

Contents

Part I Formation

1	Synthesis of Tailored Nanoparticles in Flames: Chemical Kinetics, In Situ Diagnostics, Numerical Simulation, and Process Development	3
1.1	Introduction	3
1.1.1	State of the Art in Flame-Based Synthesis of Nanoparticles	5
1.2	Principles of Particle Formation and Growth in the Gas Phase.	6
1.3	Shock-Tube Studies of Precursor Reactions	8
1.3.1	Formation of Iron Clusters From $\text{Fe}(\text{CO})_5$	9
1.3.2	Reaction of Gallium Atoms with Nitrogen and Oxygen.	11
1.4	Flame Reactor Studies of Particle Formation and Growth	13
1.4.1	Molecular-Beam Sampling.	15
1.4.2	Thermophoretic Sampling with Ex Situ Analysis	16
1.5	Laser-Based Diagnostics in Particle Synthesis Reactors.	16
1.5.1	Diagnostics for Temperature	17
1.5.2	Diagnostics for Species Concentration.	19
1.5.3	Optical Diagnostics for Particle Sizes	22
1.6	Chemistry Modeling and Simulation of Reactive Flows	23
1.6.1	Modeling and Validation of the Fe Chemistry in Flames.	25
1.6.2	CFD Simulation of Reactive Flows in Nanoparticle Synthesis	30
1.7	Examples of Flame-Synthesized Particles	32
1.7.1	Semi-Conducting Single Oxide Particles	34
1.7.2	Mixed Oxide and Composite Nanoparticles	37
1.8	Conclusions	42
	References	42

2	Chemical Vapor Synthesis of Nanocrystalline Oxides	49
2.1	Introduction	49
2.2	Influence of Pulsed Precursor Delivery on Particle Size and Size Distribution	50
2.2.1	Experimental Methodology	51
2.2.2	Results and Discussion	53
2.3	Influence of the Time-Temperature Profiles on Powder Characteristics	59
2.3.1	Experimental Methodology	60
2.3.2	Results and Discussion	61
2.4	Control of Composition by Laser Flash Evaporation: Crystal and Local Structure of Cobalt Doped Zinc Oxide Nanoparticles	64
2.4.1	Experimental Methodology	65
2.4.2	Results and Discussion	67
2.5	Summary and Conclusions.	74
	References	75
3	Nucleation, Structure and Magnetism of Transition Metal Clusters from First Principles	77
3.1	Introduction	77
3.2	Magnetism and Structural Transformations in Nanoparticles	79
3.3	Structure and Magnetism in Binary Nanoparticles	85
3.4	MAE of Clusters	89
3.4.1	MAE for Perfect Clusters	91
3.4.2	MAE for Relaxed Clusters.	93
3.5	Summary and Outlook	94
	References	95
4	Synthesis and Film Formation of Monodisperse Nanoparticles and Nanoparticle Pairs	99
4.1	Introduction	99
4.2	Synthesizing Monodisperse Nanoparticles by Means of Spark Discharge	103
4.2.1	Spark Discharge	103
4.2.2	Synthesis of Monodisperse Au Nanoparticles.	105
4.2.3	Synthesis of Ge Nanoparticles	108
4.3	Formation of Alloy and Pair Nanoparticles	110
4.3.1	Motivation and Synthesis Approach	110
4.3.2	Synthesis of Au-Ge Pair Nanoparticles	111
4.3.3	Synthesis of AuGe Alloyed Nanoparticles by Co-Sparking	114
4.4	Film Formation by Electrostatic Means.	116
	References	119

