

# Contents

## Part I Nanomaterials

<b>1</b>	<b>Introduction</b> . . . . .	3
	Sebastian Volz	
1.1	Nanostructures . . . . .	3
1.2	Scientific and Technological Stakes . . . . .	5
1.3	Physical Mechanisms . . . . .	8
1.3.1	Rarefaction, Surface Reflection and Transmission at Interfaces . . . . .	9
1.3.2	Confinement . . . . .	10
1.3.3	Densities of States and Dimensionality . . . . .	12
1.3.4	Non-Fourier Effects and Thermal Conductivity . . . . .	13
1.4	Conclusion . . . . .	15
	References . . . . .	15
<b>2</b>	<b>Nanostructures</b> . . . . .	17
	Patrice Chantrenne, Karl Joulain, and David Lacroix	
2.1	Introduction . . . . .	17
2.2	Modelling Heat Transfer . . . . .	18
2.2.1	The Physics of Phonon Transfer . . . . .	18
2.2.2	Semi-Analytic Models . . . . .	27
2.3	Nanofilms, Nanowires, and Nanotubes . . . . .	31
2.3.1	Deterministic Model: BTE and the Discrete Ordinate Method . . . . .	31
2.3.2	Statistical Model: BTE and the Monte Carlo Method . . . . .	33
2.3.3	Mechanical Model: Molecular Dynamics . . . . .	40
2.4	Comparison and Limitations of the Models . . . . .	49
2.4.1	Examples of Confinement in a Nanofilm . . . . .	50
2.4.2	Examples of Confinement in a Nanowire and a Nanotube . . . . .	54

2.5	Conclusion .....	57
	Appendix: Measuring Thermal Properties .....	58
	References .....	59
<b>3</b>	<b>Green's Function Methods for Phonon Transport Through Nano-Contacts</b> .....	<b>63</b>
	Natalio Mingo	
3.1	Introduction to Green's Functions for Lattice Thermal Transport ..	63
3.2	The Harmonic Problem .....	65
3.2.1	Dynamics of Non-Periodic Systems .....	65
3.2.2	The Heat Current .....	68
3.2.3	Different Formulas for the Transmission .....	71
3.2.4	Weak Coupling Limit: The Low Temperature Thermal Conductance of a Weak Junction .....	75
3.2.5	Upper Limits to Thermal Conductance, Entropy Flow, and Information Rates .....	77
3.3	The Anharmonic Problem .....	82
3.3.1	Many-Body Hamiltonian .....	82
3.3.2	The Heat Current .....	83
3.3.3	Computing the Interacting Phonon Green Functions .....	84
3.3.4	Another Formula for the Heat Current .....	89
3.3.5	Can We 'See' the Phonon Current? .....	90
3.4	Concluding Remarks .....	91
	References .....	93
<b>4</b>	<b>Macroscopic Conduction Models by Volume Averaging for Two-Phase Systems</b> .....	<b>95</b>
	Benoît Goyeau	
4.1	Introduction .....	95
4.2	Local Volume Averages .....	96
4.3	Averaged Equations .....	97
4.3.1	Local Thermal Equilibrium and the Single-Equation Model .....	99
4.3.2	Deviation Equations .....	100
4.3.3	Closure Problem .....	103
4.3.4	Closed Form .....	104
4.3.5	Local Thermal Non-Equilibrium .....	105
	References .....	105
<b>5</b>	<b>Heat Conduction in Composites</b> .....	<b>107</b>
	Jean-Yves Duquesne	
5.1	Microcomposites and Effective Media .....	107
5.1.1	Taking Averages .....	107
5.1.2	Particle Shell .....	110
5.1.3	Experimental Examples .....	114
5.2	Nanocomposites and Phonon Scattering .....	114
5.2.1	Limitations of Effective Medium Theories .....	114
5.2.2	Kinetic Theory of Heat Transport in Solids .....	115

