

<b>1</b>	<b>Introduction</b> .....	<b>1</b>
	S. Sadewasser and Th. Glatzel	
	References .....	<b>3</b>
 <b>Part I Technical Aspects</b>		
<b>2</b>	<b>Experimental Technique and Working Modes</b> .....	<b>7</b>
	S. Sadewasser	
2.1	Introduction .....	7
2.2	Non-Contact Atomic Force Microscopy .....	8
2.3	Kelvin Probe Force Microscopy .....	12
2.4	AM-KPFM .....	14
2.5	FM-KPFM .....	15
2.6	Comparison of AM- and FM-KPFM .....	16
2.7	Technical Realization .....	19
2.8	Other Modes and Additional Experimental Options.....	20
2.9	Additional Remarks .....	22
	References .....	24
<b>3</b>	<b>Capacitive Crosstalk in AM-Mode KPFM</b> .....	<b>25</b>
	H. Diesinger, D. Deresmes, and T. Mélin	
3.1	Introduction .....	25
3.2	AM-KPFM in Ultrahigh Vacuum.....	26
3.2.1	Self-Oscillating AFM Configuration .....	26
3.2.2	Electrostatic Excitation Dependence on dc Bias .....	28
3.2.3	Measurement of the Crosstalk .....	29
3.2.4	Active Compensation at the Cantilever Frequency .....	31
3.2.5	Crosstalk Reduction by Filtering .....	33
3.2.6	PLL Controlled AFM Setup .....	34
3.2.7	Comparison of the Countermeasures in UHV KPFM ....	35

3.3	AM-KPFM in Air .....	35
3.3.1	Crosstalk Determination by Resonance Curve Fitting ....	35
3.3.2	Crosstalk Compensation .....	38
3.4	Crosstalk Effect on Complementary Measurements.....	38
3.4.1	$V_{dc}$ Sweep of the Oscillation Amplitude.....	39
3.4.2	Phase Dependent KPFM Reading .....	41
3.5	Comparison of Crosstalk Compensation in Vacuum and in Air ...	43
	References.....	43
<b>4</b>	<b>The Effect of the Measuring Tip and Image Reconstruction .....</b>	<b>45</b>
	Y. Rosenwaks, G. Elias, E. Strassbourg, A. Schwarzman, and A. Boag	
4.1	Introduction.....	45
4.2	Tip-Sample Electrostatic Interaction: A Review .....	46
4.2.1	Conducting Surfaces.....	46
4.2.2	Semiconducting Surfaces .....	49
4.3	Deconvolution and Image Restoration .....	52
4.3.1	Accurate Algorithm for Image Restoration .....	52
4.3.2	Tip Oscillation and the Effect of the Cantilever.....	56
4.3.3	The Effect of Nano Scale Tip Protrusions .....	59
4.3.4	Comparison with Experimental Results .....	63
4.4	Summary and Conclusions .....	66
	References.....	67
<b>5</b>	<b>Contribution of the Numerical Approach to Kelvin Probe Force Microscopy on the Atomic-Scale .....</b>	<b>69</b>
	L. Nony, F. Bocquet, A. Foster, and Ch. Loppacher	
5.1	Atomic-Scale Contrast in KPFM: Relevance of the Numerical Approach .....	69
5.2	Prerequisite: The nc-AFM Simulator.....	73
5.2.1	Overview of the Numerical Implementation .....	75
5.2.2	Numerical Schemes .....	76
5.2.3	Main Results .....	80
5.3	Numerical Implementation of the KPFM Methods: The nc-AFM/KPFM Simulator .....	80
5.3.1	Amplitude-Modulation KPFM (AM-KPFM) .....	81
5.3.2	Frequency Modulation KPFM (FM-KPFM) .....	84
5.3.3	Methodology with the nc-AFM/KPFM Simulator .....	85
5.4	Atomistic Simulations of Bias Voltage-Dependent Force Fields.....	87
5.4.1	Madelung Surface Potential of an Alkali Halide.....	87
5.4.2	Atomistic Simulations of the Bias Voltage-Dependent Force Field .....	88
5.5	Results with the nc-AFM/KPFM Simulator .....	92
5.5.1	Spectroscopic Curves.....	92
5.5.2	Topography and LCPD Images .....	93

