

Contents

Preface XV

List of Contributors XVII

Part 1 **Material Properties** 1

1 **Introduction** 3

Joachim Piprek

- 1.1 A Brief History 3
- 1.2 Unique Material Properties 4
- 1.3 Thermal Parameters 5
- References 10

2 **Electron Bandstructure Parameters** 13

Igor Vurgaftman and Jerry R. Meyer

- 2.1 Introduction 13
- 2.2 Band Structure Models 14
- 2.3 Band Parameters 17
 - 2.3.1 GaN 19
 - 2.3.2 AlN 25
 - 2.3.3 InN 28
 - 2.3.4 AlGa_N 30
 - 2.3.5 InGa_N 32
 - 2.3.6 InAlN 34
 - 2.3.7 AlGaIn_N 34
 - 2.3.8 Band Offsets 35
- 2.4 Conclusions 36
- References 37

3	Spontaneous and Piezoelectric Polarization: Basic Theory vs. Practical Recipes	49
	<i>Fabio Bernardini</i>	
3.1	Why Spontaneous Polarization in III-V Nitrides?	49
3.2	Theoretical Prediction of Polarization Properties in AlN, GaN and InN	51
3.3	Piezoelectric and Pyroelectric Effects in III-V Nitrides Nanostructures	54
3.4	Polarization Properties in Ternary and Quaternary Alloys	58
3.5	Orientalional Dependence of Polarization	64
	References	67
4	Transport Parameters for Electrons and Holes	69
	<i>Enrico Bellotti and Francesco Bertazzi</i>	
4.1	Introduction	69
4.2	Numerical Simulation Model	70
4.2.1	Scattering in the Semi-Classical Boltzmann Equation	72
4.3	Analytical Models for the Transport Parameters	76
4.4	GaN Transport Parameters	79
4.4.1	Electron Transport Coefficients	79
4.4.2	Hole Transport Coefficients	81
4.5	AlN Transport Parameters	84
4.5.1	Electron Transport Coefficients	84
4.5.2	Hole Transport Coefficients	86
4.6	InN Transport Parameters	87
4.6.1	Electron Transport Coefficients	88
4.6.2	Hole Transport Coefficients	89
4.7	Conclusions	91
	References	91
5	Optical Constants of Bulk Nitrides	95
	<i>Rüdiger Goldhahn, Carsten Buchheim, Pascal Schley, Andreas Theo Winzer, and Hans Wenzel</i>	
5.1	Introduction	95
5.2	Dielectric Function and Band Structure	95
5.2.1	Fundamental Relations	95
5.2.2	Valence Band Ordering, Optical Selection Rules and Anisotropy	97
5.3	Experimental Results	99
5.3.1	InN	99
5.3.2	GaN and AlN	102
5.3.3	AlGaN Alloys	105
5.3.4	In-rich InGaN and InAlN Alloys	107

5.4	Modeling of the Dielectric Function	108
5.4.1	Analytical Representation of the Dielectric Function	109
5.4.2	Calculation of the Dielectric Function for Alloys	111
5.4.3	Influence of Electric Fields on the Dielectric Function	112
	References	114
6	Intersubband Absorption in AlGaIn/GaN Quantum Wells	117
	<i>Sulakshana Gunna, Francesco Bertazzi, Roberto Paiella, and Enrico Bellotti</i>	
6.1	Introduction	117
6.2	Theoretical Model	118
6.2.1	Spontaneous and Piezoelectric Polarization	122
6.3	Numerical Implementation	123
6.3.1	Achieving Self-consistency: The Under-Relaxation Method	127
6.3.2	Predictor–Corrector Approach	128
6.4	Absorption Energy in AlGaIn-GaN MQWs	129
6.4.1	Numerical Analysis of Periodic AlGaIn-GaN MQWs	130
6.4.2	Numerical Analysis of Non-periodic AlGaIn-GaN MQWs and Comparison with Experimental Results	138
6.5	Conclusions	141
	References	142
7	Interband Transitions in InGaIn Quantum Wells	145
	<i>Jörg Hader, Jerome V. Moloney, Angela Thränhardt, and Stephan W. Koch</i>	
7.1	Introduction	145
7.2	Theory	146
7.2.1	Bandstructure and Wavefunctions	146
7.2.2	Semiconductor Bloch Equations	149
7.2.3	Semiconductor Luminescence Equations	151
7.2.4	Auger Recombination Processes	152
7.3	Theory–Experiment Gain Comparison	154
7.4	Absorption/Gain	156
7.4.1	General Trends	156
7.4.2	Structural Dependence	159
7.5	Spontaneous Emission	161
7.6	Auger Recombinations	164
7.7	Internal Field Effects	164
7.8	Summary	166
	References	167