5.2.3	Phonon Scattering by Particles	118
5.2.4	Example of a Pure Bulk Material	118
5.2.5	Example of a Disordered Alloy	120
5.3	Conclusion	122
	Appendix A. Demonstration of (5.7)	122
	Appendix B. Effective Medium and Interface Resistance	123
	Appendix C. Calculation Parameters for Scattering by Particles	125
	References	126
<b>6</b>	<b>Optical Generation and Detection of Heat Exchanges in Metal–Dielectric Nanocomposites</b>	<b>127</b>
	Bruno Palpant	
6.1	Optical Properties of Noble Metal Nanoparticles and Nanocomposite Media	128
6.1.1	Dielectric Function of Noble Metals	128
6.1.2	Optical Response of Nanocomposite Media	131
6.2	Thermo-Optical Response	132
6.2.1	Noble Metals	132
6.2.2	Nanocomposites	133
6.2.3	Calculation	134
6.3	Heat Exchange Dynamics	136
6.3.1	Athermal Regime and the Boltzmann Equation	136
6.3.2	Thermal Regime and the Three-Temperature Model	139
	References	147
<b>7</b>	<b>Mie Theory and the Discrete Dipole Approximation. Calculating Radiative Properties of Particulate Media, with Application to Nanostructured Materials</b>	<b>151</b>
	Franck Enguehard	
7.1	Introduction	151
7.2	Absorption and Scattering by a Particle of Arbitrary Shape and by a Population of Such Particles	153
7.2.1	Incident Electromagnetic Field, Poynting Vector, and Associated Power	153
7.2.2	Electromagnetic Fields Within and Scattered by the Particle	154
7.2.3	Extinction, Absorbed, and Scattered Power	155
7.2.4	Expressing the Extinction and Scattered Powers in Terms of the Incident and Scattered Electric Fields	157
7.2.5	Extinction, Absorption, and Scattering Cross-Sections. Associated Efficiencies and Scattering Phase Function	159
7.2.6	Directions of Propagation and Polarisation	160
7.2.7	Radiative Properties of a Population of Particles	162
7.3	Mie Theory	163
7.3.1	Analytic Solution to Mie's Electromagnetic Problem	163
7.3.2	Extinction and Scattering Cross-Sections. Scattering Phase Function	165

7.3.3	A Special Case: Rayleigh Scattering . . . . .	167
7.3.4	Numerical Considerations . . . . .	169
7.3.5	Radiative Response of a Population of Spherical Particles . . . . .	170
7.3.6	Application of Mie Theory to the Radiative Response of a Cloud . . . . .	173
7.4	Discrete Dipole Approximation (DDA) . . . . .	175
7.4.1	The Theory of the DDA . . . . .	176
7.4.2	Models for Polarisability . . . . .	187
7.4.3	Applying the Discrete Dipole Approximation . . . . .	191
7.5	Summary . . . . .	205
	Appendix: Analytical Solution of Mie's Electromagnetic Problem . . . . .	205
	References . . . . .	211
<b>8</b>	<b>Thermal Conductivity of Nanofluids . . . . .</b>	<b>213</b>
	Pawel Keblinski	
8.1	Introduction . . . . .	213
8.2	Excitement, Controversy, and New Physics . . . . .	214
8.2.1	Brownian Motion . . . . .	214
8.2.2	Interfacial Liquid Layer . . . . .	215
8.2.3	Interfacial Thermal Resistance . . . . .	216
8.2.4	Near Field Radiation . . . . .	216
8.2.5	Particle Clustering . . . . .	217
8.3	Discussion . . . . .	218
	References . . . . .	219
<b>Part II Nanosystems</b>		
<b>9</b>	<b>Nanoengineered Materials for Thermoelectric Energy Conversion . . . . .</b>	<b>225</b>
	Ali Shakouri and Mona Zebarjadi	
9.1	Introduction . . . . .	225
9.2	Thermoelectric Energy Conversion . . . . .	226
9.3	Theoretical Modelling . . . . .	230
9.3.1	Boltzmann Transport and Thermoelectric Effects . . . . .	230
9.3.2	Theory of Thermoelectric Transport in Multilayers and Superlattices . . . . .	233
9.3.3	Monte Carlo Simulation of Electron Transport in Thermoelectric Layers . . . . .	235
9.3.4	Non-Equilibrium Green Function for Thermoelectric Transport . . . . .	236
9.3.5	Phonon Transport . . . . .	237
9.3.6	Thermoelectric Transport in Strongly Correlated Systems . . . . .	238
9.3.7	Wave or Particle Picture for Electrons and Phonons? . . . . .	239
9.3.8	Why Is There a Trade-off Between Electrical Conductivity and Seebeck Coefficient? . . . . .	240
9.3.9	Low-Dimensional Thermoelectrics . . . . .	241

