

# Contents

<b>Theoretical Approach to Polarization Effects in Semiconductors</b> . . . . .	1
Piotr Boguslawski and J. Bernholc	
1 Introduction . . . . .	1
2 Basic Electrostatics . . . . .	2
3 Polarization . . . . .	4
4 <i>Ab Initio</i> Calculations of the Electronic Structure . . . . .	5
5 Modern Theory of Polarization . . . . .	6
6 Polarization at Interfaces: Interface Dipoles . . . . .	10
6.1 Averaging Microscopic Charges and Field . . . . .	10
6.2 AlAs/GaAs Superlattice . . . . .	11
7 Spontaneous Polarization in the Wurtzite Structure: BeO . . . . .	12
8 GaN/AlN Superlattice: Spontaneous Polarization and Piezoelectricity . . . . .	13
9 Electric Field-Driven Diffusion and Segregation of Dopants in Superlattices . . . . .	16
9.1 Introduction . . . . .	16
9.2 Interfacial Segregation . . . . .	17
9.3 Profile of H in AlN/GaN Superlattice . . . . .	19
10 Summary . . . . .	23
References . . . . .	24
<b>Polarization Induced Effects in GaN-based Heterostructures and Novel Sensors</b> . . . . .	27
O. Ambacher and V. Cimalla	
1 Introduction . . . . .	27
2 First-Principles Prediction of Structural and Pyroelectric Properties	29
3 Lattice Constants, Average Bond Length and Bond Angles in Ternary Compounds . . . . .	30
4 Polarity . . . . .	40
5 Growth of Undoped AlGaN/GaN, InGaN/GaN and AlInN/GaN Hetero- and Nanostructures . . . . .	41

5.1	AlGaN/GaN Heterostructures .....	41
5.2	InGaN/GaN Heterostructures .....	42
5.3	AlInN/GaN Heterostructures .....	42
6	Non-Linear Spontaneous and Piezoelectric Polarization in Group-III-Nitrides .....	42
6.1	Spontaneous Polarization .....	43
6.2	Piezoelectric Polarization .....	45
7	Polarization Induced Surface and Interface Charges .....	56
8	Sheet Carrier Concentration of Polarization Induced 2DEGs .....	61
8.1	2DEGs Confined at Interfaces of Undoped Ga-face AlGaN/GaN Heterostructures .....	63
8.2	2DEGs Confined at Interfaces of Undoped, Ga-face AlInN/GaN Heterostructures .....	65
8.3	2DEGs Confined in InGaN/GaN Single Quantum Wells ..	69
9	Sensors Based on Polarization Induced 2DEGs .....	74
9.1	Overview .....	74
9.2	Surface Sensitive Sensors .....	75
9.3	Mechanical Sensors .....	92
9.4	Sensor for Electromagnetic Fields .....	98
10	Summary .....	100
	References .....	103

### **Lateral and Vertical Charge Transport in Polar Nitride**

	<b>Heterostructures:</b> .....	111
	Yuh-Renn Wu, Madhusudan Singh, and Jasprit Singh	
1	Polar Heterostructures: What Do They Offer? .....	111
1.1	Polar Heterostructures: Undoped Electronics .....	112
1.2	The Applications of Nitrides .....	113
1.3	Transport Issues in Nitride Device .....	115
1.4	Polar Materials: Use in Sensor Technology–Potential of Merging Polar Materials with Semiconductors .....	115
2	Theoretical Approach .....	117
2.1	Polarization by Strain .....	117
2.2	Vertical Junction Transport .....	119
2.3	Lateral Transport in Undoped HEMTs .....	123
2.4	$k \cdot p$ Method for Strained Nitride Quantum Wells and Quantum Dots .....	127
3	Tailoring of Vertical Junctions .....	128
3.1	Gate Leakage Suppression .....	129
3.2	Forming Ohmic Contacts by Using Polarization Effects ..	132
4	Nitride HFETs: Transport Issues .....	134
4.1	Nonlinear Access Resistance and GaN Device Operation	135
4.2	Scaling Issues in Nitride HEMTs .....	139
5	Smart HFETs: Multi-Functional Devices .....	142
5.1	Stress and Strain Calculation .....	145
5.2	Pyroelectricity .....	146

5.3	Strain Sensor FETs: Results .....	147
5.4	Thermal Sensor FETs .....	150
5.5	Effects of Defects .....	152
6	Conclusions .....	154
	References .....	154
<b>Polarization Effects on Low-Field Transport &amp; Mobility in III-V Nitride HEMTs</b> .....		
161		
Debdeep Jena		
1	Introduction .....	161
2	Polarization-Induced 2DEGs in AlGaIn/GaN HEMTs .....	163
2.1	Polarization Effects on Charge Transport and Scattering .	163
2.2	Charge Control .....	164
2.3	Survey of Experimental 2DEG Mobility Data .....	169
2.4	Theoretical Tools to Address AlGaIn/GaN 2DEG Mobilities .....	171
3	Scattering Mechanisms .....	171
3.1	Typical AlGaIn/GaN 2DEG Structures .....	171
3.2	Traditional Scattering Mechanisms .....	172
3.3	Novel Scattering Mechanisms in AlGaIn/GaN 2DEGs ...	182
4	Using Theory to Explain Experimental Data .....	194
5	Summary and Conclusions .....	198
6	Appendix on the Theory of Low-Field Transport & Mobility .....	198
6.1	The Boltzmann Transport Equation .....	199
6.2	Mobility-Basic Theory .....	203
6.3	Statistics for Two- and Three-Dimensional Carriers .....	206
6.4	Screening by Two- and Three-Dimensional Carriers .....	207
6.5	Mobility of 2DEGs .....	208
6.6	Material Properties of III-V Nitrides Relevant to Transport .....	211
	References .....	214
<b>Local Polarization Effects in Nitride Heterostructures and Devices</b> .....		
217		
E. T. Yu and P. M. Asbeck		
1	Introduction .....	217
1.1	Basic Physics of Polarization Effects .....	217
1.2	Experimental Determination of Polarization Charge Densities .....	219
1.3	Consequences for Heterostructures, Defects, and Devices	224
2	Polarization-Based Engineering of Nitride Heterostructures .....	225
2.1	Enhancement of Schottky Barrier Height in HFET Structures .....	229
2.2	Polarization-Based Energy Barrier Engineering .....	230
2.3	Residual Stress and Piezoelectric Effects in GaN HFETs .	235
2.4	Polarization Effects in Nitride-Based HBTs and p-Type Structures .....	238