5.6	Conclusions and Outlook .....	94
	References.....	95

## Part II Selected Applications

<b>6</b>	<b>Electronic Surface Properties of Semiconductor Surfaces and Interfaces .....</b>	<b>101</b>
	R. Shikler	
6.1	Introduction.....	101
6.2	KPFM Measurements of <i>pn</i> Junctions.....	105
6.3	KPFM Measurements of Thin Film Solar Cells, the Role of Grain Boundaries .....	109
6.4	KPFM Measurements on Organic Materials.....	111
6.5	Concluding Remarks .....	113
	References.....	114
<b>7</b>	<b>Surface Properties of Nanostructures Supported on Semiconductor Substrates .....</b>	<b>117</b>
	F. Krok, J. Konior, and M. Szymonski	
7.1	Introduction.....	117
7.2	Experimental .....	118
7.3	Self-Assembling on Semiconductor Surfaces.....	120
	7.3.1 Epitaxial Au Nanostructures Assembled on InSb(00 1) .....	120
	7.3.2 Semiconductor Nanostructures Grown on Lattice-Mismatched Semiconductor Substrates .....	124
7.4	Surface Modification and Nanostructuring Induced by Laser Ablation and Ion Beams .....	127
7.5	Dielectric Structures Grown on InSb(00 1) .....	131
	7.5.1 Accuracy of KPFM Signal Measurements .....	133
	7.5.2 Theoretical Model of Electrostatic Tip-Sample Interaction.....	135
	7.5.3 Numerical Simulation of KPFM Contrast.....	140
7.6	High Resolution KPFM Measurements .....	142
	7.6.1 Limits of Lateral Resolution in FM-KPFM.....	142
	7.6.2 Characterization of the Short-Range Bias Dependent Interactions: Quasispectroscopic KPFM Measurements .....	144
7.7	Summary.....	147
	References.....	148
<b>8</b>	<b>Optoelectronic Studies of Solar Cells.....</b>	<b>151</b>
	S. Sadewasser	
8.1	Introduction to Solar Cells .....	151
8.2	Nanometer Optoelectronic Surface Studies .....	154
	8.2.1 Cu(In,Ga)(S,Se) <sub>2</sub> -Based Solar Cells.....	154
	8.2.2 Organic Solar Cells .....	159

8.3	Grain Boundaries in Thin Film Solar Cells .....	160
8.3.1	Si-Based Solar Cells .....	160
8.3.2	Cu(In,Ga)(S,Se) <sub>2</sub> -Based Solar Cells .....	161
8.3.3	CdTe-Based Solar Cells .....	164
8.4	Cross-Sectional Device Characterization .....	165
8.4.1	Si-Based Solar Cells .....	165
8.4.2	Cu(In,Ga)(S,Se) <sub>2</sub> -Based Solar Cells .....	166
8.4.3	III-V-Based Solar Cells .....	170
8.5	Summary .....	171
	References .....	171

## **9 Electrostatic Force Microscopy Characterization of Low Dimensional Systems .....**

	Yoichi Miyahara, Lynda Cockins, and Peter Grütter	
9.1	Fluctuations of the Electrostatic Potential in Semiconductor Low-Dimensional Structures .....	175
9.1.1	Kelvin Probe Force Microscopy on Semiconductor Heterostructures .....	177
9.1.2	Large Spatial Fluctuations in Electrostatic Potential on Epitaxially Grown InAs/InGaAs/InP Heterostructures Observed by FM-AFM .....	178
9.2	Temporal Fluctuations of the Surface Potential Under Light Illumination .....	187
9.3	Single-Electron Sensitive Electrostatic Force Microscopy/Spectroscopy .....	189
9.3.1	Single-Electron Electrostatic Force Microscopy/Spectroscopy on Quantum Dots .....	189
9.3.2	Single-Electron Tunneling Force Microscopy/Spectroscopy on Insulator Surfaces .....	192
9.4	Related Scanning Probe Techniques .....	192
9.4.1	Scanning Single Electron Transistor Microscopy .....	192
9.4.2	Scanning Charge Accumulation Microscopy .....	194
9.5	Conclusion .....	194
	References .....	195