9.4	Thermionic Energy Conversion . . . . .	244
9.4.1	Vacuum Thermionic Energy Conversion . . . . .	244
9.4.2	Nanometer Gaps and Thermotunneling . . . . .	244
9.4.3	Inverse Nottingham Effect and Carbon Nanotube Emitters . . . . .	245
9.4.4	Single Barrier Solid-State Thermionic Energy Conversion . . . . .	246
9.4.5	Multilayer Solid-State Thermionic Energy Conversion . .	247
9.4.6	Conservation of Transverse Momentum in Thermionic Emission . . . . .	248
9.4.7	Electron Group Velocity and the Electronic Density of States . . . . .	249
9.4.8	Reversible Thermoelectrics . . . . .	251
9.5	Reduction of Phonon Thermal Conductivity . . . . .	251
9.5.1	Thermal Conductivity of Superlattices . . . . .	252
9.5.2	Thermal Conductivity of Nanowires . . . . .	255
9.6	Applications . . . . .	255
9.6.1	Heterostructure Integrated Thermoelectric/Thermionic Microrefrigerators on a Chip . . . . .	255
9.6.2	SiGe and SiGeC Superlattice Optimization . . . . .	262
9.6.3	Potential Metal/Semiconductor Heterostructure Systems .	264
9.6.4	InGaAlAs Embedded with ErAs Nanoparticles . . . . .	265
9.6.5	Metal/Semiconductor Multilayers Based on Nitrides . . .	270
9.7	Scaling up Production . . . . .	271
9.7.1	Thin-Film Power Generation Modules . . . . .	272
9.7.2	Optoelectronic and Electronic Applications . . . . .	273
9.8	System Requirements for Power Generation . . . . .	275
9.9	Graded Materials . . . . .	277
9.10	Characterization Techniques . . . . .	278
9.10.1	Cross-Plane Seebeck Measurement . . . . .	279
9.10.2	Transient $ZT$ Measurement . . . . .	280
9.10.3	Suspended Heater and Nanowire Characterization . . . . .	281
9.11	Thermoelectric/Thermionic vs. Thermophotovoltaics . . . . .	282
9.12	Ballistic Electron and Phonon Transport Effects . . . . .	283
9.13	Nonlinear Thermoelectric Effects . . . . .	285
9.14	A Refrigerator Without the Hot Side . . . . .	286
9.15	Conclusion . . . . .	287
	References . . . . .	287
<b>10</b>	<b>Molecular Probes for Thermometry in Microfluidic Devices . . . . .</b>	<b>301</b>
	Charlie Gosse, Christian Bergaud, and Peter Löw	
10.1	Microlaboratories and Heat Transfer Issues . . . . .	301
10.1.1	Historical Context . . . . .	301
10.1.2	Electrokinetic Separation . . . . .	302
10.1.3	DNA Amplification by PCR . . . . .	303
10.1.4	Thermodynamic and Kinetic Measurements . . . . .	305

10.2	Microfluidics and Thermometry .....	308
10.2.1	Electrical Methods .....	308
10.2.2	Non-Spectroscopic Optical Methods .....	309
10.2.3	Molecular-Probe-Related Methods .....	310
10.3	Thermosensitive Materials .....	311
10.3.1	Liquid Crystals .....	311
10.3.2	Polymers .....	315
10.3.3	Phospholipid Membranes .....	316
10.4	Kinetic Fluorescent Probes .....	317
10.4.1	Intramolecular Charge Transfer in Organic Molecules ...	319
10.4.2	Charge Transfer in Organometallic Complexes .....	320
10.4.3	Excimer Formation .....	322
10.4.4	Delayed Fluorescence .....	323
10.5	Thermodynamic Fluorescent Probes .....	324
10.5.1	Isomerisation Between Species in Their Ground State. General Features .....	325
10.5.2	Folding of Nucleic Acid Structures .....	326
10.5.3	Chromophore Complexation by Cyclodextrins .....	327
10.5.4	Acid–Base Reactions .....	328
10.5.5	Modification of the Coordination Sphere of Metallic Ions .....	329
10.5.6	Thermalisation Between Excited States. General Features and Examples .....	330
10.6	Procedures for Fluorescence Microscopy .....	331
10.6.1	Single-Wavelength Intensity Measurement .....	331
10.6.2	Ratiometric Intensity Measurement .....	332
10.6.3	Lifetime Measurement .....	333
10.7	Other Forms of Spectroscopy for Probing Thermodynamic Equilibria .....	333
10.7.1	Raman Spectroscopy .....	334
10.7.2	Nuclear Magnetic Resonance .....	334
10.8	Conclusion and Prospects .....	335
10.8.1	Fluorescent Probes .....	336
10.8.2	Microscopic Techniques .....	336
	References .....	337
<b>11</b>	<b>Cell Targeting and Magnetically Induced Hyperthermia .....</b>	<b>343</b>
	Etienne Duguet, Lucile Hardel, and Sébastien Vasseur	
11.1	Introduction .....	343
11.1.1	Nanomedicine. An Application of Nanoscience and Nanotechnology ...	343
11.1.2	An Incomplete and Complex Set of Requirements .....	344
11.2	In Vivo Applications of Nanoparticles .....	344
11.2.1	Nanoparticles in the Blood Compartment .....	344
11.2.2	Designing Particles with Extended Vascular Lifetime ...	345
11.2.3	Active Targeting by Coupling with Molecular Recognition Ligands .....	346

