Crystal Properties via Group Theory

Arthur S. Nowick
(Cambridge University Press, Cambridge, 1995)
xv + 228 pages, $80.00
ISBN 0-521-41945X

Properties of a crystal may be expressed by single scalars and then can be defined regardless of the crystal class and orientation. But often the response of a crystal to an external excitation depends not only on the magnitude of that excitation but also on its orientation relative to the crystal axes. The corresponding properties must then be expressed by vectors or tensors. As some examples, pyroelectric or magnetocaloric effects are tensors of rank 1; diffusivity, electrical conductivity, Hall effect or magnetoelectric effects are tensors of rank 2; piezoelectricity or linear electro-optic tensors are of rank 3; while elastic constants or second-order Hall effect can be of rank 4 or 5 and even 6. This means that, *a priori*, properties need a large number of physical constants (components of their associated tensor) to be defined. Fortunately, the physical properties of a crystal must obey, at least, all the symmetries exhibited by the point group of the crystal. This leads to simplifications by decreasing the number of nonzero components in property tensors. All of this is well-explained in the book with its major objective to examine the consequences of these simplifications for all possible crystal symmetries, using the powerful mathematical methods of group theory with the new approach of symmetry coordinates. This allows a generalized description with different physical phenomena being treated together provided that they correspond to tensors of a given rank and type.

The book is organized in such a way that it is a self-sufficient document with chapters presenting the basic ideas on properties, symmetries, and group theory, followed by the sequential analyses of the various tensors according to their rank. Mathematical conclusions are illustrated by practical examples of materials of special interest (such as high-temperature superconductors) and even the lazy reader will be satisfied as one can jump directly to tables giving the tensor reductions for all point groups (almost all to be exact, as the icosahedral point group is sadly missing).

Well-written, well-organized, just the right size, the book will be very useful for both students and researchers in solid-state physics and materials science.

Reviewer: *Christian Janot is a professor at the University Joseph Fourier of Grenoble, France. He specializes in metal physics (structure, dynamics, and properties). He has particular interest in lattice defects, amorphous materials, and quasicrystals. He is the author or co-author of 10 books and more than 300 papers in international journals. Janot is currently visiting the University of Rome 'La Sapienza', Italy.*

Handbook of Physical Vapor Deposition (PVD) Processing

Donald M. Mattox
(Noyes Publications, Westwood, New Jersey, 1998)
xxciii + 917 pages, $125.00
ISBN 0-8155-1422-0

This is a substantial volume which clearly aims to be a definitive reference work for specialist users of physical-vapor deposition (PVD) as a thin-film deposition technique. PVD encompasses simple thermal evaporation and sputtering as well as more recent developments such as ion-beam-assisted deposition (IBAD). The work is the end-product of the author's extensive career in the coatings industry, and the book covers peripheral aspects of the deposition process in considerable detail, having substantial chapters on substrate cleaning, chamber design, pumping systems, and postdeposition analysis. Most conceivable types of pumps and vacuum gauges are covered in detail and their relative merits discussed. The book adopts a justifiably applied stance on the processes, and issues such as contamination control during sputtering are addressed in an open fashion which is missing from many standard textbooks on the subject. A single source for this type of material is certainly useful, and this book provides good reference material for graduate-level training in thin-film deposition.

However, I was disappointed by significant gaps in the information presented. The book clearly emphasizes the "low-vacuum" coating area in which the structural properties of the deposited film are of paramount importance. The quality of the coverage declines as one moves to the higher-quality vacuum end of the subject and functional properties such as resistivity and defect density begin to determine "film quality." While it is perhaps justifiable in a book of this type to omit the fundamental materials science of film growth (for example, although the Thornton zone model is covered in some detail, I have been unable to find a description of Stransky-Krastenov growth), it is less permissible to leave out areas of major technological importance, such as techniques for optimizing thickness uniformity over large areas which are being driven by the large wafer sizes now standard in the microelectronics industry. Perhaps most surprising is the cursory mention of laser ablation under the misleading heading of "flash evaporation."

Overall, this is certainly a book I will consult, but it is to be hoped that a second edition will include more details of interest to those working on precision thin-film deposition.

Reviewer: *Mark Blamire is a lecturer in device materials in the Department of Materials Science, University of Cambridge.*

CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide (Pergamon Materials Series, Vol. 1)

N. Saunders and A.P. Miodownik
(Pergamon, Oxford, 1998)
479 pages, $180.00
ISBN 0-08-042129-6

This book has the ambitious goal of covering all aspects of CALPHAD. The goal of the CALPHAD method is to describe a system in such a way that it reproduces most accurately experimental phase diagram and thermodynamic properties. It is not a basic textbook but aims at materials scientists, chemists, physicists, graduate students, and researchers who want to enhance their understanding of what is meant by the expression CALPHAD. The presentation of the various topics is logically organized in 12 chapters. The first two chapters give an introduction to the topic and cover the history of CALPHAD. The next two chapters give an overview of the underlying basic thermodynamics and various experimental techniques. These chapters are not intended to go into great depth. They indicate the key concepts of the thermodynamics employed by CALPHAD and give a brief overview of the techniques that are generally used in the experimental determination of phase diagrams and thermodynamic quantities. The next five chapters, which amount to almost half of the book, cover the various components of the CALPHAD method. The first of these chapters provides an overview of thermodynamic models for solution and compound phases. Models for four types of phases (random substitutional, sublattice, ionic, and aqueous) that are currently available in CALPHAD software programs are outlined and discussed. The second chapter in this section focuses on the thermodynamic quantities of end-member components and compounds (phase stabilities), an essential quantity needed in the CALPHAD approach. The next chapter in this section describes ordering models and gives an overview of the routes that can be used to describe systems with phase structures that have common symmetry elements and similar bonding. Aside from chemical ordering,

