

Contents

Chapter 1 **2-33**

- 1.1 Introduction: Present state of Knowledge
- 1.2 Approximation used in Lattice Dynamics
- 1.3 Secular Determinants
- 1.4 Fluorite Structure
- 1.5 CdI_2 Structure

Chapter 2 **35-53**

- 2.1 Relevant Models for Superionic Crystals
 - 2.1.1 Rigid Ion Model (RIM)
 - 2.1.2 Modified Rigid Ion Model (MRIM)
 - 2.1.3 Virtual Crystal Approximation (VCA) Model
 - 2.1.4 Pseudo-Unit-Cell Model
 - 2.1.5 Linear Chain Model
 - 2.1.6 Cluster Model
 - 2.1.7 Random Element Isodisplacement (REI) Model
 - 2.1.8 Coherent Potential Approximation (CPA) Model
 - 2.1.9 Green's Function Technique
 - 2.1.10 Microscopic Approach
- 2.2 Behavior of Mixed Crystals
 - 2.2.1 Zone Centre Mode Behavior
 - 2.2.2 One-Mode Behavior
 - 2.2.3 Two-Mode Behavior
- 2.3 Frequency Distribution Function or Phonon Density of States

| | | |
|----------------|---|----------------|
| Chapter | 3 | 55-77 |
| 3.1 | Bond Bending Rigid Ion Model (BBRIM) | |
| 3.2 | Expression for Dynamical Matrices of Fluorite Structure | |
| 3.3 | Expression for Dynamical Matrices of CdI ₂ Structure | |
| 3.4 | Evolution of Force Constant | |
| 3.5 | Lattice Equilibrium Condition | |
| | | |
| Chapter | 4 | 79-131 |
| 4.1 | One-Mode Behavior of Mixed Crystals | |
| 4.2 | Behavior of Mixed Superionic Fluorites | |
| 4.2.1 | Pb _x Cd _{1-x} F ₂ | |
| 4.2.2 | Mn _x Cd _{1-x} F ₂ | |
| 4.2.3 | Sr _{1-x} Cd _x F ₂ | |
| 4.2.4 | Sr _x Ca _{1-x} F ₂ | |
| | | |
| Chapter | 5 | 133-167 |
| 5.1 | Mixed Crystals Showing Two Mode Behavior | |
| 5.2 | Evolution of Force Constants, Interlayer and Intralayer Coupling Constants | |
| 5.3 | Phonon Dispersion of Mixed Crystals | |
| 5.3.1 | SnS _x Se _{2-x} | |
| 5.3.2 | HfS _{2-x} Te _x | |
| 5.3.3 | Hf _x Ti _{1-x} Se ₂ | |
| 5.3.4 | TiSe _{2-x} S _x and ZrTi _{1-x} Se ₂ | |
| 5.4 | Conclusion | |

List of publications

1. Lattice Dynamical Properties of $\text{Sr}_{1-x}\text{Cd}_x\text{F}_2$ published in SCITECH Vol. 4, No. 2, July-Dec. (2009) Page No. (64-68).
2. Lattice Dynamics of Superionic Crystal $\text{Mn}_x\text{Cd}_{1-x}\text{F}_2$ published in the proceedings of the national conference on “Current Concepts and Frontier Advance in Science Education Research” held at T. D. P. G. College Jaunpur (2011).
3. Lattice Dynamics of Superionic Crystal $\text{Mn}_x\text{Cd}_{1-x}\text{F}_2$ published in I. J. Materials Physics, Vol. 4, NO. 1, (2013) Page No. (23-28).