8	Electronic and Optical Properties of GaN-based Quantum Wells with (10$\bar{1}$0) Crystal Orientation	169
	<i>Seoung-Hwan Park and Shun-Lien Chuang</i>	
8.1	Introduction	169
8.2	Theory	170
8.2.1	Non-Markovian gain model with many-body effects	175
8.3	Results and Discussion	177
8.4	Summary	188
	References	189
9	Carrier Scattering in Quantum-Dot Systems	191
	<i>Frank Jahnke</i>	
9.1	Introduction	191
9.2	Scattering Due to Carrier–Carrier Coulomb Interaction	193
9.2.1	Formulation of the Problem and Previous Developments	193
9.2.2	Kinetic Equation and Scattering Rates	195
9.2.3	Results for Carrier–Carrier Scattering	198
9.3	Scattering Due to Carrier–Phonon Interaction	200
9.3.1	Perturbation Theory Versus Polaron Picture	200
9.3.2	Polaron States and Kinetics	202
9.3.3	Results for Carrier Scattering Due to LO-phonons	204
9.4	Summary and Outlook	207
	References	208
Part 2	Devices	211
10	AlGaIn/GaN High Electron Mobility Transistors	213
	<i>Tomás Palacios and Umesh K. Mishra</i>	
10.1	Introduction	213
10.2	Physics-based Simulations	216
10.2.1	Basic Material Properties	217
10.2.2	Polarization	218
10.2.3	Surface States	222
10.2.4	Electron Mobility	224
10.2.5	Breakdown Voltage	227
10.2.6	Energy Balance Models	228
10.3	Conclusions	230
	References	231
11	Intersubband Optical Switches for Optical Communications	235
	<i>Nobuo Suzuki</i>	
11.1	Introduction	235

11.2	Physics of ISBT in Nitride MQWs	236
11.2.1	Dipole Moment	236
11.2.2	Rate Equations	236
11.2.3	Absorption	238
11.2.4	Relaxation Time	239
11.2.5	Dephasing Time and Spectral Linewidth	240
11.3	Calculation of Absorption Spectra	242
11.3.1	Transition Wavelength and Built-In Field	242
11.3.2	Absorption Spectra	243
11.4	FDTD Simulator for GaN/AlGaN ISBT Switches	244
11.4.1	Model	245
11.4.2	Saturation of Absorption	246
11.4.3	Temporal Response	248
11.4.4	Future Applications	249
	References	251
12	Intersubband Electroabsorption Modulator	253
	<i>Petter Holmström</i>	
12.1	Introduction	253
12.2	Modulator Structure	256
12.2.1	Multiple-Quantum-Well Structure	256
12.2.2	Waveguide and Contacting	259
12.3	Model	261
12.3.1	Conduction Band Potential and Active Layer Biasing	261
12.3.2	Intersubband Transitions	263
12.3.3	Optical Mode and the Plasma Effect	265
12.4	Results	266
12.4.1	Electroabsorption	266
12.4.2	Chirp Parameter	269
12.4.3	Electrical Properties	270
12.4.4	Figure of Merit	271
12.4.5	Absorption Saturation	272
12.4.6	Thermal Properties and Current	273
12.4.7	Significance of the Linewidth	275
12.5	Summary	276
	References	276
13	Ultraviolet Light-Emitting Diodes	279
	<i>Yen-Kuang Kuo, Sheng-Hong Yen, and Jun-Rong Chen</i>	
13.1	Introduction	279
13.2	Device Structure	281
13.3	Physical Models and Parameters	282

13.3.1	Band Structure	283
13.3.2	Polarization Effects	285
13.3.3	Carrier Transport Model	287
13.3.4	Thermal Model	288
13.3.5	Spontaneous Emission	288
13.3.6	Ray Tracing	290
13.4	Comparison Between Simulated and Experimental Results	291
13.5	Performance Optimization	293
13.5.1	Optimal Aluminum Composition in p-AlGaN Electron Blocking Layer	293
13.5.2	Optimal Number of Quantum Wells	294
13.5.3	Lattice-matched AlInGaN Electron Blocking Layer	296
13.6	Conclusion	299
	References	300
14	Visible Light-Emitting Diodes	303
	<i>Sergey Yu. Karpov</i>	
14.1	Introduction	303
14.2	Simulation Approach and Materials Properties	304
14.3	Device Analysis	309
14.3.1	Band Diagrams, Carrier Concentrations, and Partial Currents	310
14.3.2	Internal Quantum Efficiency and Carrier Leakage	312
14.3.3	Emission Spectra	315
14.3.4	Polarity Effects	317
14.4	Novel LED Structures	320
14.4.1	LED with Indium-free Active Region	320
14.4.2	Hybrid ZnO/AlGaN LED	321
14.5	Conclusion	323
	References	324
15	Simulation of LEDs with Phosphorescent Media for the Generation of White Light	327
	<i>Norbert Linder, Dominik Eisert, Frank Jermann, and Dirk Berben</i>	
15.1	Introduction	327
15.2	Requirements for a Conversion LED Model	328
15.3	Color Metrics for Conversion LEDs	330
15.4	Phosphor Model	332
15.4.1	Phosphor Materials	332
15.4.2	Luminescence and Absorption of Phosphor Particles	334
15.4.3	Scattering of Phosphor Particles	335
15.4.4	Determination of Material Parameters	341
15.4.5	LED Ray Tracing Model	344

