

Springer Series in Materials Science

Volume 197

Series editors

Robert Hull, Charlottesville, USA
Chennupati Jagadish, Canberra, Australia
Richard M. Osgood, New York, USA
Jürgen Parisi, Oldenburg, Germany
Shin-ichi Uchida, Tokyo, Japan
Zhiming M. Wang, Chengdu, China

For further volumes:
<http://www.springer.com/series/856>

The Springer Series in Materials Science covers the complete spectrum of materials physics, including fundamental principles, physical properties, materials theory and design. Recognizing the increasing importance of materials science in future device technologies, the book titles in this series reflect the state-of-the-art in understanding and controlling the structure and properties of all important classes of materials.

Bernard Gil

Physics of Wurtzite Nitrides and Oxides

Passport to Devices

 Springer

Bernard Gil
Institut de Physique de Montpellier
University of Montpellier 2
Montpellier, Cedex
France

ISSN 0933-033X ISSN 2196-2812 (electronic)
ISBN 978-3-319-06804-6 ISBN 978-3-319-06805-3 (eBook)
DOI 10.1007/978-3-319-06805-3
Springer Cham Heidelberg New York Dordrecht London

Library of Congress Control Number: 2014940318

© Springer International Publishing Switzerland 2014

This work is subject to copyright. All rights are reserved by the Publisher, whether the whole or part of the material is concerned, specifically the rights of translation, reprinting, reuse of illustrations, recitation, broadcasting, reproduction on microfilms or in any other physical way, and transmission or information storage and retrieval, electronic adaptation, computer software, or by similar or dissimilar methodology now known or hereafter developed. Exempted from this legal reservation are brief excerpts in connection with reviews or scholarly analysis or material supplied specifically for the purpose of being entered and executed on a computer system, for exclusive use by the purchaser of the work. Duplication of this publication or parts thereof is permitted only under the provisions of the Copyright Law of the Publisher's location, in its current version, and permission for use must always be obtained from Springer. Permissions for use may be obtained through RightsLink at the Copyright Clearance Center. Violations are liable to prosecution under the respective Copyright Law. The use of general descriptive names, registered names, trademarks, service marks, etc. in this publication does not imply, even in the absence of a specific statement, that such names are exempt from the relevant protective laws and regulations and therefore free for general use.

While the advice and information in this book are believed to be true and accurate at the date of publication, neither the authors nor the editors nor the publisher can accept any legal responsibility for any errors or omissions that may be made. The publisher makes no warranty, express or implied, with respect to the material contained herein.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

This book aims at offering the master students—and probably to other ones—who are studying the physics of wide bandgap semi-conductors, the elements required to rapidly grasp the concept of solid state physics that are needed to start a formation or a research activity at the boarder between physics, chemistry, electrical engineering.

This field has known tremendous developments during the past 20 years, and it will probably continue to be very exciting: so many applications are possible to wide band gap semi-conductors and so few have been satisfied to date.

I have been routinely working on optical properties of wide band gap semi-conductors, of their heterostructures, of their nanostructures since 1991 and I could attend every year a lot of scientific international conferences. Each time was the opportunity for me to meet new faces, sometimes very young ones. Most of these newcomers had received a formation in chemistry, electronics, physics, mathematics, or another one, sometimes including astronomy. They are often launched into the international scientific arena just after having spent a few weeks or months in immersion into a research group, and they have to accommodate a lot of concepts in very different domains. This is not so easy for them. I had a lot of opportunities to chat with many of these newcomers. I got convinced as many of my colleagues are now, too, that there is a need for a general book in which they could find gathered most of the concepts that they need to know. When Claus Ascheron from Springer asked me to write such book, I accepted it without having in mind the challenging proposal he had made to me. You are holding such a book in your hands. The field is wide and necessarily unexhaustively addressed, but I hope this monograph contains a strong enough message for being of value for a lot of my young colleagues.

This book is declined along five chapters: basic symmetry and physical properties linked to it, basics of growth and structural characterization methods, band structure effects and lattice vibrations, optical properties of bulk materials, and finally physics and optical properties of low-dimensional systems. Photonics, quantum optics, plasmonics, and transport properties are not treated; they are from very much specialized areas and are addressed or in the way of being addressed in specialized research books.

