

WILEY-VCH

Edited by Vera V. Myasoedova, Sabu Thomas,
and Hanna J. Maria

Chemical Physics of Polymer Nanocomposites

Processing, Morphology, Structure,
Thermodynamics, Rheology

Volumes 1–3



Chemical Physics of Polymer Nanocomposites

Chemical Physics of Polymer Nanocomposites

Processing, Morphology, Structure, Thermodynamics,
Rheology

Volume I

Edited by

Vera V. Myasoedova, Sabu Thomas, and Hanna J. Maria

Editors

Prof. Vera V. Myasoedova

Semenov Federal Research Center
for Chemical Physics
119991, Moscow, Kosygin Str., 4
Russia

Dr. Sabu Thomas

Mahatma Gandhi University
Priyadarshini Hills
Kottayam, Kerala
India

Dr. Hanna J. Maria

Mahatma Gandhi University
Priyadarshini Hills
Kottayam, Kerala
India

Cover Image: © BAIVECTOR/
Shutterstock

■ All books published by **WILEY-VCH** are carefully produced. Nevertheless, authors, editors, and publisher do not warrant the information contained in these books, including this book, to be free of errors. Readers are advised to keep in mind that statements, data, illustrations, procedural details or other items may inadvertently be inaccurate.

Library of Congress Card No.: applied for

British Library Cataloguing-in-Publication Data

A catalogue record for this book is available from the British Library.

Bibliographic information published by the Deutsche Nationalbibliothek The Deutsche Nationalbibliothek lists this publication in the Deutsche Nationalbibliografie; detailed bibliographic data are available on the Internet at <<http://dnb.d-nb.de>>.

© 2024 WILEY-VCH GmbH, Boschstraße 12,
69469 Weinheim, Germany

All rights reserved, including rights for text and data mining and training of artificial technologies or similar technologies (including those of translation into other languages). No part of this book may be reproduced in any form – by photoprinting, microfilm, or any other means – nor transmitted or translated into a machine language without written permission from the publishers. Registered names, trademarks, etc. used in this book, even when not specifically marked as such, are not to be considered unprotected by law.

Print ISBN: 978-3-527-35163-3

ePDF ISBN: 978-3-527-83700-7

ePub ISBN: 978-3-527-83701-4

oBook ISBN: 978-3-527-83702-1

Typesetting Straive, Chennai, India

We would like to dedicate Chapter 27 to Prof. Akhilesh Rai.

Contents

Volume I

Preface *xvii*

- 1 Classification of Nanofillers, Nano-Objects, Nanomaterials, and Polymer Nanocomposites Based on Chemical Nature and Identity 1**
Lan Chen
 - 1.1 Classification of Nanocomposites 1
 - 1.2 Classification of Nanofillers 2
 - 1.3 Classification of Nano-Objects and Nanomaterials 3
 - 1.4 Production Method and Existing Form of Nano-Objects 6
 - 1.5 Classification of Polymer Nanocomposites 9
 - 1.6 Summaries 12List of Abbreviations 13
References 13

- 2 Biological and Chemical Synthesis of Nanoparticles 15**
Atta Ullah Khan, Abdul Waris, Doaa Zamel, Vestince Balidi Mbayachi, Abdul Muhaymin, Ammara Safdar, Zarfashan Shahid, Mohammed Al Dalawi, Umm y Umna, and Maria Khalil
 - 2.1 Introduction 15
 - 2.2 Synthesis Approach of Nanoparticles 16
 - 2.2.1 Bottom-Up Approach 16
 - 2.2.1.1 Non-Biological Synthesis of Nanoparticles 18
 - 2.2.2 Top-Down Approach 19
 - 2.2.2.1 Spinning Methods 19
 - 2.2.2.2 Template Based Synthesis 20
 - 2.2.2.3 Chemical Vapor Deposition 21
 - 2.2.2.4 Laser Pyrolysis Synthesis of Nanoparticles 22
 - 2.2.2.5 Flame Spray Pyrolysis Synthesis of Nanoparticles 25
 - 2.2.2.6 Inert Gas Condensation 26
 - 2.2.2.7 Laser Ablation 27
 - 2.2.2.8 Mechanical Milling 28

2.2.2.9	Chemical Etching	29
2.2.2.10	Electro-Explosion of Wire	29
2.2.3	Biological Synthesis of Nanoparticles	30
2.2.3.1	Bacteria Mediated Nanoparticles	30
2.2.3.2	Fungi Mediated Nanoparticles	31
2.2.3.3	Yeasts Mediated Nanoparticles	31
2.2.3.4	Algae Mediated Nanoparticles	31
2.2.3.5	Plant-Mediated Nanoparticles	32
2.3	Conclusion	33
	List of Abbreviations	33
	References	33
3	Using In situ Polymerization for Manufacturing of Polymer Nanocellulose	45
	<i>Stephen Chinenyeze Agwuncha, Chukwu Felix Oyemaechi, Chioma Grace Anusionwu, Tochukwu Perpetua Okonkwo, Osemudiamhen Destiny Amienghemhen, and Mamookho Elizabeth Makhatha</i>	
3.1	Introduction	45
3.2	<i>In situ</i> Polymerization	46
3.3	Cellulose Nanoparticles	48
3.4	Polymer Nanocellulose	48
3.5	Method of Polymer Nanocomposite Processing	50
3.5.1	Solvent Casting and Evaporation	51
3.5.2	Coating Polymerization Process	52
3.5.3	Melt Processing	53
3.5.4	Radical Polymerization	53
3.5.5	Other Methods	54
3.6	Applications of <i>In situ</i> Polymerization Methods for the Production of Nanocellulose Materials	54
3.7	Future of <i>In situ</i> Polymerization Manufacturing Processes	57
3.8	Conclusion	57
	List of Abbreviations	58
	References	58
4	Manufacturing of Nanocomposites by Electrospinning	67
	<i>Fariborz Sharifanajazi, Amirhossein Esmailkhanian, Mehdi Reisi Nafchi, Leila Bazli, Poursan Pourhakkak, Hosein Rostamani, Mohammad Yusuf, Zahra Moazzami Goudarzi, Samad Khaksar, and Ali Farahani</i>	
4.1	Introduction	67
4.2	Electrospinning Process	68
4.2.1	Principles of the Process	68
4.2.2	Solution Parameters	70
4.2.2.1	Concentration and Viscosity of Solution	70
4.2.2.2	Surface Tension	70

