

Contents

Part I Dusty Plasmas

1 Phase Transitions in Dusty Plasmas	3
Hauke Thomsen, Jan Schablinski and Michael Bonitz	
1.1 Introduction	4
1.1.1 Melting as a Loss of Order	6
1.1.2 Coupling Strength and Coupling Parameter	7
1.1.3 The Specific Heat Capacity	10
1.1.4 The Radial Pair Distribution Function	12
1.2 Phase Transitions in Finite Systems	13
1.2.1 Coupling Parameter of Finite Systems	15
1.2.2 The Specific Heat Capacity of Finite Systems	16
1.2.3 Radial Pair Distribution Function in Finite Systems	18
1.2.4 The Center-Two-Particle Correlation Function	20
1.3 Simulation Methods	24
1.3.1 Dimensionless System of Units	24
1.3.2 Metropolis Monte Carlo (MC) Sampling	25
1.3.3 Molecular Dynamics Simulations	30
1.3.4 Langevin Molecular Dynamics Simulations	33
1.4 Experimental Realization of Heating and Phase Transitions	35
1.4.1 Variation of the Dust Kinetic Temperature in Experiments	35
1.4.2 Experimental Realization of the Laser Heating of Dusty Plasmas	36
1.4.3 Modeling Laser Heating	39
1.5 Melting Parameters with Focus on Application in Simulations and Experiments	41
1.5.1 Lindemann-Type Melting Parameters	41
1.5.2 Bond Angular Order Parameter	44
1.6 Summary and Conclusion	45
References	46

2	Introduction to Streaming Complex Plasmas A: Attraction of Like-Charged Particles.	51
	André Schella, André Melzer, Patrick Ludwig, Hauke Thomsen and Michael Bonitz	
2.1	Introduction	51
2.2	Ion Focus and Wakefield	53
2.2.1	Phenomenological Description of the Ion Focus	54
2.2.2	Biasing Wakes in the Experiment	56
2.3	Wakefield Effects in Dusty Plasma Experiments	57
2.3.1	Experimental Setup	57
2.3.2	Structure of Ion-Focus Affected 3D Dust Clusters	59
2.3.3	Dynamics of Ion-Focus Affected 3D Dust Clusters	61
2.4	Summary and Outlook	66
	References	66
3	Introduction to Streaming Complex Plasmas B: Theoretical Description of Wake Effects	73
	Patrick Ludwig, Christopher Arran and Michael Bonitz	
3.1	Introduction	74
3.2	Simulation Approaches to Streaming Multi-Component Plasmas	75
3.2.1	Particle-in-Cell Simulations of Plasma Wakes	76
3.2.2	Multiscale Approach to the Dynamics of Complex Plasmas	76
3.3	Introduction to the Kielstream Program	81
3.3.1	Code Structure	82
3.3.2	Performance and Runtimes	84
3.3.3	Estimation of Numerical Errors	89
3.4	Simulation Results	90
3.4.1	Wake Structure Around a Single Grain	90
3.4.2	Many-Particle Langevin Dynamics Simulations	95
3.5	Synopsis	97
	References	98
Part II Quantum Plasmas		
4	Quantum Hydrodynamics	103
	Shabbir A. Khan and Michael Bonitz	
4.1	Introduction	104
4.2	Basics of Quantum Hydrodynamics	109
4.2.1	The Time-Dependent Schrödinger Equation	109
4.2.2	Quantum Mixed State Description: Wigner Function	111

4.2.3	Moments of the Wigner Function: Hydrodynamics	114
4.2.4	Examples and Test of the Assumption $A_i(x, t) = A(x, t)$	118
4.2.5	Main Assumptions and Applicability Conditions of QHD	120
4.2.6	Linearized QHD: Linear Waves of Quantum Plasmas	122
4.2.7	Nonlinear Waves in Quantum Plasmas	134
4.2.8	Magnetized Quantum Plasmas	137
4.3	Interaction and Spin Effects in Quantum Plasmas	144
4.3.1	Prediction of Attractive Forces Between Protons in Quantum Plasmas	144
4.3.2	Spin Effects in Quantum Plasmas	146
4.4	Conclusion and Outlook	148
	References	149
5	Introduction to Configuration Path Integral Monte Carlo	153
	Tim Schoof, Simon Groth and Michael Bonitz	
5.1	Introduction	154
5.2	Monte Carlo	155
5.2.1	Metropolis Algorithm	155
5.2.2	Error in the Monte Carlo Simulation	158
5.3	Second Quantization	160
5.3.1	(Anti-)Symmetric Many-Particle States	161
5.3.2	Occupation Number Representation	163
5.3.3	Creation and Annihilation Operators	165
5.3.4	Operators in Second Quantization	168
5.4	The Density Operator	172
5.5	Configuration Path Integral Monte Carlo in the Interaction Representation	174
5.5.1	Expansion of the Partition Function	175
5.5.2	Estimators for Many-Particle Observables	178
5.5.3	CPIMC Procedure: Monte Carlo Steps	180
5.5.4	Acceptance Probabilities of the Monte Carlo Steps	183
5.6	Results for Interacting Fermions in a One-Dimensional Harmonic Trap	185
5.6.1	The System	186
5.6.2	Numerical Results	187
5.6.3	Fermion Sign Problem	190
5.7	Summary and Outlook	191
	References	193