11.2.4	Alternatives to Active Targeting .....	347
11.2.5	Overview of Commercially Available and Forthcoming Formulations .....	348
11.2.6	Relative Importance of Toxicity .....	352
11.3	Magnetically Induced Hyperthermia .....	353
11.3.1	Therapeutic Advantages of Heat .....	353
11.3.2	Different Methods and Their Limitations .....	353
11.3.3	Mechanisms for Induction Losses in Magnetic Materials .....	354
11.3.4	Comparing Theory and Experiment .....	356
11.3.5	Physiological Constraints .....	357
11.3.6	Some Formulations Under Development or Undergoing Clinical Assessment .....	359
11.4	Short and Mid-Term Prospects .....	360
11.4.1	Mediators .....	361
11.4.2	Physics of Magnetic Dissipation Phenomena and Modelling the in Vivo Temperature Distribution ....	362
11.4.3	Targeting Strategies .....	362
11.4.4	System Applying the Alternating Magnetic Field .....	362
	References .....	363
<b>12</b>	<b>Accounting for Heat Transfer Problems in the Semiconductor Industry .....</b>	<b>367</b>
	Christian Brylinski	
12.1	Introduction .....	367
12.2	General Trends .....	368
12.2.1	Miniaturisation .....	368
12.2.2	Rising Frequencies .....	369
12.2.3	Heterogeneous Integration .....	370
12.3	Heat Transport .....	370
12.3.1	Heat Conduction .....	370
12.3.2	Microscopic Order in the Semiconductor .....	371
12.3.3	The Substrate .....	372
12.4	Problems and Predictions for the Main Chip Types .....	378
12.4.1	Components for Controlling Electrical Energy .....	378
12.4.2	Processor and Memory .....	381
12.4.3	Light-Emitting Components .....	383
12.4.4	Trends in Heat Transfer Features of Semiconductor Components in the Coming Decades ..	384
	References .....	385
<b>Part III Advanced Thermal Measurements at Nanoscales</b>		
<b>13</b>	<b>Photothermal Techniques .....</b>	<b>389</b>
	Gilles Tessier	
13.1	Introduction .....	389
13.1.1	Problems Specific to Structures Made by a Top-Down Approach .....	390
13.1.2	Thermorefectance and CCD Cameras .....	391

13.2	Thermoreflectance Imaging . . . . .	392
13.2.1	The Underlying Phenomenon . . . . .	392
13.2.2	Measurement Methods . . . . .	393
13.3	Thermoreflectance Under Visible Illumination . . . . .	395
13.3.1	Spectroscopy of $dR/dT$ . . . . .	395
13.3.2	Modelling . . . . .	396
13.3.3	Calibration . . . . .	398
13.4	Thermoreflectance Under Ultraviolet Illumination . . . . .	401
13.5	Thermoreflectance in the Near Infrared. Rear Face Imaging . . . . .	403
13.5.1	Near-Infrared Thermoreflectance with Laser Illumination . . . . .	403
13.5.2	Near-Infrared Thermoreflectance with Incoherent Illumination . . . . .	404
13.5.3	Improving Resolution with a Solid Immersion Lens . . . . .	405
	References . . . . .	407
<b>14</b>	<b>Thermal Microscopy with Photomultipliers and UV to IR Cameras . . . . .</b>	<b>411</b>
	Bernard Cretin and Benjamin Rémy	
14.1	Basic Physics . . . . .	412
14.1.1	Radiometry . . . . .	412
14.1.2	Black Body Emission and Planck's Law . . . . .	415
14.1.3	Short Wavelength Measurements. Photon Flux . . . . .	417
14.1.4	Random Nature of the Photon Flux . . . . .	419
14.1.5	Multispectral Measurements . . . . .	420
14.2	Measurement by Photomultiplier and UV to NIR Camera . . . . .	421
14.2.1	Principle of Photomultipliers and Cameras . . . . .	422
14.2.2	Experimental Setup for the UV Thermal Microscope . . . . .	425
14.2.3	Experimental Setup for the Silicon CCD Camera . . . . .	430
14.3	Conclusion . . . . .	436
	References . . . . .	437
<b>15</b>	<b>Near-Field Optical Microscopy in the Infrared Range . . . . .</b>	<b>439</b>
	Yannick De Wilde, Paul-Arthur Lemoine, and Arthur Babuty	
15.1	Introduction . . . . .	439
15.2	Resolution Limit in Conventional Microscopy . . . . .	441
15.3	Near-Field Microscopy . . . . .	444
15.3.1	Basic Idea . . . . .	444
15.3.2	Aperture SNOM . . . . .	445
15.3.3	Apertureless or Scattering SNOM . . . . .	448
15.4	Thermal Radiation STM . . . . .	456
15.4.1	Introduction . . . . .	456
15.4.2	TRSTM Setup and Operation . . . . .	457
15.4.3	First Example Application of TRSTM . . . . .	458
15.4.4	Prospects . . . . .	463
	References . . . . .	465