4.2.2.3	Conductivity of Solution	71
4.2.2.4	Polymer Molecular Weight	71
4.2.2.5	Addition of Inorganic Components	71
4.2.2.6	Applied Voltage	72
4.2.2.7	Receiving Distance	72
4.2.2.8	Feed Rate	72
4.2.2.9	Electrospinning Type/Principle/Spinneret	73
4.2.2.10	Receiver Morphology/Specification	73
4.2.3	Environmental Parameters	73
4.2.3.1	Temperature	73
4.2.3.2	Humidity	74
4.3	Fiber Type	74
4.3.1	Organic Polymers (Natural Polymers, Synthetic Polymers)	74
4.3.1.1	Natural Polymers	74
4.3.1.2	Synthetic Polymers	75
4.3.2	Inorganic Materials	75
4.3.2.1	Carbon Nanofibers	76
4.3.2.2	Metal Oxide Nanofibers	76
4.3.2.3	Metal Nanofibers	76
4.4	Electrospinning of Nanocomposite	77
4.4.1	Polymer/Polymer	77
4.4.2	Polymer/Inorganic	77
4.4.3	Inorganic/Inorganic	78
4.5	Application	79
4.5.1	Filtration	79
4.5.2	E-spun Nanofibers for Hazardous Substances Adsorption	80
4.5.3	E-spun Nanofibers for Bioengineering Separation	80
4.5.4	E-spun Nanofibers for Insulation	81
4.5.5	Medical/Biological Applications	81
4.5.6	Catalysis	82
4.5.7	Energy Conversion and Storage	82
4.5.8	Triboelectric Nanogenerator	83
4.6	Summary and Outlook	83
	References	83
5	Polymer Nanocomposites Based on Metal Oxide Nanoplatelets	95
	<i>Usisipho Feleni, Xolile Godfrey Fuku, and Kutloano Edward Sekhosana</i>	
5.1	Introduction	95
5.2	Polymers	95
5.2.1	Polymer Structure	96
5.2.2	Design Approaches to Polymers	97
5.2.2.1	Surface-initiated Atom-Transfer Radical Polymerization (SI-ATRP)	98
5.2.2.2	Surface-initiated Reversible Addition–Fragmentation Chain-Transfer (SI-RAFT) Strategy	99

5.3	Properties of Nanoplatelets (NPLs)	99
5.3.1	Applications of Nanoplatelets	101
5.4	Polymer–Metal Oxide Nanocomposite Materials	104
5.4.1	Properties of Polymer–Metal Oxide Nanocomposites	105
5.4.1.1	Electrical Properties	105
5.4.1.2	Optical Properties	106
5.4.1.3	Thermal Properties	107
5.4.1.4	Mechanical Properties	107
5.4.2	Designs of Polymer–Metal Oxide Composites	108
5.4.3	Synthesis Methods of Polymer–Metal Oxide Composites	109
5.4.3.1	Blending/Mixing	109
5.4.3.2	In situ polymerization	110
5.4.3.3	Sol–Gel Process	111
5.5	General Applications of Polymer–Metal Oxide Composites	112
5.5.1	Applications of Polymer–Metal Oxide Composites in Sensors	112
5.5.2	Applications of Polymer–Metal Oxide Composites in Supercapacitors	113
5.6	Conclusion	116
	Acknowledgments	117
	References	117
6	Polymer Nanocomposites Filled in Carbon Nanotubes: Properties and Applications	133
	<i>Natália Ferreira Braga, Erick Gabriel Ribeiro dos Anjos, Nayara Koba de Moura, Thais Ferreira da Silva, and Fabio Roberto Passador</i>	
6.1	Introduction	133
6.1.1	Polymer Nanocomposites	133
6.1.2	Carbon Nanotubes	135
6.1.2.1	Functionalization of CNTs	138
6.1.3	Potential Uses of CNT-based Polymer Nanocomposites	139
6.1.4	Some Examples of Thermoplastics Used as Nanocomposite Matrix	141
6.1.4.1	Poly (Trimethylene Terephthalate)	141
6.1.4.2	Acrylonitrile Butadiene Styrene	142
6.1.4.3	Polycarbonate	143
6.1.4.4	Poly (Lactic Acid)	144
6.2	Experimental Section: Production of Nanocomposites Filled CNT	144
6.2.1	CNT Functionalization	144
6.2.2	Polyester-based CNT Nanocomposites: PTT/CNT	145
6.2.3	Blend-based CNT Nanocomposites: PTT/ABS/CNT	145
6.2.4	Blend-based CNT Nanocomposites: PC/ABS/CNT	145
6.2.4.1	Injection Molding Process	145
6.2.5	Mechanical, Electrical Characterization and Morphology	146
6.3	Results and Discussion	146
6.3.1	CNT Functionalization	146

