

1. Record Nr.	UNINA9910449824503321
Autore	Saunders N (Nigel)
Titolo	CALPHAD (calculation of phase diagrams) [[electronic resource]] : a comprehensive guide // by N. Saunders and A.P. Miodownik
Pubbl/distr/stampa	Oxford ; ; New York, : Pergamon, c1998
ISBN	1-281-05911-0 9786611059118 0-08-052843-0
Descrizione fisica	1 online resource (497 p.)
Collana	Pergamon materials series ; ; v. 1
Altri autori (Persone)	MiodownikA. P (A. Peter)
Disciplina	530.4/74
Soggetti	Phase diagrams - Data processing Thermochemistry - Data processing Electronic books.
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and indexes.
Nota di contenuto	Front Cover; CALPHAD Calculation of Phase Diagrams: A Comprehensive Guide; Copyright Page; Contents; Series preface; Preface; Foreword; CHAPTER 1. INTRODUCTION; CHAPTER 2. History of CALPHAD; 2.1. Introduction; 2.2. The Early Years; 2.3. The Intermediate Years; 2.4. The Last Decade; 2.5. The Current Status of CALPHAD; References; CHAPTER 3. BASIC THERMODYNAMICS; 3.1. Introduction; 3.2. The First Law of Thermodynamics; 3.3. The Second Law of Thermodynamics; 3.4. The Third Law of Thermodynamics; 3.5. Thermodynamics and Chemical Equilibrium; 3.6. Solution Phase Thermodynamics 3.7. Thermodynamics of Phase Equilibria and Some Simple Calculated Phase DiagramsReferences; CHAPTER 4. EXPERIMENTAL DETERMINATION OF THERMODYNAMIC QUANTITIES AND PHASE DIAGRAMS; 4.1. Introduction; 4.2. Experimental Determination of Thermodynamic Quantities; 4.3. Experimental Determination of Phase Diagrams; References; CHAPTER 5. THERMODYNAMIC MODELS FOR SOLUTION AND COMPOUND PHASES; 5.1. Introduction; 5.2. Stoichiometric Compounds; 5.3. Random Substitutional Models; 5.4. Sublattice Models; 5.5. Ionic Liquid Models; 5.6. Aqueous Solutions;

References; CHAPTER 6. PHASE STABILITIES

6.1. Introduction; 6.2. Thermochemical Estimations; 6.3. Ab Initio Electron Energy Calculations; 6.4. The Behaviour of Magnetic Elements; 6.5. The Effect of Pressure; 6.6. Determination of Interaction Coefficients for Alloys and Stability of Counter-Phases; 6.7. Summary;

References; CHAPTER 7. ORDERING MODELS; 7.1. Introduction; 7.2. General Principles of Ordering Models; 7.3. Features of Various Ordering Models; 7.4. Empirical Routes; 7.5. Role of Lattice Vibrations; 7.6. Integration of Ordering into Phase Diagram Calculations

7.7. Comments on the use of ordering treatments in CALPHAD calculations; References; CHAPTER 8. THE ROLE OF MAGNETIC GIBBS ENERGY; 8.1. Introduction; 8.2. Derivation of the Magnetic Entropy; 8.3.

Derivation of Magnetic Enthalpy, H_{mag} ; 8.4. Derivation of Magnetic Gibbs Energy; 8.5. The Effect of Alloying Elements; 8.6. The Estimation of Magnetic Parameters; 8.7. Multiple Magnetic States; 8.8. Changes in Phase Equilibria Directly Attributable to G_{mag} ; 8.9. Interaction with External Magnetic Fields; References; CHAPTER 9. COMPUTATIONAL METHODS; 9.1. Introduction

9.2. Calculation of Phase Equilibria; 9.3. Thermodynamic Optimisation of Phase Diagrams; References; CHAPTER 10. THE APPLICATION OF CALPHAD METHODS; 10.1. Introduction; 10.2. Early CALPHAD Applications; 10.3. General Background to Multi-Component Calculations; 10.4. Step-by-Step Examples of Multi-Component Calculations; 10.5. Quantitative Verification of Calculated Equilibria in Multi-Component Alloys; 10.6. Selected Examples; 10.7. Summary; References; CHAPTER 11. COMBINING THERMODYNAMICS AND KINETICS; 11.1. Introduction; 11.2. The Calculation of Metastable Equilibria

11.3. The Direct Coupling of Thermodynamics and Kinetics

11.3. The Direct Coupling of Thermodynamics and Kinetics

Sommario/riassunto

This monograph acts as a benchmark to current achievements in the field of Computer Coupling of Phase Diagrams and Thermochemistry, often called CALPHAD which is an acronym for Computer CALculation of PHase Diagrams. It also acts as a guide to both the basic background of the subject area and the cutting edge of the topic, combining comprehensive discussions of the underlying physical principles of the CALPHAD method with detailed descriptions of their application to real complex multi-component materials. Approaches which combine both thermodynamic and kinetic models to
