

Contents

Preface XV

List of Contributors XIX

1	Polymer Nanocomposites: Synthesis, Microstructure, and Properties	1
	<i>Vikas Mittal</i>	
1.1	Introduction	1
1.2	Means of Synthesis and Microstructure	3
1.3	Importance of Thermogravimetric Analysis and X-Ray Diffraction for Filler and Nanocomposite Microstructure Characterization	6
1.4	Polar and Nonpolar Polymer Systems	9
1.5	Advances in Filler Surface Modifications	14
1.6	Prediction of Composite Properties	15
	References	17
2	Morphology Development in Thermoset Nanocomposites	21
	<i>Peter J. Halley</i>	
2.1	Introduction	21
2.2	Epoxy Nanocomposite Systems	22
2.3	Effects of Processing and Aging	27
2.4	Other Thermoset Nanocomposite Systems	30
2.5	Recent Advances in Thermoset Nanocomposites	33
2.5.1	Epoxy-HBP Nanostructured Systems	33
2.5.2	Ternary Nanostructured Systems and Multiscale Composites	34
2.5.3	Novel Characterization Methods	36
2.5.4	Modeling Thermoset Nanocomposite Systems	36
2.6	Summary	38
	References	38

3	Morphology and Interface Development in Rubber–Clay Nanocomposites	41
	<i>Yong-Lai Lu and Li-Qun Zhang</i>	
3.1	Introduction	41
3.2	Melt Compounding	42
3.2.1	Mechanism and Influencing Factors	42
3.2.1.1	The Organic Modification	43
3.2.1.2	The Features of Rubber and Compatibilizers or Coupling Agents	44
3.2.1.3	Melt-Compounding Conditions	44
3.2.2	Evolution of Morphology and Interface during Vulcanization of RCNs	44
3.2.2.1	Changes in the Local Microstructure of Clay Particles	44
3.2.2.2	Change in the Spatial Distribution of Clay Particles	45
3.3	Latex Compounding	57
3.3.1	Mechanism and Influencing Factors	57
3.3.2	Interface Enhancement	60
	References	65
4	Morphology Development in Polyolefin Nanocomposites	67
	<i>Mitsuyoshi Fujiyama</i>	
4.1	Introduction	67
4.2	Intercalation, Exfoliation, and Dispersion of MMT	68
4.2.1	Manufacturing Processes	68
4.2.2	Dispersion (Exfoliation) State of Nanoclays	69
4.2.3	Exfoliation Process of Nanoclays	72
4.2.4	Control of Exfoliation/Dispersion of Nanoclays	75
4.2.4.1	Raw Materials	75
4.2.4.2	Mixing Methods	78
4.2.4.3	Mixing Conditions	82
4.2.5	Morphology of Base Polymers	82
4.3	Crystallization and Crystalline Structure of Matrix Polymers	83
4.3.1	Crystallization	83
4.3.1.1	Quiescent Crystallization	83
4.3.1.2	Flow-Induced Crystallization	84
4.3.2	Crystalline Structure	84
4.3.2.1	Quiescent Crystallization	84
4.3.2.2	Flow-Induced Crystallization	86
4.4	Morphology Development in Processing	86
4.4.1	Injection Molding	87
4.4.1.1	Conventional Injection Molding	87
4.4.1.2	Dynamic Packing Injection Molding	88
4.4.2	Sheet Extrusion	89

