1. Record Nr. UNINA9910808641803321

Titolo	A study of ion cluster theory of molten silicates and some inorganic substances / / edited by Jiang GuoChang [and three others]
Pubbl/distr/stampa	Stafa-Zuerich ; ; Enfield, New Hampshire : , : Trans Tech, , [2009] ©2009
ISBN	3-03813-324-8
Descrizione fisica	1 online resource (282 p.)
Collana	Materials science foundations, , 1422-3597 ; ; volumes 52-53
Disciplina	549.6
Soggetti	Silicates Ionic structure Inorganic compounds Raman spectroscopy
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.
Nota di contenuto	A Study of Ion Cluster Theory of Molten Silicates and some Inorganic Substances; Preface; Table of Contents; Table of Contents; 1. Significance of Studying Molten State in Metallurgy/Ggeometry/Ceramics; 1.1. Why it Is Important to Interconnect Micro Structure with Relevant Macroscopic Properties; 1.2. Two Aspects of the Studying Approach. Ref.1.; 2. Development of High Temperature Raman Spectroscopy in Shanghai University; 2.1. Selection of Experiment Method in Studying Micro Structure of Molten Silicate; 2.2. Summary of Raman Spectroscopy 2.3. Characteristics of Diverse High Temperature Raman Spectroscopy (HTRS)2.4. The First Set of HTRS Developed in Shanghai University (SU-HTRS); 2.5. The Second Set of HTRS Developed in Shanghai University, SU-HTRS(T/S); Ref. 2; 3. Micro Structure of Diverse Hierarchy in Silicates and Aluminates; 3.1. Micro Structure of Silicates in Phenomenology; 3.2. Elementary Micro Structure of Silicates; 3.3. Second and Multi Order Micro Structure of Silicates; 3.4. Discrepancy of Micro Structure between Silicate Melt and Silicate Glass 3.5. Coordination Bond of Al in Ai-O Tetrahedron, and the Oxygen with Three Bonds3.6. Al-O Tetrahedra in Aluminates; Ref. 3; 4. SiOT Model

Used to Calculate the Raman Spectroscopy of Molten Silicates; 4.1. Survey of the Theoretical Description of HTRS of Molten Silicate; 4.2. Gist of the Model; 4.3. Application of SiOt Model; 4.4. Characteristics and Function of SiOt Model; Ref.4; 5. Interconnection of Micro Structure and Thermodynamic Properties ---CEMS Model; 5.1. CEMS Model; 5.2. Self-Consistent Calcuation of CEMS Model; 5.3. A Discussion on the Reliability of CEMS Model
5.4. Calculation of Thermodynamic Properties5.5. Characteristics and Function of CEMS Model; Ref. 5; 6. Ab Initio Calculation of Raman Spectra of Silicate; 6.1. A Brief Introduction of Ab Initio calculation; 6.2. Use of Gaussian 98 Software in Raman Spectrum Calculation; 6.3. Raman Spectra of Na2O-SiO2 System Crystals Calculated with G98 Software; 6.4. Prediction of Micro Structure in Glass and Melt According to the Result for Crystal; 6.5. Error and Applicable Limit of Ab Initio Calculation; Ref. 6.; 7. Raman Spectra of some Inorganic Glasses and Compounds
7.1. Influence of Composition on Raman Spectra of Silicate Glasses7.2. Raman Spectra of some Aluminosilicate Minerals; 7.3. Raman Spectra of Binary Na2O-P2O5 System; 7.4. Raman Spectra of Borate; 7.5. Summary of the Study on Phase Transformation by Means of HTRS. 7.6. Raman Spectra of TiO2 and Nano-PbTiO3; 7.7. Solid-Liquid Boundary during the Growing Process of TeO2 Crystal; Ref.7; 8. Ion Cluster Theory in Thermodynamics---the High Order Subregular Model of Melt; 8.1. SReM Model; 8.2. Relationships between the Parameters in Quaternary and Quinary System
8.3. Parameter Fitting Procedures in the SReM Model

Sommario/riassunto

The first part of this monograph consists of a discussion of the microstructures of molten silicates and other inorganic substances. It is made up of seven chapters. Chapter 1 considers developments in ion-cluster theory. Chapter 2 introduces experimental approaches to the direct monitoring of a molten sample, such as hightemperature Raman spectroscopes which have successfully recorded Raman spectra from melts at temperatures of 2000K or more. Chapter 3 shows that five types of Si-O tetrahedron are appropriate microstructural units for setting up structural models. Chapter 4 confirms the SiOT