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Nota di contenuto	Thermodynamic Properties of Solids: Experiment and Modeling; Contents; Preface; List of Contributors; Abbreviations; 1 Thermodynamic Properties of Solids: Experiment and Modeling; 1.1 Introduction; 1.2 Spectroscopic Techniques and Semiempirical Theoretical Methods; 1.3 Thermal Measurement Techniques; 1.4 First-Principles Quantum Mechanical Methods; 1.5 Outlook; References; 2 Optical Spectroscopy Methods and High-Pressure-High-Temperature Studies; 2.1 Methods and Principles: Ambient Conditions; 2.1.1 Semiconductors; 2.1.2 q~0 Optical Modes: Concept of Polaritons [4, 5] 2.1.2.1 Maxwell Equations2.1.2.2 Mechanical Equations; 2.1.2.3 Lorentz Approach; 2.1.2.4 Effective Charge/Force Constant; 2.1.2.5 Combined Electrical/Mechanical Equations: Dispersion of Polaritons Modes; 2.1.3 Vibration Spectra; 2.1.3.1 IR Spectroscopies: A Direct Light/Optical-Mode Interaction [4, 5, 11]; 2.1.3.2 Raman Scattering: An

Indirect Light/Optical-Mode Interaction [13, 14]; 2.1.3.3 Brillouin Scattering: An Indirect Light/Acoustical-Mode Interaction; 2.1.4 Some Particular Cases; 2.1.4.1 Multioscillator System; 2.1.4.2 Multilayer System [12]

2.1.4.3 Multicomponent System (Composite) [22] 2.1.5 Selection Rules [5, 17]; 2.1.5.1 Raman Scattering; 2.1.5.2 IR Absorption; 2.1.5.3 Brillouin Scattering; 2.1.6 When Departing from Pure Crystals . . .; 2.2 Optical Vibrational Spectroscopies Under Extreme Conditions; 2.2.1 A Specific Impact/Identity in the Field; 2.2.1.1 Solid-State Physics; 2.2.1.2 Earth Sciences; 2.2.2 Specificities and Instrumentation for High-Temperature and High-Pressure Investigations; 2.2.2.1 Temperature and Emissivity; 2.2.2.2 High-Pressure Optical Cells, Diamond-Anvil Cells; 2.2.2.3 High-Temperature Instrumentation

2.2.2.4 Brillouin Devices 2.2.2.5 Raman Devices; 2.2.2.6 Infrared Devices: Emissivity Measurements (Temperature and Pressure); 2.2.3 Acoustical Modes; 2.2.3.1 General Presentation; 2.2.3.2 Examples; 2.2.4 Optical Modes; 2.2.4.1 Pressure Aspect; 2.2.4.2 Temperature Aspect; 2.3 Perspectives; 2.3.1 Instrumentation; 2.3.1.1 Natural Development of Existing Setups; 2.3.1.2 Innovative Combinations of X-ray and Vibrational Spectroscopies; 2.3.2 Physical Phenomena; 2.3.2.1 Phonons (Zone-Center): A Natural .Mesoscope. into the Alloy Disorder 2.3.2.2 Elucidation of the Mechanism of the Pressure-Induced Phase Transformations 2.3.2.3 Glasses; References; 3 Inelastic Neutron Scattering, Lattice Dynamics, Computer Simulation and Thermodynamic Properties; 3.1 Introduction; 3.2 Lattice Dynamics; 3.2.1 Theoretical Formalisms; 3.3 Computational Techniques; 3.4 Thermodynamic Properties of Solids; 3.5 Theory of Inelastic Neutron Scattering; 3.5.1 Inelastic Neutron Scattering from Single Crystals: Phonon Dispersion Relations; 3.5.2 Inelastic Neutron Scattering from Powder Samples: Phonon Density of States

3.6 Experimental Techniques for Inelastic Neutron Scattering

Sommario/riassunto

Recent years have seen a growing interest in the field of thermodynamic properties of solids due to the development of advanced experimental and modeling tools. Predicting structural phase transitions and thermodynamic properties find important applications in condensed matter and materials science research, as well as in interdisciplinary research involving geophysics and Earth Sciences. The present edited book, with contributions from leading researchers around the world, is aimed to meet the need of academic and industrial researchers, graduate students and non-specialists working in these
