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Nota di contenuto	1 Introduction -- 2 General overview of crystallography and thermodynamics -- 3 Basic crystallography for thermodynamic modeling -- 4 Basic thermodynamics: From Principles to Phase equilibria -- 5 Ab initio calculations for thermodynamics -- 6 The thermodynamic approach to phase diagrams -- 7 The modern description of phase diagrams -- 8 The relationships between phase diagrams, phase equilibria and phase stability -- 9 Conclusion -- Appendix -- Index.
Sommario/riassunto	This book provides expert treatment of the use of the Calphad calculations for the study of crystal structures and thermodynamics relationships in phase diagram determination. After a short review of

the relationships between crystal structures and the thermodynamics of materials, including all possible phase transformations, the book proceeds to a brief discussion of the methods for solving the stability hierarchy of different phases. Coverage includes both theoretical calculations and experimental methods based on classical thermodynamics, with emphasis on the latter. The experimental approach is mainly carried out using heat-exchange data associated with the transition of one form into another. It is demonstrated that the crystallographic properties must be associated with the phase transformations and should be taken into account. The role of X-ray crystallography therein is also discussed. Readers interested in carrying out related research will appreciate the detailed discussion and critical analysis of key results obtained by the author and his colleagues over the past five years.