

Contents

1. Aerosol Chemical Physics. By W.H. Marlow	1
1.1 Aerosol Microphysics	1
1.2 Chemical Physics of Microparticles	2
1.2.1 Isolated Particles and Clusters	2
1.2.2 Physical Transformations and Thermodynamics	4
References	6
2. Physics of Microparticles	
By H.P. Baltes and E. Šimánek (With 11 Figures)	7
2.1 Introductory Remarks	8
2.1.1 How Small is Small?	8
2.1.2 Exemplary Size Effects	10
2.1.3 Overview and Guide to the Literature	14
2.2 Perfect Gases in Finite Boxes of Regular Shape	15
2.2.1 Weyl's Problem	15
2.2.2 Vibrational Specific Heat	17
2.2.3 Radiation Laws	19
2.2.4 Electronic Magnetic Moments	20
2.2.5 Thermodynamic Relations and Bose-Einstein Condensation	21
2.3 Optical Phonons in Dielectric Microparticles	23
2.3.1 Dispersion Scheme and Gap Modes	23
2.3.2 Summary of Theoretical Results	24
2.3.3 Far-Infrared Measurements	26
2.4 Electronic Heat Capacity and Magnetic Susceptibility of Metallic Microparticles	26
2.4.1 Historical Background	27
2.4.2 Free Energy of an "Even" Particle	28
2.4.3 Free Energy of an "Odd" Particle	30
2.4.4 Thermodynamic Properties of a Single Metallic Microparticle	31
2.4.5 Ensemble Averaging	32
2.4.6 Electronic Heat Capacity	34
2.4.7 Spin Susceptibility and NMR Shift	35
2.4.8 Spin-Orbit Coupling and Electron-Spin Resonance	36

2.5	Electromagnetic Properties of Metallic Microparticles	38
2.5.1	Electric Polarizability	39
2.5.2	Gorkov-Eliashberg Anomaly	39
2.5.3	Plasma Resonance Absorption	40
2.5.4	Far-Infrared Absorption	42
2.6	Superconducting Properties	43
2.6.1	Fluctuations of the Order Parameter	43
2.6.2	Magnetic Susceptibility	45
2.6.3	Specific Heat	45
2.6.4	Ultrasonic Attenuation	46
2.6.5	Nuclear Spin Relaxation	47
2.6.6	Transition Temperature	48
	References	50
3.	Electronic Structure Studies of Overlayers Using Cluster and Slab Models	
	By I.P. Batra (With 14 Figures)	55
3.1	Theoretical Background	57
3.1.1	Hartree-Fock Approximation	58
3.1.2	Statistical Exchange Approximation	60
3.1.3	SCF- x_α -SW Method	61
3.1.4	LCAO- x_α Method	62
3.2	ETB- x_α Method	63
3.2.1	Crystal Potential and Matrix Elements	65
3.2.2	ETB-Slab Model	67
3.3	Oxygen Chemisorption on Aluminum	68
3.3.1	Cluster Approach	68
3.3.2	Band Structure Approach and Experimental Results	73
3.3.3	Unresolved Issues	80
	Appendix 3.A	82
	Appendix 3.B	83
	Appendix 3.C	86
	Appendix 3.D	91
	References	95
4.	Computer Experiments on Heterogeneous Systems	
	By B.J. Berne and R.V. Mikkilineni (With 13 Figures)	99
4.1	Methodology	99
4.1.1	Molecular Dynamics	101
4.1.2	Stochastic Molecular Dynamics	104
4.1.3	Monte Carlo Method	105

4.2	Computer Simulation of Planar Interfaces in a Lennard-Jones Fluid	106
4.2.1	Flat Interfaces	107
	a) Preparation of the Planar Interface	107
	b) Density Profile	108
	c) Transverse Correlations	109
	d) Pressure Tensor	111
4.2.2	Thermodynamics of Microclusters and Nucleation in a Finite System	115
	a) Preparation of Droplet in Computer Simulation	118
	b) Cluster Distribution	120
	c) The Density Profile of a Droplet	121
4.3	Computer Simulation of Idealized Interfaces	122
4.3.1	Lattice Gas Models	122
4.3.2	Nucleation in Two-Dimensional Square-Well Fluids	123
4.4	Conclusion	124
	References	125
5.	Aerosol Growth by Condensation. By P.E. Wagner (With 12 Figures)	129
5.1	Statement of the Problem	129
5.2	Quasistationary Fluxes to a Single Droplet in the Continuum Regime	132
	5.2.1 Conservation Laws	133
	5.2.2 Phenomenological Equations	134
	5.2.3 Calculation of Heat and Mass Flux	138
	a) Heat Flux Q_c in the Continuum Regime	139
	b) Mass Flux I_c in the Continuum Regime	142
5.3	Quasistationary Fluxes to a Single Droplet in the Transition Regime	144
	5.3.1 Knudsen Numbers	146
	5.3.2 Expressions for Mass and Heat Flux	149
	5.3.3 Jumps of Density and Temperature	151
5.4	Quasistationary Droplet Growth and Evaporation	152
	5.4.1 Mass Flux to a Single Droplet	152
	5.4.2 Mass and Heat Balance in a Monodispersed Droplet Aerosol .	154
	5.4.3 Calculation of Droplet Growth and Evaporation	156
5.5	Experimental Results	158
	5.5.1 Measurements of Particle Evaporation	158
	5.5.2 Measurements of Particle Growth	159

5.6	Comparison of Numerical Growth Calculations with Recent Expansion Chamber Experiments	166
5.7	Conclusions and Outlook	173
References		175
Additional References with Titles		179
Subject Index		181