who described interparticle bonding by means of hooks as holders, and continues to the concepts currently used in electron-density analysis, such as atomic charges and pseudoatomic moments, deformation densities and the topology of the total electron distribution. The final chapter (Chapter 7) deals with the derivation of crystal properties from the electron density, including the electrostatic potential, the Coulombic interaction energy and the electric field gradient at the nuclear positions. The theoretical chapters frequently give an insight not found in many other books, though, as is probably unavoidable given the nature of this volume, other theoretical texts will be needed to fill in the details. It should be noted that the experimental chapters cover many interesting Russian contributions, some of which are less known to Western readers. Chapters 4 and 5 have been written by Professor Ozerov, the remainder, constituting the main body of the book, by Professor Tsirelson. Some appendices on related topics, again divided among the authors, conclude the book. Since the book contains an extensive review of the literature through 1993, and a number of references to work published in 1994 and 1995, it will find use as a source of information on past work. For this purpose, it is important that the index be detailed and easy to use. In this respect I was disappointed. Several important subjects are not referred to, or appear only once, even when they are discussed several times in the text. To give two examples, a central concept such as the multipole model, discussed several times in the text, is not listed in the index, while a student looking for a reference to crystal field theory is referred to page 244, though a much more detailed description of the concept appears on page 312. Chemical names or formulas are also omitted from the index, which one hopes will be improved in any later edition of the book, which should also be priced so as to make it more broadly accessible to beginning researchers in the field. Notwithstanding these drawbacks, the authors have produced a highly interesting volume that should be useful for many years, and will find its place on the bookshelves of many scientists interested in this central subject.

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**Industrial crystallization – Process simulation, analysis and design.** By N. S. TAVARE. Pp. xxviii + 527. New York: Plenum Publishing Corporation, 1995. Price US \$95.00. ISBN 0-306-44861-0.

An explosion of papers developing the design-oriented theories of industrial crystallization over the past decades has created a need to summarize what has been accomplished. Thus, several textbooks on this topic have appeared recently that merit mention. These include the completely rewritten third edition of *Crystallization*, by J. W. Mullin (Butterworth-Heinemann, Oxford, 1993), an extensive and instructive general survey of the field of crystallization; *The Kinetics of Industrial Crystallization*, by J. Nývlt, O. Sohnel, M. Matuchova & M. Broul (Elsevier, Amsterdam, 1985), dealing mainly with the effects of various parameters on the kinetics of individual steps in the crystallization process; *Design of Crystallizers*, also by J. Nývlt (CRC Press, Boca Raton, 1992), focuses on the application of kinetics to develop the relationships between the volumes of various types of crystallizer and the resulting product crystal size. Two other books, *Crystallization Technology Handbook*, edited by A. Mersmann (Marcel Dekker, New York, 1995), and *Precipitation*, edited by O. Sohnel & J. Garside (Butterworth-Heinemann, Oxford, 1992), summarize, respectively, our knowledge of design-oriented processes and the role of thermodynamics in the precipitation of less soluble compounds. Now comes this new book by N. S. Tavare, the main thrust of which is the application of mathematical methods to modelling the crystallization process.

The book has twelve chapters. Chapter 1 is a brief introduction to the problem. Chapter 2 deals with phase equilibria in various systems and with the materials balance of crystallization; the chapter is a good survey of the shapes of phase diagrams but, surprisingly, provides almost no hints as to their mathematical description and their practical uses. Chapter 3 gives a very brief survey of the fundamental concepts of nucleation and crystal growth and of the fundamental equations used for chemical-engineering descriptions of the processes. Most interesting are tables showing the range of typical kinetic parameters, with most probable estimates. However, the effects of several other parameters (*e.g.* solution purity, agitation, temperature *etc.*) are not mentioned. Chapter 4 is devoted to crystal-size distribution; important, because that is the basis of most modelling and design methods. The survey of the various distribution functions is very brief, with only a weak emphasis on the advantages of  $\gamma$ -distribution. The main value of this chapter is in its general presentation of the population balance problem and methods of solving it. Chapter 5 illustrates methods of process representation, of operating modes of batch crystallizers, and of process analysis. This chapter, and the related Chapter 6, on characterization of crystallization kinetics from batch experiments, are certainly of great value for those research workers dealing with batch crystallization and, together, the two chapters occupy about 100 pages. Chapter 7 deals mainly with precipitation processes and, perhaps a little inconsistently, with other processes such as Ostwald ripening and agglomeration.