- 6.3.2 Electrical and Mechanical Properties of CNT/Polymer Nanocomposites 147
- 6.3.3 Electrical and Mechanical Properties of Polymer Blends-based CNT Nanocomposites 150
 - 6.3.3.1 PTT/ABS/MWCNT Films 151
 - 6.3.3.2 PC/ABS/MWCNT Injection Molded Samples 152
- 6.4 Conclusions 153
 - Acknowledgments 153
 - List of Abbreviations 154
 - References 155
- 7 Polymer Nanocomposites Filled in Nanocellulose and Cellulose-whiskers 165**
Marcelo Bruno de Oliveira Silva, Paulo Henrique Camani, and Derval dos Santos Rosa
 - 7.1 Introduction 165
 - 7.2 Nanocellulose: Extraction, Types, and Application 166
 - 7.3 Polymers Nanocomposites 169
 - 7.3.1 Thermoplastic 169
 - 7.3.2 Thermosetting 172
 - 7.3.3 Elastomers 174
 - 7.4 Nanocellulose Nanocomposite Applications 175
 - 7.5 Processing: Different Approaches and Dispersion Methods of Nanocellulose 178
 - 7.6 Future Trends and Perspectives 183
 - Acknowledgments 185
 - List of Abbreviations 185
 - References 186
- 8 Polymer Nanocomposites Based on Nano Chitin 199**
Jun-ichi Kadokawa
 - 8.1 Introduction 199
 - 8.2 Top-Down Approach for the Preparation of Nanochitins 201
 - 8.3 Top-Down Approach for the Preparation of Nanochitin/Polymer Composites 205
 - 8.4 Bottom-Up Approach for the Preparation of Nanochitins 210
 - 8.5 Bottom-Up Approach for the Preparation of Nanochitin/Polymer Composites 213
 - 8.6 Conclusions 219
 - Acknowledgment 220
 - References 220
- 9 Nanostarch-Filled Polymer Nanocomposites 229**
Paula Gonzalez-Seligra, Lucía M. Quintero-Borregales, Laura Ribba, Lucía Famá, and Silvia Goyanes
 - 9.1 Introduction 229

9.2	Nanostarch	230
9.2.1	Starch Nanocrystals (SNCs)	231
9.2.2	Amorphous Starch Nanoparticles (SNPs)	233
9.2.3	Nanostarch Functionalization	234
9.3	Nanostarch-Filled Nanocomposites from Synthetic Polymers	235
9.4	Nanostarch-Filled Nanocomposites from Natural Polymers	237
9.4.1	Nanostarch-Filled Starch-Based Nanocomposites	240
9.4.1.1	Applications of Nanostarch–Starch Nanocomposites in Food Packaging	244
9.5	Regulatory Aspects	245
9.6	Summary and Future Perspectives	246
	List of Abbreviations	247
	References	247

10 Polymer Nanocomposites Based on Nanolignin: Preparation, Properties, and Applications 257

Vidhukrishnan Naiker, Meera Balachandran, P.S. Sari, Mrudul Vijay Supekar, Peter Samora Owuor, Vijay Kumar Thakur, Ramiro Rafael Ruiz-Rosas, and Prasanth Raghavan

10.1	Introduction	257
10.2	Extraction of Lignin	259
10.3	Preparation of Nanolignin and Lignin Nanoparticles	259
10.3.1	Antisolvent Precipitation	261
10.3.1.1	Acid Solution as Antisolvent	261
10.3.1.2	Supercritical CO ₂ as Antisolvent	261
10.3.2	Physiochemical Preparation of Lignin Nanoparticles	262
10.3.2.1	Homogenization	263
10.3.2.2	Ultrasonication	263
10.3.3	Ice Segregation-induced Self-assembly	263
10.3.4	Electrospinning of Solutions	264
10.3.5	Aerosol Flow Synthesis	264
10.4	Properties of Nanolignin	265
10.5	Nanolignin Based Nanocomposites	266
10.5.1	Thermoplastic–Lignin Nanocomposites	266
10.5.2	Thermoset–Lignin Nanocomposites	269
10.5.2.1	Formaldehyde-Based Thermoset–Lignin Nanocomposite	269
10.5.2.2	Epoxy-Based Thermoset–Lignin Nanocomposite	271
10.5.3	Elastomer–Lignin Nanocomposites	272
10.5.3.1	Natural Rubber-Based Elastomer–Lignin Nanocomposite	273
10.5.3.2	Synthetic Rubber-Based Elastomer–Lignin Nanocomposite	274
10.6	Applications of Nanolignin and Lignin Nanocomposites	276
10.6.1	Antibacterial Effect	277
10.6.2	Reinforcing Materials	278
10.6.3	Anti-ultraviolet Effect	279
10.6.4	Food Packaging Films	280

- 10.6.5 Green Synthesis of Phenol-formaldehyde 280
- 10.6.6 Lignin Composite Foam 281
- 10.6.7 Future Trends 283
- 10.7 Conclusions 283
- References 283

- 11 Polymer Nanocomposites Based on Talc 295**
Luciana A. Castillo and Silvia E. Barbosa
- 11.1 Introduction 295
- 11.2 Talc 298
- 11.2.1 General Aspects 298
- 11.2.2 Geology 301
- 11.3 Talc/Polymer Nanocomposites Compounding 303
- 11.4 Influence of Talc Characteristics and Concentration on Polymer Nanocomposites Properties 306
- 11.4.1 Particle Morphology 308
- 11.4.2 Particle Size 318
- 11.4.3 Degree of Purity 319
- 11.4.4 Nucleating Capability 320
- 11.4.5 Particle Concentration 321
- 11.5 Chemical Modifications of Talc 322
- 11.6 Influence of Talc Surface Treatments on Polymer Nanocomposites Properties 324
- 11.7 Industrial Applications 328
- 11.8 Concluding Remarks 330
- References 331

Volume II

Preface xvi

- 12 Polymer Nanocomposites Based on Graphene and Graphene Oxide 343**
Eduardo A. Takara, Claudio F. Jofre, Sofia V. Piguillem, María L. Scala-Benuzzi, Julio Raba, Franco A. Bertolino, Sirley V. Pereira, and Germán A. Messina

- 13 Polymer Nanocomposites Based on Nano Alumina 373**
Christian Chapa González

- 14 Polymer Nanocomposites Based on Nano Magnesium Hydroxide 423**
Yue Zhang, Haotian Wu, Wuxiang Zhang, and Fu Yang

- 15 Polymer Nanocomposites Based on Nanosilica 471**
Vadim V. Potapov and Roman S. Fediuk