3	Localized Effects of Polarization .....	243
3.1	Dislocation-induced Polarization Fields .....	244
3.2	Scanning Capacitance Microscopy .....	245
3.3	Threshold Voltage Variations in AlGaIn/GaN HEMT Structures .....	246
3.4	Nanoscale Electronic Structure in InGaIn/GaN Quantum Wells .....	251
	References .....	260
<b>Polarization in Wide Bandgap Semiconductors and their Characterization by Scanning Probe Microscopy .....</b>		
Goutam Koley, MVS Chandrashekhar, Christopher I. Thomas, Michael G. Spencer		
1	Introduction .....	265
1.1	Polarization in III-N .....	266
1.2	Polarization in Silicon Carbide .....	268
2	III-N and SiC Heterostructures .....	269
2.1	III-N Based Heterostructures .....	269
2.2	SiC Based Heteropolytype Structures .....	271
3	Interface and Surface Charge in SiC and III-N Heterojunctions ...	274
3.1	Charges at the Interface and Surface .....	274
3.2	Surface States and Their Significance .....	284
4	SPM Characterization of Heterostructures .....	285
4.1	Basics of Kelvin Probe Microscopy .....	286
4.2	Characterization of Charge Instability .....	287
4.3	Surface States Characterization and Passivation .....	299
5	Summary .....	302
	References .....	303
<b>Functionally Graded Polar Heterostructures: New Materials for Multifunctional Devices .....</b>		
Debdeep Jena, S. Pamir Alpay, and Joseph V. Mantese		
1	Introduction .....	307
2	Graded Polar Nitride Semiconductor Heterostructures .....	308
2.1	Polarization in Nitrides: A Tutorial .....	308
2.2	Electrostatics and Dipole-Engineering .....	321
2.3	Epitaxial Growth and Structural Properties .....	324
2.4	Electronic Properties .....	326
2.5	Transport Properties of Polarization-induced 3D Electron Slabs .....	328
2.6	Quantum Magnetotransport Properties .....	333
2.7	Device Applications of Polarization-‘Doped’ Graded Nitride Layers .....	340
3	Universal Physics of Functionally Graded Ferroelectric and Ferromagnetic Alloys .....	345

3.1	Order Parameters in Ferroic (Ferroelectric, Ferromagnetic, & Ferroelastic) Materials . . . . .	345
3.2	Functionally Graded Electrets and Magnets . . . . .	352
3.3	Functionally Graded Ferromagnets . . . . .	366
4	Summary and Challenges . . . . .	368
	References . . . . .	368
<b>Polarization in GaN Based Heterostructures and Heterojunction Field Effect Transistors (HFETs) . . . . . 373</b>		
Hadis Morkoç and Jacob Leach		
	Introduction . . . . .	373
1	Heterojunction Field Effect Transistors (HFETs) . . . . .	376
1.1	Polarization Issues as Pertained to HFETs . . . . .	379
1.2	Analytical Description of HFETs . . . . .	397
1.3	Numerical Modeling of Sheet Charge and Current . . . . .	409
1.4	Calculated I-V Characteristics . . . . .	418
1.5	Experimental Considerations . . . . .	419
2	AlGaIn/GaN HFET Performance . . . . .	424
2.1	Evolution of GaN FET Performance . . . . .	430
2.2	Drain Voltage and Drain Breakdown Mechanisms . . . . .	442
2.3	Anomalies in GaN MESFETs and AlGaIn/GaN HFETs . . . . .	453
	References . . . . .	457
<b>Effects of Polarization in Optoelectronic Quantum Structures . . . . . 467</b>		
Raphaël Butté and Nicolas Grandjean		
1	Introduction . . . . .	467
2	Basic Elements of the Theory of Polarization in III-V Nitride Heterostructures . . . . .	468
2.1	The Wurtzite Structure . . . . .	469
2.2	Strain and Internal Electric Field in III-Nitride Heterostructures . . . . .	470
2.3	Effects of Polarization Fields on Optical Properties of III-V Nitride Quantum Heterostructures . . . . .	484
3	Experimental Manifestation of Polarization Fields in Group-III Nitride Based Nanostructures . . . . .	494
3.1	Experimental Evidence of Polarization Fields . . . . .	494
3.2	Polarization Field Measurement . . . . .	496
3.3	Optical Properties of GaN/AlGaIn Quantum Wells . . . . .	498
3.4	Optical Properties of GaN/AlN Quantum Dots . . . . .	502
3.5	InGaIn/GaN Quantum Wells: The Heart of Nitride Based Optoelectronic Devices . . . . .	504
4	Conclusion . . . . .	506
	References . . . . .	507
<b>Index . . . . . 513</b>		