15.5	Simulation Examples	346
15.6	Conclusions	350
	References	350
16	Fundamental Characteristics of Edge-Emitting Lasers	353
	<i>Gen-ichi Hatakoshi</i>	
16.1	Introduction	353
16.2	Basic Equations for the Device Simulation	354
16.2.1	Electrical and Optical Simulation	354
16.2.2	Simulation Model for Thermal Analysis	357
16.3	Simulation for Electrical Characteristics and Carrier Overflow Analysis	359
16.4	Perpendicular Transverse Mode and Beam Quality Analysis	366
16.5	Thermal Analysis	370
16.6	Conclusions	378
	References	378
17	Resonant Internal Transverse-Mode Coupling in InGaN/GaN/AlGaIn Lasers	381
	<i>Gennady A. Smolyakov and Marek Osiński</i>	
17.1	Introduction	381
17.2	Internal Mode Coupling and the Concept of “Ghost Modes”	382
17.3	Device Structure and Material Parameters	384
17.4	Calculation Technique	385
17.5	Results of Calculations	386
17.5.1	Resonant Conditions	386
17.5.2	Spatial Characteristics of Laser Emission under the Resonant Internal Mode Coupling	391
17.5.3	Spectral Effects of the Resonant Internal Mode Coupling	394
17.5.4	Carrier-Induced Resonant Internal Mode Coupling	396
17.6	Discussion and Conclusions	399
	References	401
18	Optical Properties of Edge-Emitting Lasers: Measurement and Simulation	405
	<i>Ulrich T. Schwarz and Bernd Witzigmann</i>	
18.1	Introduction	405
18.2	Waveguide Mode Stability	406
18.3	Optical Waveguide Loss	412
18.4	Mode Gain Analysis	417
18.5	Conclusion	420
	References	422

19	Electronic Properties of InGaN/GaN Vertical-Cavity Lasers	423
	<i>Joachim Piprek, Zhan-Ming Li, Robert Farrell, Steven P. DenBaars, and Shuji Nakamura</i>	
19.1	Introduction to Vertical-Cavity Lasers	423
19.2	GaN-based VCSEL Structure	424
19.3	Theoretical Models and Material Parameters	425
19.3.1	Carrier Transport	426
19.3.2	Electron Band Structure	429
19.3.3	Built-In Polarization	432
19.3.4	Photon Generation in the Quantum Wells	434
19.3.5	Optical Mode	436
19.4	Simulation Results and Device Analysis	437
19.4.1	Current Confinement	438
19.4.2	Polarization Effects	438
19.4.3	Threshold Current	440
19.4.4	AlGaIn Doping	442
19.4.5	AlGaIn Composition	443
19.5	Summary	443
	References	443
20	Optical Design of Vertical-Cavity Lasers	447
	<i>Włodzimierz Nakwaski, Tomasz Czystanowski, and Robert P. Sarzała</i>	
20.1	Introduction	447
20.2	The GaN VCSEL Structure	449
20.3	The Scalar Optical Approach	453
20.4	The Vectorial Optical Approach	454
20.5	The Self-consistent Calculation Algorithm	458
20.6	Simulation Results	460
20.7	Discussion and Conclusions	464
	References	465
21	GaN Nanowire Lasers	467
	<i>Alexey V. Maslov and Cun-Zheng Ning</i>	
21.1	Introduction	467
21.2	Nanowire Growth and Characterization	469
21.3	Nanowire Laser Principles	470
21.4	Anisotropy of Material Gain	471
21.5	Guided Modes	475
21.5.1	Guided Modes, Dispersions, and Mode Spacing	476
21.5.2	Reflection from Facets	479
21.5.3	Far-field Pattern	481
21.5.4	Confinement Factors for Anisotropic Nanowires	483

21.5.5	Spontaneous Emission Factors	486
21.6	Modal Gain and Threshold	488
21.7	Conclusion	489
	References	490
	Index	493