<b>16 PhotoThermal Induced Resonance.</b>	
<b>Application to Infrared Spectromicroscopy</b>	469
Alexandre Dazzi	
16.1 Infrared Spectroscopy and Microscopy	469
16.1.1 Optical Index and Absorption	469
16.1.2 Infrared Spectrometers	471
16.1.3 Confocal Microscopes	473
16.2 The PTIR Technique	475
16.3 Photothermoelastic Phenomena	477
16.4 Time Scales	477
16.5 Thermoelastic Deformation	481
16.6 AFM Contact Resonance Mode	482
16.7 Absorption Measurement by Contact Resonance	485
16.8 PTIR Lateral Resolution	488
16.8.1 Resolution of an Object Placed on a Surface	489
16.8.2 Resolution of a Buried Object	489
16.9 Experimental Illustration	492
16.9.1 Candida Albicans	492
16.9.2 Escherichia Coli and Its Bacteriophage T5	493
16.9.3 Ultralocalised Infrared Spectroscopy	494
16.9.4 Chemical Mapping at the Nanoscale	498
16.10 Conclusion	502
References	503
<b>17 Scanning Thermal Microscopy with Fluorescent Nanoprobes</b>	505
Lionel Aigouy, Benjamin Samson, Erika Saïdi, Peter Löw, Christian Bergaud, Jessica Labéguerie-Egéa, Carine Lasbruggas, and Michel Mortier	
17.1 Luminescence	505
17.1.1 Introduction to Luminescence	505
17.1.2 Effect of Temperature on Light Emission	507
17.2 Luminescent Materials Used in Thermometry	508
17.2.1 Organic Molecules. Intensity Variations	508
17.2.2 Materials Containing Rare Earth Ions	509
17.2.3 Materials Containing Transition Ions. Intensity Variations and Lifetimes	512
17.2.4 Semiconducting Quantum Dots. Intensity and Wavelength Variations	513
17.3 Development of a Scanning Fluorescent Probe for Temperature Measurements	515
17.3.1 Choice of Material. Reversibility	515
17.3.2 Making the Probes	516
17.3.3 Experimental Setup for Fluorescent SThM	518
17.4 Applications	519
17.4.1 Direct Current Measurements	520

17.4.2	Alternating Current Measurements . . . . .	527
17.4.3	Measuring Tip–Sample Heat Transfer . . . . .	531
17.5	Conclusion and Prospects . . . . .	533
	References . . . . .	533
<b>18</b>	<b>Heat Transfer in Low Temperature Micro- and Nanosystems . . . . .</b>	<b>537</b>
	Olivier Bourgeois	
18.1	Introduction . . . . .	537
18.2	Thermal Physics at Low Temperatures . . . . .	538
18.2.1	Equilibrium Thermodynamics . . . . .	539
18.2.2	Quasi-Steady State Nonequilibrium Heat Transfer . . . . .	544
18.3	Probing Thermal Properties by Electrical Measurements . . . . .	551
18.3.1	Thermometry . . . . .	551
18.3.2	Low Temperature Specific Heat Measurements at the Nanoscale . . . . .	555
18.3.3	Thermal Conductance Measurements on Nanoscale Samples . . . . .	559
18.4	Conclusions . . . . .	565
	References . . . . .	566
	<b>Index . . . . .</b>	<b>569</b>

Thermal Nanosystems and Nanomaterials

Volz, S. (Ed.)

2009, XX, 588 p. 50 illus., Hardcover

ISBN: 978-3-642-04257-7