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book reviews

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Physics meets mineralogy: condensed matter physics in the geosciences. Edited by H. Aoki, Y. Syono & R. J. Hemley. Pp. xi + 397. Cambridge University Press, 2000. Price £65.00, US $100.00. ISBN 0-521-64342-2.

This book is of great importance and relevance for mineralogists and crystallographers, in particular for those who are interested in high-pressure and high-temperature solid-state physics as well as geophysics and the study of the deep earth interior. Much scientific progress has recently been made through advances in theoretical and computational solid-state physics using supercomputers and through advances in high-pressure and high-temperature experimental mineralogy using multianvil apparatus and diamond anvil cells. The book is an excellent review of the current interaction between solid-state physics and mineralogy, which has had a high impact on geoscience as well as on materials science. It is dedicated to Professor Y. Matsui, to honour his scientific work, and consists of contributions by internationally recognized researchers. It is an excellent basis for those who want to start their own research in experimental and theoretical high-pressure geophysics and is a relevant presentation for those who are already experts in other fields of geoscience or of crystallography (Part I).

Part II deals with advances in theoretical and experimental techniques and starts with a review by L. Stixrude on the applications of density functional theory with the main focus on local density approximation (LDA) methods and the linearized augmented plane-wave (LAPW) technique, to calculate total energies, equations of state, crystal structures, phase stabilities, and elasticity of some geophysically important oxides and silicates. T. Matsumoto introduces crystallographic orbits of space groups for the description of crystal structures, in particular those related to the fluorite type. L. Finger discusses possible sources of errors in powder diffraction measurements, especially those obtained in energy-dispersive diffraction with synchrotron radiation, often used for *in situ* high-pressure experiments. Three-dimensional diffraction techniques nowadays allow such studies of elasticity, rheology, texture and strength of minerals at high pressures. A statistical method based on a generalized linear model is presented by A. Kavner *et al.* to provide best fit phase boundaries to experimentally determined phase diagram data. The melting curve of platinum is analysed as an example.

Part III reviews new findings in oxides and silicates. Using first-principles molecular-orbital (MO) calculations, G. V. Gibbs *et al.* come to the conclusion that the bond strength of metal-to-oxygen bonds correlates with covalency: the greater the bond strength, the more covalent the bond. R. E. Cohen applies first-principles theory to the ionic mineral MgO and calculates the electronic structure, bonding, thermal equation of state, elasticity, melting, thermal conductivity and diffusivity of this mineral, which can be considered as a model compound providing fundamental information on the high-pressure behaviour of other minerals in the deep earth. Z. Fang *et al.* report on the phase stability and the various polymorphic structures of MnO and FeO occurring under ultra-high pressure, using first-principles calculations based on the non-local density functional theory. A. Patel *et al.* review their computer-simulation studies of the lower mantle phases $MgSiO_3$, perovskite and MgO with respect to their thermoelastic properties and diffusion behaviour and outline the geophysical significance of these calculations.

Part IV is dedicated to transformations in crystalline and amorphous silica up to megabar pressures. R. J. Hemley *et al.* review theoretical advances, including first-principles methods, in the context of recent experimental results and discuss the different high-pressure structures of silica and their extensive metastability, as well as short-range order in high-pressure amorphous silica. Using molecular dynamics calculations (MD), K. Kusaba & Y. Syono report the anisotropic nature of the shock-induced phase transition of TiO_2 (rutile). T. Yamanaka & T. Tsuchiya examine both reversible and irreversible amorphization processes in silica by means of X-ray diffraction and MD simulations. T. Yagi & M. Yamakata investigate the effect of hydrostaticity on the phase transformation of cristobalite, which affects not only the transition pressure but also the structure of high-pressure phases.

Part V deals with novel structures and materials. H. Aoki outlines the diversity in crystal structures of materials, from silica to superstructures made up by building blocks at ambient or high pressures, and discusses their interesting electronic and physical properties. The application of high pressure is considered to be a unique tool for realizing novel structures. On the basis of first-principles molecular dynamics simulation, S.Tsuneyuki *et al.* propose a search for new materials to be found by compressing graphitic layered materials to give an exotic diamond-like material. On the basis of Rietveld analysis and neutron-diffraction data, J. B. Parise *et al.* reinterpret observations of order–disorder phenomena at high pressure in hydrous phases such as $Co(OH)_2$ compounds as a partial amorphization of the hydrogen sublattice.

Part VI describes melts and crystal–melt interactions and starts with an article by M. Hemmati & C. A. Angel, who have carried out a detailed comparative study of various interatomic potentials for predicting thermodynamic, structural and dynamic properties of liquid silica, and who were successful in modelling the density maximum of liquid silica as a function of temperature. B. T. Poe & D. C. Rubie report state-of-the-art experimental studies of the diffusivity of silicate liquids up to 15 GPa and 2800 K, and have observed a decrease of viscosity with increasing pressure. Y. Waseda & K. Sugiyama report the local structure (radial distribution functions) of oxide melts found by use of new X-ray diffraction techniques such as angle-dispersive, energy-dispersive and anomalous-scattering methods with new intense synchrotron sources, as a function of pressure as well as of temperature. M. Kanzaki examines trace-element partitioning between melt and crystals and calculates the partial excess enthalpy of trace-element substitution in a crystal by means of MD simulation. The partial excess enthalpy has a minimum at the host cation position and increases with increasing degree of misfit to the host ion

site. The calculation thus reproduces the partition coefficient *versus* ionic radii diagrams of Onuma.

