

Contents

1. Introduction: Surface Phenomena and Their Analysis by Scattering Experiments. By P. von Blanckenhagen and W. Schommers (With 10 Figures)	1
1.1 Surface Phenomena	1
1.1.1 Reconstruction and Relaxation	1
1.1.2 Phase Transitions	2
1.1.3 Defects	3
1.1.4 Phonons and Mean Vibrational Amplitudes	4
1.1.5 Bound Resonant States	6
1.1.6 Vibrations of Adsorbed Species	6
1.1.7 Diffusion, Adsorption and Desorption	6
1.1.8 Segregation	7
1.1.9 Interfaces and Superlattices	7
1.1.10 Magnetism and Electronic States	8
1.2 Scattering Methods for Surface Analysis	9
1.2.1 Electron Scattering	10
1.2.2 Scattering of He Atoms	12
1.2.3 Neutron Scattering	13
1.2.4 X-Ray Scattering	17
1.2.5 Scattering of Ions	17
1.2.6 Comparison of Different Scattering Methods	19
1.2.7 Conclusion and Outlook	21
1.3 On the Temperature-Dependence of Surface Properties	24
1.3.1 Pair Potentials at the Surface	24
1.3.2 Density-Functional Formalism for Nonzero Temperatures	25
1.3.3 Conclusions	26
1.4 Book Outline	27
References	28
Additional References with Titles	33
 2. Study of Surface Phonons by Means of the Green's Function Method. By L. Miglio and G. Benedek (With 18 Figures)	 35
2.1 Introductory Remarks	35
2.2 The Time-Independent Green's Function Method in Summary	36

2.3	The Green's Function Method in Surface Dynamics	41
2.4	From a Slab to a Semiinfinite Lattice: Selfconsistent Definition of the Perturbation Matrix	45
2.5	The Electronic Contribution to Surface Dynamics in the Framework of Shell Models	49
2.6	Surface Vibrations in Alkali Halides	53
2.6.1	LiF and NaF	55
2.6.2	NaCl and NaI	60
2.6.3	Potassium Halides	63
2.7	Further Developments: The Study of Surface Phonon Anomalies	67
	References	70
3.	Surface Diffusion and Layer Growth.	
	By P. von Blanckenhagen (With 20 Figures)	73
3.1	Mass Transport and Growth Phenomena at Surfaces	73
3.2	Description of Surface Diffusion	75
3.3	Experimental Methods for the Study of Surface Diffusion and Typical Results	78
3.3.1	Direct Observation of Diffusing Atoms	78
3.3.2	The Study of Particle Correlations in Equilibrium Systems	80
3.3.3	Diffusion Studies in a Concentration Gradient	83
3.3.4	Anisotropy of Surface Diffusion	86
3.3.5	Surface Diffusion Near the Melting Point	88
3.4	Growth Modes	88
3.5	Layer-Growth Techniques	93
3.6	Methods for the Examination of Growth Processes and Typical Results	93
3.6.1	Detection of Growth Modes by Electron Spectroscopy ..	96
3.6.2	Observation of Layer Growth by Diffraction Experiments ..	96
3.6.3	Examination of Surface and Interface Layers by High-Energy Ion Scattering	100
3.6.4	The Growth of Metal Layers on Semiconductor Substrates	102
3.6.5	Examination of Superlattices	102
3.7	Model Calculations and Simulations	106
3.8	Conclusion and Outlook	107
	References	108
	Additional References with Titles	113
4.	Phase Transitions on Single-Crystal Surfaces and in Chemisorbed Layers. By E. Bauer (With 24 Figures) ...	115
4.1	Background	115
4.2	Theoretical Foundations	117
4.2.1	Phases in Two Dimensions	118

