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Autore	Chen Chuangtian <1937->
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Nota di contenuto	Nonlinear Optical Borate Crystals: Principles and Applications; Contents; Preface; List of Contributors; Acknowledgments; 1 Introduction; 1.1 History of the Theoretical Understanding of Nonlinear Optical Crystals; 1.2 History of Development of NLO Borate Crystals; 1.3 History of Crystals for Frequency Conversion; 1.3.1 Frequency Conversion Efficiency of Second Harmonic Generation; 1.3.2 Methods to Obtain Higher Efficiency for Frequency Conversion; 1.3.3 Desirable Conditions for Frequency Conversion Crystals; 1.3.4 History of Crystals and Techniques for Frequency Conversion; References 2 Theoretical Basis for the Development of Borate Nonlinear Optical Crystals 2.1 The Anionic Group Theory and its Approximate Quantum Chemical Methods; 2.1.1 Theoretical Model; 2.1.2 Molecular Orbital Calculation Method; 2.1.2.1 The CNDO-Type Approximation; 2.1.2.2 The EHMO-Type Approximation; 2.2 The SHG Coefficients for Typical

NLO Crystals Calculated with the Anionic Group Theory; 2.2.1 The Perovskite and Tungsten-Bronze Type of Crystals; 2.2.1.1 Niobate Crystals; 2.2.1.2 SrTiO₃, BaTiO₃, KTaO₃ Crystals; 2.2.2 Iodate Crystals; 2.2.3 The Phosphate Crystals; 2.2.4 The Molybdate Crystals; 2.2.5 The Na₂SbF₅ Crystal; 2.2.6 KB₅O₈ · 4H₂O or K[B₅O₆(OH)₄] · 2H₂O (KB₅) Crystal; 2.2.7 The NaNO₂ Crystal; 2.3 The Relationship between the Anionic Group and the Absorption Edge of Inorganic Crystals on the UV Side; 2.3.1 The Model and Approximation; 2.3.2 Absorption Edge Calculations for the Isolated Anionic Group Type; 2.3.2.1 Electronic Structure of -BaB₂O₄ (BBO); 2.3.2.2 Electronic Structure of LiB₃O₅ (LBO); 2.3.2.3 Electronic Structure of KBe₂BO₃F₂ (KBBF); 2.3.2.4 Electronic Structure of KB₅O₈ · 4H₂O; 2.3.2.5 Electronic Structure of KH₂PO₄ (KDP); 2.3.2.6 Electronic Structure of Na₂SbF₅; 2.3.2.7 Electronic Structure of Iodate Crystals and NaNO₂ Crystal; 2.3.3 Summary; 2.4 Ab initio Calculations on the Linear and Nonlinear Optical Properties of Borate and Other Crystals; 2.4.1 Computational Methods; 2.4.2 Calculations and Analysis for Borate Crystals; 2.4.2.1 BBO and LBO Family Crystals; 2.4.2.2 KBBF, BaAlBO₃F₂ (BABF) and Sr₂Be₂B₂O₇ (SBBO) Family Crystals; 2.4.2.3 BIBO Crystal; 2.4.3 Calculations and Analysis for Other NLO Crystals; 2.4.3.1 NaNO₂; 2.4.3.2 Na₂SbF₅; 2.4.3.3 KH₂PO₄ (KDP); 2.5 The Computer-Assisted Molecular Design System for Searching New NLO Crystals; 2.5.1 Material Requirements for NLO Devices; 2.5.2 Theoretical Evaluation; 2.6 The Developments of New NLO Crystals in Borate Series; 2.6.1 The Basic Structural Units in Borate Series and Their NLO and LO Properties; 2.6.1.1 The Second-Order Susceptibilities of the Borate Groups; 2.6.1.2 The Band Gaps of the Borate Groups; 2.6.2 The Development of New NLO Borate Crystals with Molecular Engineering Approach; 2.6.2.1 The History of Discovering BBO; 2.6.2.2 From BBO to LBO; 2.6.2.3 From BBO to LBO to KBBF Crystal; 2.6.2.4 From KBBF to SBBO Family; References

3 Borate Nonlinear Optical Crystals for Frequency Conversion

Sommario/riassunto

This clear and self-contained review of the last four decades of research highlights in the hot field of nonlinear optical (NLO) crystals, particularly of borate-based ultraviolet and deep-ultraviolet NLO crystals, covers three major subjects: the structure-property relationship in borate crystals, the structural and optical characteristics of various promising borate crystals, and their fruitful applications in a wide range of scientific and technological fields. Edited by the discoverers and users of these optical borate crystals, this is a readily accessible reading for semiconductor, a