external electric and magnetic fields to the Gibbs energy. Chapter 3 deals with phase equilibria in heterogeneous systems, the Gibbs phase rule, and phase diagrams. Chapter 4 briefly covers experimental measurements of thermodynamic properties used as input for thermodynamic modeling by calculation of phase diagrams (CALPHAD).

Chapter 5 discusses the use of density functional theory to obtain thermochemical data and fill gaps where experimental data are missing. The chapter introduces the Vienna *ab initio* simulation package (VASP) for density functional theory and the YPHON code for phonon calculations. Chapter 6 introduces the modeling of Gibbs energy of phases using the CALPHAD method. Chapter 7 deals with chemical reactions and the Ellingham diagram for metal oxide systems, and presents the calculation of the maximum reaction rate from equilibrium thermodynamics. Chapter 8 is devoted to electrochemical reactions and Pourbaix diagrams with application examples. Chapter 9 concludes this volume with the application of a model of multiple microstates to Ce and Fe_3Pt. CALPHAD modeling is briefly discussed in the context of genomics of materials.

The book introduces basic thermodynamic concepts clearly and directs readers to appropriate references for advanced concepts and details of software implementation. The list of references is quite comprehensive. The authors make liberal use of diagrams to illustrate key concepts. The two appendices discuss software requirements and the file structure, and present templates for special quasi-random structures. There is also a link to download pre-compiled binary files of the YPHON code for Linux or Microsoft Windows systems. The exercises at the end of the chapters assume that the reader has access to VASP, which is not freeware. Readers without access to this code can work on a limited number of exercises. However, results from other first-principle codes can be organized in the YPHON format, as explained in the appendix. This book will serve as an excellent reference on computational thermodynamics, and the exercises provided at the end of each chapter make it valuable as a graduate level textbook.

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X-Ray Diffraction for Materials Research: From Fundamentals to Applications

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Apple Academic Press and CRC Press, 2016
302 pages, $159.95 (e-book $111.97)
ISBN 9781771882989

X-ray diffraction (XRD) is a powerful nondestructive characterization technique for determining the structure, phase, composition, and strain in materials. It is one of the most frequently employed methods for characterizing materials.

This book distinguishes itself from other books on this topic by its simplified treatment and its coverage of thin-film analysis. It largely minimizes the mathematics and is profusely illustrated, making it a good entry point for learning the basic principles of XRD. The common thin-film structures (random polycrystalline, textured) and their relationships with the substrate (strain, in-plane rotation) are defined and explained. This makes it valuable to researchers who study thin-film deposition. The book includes example problems to reinforce the concepts covered, plus problems that can be assigned as homework.

The background physics is presented first. Chapter 1 covers the properties of electromagnetic radiation, including wave-particle duality and the generation of x-rays. Chapter 2 describes crystal geometry, explaining the concept of a lattice and how Miller indices are assigned to planes and directions, reciprocal lattices, and crystal structures. The scope of this treatment is above that found in introductory materials science and engineering textbooks. The interaction of electromagnetic radiation with materials is discussed in chapter 3, including interference and diffraction. Many of these topics will be familiar to those who have taken college physics, but here they are described with an emphasis on their importance to XRD.

After establishing the basic physics, the book describes the conditions required for XRD to occur in chapter 4. Bragg's Law and the Laue equations are presented and explained. Electron diffraction and the Scherrer equation for estimating nanoparticle size are discussed. In chapter 5, the main factors controlling the intensity of diffracted x-rays are delineated. These include scattering by electrons and atoms and the specific arrangement of atoms, the material's unit cell.

Specific applications of XRD are covered in chapter 6 (thin films), chapter 7 (single crystals), and chapter 8 (powder diffraction). Rocking curves for assessing thin-film quality as well as grazing incidence XRD for enhancing the signal from the surface and diminishing signal from the substrate are introduced. The Laue method for determining the orientation of single crystals is described in detail. The procedure for identifying phases present and lattice constant values is recounted.

This book is a highly accessible introduction to XRD for materials research. It is written in concise and clear prose. The text creates a cohesive picture of XRD. After finishing this book, researchers will be able to understand the basics of many materials science and engineering research papers.

***Reviewer: J.H. Edgar** of the Department of Chemical Engineering, Kansas State University, USA.*