4.4.3	Film Extrusion Casting	90
4.5	Conclusions	90
	References	91
5	Rheological Behavior of Polymer Nanocomposites	93
	<i>Mo Song and Jie Jin</i>	
5.1	Introduction	93
5.2	Rheological Behavior of Polymer Nanocomposites in Solution State	95
5.3	Rheological Behavior of Polymer Nanocomposites in Melt State	107
5.4	Conclusions	118
	References	119
6	Mechanical Property Enhancement of Polymer Nanocomposites	123
	<i>Nourredine Ait Hocine</i>	
6.1	Introduction	123
6.2	Material Stiffness	124
6.2.1	Experimental Investigations	124
6.2.2	Analytical Modeling	125
6.3	Ultimate Mechanical Properties	129
6.3.1	Experimental Investigations	129
6.3.2	Analytical Modeling	131
6.3.2.1	Yield Stress	131
6.3.2.2	Properties at Break	132
6.4	Conclusions	135
	References	136
7	Stress Transfer and Fracture Mechanisms in Carbon Nanotube-Reinforced Polymer Nanocomposites	139
	<i>Bhabani K. Satapathy, Martin Ganß, Petra Pötschke, and Roland Weidisch</i>	
7.1	Introduction	139
7.2	Experimental Studies	142
7.2.1	Fabrication of Composites	142
7.2.2	Morphology Characterization	142
7.2.2.1	Transmission Electron Microscopy (TEM)	142
7.2.2.2	Atomic Force Microscopy (AFM)	143
7.2.2.3	2-D Wide-Angle X-Ray Diffraction	143
7.2.3	Thermal Characterization	143
7.2.3.1	Differential Scanning Calorimetry	143
7.2.3.2	Dynamical Mechanical Analysis	143
7.2.3.3	Melt Rheological Investigations	144
7.2.4	Mechanical and Fracture Mechanical Investigations	144
7.2.4.1	Tensile Testing	144
7.2.4.2	Essential-Work-of-Fracture Approach	144

7.2.4.3	Kinetics of Crack Propagation Measurement Using a Single-Specimen Technique	145
7.3	Mechanical Behavior of Polymer Nanocomposites and Stress Transfer	145
7.3.1	Amorphous Thermoplastic	145
7.3.2	Semi-Crystalline Thermoplastic	149
7.4	Fracture Mechanics of CNT-Polymer Nanocomposites	156
7.4.1	Amorphous Thermoplastic	156
7.4.2	Semi-Crystalline Thermoplastic	162
7.5	Concluding Remarks	168
	Acknowledgments	169
	References	169
8	Barrier Resistance Generation in Polymer Nanocomposites	173
	<i>Vikas Mittal</i>	
8.1	Introduction	173
8.2	Theory of Permeation	174
8.3	Barrier Generation in Polar Nanocomposites	176
8.4	Barrier Generation in Nonpolar Nanocomposites	183
8.5	Modeling of Barrier Properties of Composites	189
	References	192
9	Mechanisms of Thermal Stability Enhancement in Polymer Nanocomposites	195
	<i>Krzysztof Pielichowski, Agnieszka Leszczyńska, and James Njuguna</i>	
9.1	Introduction	195
9.2	The Mechanisms of Thermal Stability Improvement by Different Nanofillers	196
9.2.1	Clay Minerals	196
9.2.1.1	Barrier Effect	196
9.2.1.2	Restricted Thermal Motions	198
9.2.1.3	Char Forming and Catalytic Effects	198
9.2.1.4	Radical Trapping and Sorption Mechanisms	201
9.2.2	Carbonaceous Nanofillers	202
9.2.2.1	Carbon Nanotubes and Carbon Nanofibers	202
9.2.2.2	Carbon Black	205
9.2.2.3	Fullerenes	205
9.2.2.4	Graphite	205
9.2.3	Silica-Based Nanofillers	205
9.2.3.1	Silica Oxide	205
9.2.3.2	Polyhedral Oligomeric Silsesquioxane	206
9.2.4	Metals and Metal Oxides	206
9.2.5	Other Fillers	207
9.3	Concluding Remarks	207
	References	208

