Record Nr. UNINA9910845485303321 Autore Tedenac Jean-Claude Titolo Thermodynamics of Crystalline Materials [[electronic resource]]: From Nano to Macro / / by Jean-Claude Tedenac Pubbl/distr/stampa Cham:,: Springer International Publishing:,: Imprint: Springer,, 2024 **ISBN** 3-030-99027-3 Edizione [1st ed. 2024.] Descrizione fisica 1 online resource (95 pages) Collana SpringerBriefs in Materials, , 2192-1105 Disciplina 548.86 Soggetti Ceramic materials Crystallography Inorganic chemistry Thermodynamics Materials Nanochemistry Ceramics Crystallography and Scattering Methods **Inorganic Chemistry** Materials Engineering Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia 1 Introduction -- 2 General overview of crystallography and Nota di contenuto 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. This book provides expert treatment of the use of the Calphad Sommario/riassunto 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.