Chapter 8, devoted to continuous crystallizers, treats in the usual way the population balance for an ideal case, as well as for size-dependent growth rate and growth-rate dispersion. Of

particular interest are the subchapters describing the effects of the size-dependent residence time distribution and the dynamics and control of continuous crystallizers. A short paragraph deals with the plug-flow crystallizer and, again, there is a paragraph on agglomeration. Chapter 9 describes the effect of growth-rate dispersion and methods of analyzing that phenomenon. Chapter 10, on mixing, is very important as, in many cases, mixing has an enormous effect on crystallization. This chapter also includes remarks on fluid-bed crystallizers and series of agitated vessels.

Chapter 11 deals with crystallizer design and operation. It is relatively brief and, besides some general remarks, contains just a few design illustrations using published examples from the literature. The concluding Chapter 12 briefly describes other crystallization techniques, such as adductive and extractive crystallization, the use of hydrotropic additives, and freeze and emulsion crystallization. A few comments are also made on encrustations and modification of crystal habit.

The book contains a number of experimental results and numerous solved examples. In addition, it provides a good literature survey, though in many cases providing only references without detailed descriptions of the respective methods. This is understandable, however, as a more detailed treatment would have enormously expanded the book's size. The book can be recommended as an extremely useful tool for process engineers, technologists and researchers in the field, and to advanced-level students of chemical engineering.

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**Atomic and ion collisions in solids and at surfaces.**

Edited by ROGER SMITH. Pp. ix + 309. Cambridge: Cambridge University Press, 1997. Price £45.00 (US \$69.95). ISBN 0-521-44022-X.

This book provides a comprehensive survey of various theoretical/computational models available for simulating energetic collisions of atoms with surfaces. Although the book does not address traditional crystallographic methods, it provides the framework for understanding how experimental techniques such as ion scattering spectroscopy (ISS) are sensitive to surface structure. The nine chapters are well organized, and smooth transitions between the various topics demonstrate the editor's skillful coordination of contributions from seven co-authors. While citing many experimental studies along the way, the book focuses on treating the dynamics of atom/surface collisions through non-experimental methods. The text begins with a review of classical scattering theory and the origins of binary collision theory. Throughout, the authors show with clarity and rigor how various standard equations are derived from first principles. It is not assumed that the reader has an advanced degree in physics or mathematics. The authors survey

four basic approaches to modeling dynamics: binary collision theory, transport theory, Monte Carlo techniques, and molecular dynamics simulations. Because an accurate atom/surface potential is required in all computational treatments, a chapter is devoted to the most common semi-empirical methods used for calculating these potentials.

A major theme to the book is understanding the inelastic processes involved when an energetic ion penetrates a lattice. The authors review many models which describe both the excitation of electrons in the solid and the recoil of substrate nuclei brought about by a swift atomic projectile. Discussion focuses on predicting the final rest distribution of the projectiles within the lattice, the corresponding atom displacements induced in the substrate, and sputtering phenomena. Along the way, the authors evaluate many of the popular algorithms and computational packages used in the field, such as *TRIM*, *TRIDYN*, *PRAL*, *KORAL*, *VEGAS*, *MARLOWE* and *SUSPRE*. The authors demonstrate how numerical simulations of ISS, secondary ion mass spectrometry (SIMS), depth profiling, radiation damage, and ion implantation can lead to a greater understanding of the fundamental dynamics. A chapter is also devoted to simulations of the surface topographical changes induced by ion bombardment and deposition. The Editor succeeds in providing a valuable resource for researchers in academia and industry, in fields of surface science, semiconductor engineering, thin-film deposition, and particle-surface interactions, who desire a deeper understanding of the non-experimental ways to study energetic atom/surface collisions. Although the book does not include problems for students, it would make an excellent supporting text for a special topics graduate course. Those interested in structural information will find a description of forward simulations whereby computations accurately reproduce ISS data; however, the inverse problem, *i.e.* extracting a unique surface structure directly from ISS data, has yet to be solved.

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**Collected works of Dorothy Crowfoot Hodgkin. Vol.**

**I. Insulin. Vol. II. Cholesterol, penicillin and other antibiotics. Vol. III. General crystallography and essays.** Edited by G. G. DODSON, J. P. GLUSKER, S. RAMASESHAN and K. VENKATESAN. Pp. cxliii + 2230. Bangalore: Indian Academy of Sciences, 1996. Price US \$120 (Individual vols. US \$40). ISBN 81-7296-020-4.

Dorothy Crowfoot Hodgkin was arguably one of the greatest scientists of this century, and certainly one of the most influential figures in the development of crystallography. What motivates such people, and what is it that causes them to inspire