

Contents

1. Introduction.....	1
1.1 Metal–Semiconductor Contacts.....	1
1.1.1 Rectification of Metal–Semiconductor Contacts.....	1
1.1.2 Explanation of Rectification by Depletion Layers.....	4
1.1.3 Metal-Induced Gap States.....	7
1.1.4 Rules, Correlations, and Models.....	9
1.1.5 MIGS-and-Electronegativity Theory.....	14
1.2 Semiconductor Heterostructures and the IFIGS Concept.....	18
2. Depletion Layer.....	21
2.1 The Schottky Barrier.....	21
2.2 Capacitance of Schottky Barriers.....	25
2.3 Image-Force or Schottky Effect.....	27
3. Determination of Barrier Heights and Offsets.....	33
3.1 Current Transport across Schottky Contacts.....	33
3.2 Effective Barrier Height of Ideal Schottky Contacts.....	38
3.3 Effective Richardson Constant.....	39
3.4 <i>I/V</i> Characteristics of Real Schottky Contacts.....	42
3.5 Barrier Heights of Real Schottky Contacts 1: <i>I/V</i> Characteristics.....	47
3.6 Ballistic-Electron-Emission Microscopy.....	57
3.7 Barrier Heights of Real Schottky Contacts 2: BEEM $I_{\text{coll}}/V_{\text{tip}}$ Characteristics.....	61
3.8 Barrier Heights of Real Schottky Contacts 3: Internal Photoemission Yield Spectroscopy.....	63
3.9 Core-Level Photoemission Spectroscopy.....	67
3.9.1 Chemical Shifts and Interface Band-Bending Determination by PES.....	67
3.9.2 Growth Modes of Metals on Semiconductors.....	70
3.10 Barrier Heights of Real Schottky Diodes 4: XPS.....	74
3.11 Metal-Induced Core-Level Shifts and the Intrinsic Interface Electric-Dipole Layer.....	75
3.12 Determination of Band Offsets at Heterostructures.....	79
3.12.1 Internal Photoemission Yield Spectroscopy.....	79
3.12.2 Core-Level X-Ray Photoemission Spectroscopy.....	81

4. Laterally Inhomogeneous Schottky Contacts	83
4.1 Potential Distribution.....	83
4.2 Current Transport in Schottky Contacts with One Circular Patch.....	91
4.3 Current Transport in Schottky Contacts with Many Circular Patches.....	93
4.4 Test of the Patch Concept with Modified Contacts.....	97
4.5 <i>I/V</i> and BEEM Test of the Patch Concept.....	98
4.6 Origin of Lateral Barrier-Height Inhomogeneities.....	103
4.6.1 Natural or Intrinsic Nonuniformities.....	103
4.6.2 Extrinsic Nonuniformities.....	104
5. The IFIGS-and-Electronegativity Theory	107
5.1 Band-Structure Lineup and Electronegativity: A Chemical Approach.....	107
5.1.1 Barrier Heights of Schottky Contacts.....	107
5.1.2 Interface Dipoles at Semiconductor Heterostructures.....	109
5.2 Barrier Heights and Interface Dipoles: A Phenomenological Approach.....	111
5.3 Interface-Induced Gap States.....	115
5.3.1 Metal-Induced Gap States.....	115
5.3.2 Semiconductor Heterostructures.....	118
5.3.3 Valence-Band Offsets at Semiconductor Heterostructures...	119
5.4 Virtual Gap States: One-Dimensional Model.....	119
5.5 Virtual Gap States: Three-Dimensional Model.....	122
5.5.1 Mean-Value k -Points and the Dielectric Band Gap.....	122
5.5.2 Branch-Point Energy in the ViGS Continuum.....	125
5.5.3 Decay Length of the ViGS at their Branch Point.....	129
5.6 Slope Parameter of Barrier Heights.....	131
6. The MIGS-and-Electronegativity Concept: Experiment and Theory ...	135
6.1 Schottky Contacts.....	135
6.1.1 Introductory Remarks.....	135
6.1.2 Silicon Schottky contacts.....	136
6.1.3 GaAs Schottky Contacts.....	139
6.1.4 GaP Schottky Contacts.....	140
6.1.5 GaN Schottky Contacts.....	141
6.1.6 SiC Schottky Contacts.....	142
6.1.7 ZnSe Schottky Contacts.....	146
6.1.8 Schottky Contacts on Layered Ga-Chalcogenides.....	146
6.1.9 CuInSe ₂ Schottky Contacts.....	148
6.1.10 Schottky Contacts on Ternary III-V Alloys.....	149
6.1.11 Metal-Insulator Contacts.....	155
6.1.12 Direct Observations of MIGS.....	159
6.2 Heterostructures.....	160
6.2.1 Introductory Remarks.....	160
6.2.2 Non-Polar Heterostructures.....	162

6.2.3	Lattice-Matched Ternary and Quaternary III–V Alloys.....	163
6.2.4	I–III–VI ₂ Chalcopyrites.....	168
6.2.5	Layered Semiconductors.....	170
6.2.6	Metamorphic Heterostructures.....	172
6.2.7	Semiconductor–Insulator Interfaces.....	173
6.2.8	<i>Langer–Heinrich</i> Rule.....	176
7.	First-Principles Calculations of Barrier Heights and Valence-Band Offsets.....	181
7.1	Introductory Remarks.....	181
7.2	Schottky Barrier Heights.....	181
7.3	Valence-Band Offsets at Heterostructures.....	186
7.3.1	Isovalent and Lattice-Matched AlGaAs/GaAs.....	186
7.3.2	SiC Heterostructures.....	187
8.	Temperature and Pressure Effects.....	189
8.1	Temperature Effects.....	189
8.2	Pressure Effects.....	193
8.2.1	Schottky Barrier Heights.....	193
8.2.2	Valence-Band Offsets.....	196
8.3	Pseudomorphic Heterostructures.....	197
9.	Barrier Heights and Extrinsic Interface Defects.....	203
9.1	Defect-Induced Changes of Barrier Heights.....	203
9.2	Application to <i>p</i> -GaP(110) Schottky Contacts.....	206
9.3	Unified Defect Model.....	208
10.	Extrinsic Interface Dipoles.....	209
10.1	Interface Doping of Schottky Contacts.....	209
10.2	Interface Structure.....	214
10.2.1	Metal/Si(111)-(7×7) ⁱ Contacts.....	214
10.2.2	Epitaxial Silicide/Silicon Interfaces.....	217
10.2.3	Polar Heterostructures.....	224
11.	Ohmic Contacts.....	227
	Appendix.....	231
	References.....	235
	Subject Index.....	257