10	Mechanisms of Tribological Performance Improvement in Polymer Nanocomposites	211
	<i>Ga Zhang and Alois K. Schlarb</i>	
10.1	Introduction	211
10.2	Nanoparticle Reinforcements	213
10.2.1	Improvement of Wear Performance by Using Nanoparticles	214
10.2.2	Roles of Nanoparticles on Transfer Film Formation	214
10.2.3	Structure–Tribological Property Relationships	215
10.2.3.1	Effect of Grafting Treatment of Nanoparticles on Tribological Improvement of Epoxy Nanocomposites	217
10.2.3.2	Role of Nano-SiO ₂ Particles on the Mechanical and Tribological Behaviors of PEEK	218
10.3	Carbon Nanotubes	223
10.4	Synthetic Roles of Nanoparticles with Traditional Fillers	226
10.4.1	Tribological Behavior of Traditional and Nanofillers (or Sub-Micro)-Filled Epoxy	226
10.4.2	Roles of Nanoparticles on the Tribological Behavior of SCF/PTFE/Graphite-Filled PEEK	227
	References	233
11	Mechanisms of Biodegradability Generation in Polymer Nanocomposites	235
	<i>Mitsuhiko Shibata</i>	
11.1	Introduction	235
11.2	PBAT Nanocomposites	237
11.2.1	Preparation and Morphology of PBAT Nanocomposites	237
11.2.2	Mechanical Properties of PBAT Nanocomposites	241
11.2.3	Thermal Properties of PBAT Nanocomposites	243
11.2.4	Biodegradability of PBAT Nanocomposites	244
11.3	PBS Nanocomposites	245
11.3.1	Preparation and Morphology of PBS Nanocomposites	245
11.3.2	Mechanical Properties of PBS Nanocomposites	248
11.3.3	Thermal Properties of PBS Nanocomposites	252
11.3.4	Biodegradability of PBS Nanocomposites	253
11.4	Conclusions	256
	References	258
12	Self-Healing in Nanoparticle-Reinforced Polymers and other Polymer Systems	261
	<i>Stephen J. Picken, Steven D. Mookhoek, Hartmut R. Fischer, and Sybrand van der Zwaag</i>	
12.1	Introduction	261
12.2	Microstructured Self-Healing Polymer Structures	264
12.2.1	Liquid-Based Self-Healing Thermosetting Polymers	264
12.2.2	Liquid-Based Self-Healing Thermoplastic Polymers	265

12.2.3	Geometric Aspects in Encapsulation	265
12.3	Nanoparticle-Reinforced Self-Healing Polymer Systems	270
12.3.1	Modeling the Modulus of Nanoparticle-Filled Polymers	270
12.3.2	Experimental Validation for Non-Self-Healing Systems	273
12.3.3	Design of a Self-Healing Nanoparticle Composite	274
12.4	Concluding Remarks	277
	Acknowledgments	277
	References	277
13	Crystallization in Polymer Nanocomposites	279
	<i>Jyoti Jog</i>	
13.1	Introduction	279
13.2	Nanofillers	280
13.2.1	Silicates	280
13.2.2	Carbon Nanotubes	281
13.2.3	Exfoliated Graphite	281
13.2.4	Other Nanoparticles	282
13.3	Isothermal and Nonisothermal Crystallization in Polymers	282
13.3.1	Polypropylene (PP)	283
13.3.1.1	Crystallization	283
13.3.1.2	Polymorphism in PP	285
13.3.2	Poly-1-Butene (PB)	285
13.3.3	Polybutylene Terephthalate (PBT)	286
13.3.4	Polyethylene Terephthalate (PET)	287
13.3.5	Poly Trimethylene Terephthalate (PTT)	288
13.3.6	Polyethylene Naphthalate (PEN)	288
13.3.6.1	Crystallization	288
13.3.6.2	Polymorphism in PEN	289
13.3.7	Polylactic Acid (PLLA)	289
13.3.8	Polyhydroxy Alkonate (PHA)	290
13.3.9	Polyether Ether Ketone (PEEK)	290
13.3.10	Nylon 6	291
13.3.10.1	Crystallization	291
13.3.10.2	Polymorphism in Nylon 6	292
13.3.11	Nylon 66	293
13.3.11.1	Crystallization	293
13.3.11.2	Polymorphism in Nylon 66	293
13.3.12	Nylon 11	293
13.3.13	Nylon 10,10	294
13.3.14	Polyvinylidene Fluoride (PVDF)	294
13.3.14.1	Crystallization	294
13.3.14.2	Polymorphism in PVDF	294
13.3.15	Syndiotactic Polystyrene (sPS)	295