## **10 Local Work Function of Catalysts and Photoelectrodes .....**

	H. Onishi and A. Sasahara	
10.1	Introduction .....	201
10.2	Na Adatoms .....	203
10.3	Cl Adatoms .....	205
10.4	Pt Adatoms and Particles .....	207
10.5	Ni Particles .....	212
10.6	Organometallic Dye .....	212
10.7	Summary and Perspectives .....	217
	References .....	218

<b>11</b>	<b>Electronic Properties of Metal/Organic Interfaces</b> .....	221
	Christian Loppacher	
11.1	Introduction .....	221
11.1.1	Ohmic Contact .....	223
11.1.2	Schottky–Mott Contact .....	223
11.1.3	Dipole Formation at Interface .....	223
11.1.4	Macroscopic Methods .....	224
11.1.5	Nanoscopic Methods: Kelvin Probe Force Microscopy .....	226
11.2	Macroscopic Studies .....	226
11.3	Nanoscopic Studies .....	228
11.3.1	Quantitative Results by KPFM.....	228
11.3.2	Orientalional Dependence.....	231
11.3.3	Dependence on Molecular Arrangement .....	234
11.4	Conclusion .....	237
	References.....	238
<b>12</b>	<b>KPFM and PFM of Biological Systems</b> .....	243
	B.J. Rodriguez and S.V. Kalinin	
12.1	Introduction .....	244
12.1.1	Electric Potentials and Electromechanics in Biosystems .....	244
12.1.2	Voltage Modulation SPM for Electrical and Electromechanical Measurements.....	246
12.2	KPFM of Biosystems .....	250
12.2.1	Organic Molecules.....	251
12.2.2	Biomolecular Systems.....	251
12.3	PFM of Biosystems .....	263
12.3.1	Historical Background.....	263
12.3.2	PFM of Collagen .....	265
12.3.3	PFM of Other Biosystems.....	267
12.3.4	Challenges .....	269
12.4	Liquid Imaging .....	270
12.4.1	Measurements of Electric Potential in Solution.....	270
12.4.2	Piezoresponse Force Microscopy .....	273
12.4.3	At the Intersection of Electrostatics and Electromechanics .....	279
12.5	Summary and Outlook .....	282
	References.....	282
<b>13</b>	<b>Measuring Atomic-Scale Variations of the Electrostatic Force</b> .....	289
	Th. Glatzel	
13.1	Introduction .....	289
13.2	Concept of the Local Work Function .....	290
13.2.1	Mesoscopic Measurements of the Work Function .....	292
13.2.2	Molecular Variations of the Local Contact Potential Difference .....	295

13.3	Measurements at the Atomic Scale .....	300
13.3.1	The Silicon(111)-(7 × 7) Surface .....	300
13.3.2	III–V Semiconductors .....	305
13.3.3	Rutile TiO <sub>2</sub> .....	307
13.3.4	Ionic Surfaces .....	311
13.3.5	KPFM by Tuning-Fork AFM .....	313
13.4	Influence of Measurement Parameters .....	317
13.4.1	Influence of the Tunneling Current .....	317
13.4.2	Influences by $V_{ac}$ .....	319
13.4.3	The Influence of Short-Range Forces .....	322
13.4.4	Capacitive Crosstalk .....	323
13.5	Summary .....	324
	References .....	325
	<b>Index</b> .....	<b>329</b>