

## book reviews

Works intended for this column should be sent direct to the Book-Review Editor, whose address appears in this issue. All reviews are also available from **Crystallography Journals Online**, supplemented where possible with direct links to the publisher's information.

**Crystals, defects and microstructures, modeling across scales.** By Rob Phillips. Pp. vii + 780. Cambridge University Press, 2001. Price £29.95 (paperback), ISBN 0 521 79357 2; £80.00 (hardback), ISBN 0 521 79005 0.

The aim of this book is to give the reader the needed tools to model crystalline materials. The approach emphasizes both solid-state theory and the practical issues that workers face when implementing computer models based on that theory. The author promotes and discusses, though not in great detail, the finite element method as a means for numerical simulations. Adhering to this approach, he does not attempt to produce an encyclopedia of data, but prefers to give the reader a qualitative perspective on modeling, which he does well with the use of numerous illustrations and graphical presentations of numerical results. There are four main parts to the book: Part One: 'Thinking About the Material World', in which the author gives an overview of what he wants to accomplish and a helpful bag of tools; Part Two: 'Energetics of Crystalline Solids', wherein the author describes a material from a total energy viewpoint; Part Three: 'Geometric Structures in Solids: Defects and Microstructures', which contains a list of defects, grouped by their dimension and followed by some observable properties they impart to the parent material; and Part Four: 'Facing the Multiscale Challenge of Real Material Behavior', in which the author addresses modeling among multiple spatial and temporal scales.

Among its four parts, the book is divided into 13 chapters. In Part One, Chapter 1, 'Idealizing Material Response', is an overview that defines the need for accurate material modeling. Chapter 2, 'Continuum Mechanics Revisited', and Chapter 3, 'Quantum and Statistical Mechanics Revisited', provide the theoretical tools that the modeler needs, both at the continuum level (linear elasticity) and at the atomic level (quantum theory of bonding). In Part Two, Chapters 4 through 6, 'Energetic Description of Cohesion in Solids', 'Thermal and Elastic Properties of Crystals' and 'Structural Energies and Phase Diagrams',

respectively, describe the link between microscopic and macroscopic total energy formulations for a material, while contrasting the continuum and atomistic approaches. Particular emphasis is placed on the modeling of energy and observable material properties, e.g. elastic properties, from atomistic structure. In Part Three, Chapters 7 through 9, 'Point Defects in Solids', 'Line Defects in Solids' and 'Wall Defects in Solids', respectively, provide a comprehensive list of geometric defects, grouped by dimension, present in crystalline solids. Chapter 10, 'Microstructure and its Evolution' catalogs the structure of materials at a scale between the atomic and continuum scales, i.e. the microstructure scale. In Part Four, Chapter 11, 'Points, Lines and Walls: Defect Interactions and Material Response', focuses on material properties that are defined by the interactions of defects, material strengthening being the most well known example. Chapter 12, 'Bridging Scales: Effective Theory Construction', categorizes material models by the scale, or scales, on which they are appropriate, and shows the reader 'various schemes for bridging scales'. Chapter 13, 'Universality and Specificity in Materials', revisits the various themes presented by the author. At the end of each chapter, Phillips lists his favorite (most used) references and gives a commentary on each. The end of the book also contains a reference area with a full list of works cited. Problems are also included at the ends of the chapters, generally fewer than ten in number, of which a good fraction are class-tested.

The book may be used as a text for courses in solid-state (crystalline) properties, microstructural evolution or materials modeling. The small number of problems offered might weigh against its use as a senior-year undergraduate class text, but it could serve as a fine basis for graduate work; it is a text that actually teaches and I plan to require my students to own at least one copy. Graduate students outside materials science may also get a contemporary flavor of crystalline material modeling from the book. Because the arrangement of the book is logical and Phillips's claim that an experienced reader can 'jump in' anywhere in the

text is quite reasonable, the book also seems valuable as a resource for the researcher, especially one who knows one end of the scale well and wants a flavor of modeling at the other end. However, this book should not be regarded as only a specialized text on modeling, it deserves a place on the shelves of anyone active in physical or materials science.

**James M. Fitz-Gerald**

Department of Materials Science  
& Engineering  
School of Engineering and Applied Science  
University of Virginia  
Charlottesville  
VA 22904-4745  
USA

E-mail: jmf8h@virginia.edu

**The basics of crystallography and diffraction.** (Second edition.) By Christopher Hammond. (**IUCr Texts on Crystallography**, No. 3.) Pp. xv + 331. Oxford: International Union of Crystallography/Oxford University Press, 2001. Price £22.95 (paperback), ISBN 0 19 850552 3; £49.95 (hardback), ISBN 0 19 850553 1.

The first edition of this text was reviewed in this journal by Professor Abraham Clearfield [*Acta Cryst.* (1998), **A54**, 1037–1038]. This second edition has been expanded by some 80 pages and goes a long way toward meeting the several legitimate criticisms of the first edition made by Professor Clearfield. Thus, Chapter 4, dealing with crystal symmetry and point and space groups, has been revised and expanded to take account of the use of Volume A of *International Tables for Crystallography*.

The material in Chapters 9 and 10 of the first edition has been rearranged and expanded to add the topics of X-ray and neutron diffraction from simple ordered metal–alloy crystals, including the representation of preferred orientation (texture or fabric). Two new chapters have been added, one dealing with electron diffraction and its applications and the other with the stereographic projection and its uses.

Some minor defects remain in this much improved book. Unit cells of simple close-packed structures are still incorrectly defined in Chapter 1 and confusingly illustrated in Figs. 1.5 and 1.6, and  $u$ ,  $v$  and  $w$  are still retained in the old style as real-space positional coordinates in Chapter 9, as opposed to their current usage as descriptors in Patterson space.

### Robert F. Bryan

Department of Chemistry  
University of Virginia  
Charlottesville  
VA 22901  
USA

E-mail: rfb6w@virginia.edu

## books received

The following books have been received by the Editor. Brief and generally uncritical notices are given of works of marginal crystallographic interest; occasionally, a book of fundamental interest is included under this heading because of difficulty in finding a suitable reviewer without great delay.

**Chirality in liquid crystals.** Edited by Heinz-Siegfried Kitzerow and Christian Bahr. Pp. xiv + 501. Heidelberg: Springer Verlag, 2001. Price DM 259.00, US \$119.00. ISBN 0-387-98679-0. A collection of 15 papers collected to honor the 60th birthday of Professor Gerd Heppke of the Technical University of Berlin. The editors hope that the work gives 'a representative impression of the interesting questions that are being investigated in the field of chiral liquid crystals, even if some pieces are missing.'