This book is the fruit of many collaborations. I would first like to thank the many students that I contributed to train. Many of them now being colleagues in

some universities or at the National Centre of Scientific Research, my employing institution. Let me thank Philippe Boring, Pierre Bigenwald, Pierre Lefebvre, Matthieu Moret, Lionel Aigouy, Claude Boemare, Sandra Ruffenach, Andenet Alemu, Magloire Tchounkeu, Francois Demangeot, Cyril Pernot, Abdelhadi Abounadi, Amal Rajira, Tomasz Ochalski, Yves-Mathieu Le-Vaillant, Marian Zamfirescu, Mathieu Gallart, Aurelien Morel, Xue Bing Zhang, Sokratis Kalliakos, Romuald Intartaglia, Benedicte Maleyre, Richard Bardoux, Stephane Faure, Luc Beur, Daniel Rosales, Julien Selles, Huong Thi Ngo, and Rereao Hahe. I had a chance to work with a lot of handsome colleagues among which are Olivier Briot, Mathieu Leroux, Jean-Yves Duboz, Nicolas Grandjean, Eric Tournie, Benjamin Damilano, Julien Brault, Jean-Michel Chauveau, Christian Morhain, Thierry Bretagnon, Amelie Dussaigne, Jean Massies, Bernard Beaumont, Pierre Gibart, Philippe Vennegues, Pierre Ruterana, Thierry Guillet, Christelle Brimont, Pierre Valvin, Christian L'henoret, Thierry Taliercio, Didier Felbacq, Brahim Guizal, Guillaume Cassabois, Emmanuel Rousseau, Christelle Eve, Jacques Leyzat, Regine Pauzat, Bruno Daudin, ...

At the international scale, Izabella Grzegory, Hadis Morkoç, Isamu Akasaki and Shuji Nakamura have been my mentors in the early days of the nitrides. I took advantages of fruitful exchanges with Yabusiko Arakawa, Bo Monemar, Alex Zunger, Hiroshi Amano, Akihiko Yoshikawa, Yasuhi Nanishi, Yoichi Kawakami, Kazamasu Hiramatsu, Katsumi Kishino, Shigefusa Chichibu, Hideto Miyake, Alexey Kavokin, Axel Homann, Martin Stutzmann, Bruno Meyer, Juergen Christen, Jorg Neugebauer, Friedhelm Beschtadt, Alois Krost, Andreas Hangleiter, Martin Feneberg, Ruediger Goldhahn, Charles Foxon, Kevin O'Donnell, Rob Martin, Peter Parbrook, Galia Pozina, Tatiana Shubina, Serguey Ivanov, Valery Yu Davidov, Tanya Paskova, Plamen Paskov, Fernando Ponce, Russell Dupuis, Ted Moutsakas, Steven den Baars, Umesh Misra, James Speck, Zlatko Sitar, Eva Monroy, Xinqiang Wang, Piotr Perlin, Tadeusz Suski, Abderrahmane Kadri, Karima Zitouni, and so many others.

Pierre Bigenwald who carefully browsed the five chapters to expurgate them from typos deserves receiving specific acknowledgments.

Montpellier

Bernard Gil

Contents

1	Basic Crystallography and Other Properties Linked with Symmetry	1
1.1	The Hexagonal Point Symmetry Deduced from the Shape of Natural Wurtzitic Crystals	1
1.2	The Hexagonal Lattice, Its Reticular Planes and Their Description Using Simple Euclidian Geometry.	4
1.3	The Four-Index Bravais-Miller Representation of the Orientation of Reticular Planes in Hexagonal Crystals.	6
1.4	Representation of Hexagonal Crystal Directions Using Four Indices	7
1.5	The Reciprocal Lattice	8
1.6	The Orthogonal Basis Set	11
1.7	The Determination of the Lattice Parameters by X-ray Diffraction	11
1.7.1	Diffraction by a Linear Grating	12
1.7.2	Diffraction by a Linear Lattice, and by a Planar One	13
1.7.3	Diffraction by a Three-Dimensional Lattice	14
1.8	The Determination of Space Symmetry by X-ray Analysis	16
1.8.1	The First Brillouin Zone	16
1.8.2	The Structure Factor	17
1.8.3	The Perfect Wurtzite Structure	19
1.8.4	The Internal Displacement Parameter	21
1.9	The Spontaneous Polarization Along the <i>c</i> Axis	23
1.10	Defects in the Lattice	25
1.11	Piezoelectric Effects in Wurtzitic Semi-conductors	25
1.12	Stresses and Strains.	27
1.12.1	The Stress Tensor	27
1.12.2	The Strain Tensor	28
1.12.3	The Stiffness and Compliance Tensors	31
1.12.4	The Stiffness and Compliance Tensors in Wurtzitic Semi-conductors	32
1.12.5	The Energy of a Strained Crystal	34