- 16 Polymer Nanocomposites Based on Quantum Dots 561**
Shiliang Mei, Dan Yang, Zhongjie Cui, Haiyang He, Bobo Yang, and Ruiqian Guo
- 17 Decorated Carbon Nanotube/Polymer Nanocomposites 589**
Wei Wu, Bin Yu, Hui Zhao, Yi-Zhang Tong, Cheng-Fei Cao, Yang Liu, and Zhao-Xia Huang
- 18 Graphene-Based Polymer Nanocomposites 623**
Ali Raza, Asma Rafiq, Usman Qumar, and Muhammad Ikram
- 19 Decorated Quantum Dot Polymer Nanocomposites 651**
Shiliang Mei, Haiyang He, Zhongjie Cui, Dan Yang, Bobo Yang, and Ruiqian Guo
- 20 Decorated Clays for Polymer Nanocomposites 679**
Grażyna Simha Martynková, Karla Čech Barabaszová, Marianna Hundáková, Lenka Klecandová, Sylva Holešová, Jana Kupková, and Gabriela Kratošová
- Volume III**
Preface xv
- 21 Decorated Nanocellulose-Polymer Nanocomposites 711**
T.C. Mokhena, J.E. Andrew, A. Mtibe, P. Matabola, S. Nyembe, G. Ndlovu, M.J. Mochane, and S.S. Ray
- 22 Advantage of Polymer Nanocomposite for Biomedical Application 739**
Rabiatul Basria S. M. N. Mydin, Wan Nuramiera Faznie Wan Eddis Effendy, Nor Hazliana Harun, and G. Ambarasan Govindasamy
- 23 Recycling of Polymer Nanocomposites. Plastic e-waste Case Study 759**
Yamila V. Vazquez and Silvia E. Barbosa
- 24 Life Cycle Analysis of Polymer Nanocomposites 775**
Mylene Cadete, Sofia Rocha, Yiyun Wu, Maria Fonseca, and Victor Neto
- 25 Lab to Industry 797**
Haneen Hassan, Amal Elhussieny, and Irene S. Fahim
- 26 Electrical Properties of Nanocomposite Polymer Electrolytes and their Energy Storage Applications 815**
Lee Tian Khoon and Nurul Akmaliah Dzulkurnain

**27 Advanced Polymeric Nanoparticles for the Treatment of
Neurodegenerative Diseases 843**

Rafaela Ferrão and Akhilesh Rai

**28 Recent Advances in the Chemorheological Behavior of
Biobased Polyurethane Nanocomposites 887**

Chiacchiarelli Leonel Matías

29 Self-healing Stretchable Composite Conductors 919

Kyuha Park and Donghee Son

**30 Graphene/Polymer Nanocomposites for Electrical
Applications 955**

Imadeddine Benfridja, Sombel Diaham, and Tadhg Kennedy

Index 991

Preface

In this comprehensive volume titled “*Chemical Physics of Polymer Nanocomposites: Processing, Morphology, Structure, Thermodynamics, Rheology*,” we embark on an exploration of the captivating domain of polymer nanocomposites – a realm where the convergence of materials science, chemistry, and physics opens doors to limitless possibilities.

Within these pages, readers will find a treasure trove of knowledge crafted by experts from across the globe. Each chapter is a testament to the collective wisdom of eminent scholars and researchers, offering unique insights into the synthesis, characterization, manufacturing techniques, and diverse applications of polymer nanocomposites.

As we navigate through this intricate landscape, we delve into the chemical identities and intricate structures of nano fillers, nano objects, and nanomaterials, examining their seamless integration into polymer matrices. From the foundational classification of nano fillers to the sophisticated synthesis of nanoparticles, from a myriad of characterization techniques to innovative manufacturing methods such as in situ polymerization and electrospinning, this volume presents a panoramic view of the myriad approaches aimed at refining the properties and functionalities of polymer nanocomposites to cater to diverse needs.

Readers will encounter groundbreaking research on polymer nanocomposites based on an array of nanostructures, including metal oxide nanoplatelets, carbon nanotubes, nano cellulose, chitin, starch, lignin, talc, graphene, nanoalumina, nano magnesium hydroxide, polymer nano silica, quantum dots, and clay, among others. In addition, the exploration of decorated nanomaterials, such as carbon nanotubes, quantum dots, clay, cellulose, and chitin, sheds light on their potential to augment performance within polymer matrices.

The applications of these advanced materials are equally diverse, spanning the realms of biomedical advancements, energy storage solutions, environmental remediation, and smart materials for industry. Through insightful discussions, we uncover the advantages of polymer nanocomposites in biomedical applications, explore strategies for recycling, conduct life cycle analysis, and chart the path from laboratory-scale innovations to industrial-scale production.

We extend our heartfelt gratitude to the contributors who have generously shared their expertise and insights, enriching this volume with a wealth of knowledge and

pioneering research. Special acknowledgment goes to Ms. Thresia Silvy John for her invaluable support during the editing process.

It is our sincere hope that this book serves as an indispensable resource for researchers, academics, and industry professionals alike, inspiring further exploration and innovation in the captivating realm of polymer nanocomposites.

17th June 2024

Vera V. Myasoedova, Russia

Sabu Thomas, India

Hanna J. Maria, India

1

Classification of Nanofillers, Nano-Objects, Nanomaterials, and Polymer Nanocomposites Based on Chemical Nature and Identity

Lan Chen

CAS Key Laboratory of Standardization and Measurement for Nanotechnology, National Center for Nanoscience and Technology, Beijing, P. R. China

1.1 Classification of Nanocomposites

Nanocomposites are materials composed of multi-heterogeneous phases and can be categorized into three classes according to the host matrix material on which they are based:

- ceramic-matrix nanocomposites (CMNC)
- polymer-matrix nanocomposites (PMNC)
- metal-matrix nanocomposites (MMNC)

However, nanocomposites can either be classified as polymer or nonpolymeric nanocomposites according to the composition of the matrix materials. PMNCs are composites with at least one polymer phase and one nanophase, where at least one of its dimensions is less than 100 nm, i.e. at the nanoscale. Therefore, polymer-based nanocomposites can further be classified as [1]:

- ceramic polymer nanocomposites
- inorganic polymer nanocomposites
- organic polymer nanocomposites
- inorganic-organic hybrid nanocomposites
- biocomposites

Inorganic nanofillers include elemental nanomaterials such as metallic, carbon, and boron nanomaterials as well as compound nanomaterials available in both synthetic and natural form while organic fillers include both synthetic and natural organics, such as cellulose, hemp, and silks as seen in Table 1.1 [2].

