



ISBN: 978-0-12-801494-3

PUB DATE: September 2018

LIST PRICE: \$200.00

FORMAT: Hardback

PAGES: c. 400 Illustrated

TRIM: 7.5w x 9.25h

AUDIENCE: Academic and industrial laboratories doing research and development in materials science, metallurgy, combustion and energy, corrosion engineering, environmental engineering, geology, glass technology, nuclear engineering and other fields of inorganic chemical and materials science and engineering. Researchers, libraries, graduate students. Professors in chemistry, chemical engineering and materials science giving graduate courses on thermodynamics and phase equilibria and/or solution modeling. Graduate students

# Phase Diagrams and Thermodynamic Modeling of Solutions

Arthur Pelton, Department of Chemical Engineering, Centre de Recherche en Calcul Thermochimique, Ecole Polytechnique de Montréal, Quebec, Canada



A systematic discussion of phase diagrams of all types, including their thermodynamics and calculation from thermodynamic databases, solution models, and more

### **KEY FEATURES**

- Presents a rigorous and complete development of thermodynamics for readers who already have a basic understanding of chemical thermodynamics
- Provides an in-depth understanding of phase equilibria
- Includes information that can be used as a text for graduate courses on thermodynamics and phase diagrams, or on solution modeling
- Covers common types of phase diagrams as well as less common types (paraequilibrium diagrams, first-melting projections, Scheil diagrams, enthalpy diagrams), and more
- Presents a comprehensive in-depth review of current solution models

#### DESCRIPTION

*Phase Diagrams and Thermodynamic Modeling of Solutions* provides readers with an understanding of thermodynamics and phase equilibria that is required to make full and efficient use of these tools. The book systematically discusses phase diagrams of all types, the thermodynamics behind them, their calculation from thermodynamic databases, and the structural models of solutions used in the development of these databases. Featuring examples from a wide range of systems including metals, salts, ceramics, refractories, and aqueous solutions, *Phase Diagrams and Thermodynamic Modeling of Solutions* is a vital resource for researchers and developers in materials science, metallurgy, combustion and energy, corrosion engineering, environmental engineering, geology, glass technology, nuclear engineering. Additionally, experts involved in developing thermodynamic databases will find a comprehensive reference text of current solution models.

Please visit <u>elsevier.com/books/isbn/9780128014943</u> Enter code CHEMENG318 for up to 30% off and free shipping!



M

# TABLE OF CONTENTS

### Part I – Phase Diagrams and Thermodynamics

- 1. Introduction
- 2. Thermodynamics fundamentals
- 3. The Gibbs Phase Rule
- 4. Fundamentals of the thermodynamics of solutions
- 5. Thermodynamic origin of phase diagrams
- 6. Ternary temperature-composition phase diagrams
- 7. General phase diagram sections
- 8. Equilibrium and Scheil-Gulliver solidification
- 9. Paraequilibrium phase diagrams and minimum Gibbs energy diagrams
- 10. Second-order and higher-order transitions
- 11. Phase diagrams of systems with an aqueous phase
- 12. Bibliography on phase diagrams

## Part II – Thermodynamic Modeling of Solutions

- 13. Introduction
- 14. Single-sublattice random-mixing (Bragg- Williams-BW) models
- 15. Multiple-sublattice random-mixing (Bragg- Williams-BW) models
- 16. Single-lattice models with short-range ordering (SRO)
- 17. Modeling short-range ordering with two sublattices
- 18. Some applications

### Exercises

19. Exercises with solutions