1.13	Basic Elements of Group Theory	34
1.13.1	The Concept of Algebraic Groups	34
1.13.2	Representations of Finite Groups by Matrices.	36
1.13.3	Character Tables and Irreducible Representations.	38
1.13.4	The Point Group C_{6v}	40
1.13.5	Application of Group Theory to the Calculation of Integrals.	41
1.13.6	Group Theory and Perturbations	43
1.13.7	Angular Momenta and Group Theory: Simple and Double Groups	44
1.13.8	Character Tables, Compatibility Table and Multiplication Tables.	45
1.13.9	The Translation Group.	47
1.13.10	The Space Group	47
	References	48
2	Basics of Growth and Structural Characterization.	49
2.1	Growth of Bulk Crystals	49
2.2	Principle of Epitaxial Growth Methods	52
2.2.1	Hydride Vapor Phase Epitaxy.	53
2.2.2	Metal-Organic Vapor Phase Epitaxy	53
2.2.3	Molecular Beam Epitaxy	54
2.2.4	The Growth of (001)-Oriented GaN on Sapphire Using a Low-Temperature-Grown Thin Buffer Layer	56
2.3	Epitaxial Lateral Overgrowth Techniques	62
2.4	Epitaxial Growth of Heterostructures.	62
	References	64
3	Electrons and Phonons in Wurtzitic Semi-conductors	65
3.1	Electrons in a Periodic Potential.	65
3.1.1	The Born-Oppenheimer Adiabatic Approximation	65
3.1.2	The One-Electron Approximation	68
3.1.3	The Free Electron Model	69
3.1.4	The Effect of a Periodic Lattice: The Bloch Theorem.	71
3.1.5	The Born-von Karman Cycling Conditions and the Concept of Spatial Folding	74
3.1.6	The Effect of a Periodic Lattice: The Formation of Energy Gaps at the Edges of the Brillouin Zone.	75
3.1.7	The Concept of the Effective Mass	77
3.1.8	The Tight-Binding Method.	78

3.1.9	Band Structure of Wurtzite Semi-conductors in the Context of a Spinless Tight-Binding Description. . .	81
3.2	The Semi-classical Theory of the Dielectric Function in Crystals	86
3.2.1	Intuitive Description	86
3.2.2	Microscopic Theory of the Dielectric Constant.	87
3.2.3	Experimental Values of the Spectral Dependence of the Dielectric Constants of Nitrides.	90
3.2.4	Excitonic Contributions to the Dielectric Constant.	91
3.3	The Spin-Orbit Interaction	94
3.4	The $\vec{k} \cdot \vec{p}$ Method and the Description of Band Dispersion at Zone Center in Wurtzitic Semi-conductors.	101
3.4.1	The Simplest Spinless Description of Conduction and Valence Bands Dispersions at Zone Center in Wurtzitic Semi-conductors	101
3.4.2	The Simplest (6×6) $\vec{k} \cdot \vec{p}$ Description for Valence Band Dispersions at Zone Center in Wurtzitic Semi-conductors	102
3.4.3	Including Strain Field to the $\vec{k} \cdot \vec{p}$ Description of Band Dispersion in Wurtzitic Semi-conductors . . .	104
3.4.4	The Simplest (8×8) $\vec{k} \cdot \vec{p}$ Description of Valence Band Dispersions at Zone Center in Wurtzitic Semi-conductors	105
3.5	Phonons in Wurtzitic Semi-conductors	106
3.5.1	Longitudinal and Transverse Waves in Continuous Media	106
3.5.2	The Classical Model and the Concept of Normal Coordinates.	107
3.5.3	Group Theory and Normal Modes.	110
3.5.4	The Linear Mono-atomic Lattice.	110
3.5.5	The Linear Lattice with Two Different Atoms: Acoustic and Optical Branches.	114
3.5.6	Quantum Theory of Lattice Vibrations.	115
3.5.7	Phonons in Wurtzitic Crystals.	118
3.5.8	Contribution of Phonons to the Dielectric Constant in Bulk Wurtzitic Semi-conductors	121
3.5.9	Phonon Energies in Bulk Wurtzitic Semi-conductors	125
3.5.10	Phonons in Strained Wurtzitic Semi-conductors . . .	126
3.5.11	Interaction of Phonons with Plasmons in Doped Wurtzitic Semi-conductors.	127
	References	128