13.3.15.1	Crystallization	295
13.3.15.2	Polymorphism in sPS	296
13.4	Conclusions	296
	References	297
14	Prediction of the Mechanical Properties of Nanocomposites	301
	<i>Qinghua Zeng and Aibing Yu</i>	
14.1	Introduction	301
14.1.1	Nanocomposites	301
14.1.2	Some Issues in Nanocomposites	301
14.1.2.1	Dispersion of Nanoparticles	301
14.1.2.2	Interface	303
14.1.2.3	Crystallization	303
14.1.3	Property Predictions	304
14.2	Analytical and Numerical Techniques	305
14.2.1	Analytical Models	305
14.2.1.1	Rule of Mixtures	305
14.2.1.2	Halpin–Tsai Model	306
14.2.1.3	Mori–Tanaka Model	306
14.2.1.4	Equivalent-Continuum Approach	307
14.2.1.5	Self-Similar Approach	307
14.2.2	Numerical Methods	307
14.2.2.1	Molecular Dynamics	308
14.2.2.2	Monte Carlo	309
14.2.2.3	Brownian Dynamics	309
14.2.2.4	Dissipative Particle Dynamics	310
14.2.2.5	Lattice Boltzmann	310
14.2.2.6	Time-Dependent Ginzburg–Landau Method	311
14.2.2.7	Dynamic Density Functional Theory	311
14.2.2.8	Finite Element Method	312
14.2.2.9	Boundary Element Method	312
14.2.3	Multiscale Modeling	313
14.2.3.1	Challenges	313
14.2.3.2	Sequential and Concurrent Approaches	313
14.2.3.3	Applications in Polymer Nanocomposites	314
14.3	Prediction of Nanocomposite Properties	314
14.3.1	Mechanical Properties	316
14.3.1.1	Stiffness and Strength	316
14.3.1.2	Stress Transfer	320
14.3.1.3	Mechanical Reinforcement	321
14.3.1.4	Interfacial Bonding	323
14.3.1.5	Viscoelasticity	323
14.3.2	Mechanical Failure	324
14.3.2.1	Buckling	324

14.3.2.2	Fatigue	325
14.3.2.3	Fracture	325
14.3.2.4	Wear	326
14.3.2.5	Creep	327
14.4	Conclusions	327
	Acknowledgments	328
	References	329
15	Morphology Generation in Polymer Nanocomposites Using Various Layered Silicates	333
	<i>Kenji Tamura and Hirohisa Yamada</i>	
15.1	Introduction	333
15.2	Aspects of Layered Silicates	334
15.2.1	General Structure	334
15.2.2	Various Types of Layered Silicates	335
15.3	Conventional Layered Silicate Polymer Nanocomposites using Smectite and Expandable Synthetic Fluoro-Mica	338
15.3.1	Relationship Between Morphology and Properties	338
15.3.2	Properties of Conventional Layered Silicate/Polymer Nanocomposites	339
15.4	Aspect Ratio Variation Using Various Layered Silicates	344
15.4.1	Exfoliation of High Crystallinity Nonexpandable Mica	344
15.4.2	Controlling the Number of Nanolayers (in the Dispersed Platelets): Interstratified Layered Silicate/Polymer Nanocomposites	347
15.5	Summary	348
	References	349
16	Thermomechanical Properties of Nanocomposites	351
	<i>Lucia Helena Innocentini-Mei</i>	
16.1	Introduction	351
16.2	Thermomechanical Analysis	352
16.3	Dynamic Mechanical Analysis and the Principle of Time-Temperature Superposition	354
16.4	Nanoclays and Their Influence on the Thermomechanical Properties of Polymer Composites: Some Case Studies	355
16.5	Conclusions	366
	References	367
17	Effect of Processing Conditions on the Morphology and Properties of Polymer Nanocomposites	369
	<i>Michele Modesti, Stefano Besco, and Alessandra Lorenzetti</i>	
17.1	Introduction	369
17.2	Melt-Intercalation of Polymer Nanocomposite Systems	370
17.2.1	Melt Intercalation of Polymer/Clay Systems	370
17.2.1.1	Effects of Temperature, Shear, and Residence Time	370

- 17.2.1.2 Effects of Extruder Configuration and Screw Profiles 374
- 17.2.1.3 Effect of Processing Route 377
- 17.2.2 Melt-Intercalation of Polymer/CNT Systems 378
- 17.3 Solution-Intercalation of Polymer Nanocomposites 380
- 17.4 Progress in Polymer Nanocomposites Processing 385
 - 17.4.1 Water Injection-Assisted Melt-Compounding 385
 - 17.4.2 Supercritical CO₂-Assisted Melt-Compounding 388
 - 17.4.3 Ultrasound-Assisted Melt-Compounding 391
- 17.5 Processing of Thermoset Nanocomposites 394
- 17.6 Conclusions 399
- References 400

Index 407