4.2.2	Origin of Surface Phases and Relation to Magnetic Models	119
4.2.3	Models and Nomenclature	122
4.2.4	Continuous Order-Disorder Transitions	126
	a) Critical Behaviour and Exponents, Universality and Scaling Laws	126
	b) Symmetry Analysis and Symmetric Lattice Models	130
	c) Asymmetric and Anisotropic Models	131
4.2.5	Order-Order Transitions	132
4.2.6	Commensurate-Incommensurate Transitions	133
4.2.7	Melting in Two Dimensions	137
4.2.8	Interface Delocalization Transitions in Two Dimensions	141
4.2.9	Systems with Long-Range Repulsive Interactions	143
4.2.10	Systems with Purely Attractive Interactions	144
4.3	Experimental Techniques	146
4.3.1	Diffraction Methods	146
4.3.2	Scattering Methods	151
4.3.3	Work Function Change Measurement	152
4.3.4	Thermal Desorption Methods	152
4.3.5	Electron Microscopy	153
4.3.6	Experimental Limitations	154
4.4	Results	155
4.4.1	Clean Surfaces	155
	a) The Si(111)-(7 × 7) ↔ (1 × 1) Transition	155
	b) The Au(110)-(1 × 2) ↔ (1 × 1) Transition	157
	c) W(100)-c(2 × 2) ↔ (1 × 1) Transition	157
	d) Other Transitions on Clean Surfaces	159
4.4.2	Chemisorbed Layers with Repulsive Nearest-Neighbour Interactions	161
	a) Two-Dimensionally Densely Packed Surfaces	161
	b) One-Dimensionally Densely Packed Surfaces (p2mm)	167
	c) Open Surfaces	168
4.4.3	Chemisorbed Layers with Attractive Nearest-Neighbour Interactions	169
4.5	Concluding Remarks and Outlook	170
	References	171
	Additional References with Titles	178
5.	Solid and Liquid Surfaces Studied by Synchrotron X-Ray Diffraction. By J. Als-Nielsen (With 32 Figures)	181
5.1	Reflectivity and Density Profile	183
5.1.1	Master Formula	183
5.1.2	Fresnel Reflectivity	184
5.1.3	Derivation of Master Formula	185
5.1.4	Traditional Calculation Scheme for R(Q)	186

5.2	Experimental Reflectivity Set Up	187
5.2.1	General Wave-Vector Transfer	188
5.2.2	Resolution	191
5.3	Examples of Reflectivity Measurements	194
5.3.1	Thermal Roughness	194
5.3.2	Smectic Layering on Liquid Crystal Surfaces	196
	a) Smectic Layering in the Isotropic Phase	197
	b) Layer Penetration in the Nematic Phase	199
	c) Antiferroelectric Surface Layers	201
5.4	In-Plane Structures	202
5.4.1	Grazing Incidence Geometry	203
	a) Penetration Depth	203
	b) Field Strength	205
	c) Summary of Grazing Incidence	206
5.4.2	Principles of Surface Crystallography	206
	a) Bragg Scattering	206
	b) Unit Cell in Surface Geometry, InSb(111)	208
	c) Reciprocal Lattice. Bragg Points	209
	d) Reconstructed ($n \times m$) Surface Structure.	
	Bragg Rods	211
	e) Bragg Rods from Termination at Surface	211
	f) Patterson Function	213
5.4.3	Reconstructed Surface of InSb(111)-(2×2)	215
	a) Diffractometer Set Up	215
	b) Sample Preparation	216
	c) Results	216
5.4.4	Surface Structures Revealed by X-Ray Diffraction	220
	References	221
6.	Statistical Mechanics of the Liquid Surface and the Effect of Premelting. By W. Schommers (With 26 Figures)	223
6.1	The Structure of the Liquid Surface	223
6.1.1	General Remarks	224
6.1.2	Bulk Liquids	225
6.1.3	Liquid Surfaces	227
	a) Single-Particle Distribution Function	227
	b) The Two-Particle Distribution Function	233
6.1.4	Surface Thermodynamic Properties	236
6.1.5	Liquid Metals	239
6.2	Dynamics of the Liquid Surface	241
6.3	The Effect of Premelting. A Study for Krypton	245
6.3.1	Model	245
6.3.2	Results for the Distribution Functions	245
	a) Single-Particle Distribution Functions for Krypton	245
	b) Pair Correlation Function for Krypton	247