Part III Low-Temperature Plasmas

6	Calorimetric Probes for Energy Flux Measurements in Process Plasmas	197
	Sven Bornholdt, Maik Fröhlich and Holger Kersten	
6.1	Introduction	198
6.2	Calorimetric Probes	200
6.2.1	THORNTON'S "Heat Flux Probe"	201
6.2.2	GARDON'S Radiometer	207
6.2.3	Other Examples	210
6.3	Contributions to the Total Energy Influx	211
6.3.1	Particle Impact	212
6.3.2	Surface Processes	216
6.3.3	Radiation	218
6.3.4	Particle Emission from Surfaces	219
6.3.5	Total Energy Influx	221
6.4	Examples of Application	221
6.4.1	Ion Beam	221
6.4.2	Magnetron Sputtering	224
6.4.3	Non-Thermal Atmospheric Pressure Plasma Jet	228
6.5	Summary and Conclusion	231
	References	231
7	Fundamental and Applied Studies of Molecular Plasmas Using Infrared Absorption Techniques	235
	J. Röpcke, P. B. Davies, J. H. van Helden, M. Hübner, N. Lang and S. Welzel	
7.1	Introduction	236
7.2	Studies of Molecular Plasmas Using Frequency Mixing, FTIR and TDL Techniques	239
7.2.1	On Ethylene Destruction in a Dielectric Packed-Bed Plasma Reactor Using FTIR Spectroscopy	239
7.2.2	Studies of Hydrocarbon RF Plasmas Using a Difference Frequency Laser Source	241
7.2.3	Chemical and Kinetic Studies in Dust Producing RF Plasmas Using TDLAS	242
7.3	Quantum Cascade Laser Absorption Spectroscopy for Plasma Diagnostics and Control	246
7.3.1	General Considerations	246
7.3.2	Application of Pulsed QCLs	247
7.3.3	Application of cw QCLs	254
7.3.4	Applications of EC-QCLs	257
7.4	Summary and Conclusions	263
	References	264

8	Surface Electrons at Plasma Walls	267
	Rafael Leslie Heinisch, Franz Xaver Bronold and Holger Fehske	
8.1	Introduction	267
8.2	Electron Surface Layer	269
8.3	Electron Physisorption	279
8.4	Mie Scattering by a Charged Particle	287
8.5	Summary	296
	References	297
9	Characterization of Local Structures in Plasma Deposited Semiconductors by X-ray Absorption Spectroscopy	299
	M. Alper Sahiner	
9.1	Introduction	299
9.2	EXAFS	300
9.2.1	EXAFS Experimental Set-up	301
9.2.2	EXAFS Data Analysis	302
9.3	Local Structural Information in Arsenic Ultra Shallow Junctions by EXAFS	304
9.3.1	DFT Calculations	305
9.3.2	Electrical Data and EXAFS Results	306
9.3.3	Arsenic PIII Structures by EXAFS	310
9.4	Local Structural Information in High-k Dielectrics by EXAFS	311
9.5	Summary	317
	References	319
10	Kinetic Monte Carlo Simulations of Cluster Growth and Diffusion in Metal-Polymer Nanocomposites	321
	Lasse Rosenthal, Thomas Strunskus, Franz Faupel, Jan Willem Abraham and Michael Bonitz	
10.1	Introduction	322
10.1.1	Physical Aspects of Polymer Metallization	323
10.1.2	Chapter Overview	328
10.2	Theoretical Foundations of Kinetic Monte Carlo Methods	329
10.2.1	Fundamental Terms of Probability Theory	329
10.2.2	Continuous-Time Markov Chains	332
10.2.3	Two Algorithmic Constructions of Continuous-Time Markov Chains	336
10.3	Description of the Simulations	338
10.3.1	Modeling the Metal-Polymer Nanocomposite	339
10.3.2	The Simulation Algorithm	344
10.4	Formation of Metal-Polymer Interfaces	346
10.4.1	Complete Condensation without Surface Defects	346
10.4.2	Complete Condensation with Surface Defects	351

