

Contents

Preface	vii
-------------------	-----

Chapter 1 (R.H. Williams)

Surface science and electronic materials. An overview	1
1. Introduction	1
2. Semiconductor surfaces and interfaces	3
2.1 Surface states and space charge layers	3
2.2 Clean semiconductor surfaces	5
2.3 Normal semiconductor surfaces	12
3. Metal–semiconductor interfaces	15
3.1 Schottky barriers on semiconductors	16
3.2 Ohmic contacts	21
3.3 Metals on oxidised semiconductor surfaces	23
4. Semiconductor–semiconductor interfaces	24
4.1 Crystal growth	26
4.2 Band discontinuities	29
4.3 Insulators on semiconductors	31
References	33

Chapter 2 (M. Schluter)

Structural and electronic properties of elemental semiconductors and surfaces	37
1. Introduction	37
2. Bonding and electronic states in bulk silicon	38
3. The atomic geometry of the Si(100) (2×1) surface	43
4. The atomic geometry of the cleaved Si(111) (2×1) surface.	48
5. The atomic geometry of the equilibrium Si(111) (7×7) surface.	54
6. The “new” reconstructions	61
Acknowledgements	63
References	64

Chapter 3 (C.B. Duke)

Atomic geometry and electronic structure of tetrahedrally coordinated compound semiconductor interfaces.	69
1. Introduction	69
2. Zincblende(110)	71
2.1 Nomenclature and background	71
2.2 Structural chemistry	74
2.3 Theory.	75
2.4 GaAs	80
2.5 Other binary semiconductors	88
3. Adsorbate structures on zincblende(110).	95
3.1 Al on GaAs(110). Reactive chemisorption	96
3.2 Sb on III–V(110). Saturated chemisorption	99
4. Polar surfaces of zincblende structure materials	103
4.1 GaAs(111)–(2×2)	105
4.2 GaAs(001)	106
4.3 GaAs(311)	106
5. Wurtzite structure materials. ZnO	109

6. Synopsis	113
Acknowledgements	114
References	114

Chapter 4 (L.J. Brillson and G. Margaritondo)

Adsorption and Schottky barrier formation on compound semiconductor surfaces	119
1. Introduction	119
2. Gas-phase adsorption.	120
2.1 III-V substrates	120
2.1.1 Oxygen adsorption on GaAs	120
2.1.2 Oxygen adsorption on other III-V compounds	123
2.1.3 Catalytic effects in oxidation processes.	124
2.1.4 Hydrogen adsorption	127
2.1.5 Adsorption of chlorine and of other species.	129
2.2 Other compound semiconductor substrates.	131
2.2.1 Binary II-VI compounds.	131
2.2.2 Mercury cadmium telluride	132
2.3 Future directions in gas-phase adsorption	133
3. Semiconductor adsorption on semiconductor substrates. Heterojunction interfaces	134
3.1 Band lineups. Theoretical aspects	136
3.2 Future directions. Band lineup control	137
4. Adsorption of metals. Schottky barrier formation	139
4.1 Historical background. A synopsis	139
4.1.1 Localized charge at interfaces	139
4.1.2 Role of interface chemical reactions and diffusion	140
4.1.3 Current models of Schottky barrier formation	141
4.2 The extended metal-semiconductor interface.	142
4.2.1 Interface reaction and diffusion. Systematics of Si and binary compounds	142
4.2.2 Reaction and diffusion. Evolution of new chemical phases.	142
4.2.3 Atomic modification of interface chemistry	145
4.2.4 Interface chemical activity of ternary compounds.	146
4.2.5 Interface phase formation by thermal processing	148
4.3 Fermi level stabilization at clean interfaces	149
4.3.1 Binary III-V compounds.	149
4.3.2 Ternary III-V compounds	154
4.3.3 Binary II-VI compounds.	156
4.3.4 Ternary II-VI compounds	157
4.3.5 III-VI compounds	157
4.3.6 IV-VI semiconductors.	158
4.4 Buried metal-semiconductor interfaces	158
4.4.1 Correlation between surface science and electrical barrier measurements	158
4.4.2 Compound and defect formation	161
4.4.3 Metal-induced interface states	162
4.4.4 Structural evolution.	164
4.5 Control of interface electronic properties by atomic-scale techniques	166
4.5.1 Metal interlayers	166
4.5.2 Anions	168
4.5.3 Laser-annealed phases.	169
4.5.4 Gases.	169
4.5.5 Photochemical processing	170
4.6 Perspectives on Schottky barrier formation	171
4.6.1 The extended interface. Complexities and systematics.	171

4.6.2 Role of bulk imperfections	172
4.6.3 Future challenges	173
Acknowledgements	173
References	174

Chapter 5 (H. Froitzheim)

Adsorption on elemental semiconductors	183
1. Introduction	183
2. Preparation of clean surfaces	184
3. Intrinsic structure of Si surfaces	185
3.1 Structure model for Si(111) 2×1	187
3.2 Structure model for Si(111) 7×7	187
3.3 Structure model for Si(100)	190
4. Intrinsic structure of Ge surfaces	191
5. Adsorption on Si	191
5.1 The adsorption of hydrogen on Si	191
5.2 The adsorption of oxygen on Si	202
5.3 The adsorption of water on Si	210
5.4 The adsorption of fluorine on Si	214
5.5 The adsorption of noble gases on Si	217
6. Adsorption on Ge	222
6.1 The adsorption of hydrogen on Ge	222
6.2 The adsorption of oxygen on Ge	224
6.3 The adsorption of water on Ge	227
7. Summary	228
Acknowledgements	230
References	231