6.3.3	Discussion of the Results for the Distribution Functions	249
a)	Single-Particle Distribution Function for the Outermost Layer at $T=7$ K	249
b)	The Dynamics of the Particles of the Outermost Layer at $T=102$ K	250
c)	Melting Mechanism: Description at the Atomic Level	252
6.4	Final Remarks	254
	References	255
	Additional References with Titles	257
7.	The Roughening Transition. By H. van Beijeren and I. Nolden (With 24 Figures)	259
7.1	Background	259
7.2	Macroscopic Description of Equilibrium Crystal Shapes	263
7.2.1	The Wulff Construction	263
7.2.2	Facets, Edges and Corners	266
7.2.3	The Roughening Transition and Other Phase Transitions	270
7.3	Microscopic Description of Crystal Surfaces	270
7.3.1	The Kossel Crystal, Lattice-Gas Models, Solid-on-Solid Models	270
7.3.2	Steps and Step Free Energies	272
7.3.3	Microscopic Characterization of Roughening Transitions	274
7.3.4	Equilibrium Shapes of Facets. General Criterium for Roughening	276
7.4	Statistical Mechanics of Interface Models	279
7.4.1	Renormalization-Group Results	281
a)	Roughening Temperature	282
b)	Surface Tension	283
c)	Step Free Energies	283
d)	Correlation Length	283
e)	Height-Height Correlation Function	284
f)	Jump in Curvature and Surface Stiffness	284
7.4.2	The BCSOS Model	285
7.4.3	The Terrace-Step-Kink Model	288
7.4.4	Universal Shape of Vicinal Areas	290
7.5	Discussion	292
7.5.1	Roughening Versus Surface Melting	292
7.5.2	Are All Roughening Transitions of Kosterlitz-Thouless Type?	294
a)	Inequivalent Layers	294
b)	Impurities and Lattice Faults	294
c)	First-Order Transitions	295
7.5.3	Multilayer Adsorption and Roughening	296
	Appendix 7.A: Surface Stiffness and Universal Jump in Curvature..	296
	References	298
	Additional References with Titles	300

8. Structural and Dynamical Aspects of Adsorption and Desorption. By G. Doyen (With 4 Figures).....	301
8.1 General.....	301
8.2 Basic Experimental Facts	304
8.2.1 Elastic Scattering at Surfaces.....	304
8.2.2 Trapping and Sticking.....	305
8.2.3 Direct Inelastic Scattering.....	307
8.2.4 Desorption.....	308
8.3 Overview of the Different Theoretical Approaches.....	309
8.3.1 Classical and Classical-Stochastic Theories.....	310
8.3.2 Semiclassical Theories.....	312
8.3.3 Quantum Theories	313
8.4 Selected Problems.....	316
8.4.1 Structural and Dynamical Constraints.....	316
8.4.2 The Compensation Effect.....	320
8.4.3 The Sticking Coefficient – Definition and Zero Temperature/Zero Kinetic Energy Behaviour	322
8.4.4 Quantum Partitioning Techniques	331
8.4.5 Non-Adiabatic Adsorption and Desorption.....	337
8.5 Concluding Remarks.....	341
References	342
 9. Many-Body Description of Surface Elementary Excitations. Application to Semiconductors. By A. Muramatsu and W. Hanke (With 9 Figures)	 347
9.1 Background	347
9.2 Elementary Excitations on Surfaces	349
9.2.1 Homogeneous Bethe-Salpeter Equations	350
9.2.2 Equation of Motion in the Local-Orbital Representation	351
9.2.3 Surface Density-Response Function.....	353
9.3 Surface Electromagnetic Response.....	355
9.3.1 Surface Macroscopic Dielectric Tensor	356
9.3.2 Microscopic Formulation of the Optical Response	358
9.3.3 Microscopic Theory of Surface Reflectivity.....	361
9.4 Electron-Phonon Interaction and Microscopic Theory of Lattice Dynamics on Surfaces	364
9.4.1 Surface Lattice Dynamics	365
9.5 Applications: Si(111).....	366
9.5.1 Electronic Instabilities in an Ideal Si(111) Slab.....	367
9.5.2 Microscopic Phonon Calculations for an Ideal Si(111)Slab	370
9.6 Summary and Perspectives.....	372
References	374
 Subject Index.....	 377