10.4.3	Incomplete Condensation	352
10.4.4	Interrupted Coalescence and Percolation	353
10.5	Co-Deposition of Metal and Polymer	355
10.5.1	Concentration Profiles	356
10.5.2	Size Distributions	357
10.6	Self-Organized Formation of Metallic Nanocolumns	360
10.6.1	Simulation Details	360
10.6.2	Results	362
10.7	Summary and Outlook	367
	References	368

Part IV Technological Applications

11	Microcavity and Microchannel Plasmas: General Characteristics and Emerging Applications	373
	J. Gary Eden and Sung-Jin Park	
11.1	Introduction	373
11.2	Principles and General Properties of Microcavity Plasmas	374
11.2.1	Gas and Electron Temperatures	375
11.2.2	Electron Densities, Scaling with d	376
11.2.3	Plasma-Wall Interactions	376
11.2.4	Breakdown of pd Scaling	377
11.2.5	Electric Field Strength in the Sheath	377
11.2.6	Gas Phase Chemistry, in situ Production of Transient Molecules	378
11.3	Device Structures, Fabrication, and Modes of Operation	379
11.4	Selected Applications	390
11.5	Summary and Future Challenges	394
	References	396
12	Plasma Electrochemistry: A Novel Chemical Process for the Synthesis and Assembly of Nanomaterials	399
	Seung Whan Lee and R. Mohan Sankaran	
12.1	Introduction to Plasma Electrochemistry	399
12.2	Plasma Electrochemical Reactions in Solution	401
12.3	Fundamental Studies of Charge Transfer Reactions at the Plasma-Liquid Interface	402
12.4	Plasma Electrochemical Reactions at the Surface of Thin Films	410
12.4.1	Direct Writing Based on Scanning Microplasma	411
12.4.2	Lithographic Pattern Transfer Using Extracted Discharge	413
12.4.3	Directed Assembly from Metallosupramolecular Polymers	416

12.5	Applications of Plasma Electrochemistry to H_2O_2 Detection	421
12.6	Summary and Conclusions	423
	References	424
13	Progress in Large-Scale Ozone Generation Using Microplasmas	427
	Jose Lopez	
13.1	Introduction	427
13.2	Ozone and Its Various Applications	429
13.3	Ozone Formation with Microplasmas	430
13.3.1	Role of the Dielectric Barrier Discharge	431
13.3.2	Kinetics of Ozone Formation	433
13.4	Standard Ozone Generator Configurations	434
13.5	Recent Developments in Large-Scale Ozone Generators	438
13.6	Challenges in Large-Scale Ozone Generators	442
13.6.1	By-Product Formation in DBDs	442
13.6.2	Hydrocarbon Contamination in DBDs	444
13.6.3	The Role of Hydrocarbons	445
13.6.4	Hazards of Hydrocarbons	449
13.7	Conclusions and Future Progress	451
	References	451
14	Dental Applications of Atmospheric-Pressure Non-Thermal Plasmas	455
	WeiDong Zhu, Kurt Becker, Jie Pan, Jue Zhang and Jing Fang	
14.1	Introduction	455
14.2	Atmospheric-Pressure Plasmas and Plasma Sources	456
14.2.1	Overview	456
14.2.2	The Plasma MicroJet (PMJ) Source	458
14.2.3	The INP kINPen Source	458
14.2.4	The Plasma Pipette (PP) Source	459
14.3	Selected Dental Applications of Non-Thermal Atmospheric-Pressure Plasmas	460
14.3.1	Human Tooth	460
14.3.2	Interactions of Non-Thermal Atmospheric-Pressure Plasmas with Dental Materials	461
14.3.3	Plasma-Induced and Plasma-Assisted in vitro Teeth Bleaching	465
14.3.4	Plasma Root Canal Treatment	474
14.4	Conclusions and Outlook	482
	References	483
	Index	487