Chapter 6 (L. Braicovich)

Adsorption and reaction of metals on elemental semiconductors	235
1. Introduction	235
2. Structural evidence for the reaction at room temperature	235
3. The electronic states of silicides	236
3.1 Silicides of near noble metals	237
3.2 Silicides of refractory metals	240
3.3 Silicides of the precursors of transition metals	242
3.4 Noble metal–silicon systems	242
4. The interface reaction as seen with electronic state spectroscopy	243
5. A scheme for interface growth at room temperature	246
6. Selected topics connected with the scheme of interface growth	251
6.1 Theoretical results relevant to the incubation stage	251
6.2 The concept of critical thickness	254
6.3 The formation of clusters in interface growth	257
6.4 The importance of the substrate conditions	258
6.5 Systems with strong chemical interaction	259
6.6 Systems with weak chemical interaction	262
6.6.1 Silver and gold	262
6.6.2 Simple metals	264
6.7 Buried interfaces	265
References	266

Molecular beam epitaxy of III-V compounds. Aspects of growth kinetics and dynamics.	271
1. Introduction	271
2. The GaAs(001) surface	273
2.1 Surface stoichiometry and reconstruction	273
2.2 Surface crystallography and electronic structure.	275
3. Thermodynamic and kinetic factors involved in the MBE process	283
3.1 Surface reaction kinetics	285
3.2 Models of GaAs surface kinetics from the application of modulated beam techniques	289
4. Growth dynamics	293
4.1 Basic effects and first order models	294
4.2 Multiple scattering effects	297
4.3 Applications of the RHEED intensity oscillation technique to growth dynamic studies.	300
4.3.1 Growth and evaporation rates	300
4.3.2 Surface diffusion	301
4.3.3 Surface recovery and interrupted growth.	302
4.3.4 Two-dimensional growth effects associated with Ga overlayers	303
Acknowledgements	305
References	305

Molecular beam epitaxy of silicon and related materials	309
1. Introduction	309
2. Molecular beam epitaxy	310
3. The technology of MBE	311
3.1 The UHV system	312
3.2 Evaporation and ion sources	314
3.3 Flux distribution and deposit uniformity.	316
3.4 Diagnostic and monitoring equipment	317
4. Substrate preparation	318
4.1 Thermal annealing/reactive-beam treatment	318
4.2 Ion sputter cleaning	319
5. Crystallographic perfection.	320
5.1 Crystallographic quality	320
5.2 Evaluation of extended defects	320
6. Evaluation of undoped homoepitaxial silicon	326
7. Doping	332
7.1 Co-evaporation doping	332
7.1.1 Sb and Ga doping	332
7.1.2 B doping	335
7.1.3 As and P doping	338
7.2 Potential enhanced doping (doping by secondary implantation)	341
7.3 Low-energy dopant ion implantation	346
8. Silicides	349
8.1 Nickel disilicide	350
8.2 Cobalt disilicide	351
9. Silicon-on-insulator structures	352
9.1 Growth on insulating substrates	353
9.2 Si on porous Si.	354

9.3 Alkaline earth/Si heterostructures	355
10. The $\text{Si}_x\text{Ge}_{1-x}$ system	356
11. Device applications	360
11.1 Two-terminal devices	360
11.2 Three-terminal devices and integration	361
12. Future prospects	361
Acknowledgements	362
References	363

Chapter 9 (R.F.C. Farrow)

Molecular beam epitaxy of insulators, metastable phases and II–VI compounds	369
1. Introduction	369
2. Factors controlling the range of materials accessible to MBE growth techniques	372
2.1 General considerations	372
2.2 Epitaxy of inorganic fluorides	374
2.3 Metastable phases	378
2.4 II–VI compounds and alloys	381
3. MBE growth and properties of epitaxial insulators	384
3.1 CaF_2/Si	384
3.2 Lanthanide trifluorides on semiconductors	392
3.3 Transition-metal difluoride epitaxy	397
4. MBE growth and properties of metastable phases	399
4.1 $\alpha\text{-Sn}/\text{InSb}$ and $\alpha\text{-Sn}/\text{CdTe}$	399
4.1.1 Optical investigation of $\alpha\text{-Sn}$ films and the $\alpha \rightarrow \beta$ phase transformation	399
4.1.2 Angle-resolved photoemission spectroscopy studies of $\alpha\text{-Sn}$ films	401
4.1.3 Carrier confinement in $\alpha\text{-Sn}$ quantum wells	402
4.2 Magnetic transition metals	403
4.2.1 B.c.c. Co/GaAs	404
4.2.2 B.c.c. Cr , Mn and Ni on $\alpha\text{-Fe}$	405
4.2.3 $\gamma\text{-Fe}/\text{Cu}$	406
5. MBE growth and properties of II–VI compounds	407
5.1 MBE growth and properties of CdTe/InSb	407
5.2 MBE growth of $\text{CdTe}/\text{Cd}_{1-x}\text{Mn}_x\text{Te}$ multilayer structures	415
6. Applications and future directions	418
6.1 Epitaxial insulators	418
6.2 Metastable phases	419
6.3 II–VI compounds	421
7. Conclusions	421
Acknowledgements	422
References	422

Chapter 10 (T.M. Mayer, M.S. Ameen and D.J. Vitkavage)

Surface chemistry of dry etching processes	427
1. Introduction	427
2. Halogen atom reactions with semiconductors and metals	429
3. Ion bombardment effects	436
4. Synergistic effects	440
5. Surface compositional modification	451
6. Film formation in halocarbon discharges	456
References	461
Index	465