Part II Structure and Dynamics

5 Diffusion Enhancement in FePt Nanoparticles for L1₀ Stability 123

5.1 Introduction 123

5.2 Gas-Phase Preparation of FePt Nanoparticles 125

5.3 Diffusion Enhancement in FePt 129

5.3.1 Oxygen Mediated Destabilization of Twinned Structures 129

5.3.2 L1₀ Stabilization by Interstitial Nitriding–Denitriding 132

5.3.3 L1₀ Stabilization by the Mobility Enhancement of a Substitutional Element 135

5.4 Conclusion. 137

References 137

6 Simulation of Cluster Sintering, Dipolar Chain Formation, and Ferroelectric Nanoparticulate Systems 139

6.1 General Introduction 139

6.1.1 Methods 140

6.2 Molecular-Dynamics Simulations of the Dipolar-Induced Formation of Magnetic Nanochains and Nanorings. 142

6.3 Molecular-Dynamics Simulations of Metal Cluster Agglomeration and Sintering 146

6.3.1 Sintering of Nickel Nanoparticles. 146

6.3.2 Agglomeration of Icosahedral Iron Nanoparticles 150

6.4 Density Functional Simulations of Dielectric Nanoparticles: Agglomeration and Ferroelectric Trends 152

6.5 Summary 157

References 158

7 Nanopowder Sintering 161

7.1 Introduction 161

7.2 Particle Coalescence 163

7.2.1 Phenomenological Theory 164

7.2.2 Atomistic Modeling 167

7.2.3 Coalescence of Agglomerates. 168

7.2.4 Coalescence of Two Particles of Different Size 169

7.3 The Effect of Grain Boundaries 171

7.3.1 Rigid Body Dynamics Combined with KMC 173

7.3.2 Competition Between Reorientation and Neck Growth for Two Particles 174

7.3.3 Reorientation Effects in Porous Agglomerates 178

7.4	Conclusion and Outlook	180
	Appendix: Activation Energies Used in the KMC-RBD	
	Hybrid Model	181
	References	182
8	Material and Doping Contrast in III/V Nanowires Probed by Kelvin Probe Force Microscopy	185
8.1	Introduction	185
8.2	Instrumental Setup	187
8.3	Material and Doping Contrast in Single GaAs Based Nanowires	190
8.3.1	Material Transitions in Single GaAs Based Nanowires	190
8.3.2	KPFM on Single p-Doped GaAs Nanowires	194
8.3.3	Localization of Doping Transitions in Single p-Doped GaAs Nanowires	197
8.4	GaAs p-n Junction Nanowire Devices	200
8.5	Conclusion	204
	References	204
 Part III Properties and Applications		
9	Optical Properties of Silicon Nanoparticles	209
9.1	Introduction	209
9.2	Vibrational Properties	212
9.3	Recombination Dynamics	214
9.4	Electroluminescence	224
	References	228
10	Electrical Transport in Semiconductor Nanoparticle Arrays: Conductivity, Sensing and Modeling	231
10.1	Introduction	231
10.2	Principles of (Nano) Particle-Based Conduction Processes	233
10.3	Electrical Measurement of (Nano) Particle Arrays	235
10.3.1	Impedance Spectroscopy	235
10.3.2	Conductivity Measurements During Powder Compaction	236
10.4	Formation of Nanoparticle Arrays	237
10.4.1	Compaction of Nanoparticle Powders	237
10.4.2	Printing of Nanoparticle Thin Films	237
10.4.3	Molecular Beam-Assisted Deposition	239
10.5	Modeling of Electrical Transport in (Nano) Particulate Networks	241

10.5.1	How the Macroscopic Impedance Depends on Sample Geometry	243
10.5.2	A Simple Model for Current-Assisted Powder Compaction	246
10.6	Examples of Nanoparticle Array Conductivity and Sensitivity	250
10.6.1	Tin Dioxide	250
10.6.2	Tungsten Oxide	254
10.6.3	Zinc Oxide	259
10.6.4	Electrical Properties of Nanoscale Powders During Compaction	267
10.7	Conclusions	269
	References	270
11	Intrinsic Magnetism and Collective Magnetic Properties of Size-Selected Nanoparticles	273
11.1	Introduction	273
11.2	Structural Characterisation	276
11.2.1	Fe/Fe-Oxide Nanocubes	276
11.2.2	FePt Nanoparticles	277
11.3	Element-Specific, Site-Selective Magnetism	281
11.3.1	Influence of Local Composition and Crystal Symmetry on the Magnetic Moments	281
11.3.2	Magnetic Response of Fe on Different Lattice Sites in Fe/FeO _x Nanocubes	285
11.4	Spectro-Microscopy of Individual Nanoparticles	287
11.4.2	Magnetic Hysteresis and Spectroscopy of Monomers, Dimers, Trimers and Many Particle Configurations	288
11.5	Magnetisation Dynamics of Nanoparticle Ensembles	294
11.6	Summary	297
	References	298
12	Optical Spectroscopy on Magnetically Doped Semiconductor Nanoparticles	303
12.1	Introduction	303
12.2	Magnetically Doped ZnO Nanoparticles	304
12.2.1	ZnO Nanoparticles Doped with Chromium	305
12.2.2	ZnO Nanoparticles Doped with Cobalt	311
12.3	Magnetically Doped CdSe Nanoparticles	313
12.3.1	Characterization of Mn-Doped CdSe Nanoparticles	314
12.3.2	Exciton Magnetic Polaron Formation in Mn-Doped CdSe Nanoparticles	317

12.4	Conclusion	323
	References	324
13	Gas Sensors Based on Well-Defined Nanostructured Thin Films	329
13.1	Introduction	329
13.2	Experimental Details	330
13.3	Results and Discussion	334
13.3.1	Differential Mobility Analyser (DMA) Measurements	334
13.3.2	Sintering Behaviour of Generated SnO _x Nanoparticles	334
13.3.3	Synthesis of Monodispersed SnO _x , Pd and Ag Nanoparticles	335
13.3.4	Low Pressure Impaction (LPI)	336
13.3.5	Gas Sensor Preparation	338
13.3.6	Sensing Results on SnO _x : M Mixed Nanoparticle Layers	341
13.3.7	Pure Pd-Nanoparticle Layers for Concentration Specific H ₂ Sensing at Room Temperature	352
	References	354
14	III/V Nanowires for Electronic and Optoelectronic Applications	357
14.1	Introduction	357
14.2	Growth of III/V Nanowires	358
14.2.1	Vapour-Liquid-Solid Growth	359
14.2.2	InAs	361
14.2.3	GaAs	362
14.3	InAs Nanowire MISFET	370
14.3.1	Nanowire FET Design	370
14.3.2	Device Performance	372
14.4	Properties of GaAs Nanowire p-n Junction	375
14.4.1	Electrical Properties	375
14.4.2	Optoelectronic Properties	376
14.5	Conclusion	382
	References	382
15	Metal Oxide Thin-Film Transistors from Nanoparticles and Solutions	387
15.1	Introduction	387
15.2	Operation Principle of Thin-Film Transistors	389
15.3	TFTs with Semiconducting Metal Oxides	393

15.3.1	General Remarks	393
15.3.2	TFTs with Nanoparticles from a Carrier Gas Stream	394
15.3.3	TFTs with Nanoparticles from Dispersion	398
15.3.4	TFTs from Solutions (Liquid Precursors).	401
15.4	Summary	405
15.5	Conclusion.	406
	References	407
Index		411