

Contents

1	Introduction	1
	C. Klingshirn	
1.1	History of ZnO Research and Contents of This Book	2
1.2	Aim of This Review	4
	References	5
2	Crystal Structure, Chemical Binding, and Lattice Properties	7
	J. Geurts	
2.1	Crystal Structure and Chemical Binding	8
2.1.1	ZnO Polytype Structures	8
2.1.2	Phase Transitions	10
2.1.3	Crystal Axis Polarity	10
2.2	Thermal Properties	11
2.2.1	Thermal Expansion Coefficients	11
2.2.2	Specific Heat	12
2.2.3	Thermal Conductivity	13
2.3	The Piezoelectric Effect	14
2.3.1	Principle and Applications	14
2.3.2	The Piezoelectric Tensor	15
2.4	Lattice Dynamics	16
2.4.1	Phonon Symmetry and Eigenvectors of the Wurtzite Lattice	17
2.4.2	Phonon Dispersion Relations	18
2.4.3	Infrared Optical Phonon Spectroscopy	21
2.4.4	Raman Spectroscopy of Phonon Modes	23
2.4.5	Vibration Modes in Doped ZnO	26
2.4.6	Incorporation of Transition Metal Atoms in ZnO	28
2.4.7	Raman Scattering from ZnO Nanoparticles	30
2.5	Phonon–Plasmon Mixed States	31
2.5.1	Collective Charge-Carrier Oscillations	32
2.5.2	Coupling to Polar Longitudinal Phonons	33
	References	35

3	Growth	39
	Andreas Waag	
3.1	Bulk Growth	40
3.1.1	Vapor Phase Transport	40
3.1.2	Solvothermal Growth	41
3.2	Epitaxial Growth Techniques	42
3.2.1	Metal Organic Chemical Vapor Deposition	46
3.2.2	Molecular Beam Epitaxy	53
3.2.3	Pulsed Laser Deposition	65
3.3	Growth of Self-Organized Nanostructures	66
3.3.1	Growth Techniques for Nano Pillars	67
3.3.2	Properties of Nanopillars	67
	References	73
4	Band Structure	77
	B.K. Meyer	
4.1	The Ordering of the Bands at the Valence Band Maximum in ZnO .	77
4.2	ZnO and Its Alloys	84
4.2.1	Cationic Substitution: Mg, Cd, Be in ZnO	85
4.2.2	Anionic Substitution: S, Se in ZnO	89
4.3	Valence and Conduction Band Discontinuities	91
4.3.1	Iso-Valent Hetero-Structures	91
4.3.2	Hetero-Valent Hetero-Structures	92
	References	93
5	Electrical Conductivity and Doping	95
	Andreas Waag	
5.1	Introduction	95
5.2	Hydrogen in ZnO	97
5.3	Donors in ZnO: Al, Ga, In	98
5.4	Acceptors in ZnO	99
5.5	Mobility	104
5.6	Ohmic and Schottky Contacts on ZnO	105
5.7	Two-Dimensional Electron Gas and Quantum Hall Effect	108
5.8	High-Field Transport and Varistors	110
5.9	Photoconductivity	114
	References	117
6	Intrinsic Linear Optical Properties Close to the Fundamental Absorption Edge	121
	C. Klingshirn	
6.1	Free Excitons in Bulk Samples	121
6.1.1	Free Excitons in Bulk Samples, Epitaxial Layers, and NanoRods	125
6.1.2	Experimental Observations	129
6.2	ZnO-Based Alloys	145

6.3	Surface Exciton Polaritons	150
6.4	Excitons in Structures of Reduced Dimensionality	153
6.4.1	Excitons in Quantum Wells and Superlattices	153
6.4.2	Quantum Wires	155
6.4.3	Quantum Dots	158
6.4.4	Cavity Polaritons	162
	References	163
7	Bound Exciton Complexes	169
	B.K. Meyer	
7.1	ZnO Luminescence: An Overview	169
7.2	Neutral Donor Bound Excitons (A-Valence Band) and Their Two Electron Satellites	172
7.3	Ionized Donor Bound Excitons (A-Valence Band)	177
7.4	A Comparison of the Localization Energies with Theoretical Predictions (the Haynes Rule)	180
7.5	Excited State Properties of the Bound Excitons	183
7.6	Donor–Acceptor Pair Transitions	189
	References	197
8	Influence of External Fields	201
	M.R. Wagner and A. Hoffmann	
8.1	Excitons in Magnetic Fields	201
8.1.1	Zeeman Effect	202
8.1.2	Free and Bound Excitons	203
8.1.3	Selection Rules for Zeeman Splitting of Exciton States in Magnetic Fields	212
8.1.4	Symmetry of Exciton Hole States	213
8.2	Excitons in Strain Fields	215
8.2.1	Uniaxial Pressure	217
8.2.2	Hydrostatic Pressure	219
8.2.3	Biaxial In-Plane Strain	225
	References	229
9	Deep Centres in ZnO	233
	A. Hoffmann, E. Malguth, and B.K. Meyer	
9.1	The Green and Yellow Emission Bands	233
9.2	Transition Metal Ions	239
9.2.1	ZnO/V	241
9.2.2	ZnO/Fe	244
9.2.3	ZnO/Fe ³⁺	245
9.2.4	ZnO/Fe ²⁺	249
9.2.5	ZnO/Co	253
9.2.6	ZnO/Ni	254
9.2.7	ZnO/Cu	258
9.3	Outlook	264
	References	264

10	Magnetic Properties	267
	Andreas Waag	
10.1	General Overview of the Topic	267
10.2	Short Overview of the Situation in ZnO	269
	References	272
11	Nonlinear Optics, High Density Effects and Stimulated Emission	275
	C. Klingshirn	
11.1	Nonlinear Optics	275
11.2	High Excitation Effects	277
11.2.1	The Intermediate Density Regime	277
11.2.2	Electron–Hole Plasma	282
11.3	Processes for Stimulated Emission	285
11.3.1	Bulk Samples and Epilayers	286
11.3.2	Quantum Wells and Superlattices	293
11.3.3	Nano Rods and Their Cavity Modes	294
11.3.4	Quantum Dots and Random Lasing	296
11.3.5	Cavity Modes, Photonic Crystals and Polariton Lasers	299
	References	302
12	Dynamic Processes	307
	C. Klingshirn	
12.1	Dephasing Dynamics	308
12.2	Relaxation Dynamics	311
12.3	Recombination Dynamics	314
	References	320
13	Past, Present and Future Applications	325
	C. Klingshirn	
13.1	Past Applications	325
13.1.1	The Electro Fax Copy	325
13.1.2	Ferrite Properties	326
13.2	Present and Emerging Applications	326
13.2.1	Cement, Rubber, Paint and Glazes	326
13.2.2	Catalysts, Pharmaceuticals, Cosmetics and Food Additives	327
13.2.3	Electronics	327
13.2.4	Gas Sensors	330
13.2.5	TCO, Solar Cells and Some Further Applications	331
13.3	Visions of Future Applications	332
13.3.1	pn Junctions	333
13.3.2	Light Emitting Diodes	334
13.3.3	Field Emitters	338
13.3.4	Spintronics	338
	References	339

14 Conclusion and Outlook347
C. Klingshirn
14.1 Conclusions347
14.2 Outlook348
References349

Index351