The properties of the nanocomposites are determined by the same factors as those in traditional composites, such as composition, structure, shape, and interfacial interactions. The commonly used structure and form of the nano-objects as the fillers and reinforcing materials are listed in Table 1.2 [2]. On the other hand, the structure of nanocomposites is usually more complicated than that of traditional composites,

Table 1.1 Fillers and reinforcing materials.

Filler materials
Alumina (trihydrate)
Boron
Carbon
Clay
Calcium carbonate
Glass
Mica
Mineral
Metal
Silica
Talcum
Aramid
Cellulose
Natural organic (cotton, sisal, hemp, flax, <i>etc.</i>)
Synthetic organic (e.g. finely divided PTFE, polyimides or thermoset resins)

Table 1.2 Form or structure of fillers and reinforcing materials.

Form or structure
Nanoparticles/Nanobeads/Nanospheres
Nanopowder/Ultrafine powder
Nano ground
Nanochips/Nanocuttings
Nanorods
Nanowhiskers
Nanotubes
Nanowires
Nanofibres
Nanoribbons/Nanotapes
Monolayer 2D materials
Few layer 2D materials (usually less than 10 layers)
Nanoplates/nanosheets (usually more than 10 layers for 2D materials)

where interfacial interactions play a significant role in nanocomposites, compared to traditional ones, because of the assumedly very large interfacial area between them.

1.2 Classification of Nanofillers

Surprisingly, the surface characteristics of nanofillers are rarely determined or known; instead, they are modified in practice to improve dispersion and/or adhesion in nanofiller-reinforced polymer composites. All kinds of nanocomposites

can be prepared with *in situ* polymerization, solvent-assisted hybridization, and melt homogenization. However, non-ideal dispersion and homogeneity are major concerns in all these technologies. The properties of nanocomposites are usually far from the expectations due to insufficient homogeneity, disordered orientation, and improper adhesion.

1.3 Classification of Nano-Objects and Nanomaterials

For a typical nanocomposite as seen in Figure 1.1, nano-objects, i.e. the discrete component of the nanomaterials with one, two, or three external dimensions in the nanoscale, i.e. 1–100 nm [3] (see *ISO/TS 80004 -2:2015 Part 2* and *ISO/TS 12805:2011*), is used as the nanofillers to be dispersed into a matrix, where the matrix is a continuous phase while the nanofillers act as an interstitial phase. When the content of the nano-objects in the matrix exceeds 50%, they are more appropriately termed nanomaterials since they become the major and continuous phase and can no longer be considered as the fillers and interstitial phase.

Nanomaterials are defined as materials with any external dimension in the nanoscale or having internal or surface structure in the nanoscale, including nano-objects and nanostructured materials as seen in Figure 1.2 (see *ISO/TS 80004-1:2015 Part 1*) [4].

In reality, most nanomaterials do not exist in a pure state and are usually mixed with other phases or materials. Therefore, nanomaterial indicates a natural, incidental, or manufactured material containing particles in an unbound state, as an aggregate, or as an agglomerate and where, in more than 50% of the particles,

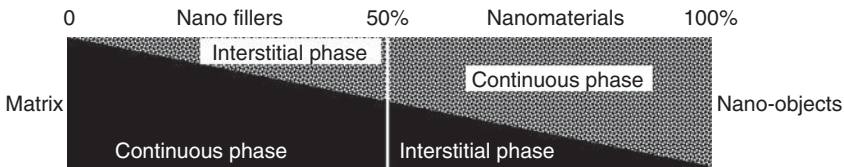


Figure 1.1 Components and composition of nanocomposites.

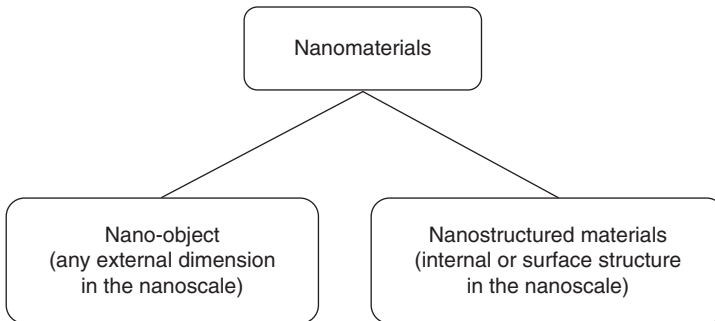


Figure 1.2 Nanomaterials framework.

one or more external dimensions is in the size range of 1–100 nm according to the definition recommended by European Commission [5]. In specific cases, and wherever warranted by concern for environment, health, safety, or competitiveness the number size distribution threshold of 50% may be replaced by a threshold between 1 and 50%. However, fullerenes, few-layered graphene, and single-wall carbon nanotubes with one or more external dimensions below 1 nm can also be considered as nanomaterial (See *ISO/TS 80004-13:2017 Part 13*).

Nano-objects are nanomaterials in pure state without either internal or surface structure in the nanoscale and can have properties that make them key components of materials and systems resulting in improved performance over their conventional counterparts. These nano-objects often have properties that are not simple extrapolations of the properties in their larger form and these novel properties are called emerging/transformational, discontinuous properties.

The nano-object size and shapes are dominant for their functions, so their description and measurement are crucial and must be treated carefully. Three types of basic shapes are illustrated in Figure 1.3 to represent different classes of structural dimensionality in categorizing nano-objects [6], however, a lot of other shapes transformed from these basic shapes also exist. In addition, the three classes of nano-objects can be further categorized into many sub-classes, such as nanosphere, nanotube, and two-dimensional (2D) material. as seen in Table 1.3 [3, 6]. The difference between a nanoparticle and a nanosphere is that the nanoparticle may have an irregular shape while the nanosphere is ideally a spherical nanoparticle. However, the nanocone can be considered as either a cone-shaped nanoparticle with a large opening angle or a cone-shaped nanofiber with a smaller opening angle.