In summary, the book is an excellent review of the recent advances in the application of modern condensed-matter physics in high-pressure and high-temperature mineralogy and the study of the deep earth interior. However, the book does not cover the whole field where physics meets mineralogy, *e.g.* physical properties of minerals such as magnetism or electrical conductivity, which also are of great geophysical importance, are not discussed very profoundly.

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Applications of neutron scattering to soft condensed matter. Edited by Barbara J. Gabrys. Pp. xii + 362. New York: Gordon and Breach Science Publishers, 2000. Price US $95, £63, EUR 105, ISBN 90-5699-300-3.

Thanks to a combination of several factors: high bulk penetrating power, the ability to manipulate local scattering amplitudes through deuteration, and having both the 'right' wavelength and energy, neutron scattering has played a key role in the exploration of the structure and dynamics of soft condensed matter over the past 25 years. This book gives a comprehensive treatment of the principles governing the application of the technique to study such systems and extends the information contained in currently available textbooks such as *Neutron, X-ray and Light Scattering; Introduction to an Investigative Tool for Colloidal and Polymeric Systems*, edited by. P. Lindner & T. Zemb [Elsevier (1991)], *Polymers and Neutron Scattering*, by J. S. Higgins & H. C. Benoit [Oxford Science Publishers (1994)] and *Methods of X-ray and Neutron Scattering in Polymer Science*, by R.-J. Roe [Oxford University Press (2000)].

The wide range of neutron-scattering applications in soft matter makes it difficult to cover all subjects of current interest in a single volume but in this book the editor offers a very useful selection of topics. An introductory chapter by W. Zajac & B. Gabrys presents the principles underlying neutron scattering and provides the background for the techniques explained in more detail in subsequent chapters. So as to complement, rather than duplicate, material that has been extensively covered elsewhere, less attention is paid to subjects such as neutron production and spectrometers *etc.* However, an updated vantage point on newer instrumentation, such as the ISIS TFXA time-of-flight focused crystal spectrometer, is given in the chapter 'Inelastic Neutron Scattering of Polymers' (S. F. Parker). As mentioned above, the main emphasis is on new material and there are chapters on 'Neutron Scattering in the Pharmaceutical Sciences' (C. Washington, M. J. Lawrence & D. Barlow) and 'The Liquid Structure of Halocarbons' (A. N. Burgess, K. A. Johnson, K. A. Mort & W. Spencer Howells) which, to my knowledge, have not been included in similar textbooks before. The emphasis on materials that are both chemically interesting and industrially important reflects the editor's concern to highlight the impact of neutron scattering on wealth creation. Similarly, the fact that two of the twelve contributors are from industry emphasizes the practical nature of many of the applications discussed.

Small-angle neutron scattering (SANS) has been widely applied to study soft matter for decades, and is perhaps the neutron-scattering technique best known to academic and industrial scientists alike. Reflectometry, the other technique that probes large-scale (1–100 nm) structures, has come to the attention of neutron scientists and users more recently but is already the second most widely used technique in industrial applications. Chapters on the 'Organization and Dynamics of Polymers at Fluid Interfaces' (S. K. Peace & R. W. Richards), 'The Structure of Surfactant Monolayers at the Air–Water Interface Studied by Neutron Reflection' (J. R. Liu & R. K. Thomas) and 'Using SANS to Study Absorbed Layers in Colloidal Dispersions' (S. M. King, P. G. Griffiths & T. Cosgrove) reflect the growing interest over the past decade in applying neutron techniques to study surface morphologies, as opposed to the bulk structures studied by SANS.

A chapter on 'Crystalline and Amorphous Polymers' reviews well documented material on a subject where the main research was performed decades ago. The author (K. Kaji) and this reviewer faced a similar problem; I recently attempted the same task and found it hard to find references to significant work after 1990! However, Kaji's chapter gives an accurate and comprehensive summary of the main findings of research on this subject over the past three decades. Chapters on 'Polymer Blends' (V. Arrighi & J. S. Higgins) and 'Scattering from Dilute Solutions and Solid State Ionomers' (A. M. Young & B. Gabrys) provide a concise but self-sufficient overview of the applications of SANS in investigations of the structure and thermodynamic properties of macromolecules in small-molecule and polymeric solvents, in bulk and at interfaces. A chapter on 'Molecular Structures Determined by Neutron Diffraction' (N. Shankland, A. J. Florence, C. C. Wilson & K. Shankland) presents the state-of-the-art in the structure refinement of crystalline materials using neutron diffraction data from powders and single-crystal samples. Almost all crystal structures are still determined by X-ray diffraction. Before neutron diffraction can take full advantage of the fact that it is much more effective for determining the positions of light atoms such as hydrogen, the technique must await the development of higher flux cameras with wider solid-angle detector banks or improvements in methods of growing crystals of sufficient volume (2–5 mm^3) for present-day instruments.

The general standard of presentation in the various articles is high and there are few typographical errors. Bibliographies for each chapter, together with an overall index at the end of the book, give the reader helpful points of entry into the relevant literature and most references cite article titles. The price of the book may limit its circulation among graduate students, which is a pity, as this is a highly commendable work, which is likely to become well worn with use in my laboratory.

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