4	Optical Properties of Wurtzitic Semiconductors and Epilayers . . .	131
4.1	Pioneering Reflectivity Experiments on Cadmium Sulfite . . .	131
4.1.1	The Valence Band Ordering in CdS	131
4.1.2	Excitons and Polaritons in CdS	134
4.2	Optical Reflectivity in Gallium Nitride	141
4.2.1	The Pioneering Work	141
4.2.2	Strain-Fields in (0001) Epilayers	141
4.2.3	Longitudinal-Transverse Splitting and Exciton-Polaritons in GaN	144
4.2.4	Excitons in GaN Epilayers Grown with Strain on M-plane or A-plane Orientations	144
4.3	Aluminum Nitride	149
4.3.1	Optical Properties of Bulk Aluminum Nitride	149
4.3.2	Strain-Fields in Aluminum Nitride Epilayers	150
4.3.3	Excitons and Polaritons in AlN	150
4.4	Zinc Oxide	150
4.4.1	Optical Properties of Bulk Zinc Oxide	150
4.4.2	Optical Properties of Zinc Oxide Heteroepitaxies	151
4.4.3	Polaritons in ZnO	154
4.5	Indium Nitride	154
4.6	Excitonic Binding Energies in Wurtzitic Materials: The Influence of Anisotropies	154
4.6.1	General Description in the Framework of the Effective Mass Approximation	154
4.6.2	Wave Functions	156
4.6.3	Numerical Values for Wurtzitic Semiconductors	157
4.7	Influence of Temperature	157
4.7.1	Bulk Materials	157
4.7.2	Reduction of the Band Gap of Bulk Materials When Increasing Temperature	159
4.7.3	Epilayers	159
4.8	Photoluminescence of Wurtzitic Semiconductors	160
4.8.1	Classical Description of the Photoluminescence Process for Free Excitons and Free Carriers	160
4.8.2	Photoluminescence of Bound Excitons and Other Extrinsic Recombination Processes	163
4.8.3	High Resolution Spectroscopy in Wurtzite Semiconductors: The GaN Case	168
4.9	Semiconductor Alloys	171
4.10	Photonics in High Quality Thin Films	174
	References	178

5 Optical Properties of Quantum Wells and Superlattices 181

5.1 Basic Theoretical Concepts Borrowed from Quantum Mechanics Text Books 181

5.1.1 Square Quantum Wells and One-Band Envelope Functions 181

5.1.2 Strained Layers, Quantum-Confined Stark Effect and One-Band Envelope Functions 188

5.1.3 Exciton Binding Energy in Quantum Wells 193

5.1.4 Effects of High Photo Injection Densities in Quantum Wells 196

5.2 Optical Properties of Polar Quantum Wells 198

5.2.1 GaN–AlGaN Polar Quantum Wells 199

5.2.2 ZnO–ZnMgO Polar Quantum Wells 208

5.2.3 GaInN-Based Polar Quantum Wells 211

5.3 Temperature: Dependent Photoluminescence Spectroscopy 214

5.4 Time-Resolved Photoluminescence 223

5.5 Optical Properties of Non Polar Quantum Wells 233

5.6 Optical Properties of Semipolar Quantum Wells 238

5.7 Optical Properties of Quantum Dots 243

5.7.1 Optical Properties of Polar Quantum Dots 246

References 255

Index 261