In addition, intense interests have arisen in graphene for both academia and industry due to its exceptional processing-relevant properties, such as abnormal electrical and thermal conductivity. More recently, other graphene-like materials have also demonstrated promising properties such as hexagonal boron nitride (*hBN*), tungsten diselenide (WSe_2), molybdenum disulfide (MoS_2), germanene, and silicene both in monolayer and few-layer forms, as well as their layered assemblies [7]. The thickness

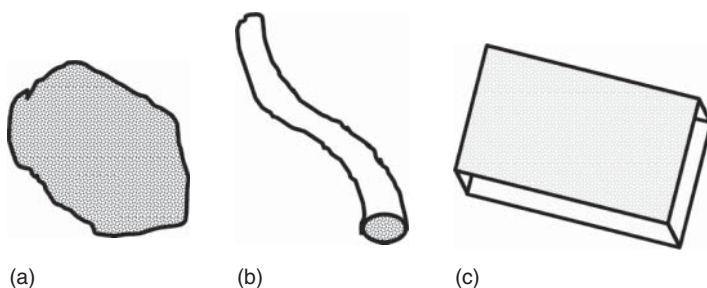


Figure 1.3 Schematic diagrams showing basic shapes of nano-objects. (a) *nanoparticle* (3 external dimensions in the nanoscale), (b) *nanofibre* (2 external dimensions in the nanoscale), (c) *nanoplate* (1 external dimensions in the nanoscale).

Table 1.3 Nano-object definition and classification.

Class of nano-objects		Definition
Nanoparticle	Nanoparticle	Nano-object with all external dimensions in the nanoscale where the lengths of the longest and the shortest axes of the nano-object do not differ significantly, usually no more than three times
	Nanosphere	Spherical nano-object, i.e. nanoparticle with equiaxial and ideal spherical shape
	Nanocapsule	Hollow nanosphere
	Nanoion	Spherical nanoparticle with multi-layer concentric structure
	Core-shell nanoparticle	Nanoparticle consisting of a core and shell(s), whose largest external dimension/length (core diameter plus shell thickness, i.e. outer diameter for spherical nanoparticles) is in the nanoscale
	Nanocone	Cone-shaped nanoparticle or nanofibre
Nanofibre	Nanofibre/ Nanofibril/ Nanofilament	Nano-object with two external dimensions in the nanoscale and the third dimension significantly larger, usually out of the nanoscale
	Nanorod	Solid nanofibre
	Nanotube	Hollow nanofibre
	Nanowire	Electrically conducting or semi-conducting nanofibre
Nanoplate	Nanoplate/ Nanoflake	Nano-object with one external nanoscale dimension and the other two significantly larger external dimensions, usually out of the nanoscale
	Nanoribbon/ Nanotape	Nanoplate with two dimensions significantly larger than the third one
	Nanofilm/ Nanosheet	Nanoplate with extended lateral dimensions
	2D Material	Material, consisting of one or several layers with the atoms in each layer strongly bonded to neighbouring atoms in the same layer, which has one dimension, i.e. its thickness, in the nanoscale or smaller and the other two dimensions generally at larger scales
Nanocrystal	All nano-objects above	Nano-objects with a crystalline structure

of these materials is restricted within nanosize or smaller, within one or a few layers. They are, thus, defined as 2D materials since they have one dimension less than 100 nm and the other two dimensions larger than the nanosize range [7]. Layered materials usually consist of several 2D layers weakly stacked (bound) together to

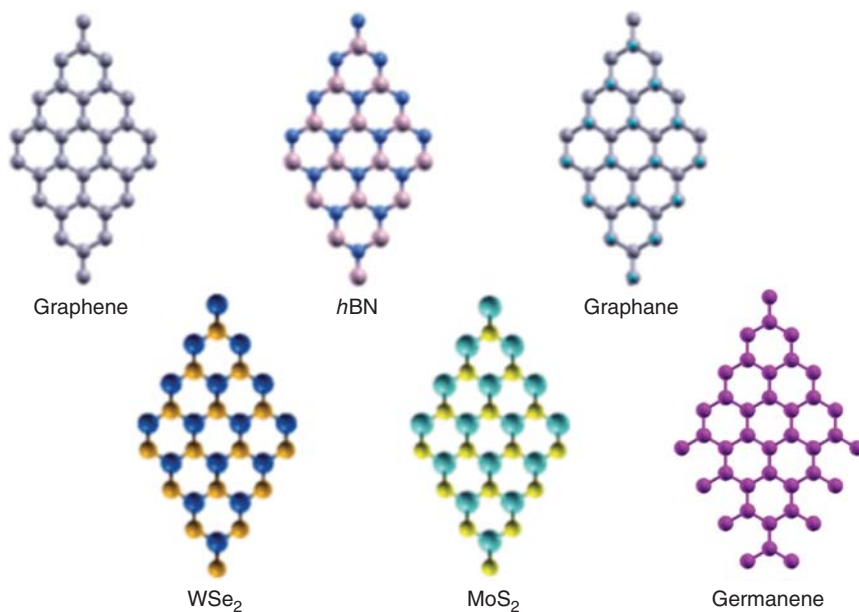


Figure 1.4 Structural scheme for different 2D materials.

form bulk structures. Several graphene-like 2D materials with distinct stacking configurations are shown in Figures 1.4 and 1.5. However, 2D materials may be not topographically flat and may be buckled somehow in reality. In addition, they can also exist in different aggregate and agglomerate morphologies. 2D materials are, therefore, considered emerging nanomaterials or their important subset.