magnetic ordering can also have a substantial effect on the Gibbs energy. Therefore, an entire chapter is dedicated to the role of magnetic Gibbs energy and various modeling approaches. The last chapter of this section presents examples of the computational methods that are employed within the CALPHAD method. In the first part of this chapter on methods for the calculation of phase diagrams by minimization of the total Gibbs energy of the system, the condition for thermodynamic equilibrium, are outlined. The second part of this chapter gives examples for the thermodynamic optimization procedures employing least-squares algorithms for the refinement of adjustable coefficients of the Gibbs energy functions.

After covering the components of the CALPHAD method, the book continues with the application of the CALPHAD method to practical problems. Two chapters are dedicated to this topic, including the combination of thermodynamics and kinetics. The first of these two chapters provides an exhaustive description of the application of the CALPHAD method to a large number of industrial alloys and other materials. This chapter draws extensively from the experience in this area of Nigel Saunders, one of the authors. The second chapter gives examples of the combination of thermodynamics and kinetics using two approaches, calculation of metastable equilibria and the direct coupling of thermodynamic and kinetic modeling. In the final chapter, the authors conclude with their views on the future development of CALPHAD.

This book provides a sound overview of the CALPHAD method and its accomplishments but it should not be mistaken as a textbook on "how to do CALPHAD" since this is not the intention of the book. It is well-written, provides the reader with the basic understanding of the principles and components of CALPHAD, and presents numerous practical examples for its application. This book will be very useful in judging whether CALPHAD can make a contribution to the reader's specific area of materials science.

Reviewer: *Ursula R. Kattner received her MS degree in mineralogy and her PhD degree in natural science (metallurgy). She worked as a research scientist at the Max-Planck-Institut für Metallforschung, Stuttgart, for three years before joining the Metallurgy division at the National Institute of Standards and Technology (then the National Bureau of Standards), Gaithersburg, in 1985, first as a guest scientist and, since 1995, as a physical scientist.*

Texture and Anisotropy: Preferred Orientations in Polycrystals and Their Effect on Materials Properties

U.F. Kocks, C.N. Tomé, and H-R. Wenk
(Cambridge University Press, Cambridge, 1998)
675 pages, $100.00
ISBN 0 521 465168

Materials Science and Engineering has a central concern with the microstructure of engineering materials, its origin in processing, and its influence on final properties. Many of the important features of the microstructure of polycrystalline materials, such as grain size, crystal defects, solute content, and second phase distribution, are reasonably easy to measure, understand, and apply to problems in materials. Despite its major importance, texture is, for many investigators, difficult to comprehend and apply. The present volume, written by three of the major figures in the field and supplemented by chapters from seven other important contributors, should go a very long way to overcoming this difficulty.

The first four chapters of the book deal with the general subject of texture, its measurement, and its description in qualitative pole figures and quantitative orientation distributions. This section includes a particularly important chapter on the various methods of measurement of texture. Here the older methods of x-ray and neutron diffraction are described and compared. These methods sample significant volumes of material but they yield no insight into the spatial relationships involved. Also described are electron diffraction techniques which, while sampling a much smaller volume of material, can capture the orientation of spatially well-defined regions. The recently developed method of orientation imaging microscopy (OIM) provides an important new technique for fully characterizing polycrystalline microstructure at the length scale of micrometers to millimeters. This is the length scale that is critically important for statistically valid structure determination and property prediction. The earlier method for local diffraction study, that of transmission electron microscopy, studied materials usually at too small a length scale to provide the needed insight.

Subsequent chapters of the book describe the textures of two major classes of materials: polycrystalline metals and ceramics, whose properties determine a major part of materials engineering—polymers have so far been less studied by texture methods. In addition, the textures in deformed rocks which can provide insight into the history of the earth's crust are also described in some detail. Rather than covering all of the material properties influenced by texture as stated in the subtitle, the book continues to a third topic, namely, the important properties of elastic and plastic deformation of high-symmetry metals and lower symmetry ceramic materials, including materials vital to geology.

The volume is, for the most part, clearly written and the topics described are well-correlated with each other, making each of the individual chapters of real value to students of the subject. The volume will be of most value to students and investigators at a postgraduate level who have reasonable mathematical expertise. Students will need to master basic crystallography, the elements of symmetry, and diffraction techniques before they can take advantage of this monograph. However, for all serious students of the structure and mechanical deformation of polycrystalline materials in the fields of materials engineering and physical geology, *Texture and Anisotropy* will be essential reading. It is difficult to think of anyone in the field who will not benefit from a detailed study of the range of topics covered here, even if they do not always agree with the conclusions drawn. In fact, disagreement with some of the conclusions is likely to help stimulate future research. The authors of the volume clearly recognize the areas of uncertainty and identify potentially fruitful areas of necessary further study.

Reviewer: *Roger Doherty is a professor of materials engineering at Drexel University. He has carried out research on the mechanisms of recrystallization processing of deformed metallic alloys.*

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