There are several parameters such as morphology, composition, surface features, and crystalline structure besides size and shape, which are also crucial to the nano-objects function and their phenomena in the microscope, such as catalytic, optical, electronic, magnetic, and other properties. Commonly, fiber or ribbon morphological nano-objects are usually easier to form the secondary structure with stronger mechanical strength and better formability than particulate nano-objects. Additionally, the composition of doped nanomaterials makes them more active in catalytic, optical, and electronic performance than their pure counterpart, particularly in the case of deeply doped materials or heterogeneous structures e.g. hybrid 2D materials. Surface features such as surface defects and roughness can significantly influence its adsorption toward the solute in solution or the gas molecules in air and the consequent functions, which may be a determining factor for the applications of nanomaterials in drug delivery and nanomedicine.

1.4 Production Method and Existing Form of Nano-Objects

According to different production methods, the nano-objects can be classified as engineered, manufactured, incidental, and natural as seen in Table 1.4 [8]. However,

- quantum dots/polymer nanocomposites
(*contd.*)
- mechanical properties 572
 - optical property 571
 - sensors 577–578
 - solar cells 575
 - stability 573
- quantum dot sensitized solar cells (QDSC)
656
- r**
- radial breathing modes (RBM) 596
 - radiation-modified MH/PS 444
 - radical polymerization 53–54
 - RA-encapsulated polymeric NPs 862
 - Raman spectroscopy 100, 349, 595, 596,
664, 699
 - Rayleigh's law 242
 - reaction injection moulding (RIM) 891
 - ReCiPe endpoint method 784, 787, 788
 - ReCiPe midpoint method 784, 787, 788
 - reduced graphene oxide aerogel
membranes (rGOAM) 347
 - reinforcement/filler 133
 - renewable resources
 - isocyanates from 893–894
 - polyols from 893
 - rhodamine-labelled PEGylated poly(alkyl
cyanoacrylate) copolymer 866
 - rhodamine modified NPs 860
 - rigid polyurethane foams (RPUFs) 887,
892
 - rivastigmine 846, 860, 861
 - RVG-Chitosan-NC intravenous
administration 865
- s**
- SAN-nAl₂O₃ composite 403, 410
 - scanning electron microscopy (SEM)
101, 146, 203, 348, 436, 500, 548,
597, 765
 - scanning tunneling microscopy (STM)
598
 - Schiff-base DCB 922
 - schisantherin A-loaded PLGA NPs 862
 - Sustainable Development Goals (SDG)
184
 - selegiline-functionalized copolymer 866
 - self-assembly approach 210, 607
 - self-healing mechanisms
 - advanced devices 933–939
 - coordination-bonding-based
autonomous 928–932
 - dynamic covalent bonding 921–922
 - hydrogen-bonding 932–933
 - ionogel 925–927
 - liquid-metal-based reconfigurable
927–928
 - macrocyclic host–guest interaction
922–925
 - self-healing properties 54, 921, 930–932,
954
 - self-healing stretchable composite
conductors (SSCCs) 921
 - self-healing/shape-memory polymers
(SHSMPs) 922
 - semi-IPN 47
 - shape-morphing LM–LCE SSCC 928
 - Shrimp–shell chitin 203
 - silane cross-linking method 435, 447
 - silane grafting 659, 662
 - silanization 171, 180, 181
 - silicone-based surfactants 890
 - silver nanoparticles (AgNPs) 31, 277,
278, 681, 724, 976
 - SimaPro software 783, 786
 - SiO₂ nanoparticles
 - dynamic light scattering determination
486
 - membrane selectivity for 489
 - OSA nucleation and growth 485
 - sample of sol, transmission electron
microscopy 487
 - solid deposits of 484, 485
 - surface electric layer of 491
 - UF-220 sample 487
 - siREST-silencing lipid nanocapsules 868
 - snap-cure thermosetting polyurethane
system 903
 - soda lignins 259

- sodium alginate-hydroxyapatites-silicon quantum dots (SA-nHA-Si QDs) 577
- sodium dodecylbenzenesulfonate (SDBS) 385
- sodium dodecyl sulfate (SDS) 267, 430, 440, 445, 851
- solar cells 25, 68, 82, 96, 106, 114, 452, 563, 574, 575, 578, 636, 641, 656, 666, 667, 938, 939, 957, 975–976
- sol-gel method 19, 111, 380, 384–386, 424, 431, 569, 822
- solution blending 109, 110, 135, 404, 964–965
- solution casting 55, 179, 206–209, 432, 449, 592, 731, 819
- solution-induced intercalation 403
- solution intercalation 350, 433, 439, 433, 713
- solution mixing 110, 449, 591–593, 611, 624, 698
- Solvmix processing route 901
- solvothermally reduced graphene (SRG) nanocomposites 968
- solvothermal method 424, 428–429
- soybased polyols 893
- soy protein isolate (SPI) plastics 207
- spinning methods 19–20, 67, 433
- stability dispersion, of MWCNT 146
- starch nanocrystals (SNCs) 230–233, 238
- starch nanoparticles (SNPs) 229, 230, 233–234, 238
- structure-properties-processing 210
- styrene-butadiene rubber (SBR) 275, 461, 770
- styrene-ethylene-butylene-styrene (SEBS) 609, 762
- submicrometer 233
- Sugar Cane Bagasse (SCB)
 Bagasse constitutes 806–807
 industrial potentials 807
 utilization advantages 805–806
- sugarcane fiber cellulose (SCFC) 811
- sugarcane in Egypt
 composition 798
 consumption 799–800
 food and beverage products 797
 harvesting phase wastes 802–803
 import 800–801
 production 798–801
 subtropical and tropical climates 797
 sugar production phase wastes 803–804
- sulfonated
 styrene-ethylene/butylene-styrene 347
- supercritical CO₂ 261–262
- supramolecular zwitterionic-network ionic-elastomer-based SSCC 933
- surface-initiated atom-transfer-radical polymerization (SI-ATRP) 98–99, 181
- surface-initiated reversible addition-fragmentation chain-transfer (SI-RAFT) strategy 99
- surface properties
 of polymer 657
 of quantum dots
 optical properties 655–656
 oxidative reactions 657
 quantum dot crystal facets and atom coordination 653–654
 quantum dot ligand coordination 654–655
 surface chemistry and charge/energy transfer 656–657
- surfactant-based modifications 180, 182
- synthetic polymers 75, 235–237, 739
- synthetic rubber-based elastomer-lignin nanocomposite 274–276
- t**
- talc
 aspect ratio 301
 chemical formula 297
 chemical modifications of 322–324
 composites and nanocomposites 297
 definition 297
 distinctive properties 298

- talca (*contd.*)
- elemental structure of 298
 - geology 301–303
 - global market size 298
 - hydrophobic character of 300
 - industrial applications 300, 328–330
 - laminae 300, 301
 - macro and micro crystals 299
 - polymer nanocomposites compounding 303–306
 - polymer nanocomposites properties
 - degree of purity 319–320
 - interface and interphase 307
 - morphology 308–318
 - nucleating capability 320–321
 - particle concentration 321–322
 - particle size 318–319
 - surface treatments on 324–328
 - purity 300–301
 - sheet's surface 299
 - surface chemical composition of 300
 - surface properties 299
 - three-dimensional structure of 299
 - uses 298
- tapioca starch (TS) 811
- TDS_{SiO₂} nanoparticles 491
- Teflon-lined autoclave 381
- telorogenic therapies 867
- template-based synthesis 20–21
- TEMPO-mediated oxidation 203, 204, 219
- TEMPO-oxidized cellulose nanofiber (TOCNF)-graphene (GN) hydrogel-based SSCC 931
- tensile strength 45, 107, 148, 149, 168, 170, 172, 174, 175, 177, 179, 199, 206–209, 218, 219, 236, 237, 239, 241, 267, 269, 271, 272, 275, 295, 304, 317, 322, 325, 352, 409, 410, 434, 435, 437, 446, 449, 520, 526, 573, 605, 607, 609, 611, 630, 632, 679, 685, 686, 691, 714, 721, 722, 728, 762, 806
- ternary polymer-based SSCC 931
- 2,2,6,6-tetramethylpiperidine-1-oxyl radical (TEMPO) 48
- therapeutic agent-loaded polymeric NPs
- Alzheimer's disease treatment 860–862
 - amyotrophic lateral sclerosis treatment 863–864
 - Huntington's disease treatment 863
 - multiple sclerosis treatment 863
 - Parkinson's disease treatment 862–863
- thermal conductivity 4, 49, 81, 141, 177, 281, 300, 344, 345, 360, 380, 404, 500, 589, 590, 598, 609–611, 627–628, 957
- thermal reduction 962, 970
- thermal stability, flame retardancy and 602–609
- thermogravimetric analysis (TGA) 323, 436, 437, 518, 598, 699, 719, 764
- thermoplastic elastomers (TPE) 175
- thermoplastic–lignin nanocomposites 266–269
- thermoplastic polyurethanes (TPU) 360, 609, 887, 891
- thermoplastics 169–172
- IPN 47
 - as nanocomposite matrix
 - acrylonitrile butadiene styrene 142–143
 - polycarbonates 143
 - poly (lactic acid) 144
 - poly (trimethylene terephthalate) 141–142
- thermoset–lignin nanocomposites 269–272
- theta alumina 376
- three-dimensional polymer 19, 265
- 3D printed bioactive scaffolds 455
- 3D printing 53, 594–595, 715, 922, 927, 929
- toluene diisocyanate (TDI) 889
- top-down approach 234
- nanochitin/polymer composites 205–210

nanochitins 201–205
 Total Hip Arthroplasty (THA)
 409, 779
 transmission electron microscopy (TEM)
 100, 348, 436–437, 487, 512, 597,
 699, 716
 transparent ionic-conductive SSCC 925,
 926
 triboelectric nanogenerator (TENG) 82,
 83, 976
 twin-screw compounders 304
 two-dimensional (2D) filler 134
 two-dimensional (2D PNC) 740

U

UF-220 sample 487, 491, 493, 500, 502,
 505–507, 509, 510, 513
 ultrafiltration membrane 486, 493, 495,
 498, 500, 523, 554
 ultrasonication 53, 110, 139, 168, 182,
 183, 201, 212, 233, 234, 262, 263,
 346, 592, 599, 631, 905, 961, 965,
 970, 972
 ultrasound 146, 233, 262, 263, 385, 404,
 850, 851, 870
 urban mining 759
 uretonimine modified MDI 889
 UV-cured waterborne polyurethane
 nanocomposite 907
 UVSL-2 installation 500, 504

V

vacuum sublimation apparatus 499
 vasoactive intestinal peptide (VIP)
 conjugated PEG-PLA NPs 865
 Verkhne–Mutnovskii geoelectric power
 station 475
 vermiculite (VMT) 681, 684–686, 689,
 696–698
 virgin e-plastic vs plastic e-waste
 763–768
 4-VPBA/AMPSLi-based ionic/DCB
 conductor 922

W

waste electrical and electronic equipment
 (WEEE)
 definition 759
 HIPS/ABS blends 760–762
 plastic 759
 sustainable recycling approaches for
 plastic e-waste 768–770
 virgin e-plastic vs plastic e-waste
 763–768
 waterborne nanocomposite film
 451–452
 waterborne polyurethane (WPU) 236,
 906, 907, 925
 water contact angle (WCA) 181, 236,
 243, 685, 719
 water-induced PVA/CQDs shape memory
 polymer composite 576
 water-soluble, low-toxic QDs 577
 wear resistance, of polymeric materials
 780
 WPU-Fc/CD/Ag composite 925

X

X-ray diffraction (XRD) 203, 309, 348,
 349, 379, 386, 597, 699
 X-ray photoelectron spectroscopy (XPS)
 182, 349, 436, 595, 717

Y

yeasts mediated nanoparticles 31
 Young's modulus 49, 56, 148, 170–172,
 174, 179, 182, 207–209, 219, 235,
 236, 239, 241, 271, 321, 520, 611,
 630, 632, 664, 685, 686

Z

zero-band-gap semiconductor 957
 zero-dimensional (0D PNC) 740
 zero-dimensional filler (0D) 134
 zero-dimensional fullerenes 955
 ZnO(PEGME) colloids 569
 ZnO/V nanocomposite materials 685