

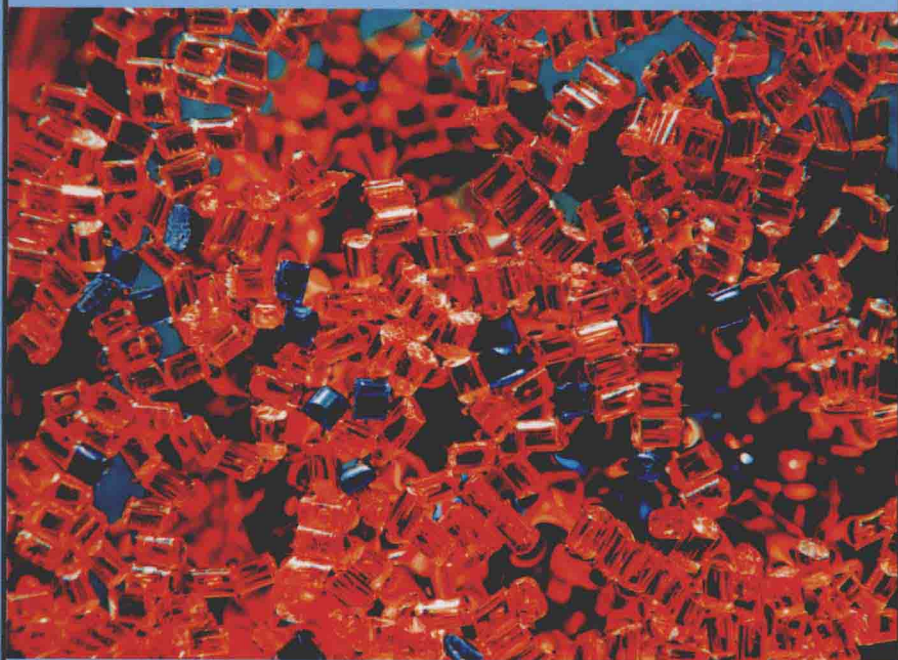
Nanomaterials and Nanotechnology for Composites

上海交通大学图书馆



E1256735

Design, Simulation, and Applications



Editors

A. K. Haghi, PhD • Sabu Thomas, PhD

Ali Pourhashemi, PhD • Abbas Hamrang, PhD

Ewa Kłodzińska, PhD

AAP | APPLE
ACADEMIC
PRESS

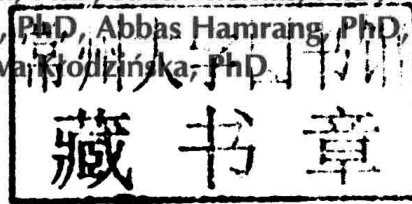
CRC | CRC Press
Taylor & Francis Group

NANOMATERIALS AND NANOTECHNOLOGY FOR COMPOSITES

Design, Simulation, and Applications

Edited by

A. K. Haghi, PhD, Sabu Thomas, PhD,
Ali Pourhashemi, PhD, Abbas Hamrang, PhD, and
Ewa Kłodzńska, PhD.



AAP | APPLE
ACADEMIC
PRESS

Apple Academic Press Inc. | Apple Academic Press Inc.
3333 Mistwell Crescent | 9 Spinnaker Way
Oakville, ON L6L 0A2 | Waretown, NJ 08758
Canada | USA

©2015 by Apple Academic Press, Inc.

Exclusive worldwide distribution by CRC Press, a member of Taylor & Francis Group

No claim to original U.S. Government works

International Standard Book Number-13: 978-1-77188-065-7 (Hardcover)

All rights reserved. No part of this work may be reprinted or reproduced or utilized in any form or by any electric, mechanical or other means, now known or hereafter invented, including photocopying and recording, or in any information storage or retrieval system, without permission in writing from the publisher or its distributor, except in the case of brief excerpts or quotations for use in reviews or critical articles.

This book contains information obtained from authentic and highly regarded sources. Reprinted material is quoted with permission and sources are indicated. Copyright for individual articles remains with the authors as indicated. A wide variety of references are listed. Reasonable efforts have been made to publish reliable data and information, but the authors, editors, and the publisher cannot assume responsibility for the validity of all materials or the consequences of their use. The authors, editors, and the publisher have attempted to trace the copyright holders of all material reproduced in this publication and apologize to copyright holders if permission to publish in this form has not been obtained. If any copyright material has not been acknowledged, please write and let us know so we may rectify in any future reprint.

Trademark Notice: Registered trademark of products or corporate names are used only for explanation and identification without intent to infringe.

Library of Congress Control Number: 2015935139

Library and Archives Canada Cataloguing in Publication

Nanomaterials and nanotechnology for composites: design, simulation, and applications /
edited by A.K. Haghi, PhD, Sabu Thomas, PhD, Ali Pourhashemi, PhD, Abbas Hamrang, PhD,
and Ewa Klodzińska, PhD.

Includes bibliographical references and index.

ISBN 978-1-77188-065-7 (bound)

1. Nanocomposites (Materials). 2. Nanoparticles.

3. Nanotechnology. I. Hamrang, Abbas, editor II. Thomas, Sabu, editor III. Haghi, A. K.,
author, editor IV. Pourhashemi, Ali, editor
V. Klodzińska, Ewa, editor

TA418.9.N35N27 2015

620.1'18

C2015-901600-2

Apple Academic Press also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic format. For information about Apple Academic Press products, visit our website at www.appleacademicpress.com and the CRC Press website at www.crcpress.com



Printed and bound in Great Britain by
TJ International Ltd, Padstow, Cornwall

NANOMATERIALS AND NANOTECHNOLOGY FOR COMPOSITES

Design, Simulation, and Applications

ABOUT THE EDITORS

A. K. Haghi, PhD

A. K. Haghi, PhD, holds a BSc in urban and environmental engineering from the University of North Carolina (USA); a MSc in mechanical engineering from North Carolina A&T State University (USA); a DEA in applied mechanics, acoustics and materials from Université de Technologie de Compiègne (France); and a PhD in engineering sciences from Université de Franche-Comté (France). He is the author and editor of 165 books and has published 1000 research papers in various journals and conference proceedings. Dr. Haghi has received several grants, consulted for a number of major corporations, and is a frequent speaker to national and international audiences. Since 1983, he served as a professor at several universities. He is currently Editor-in-Chief of the *International Journal of Chemoinformatics and Chemical Engineering* and *Polymers Research Journal* and on the editorial boards of many international journals. He is a member of the Canadian Research and Development Center of Sciences and Cultures (CRDCSC), Montreal, Quebec, Canada.

Sabu Thomas, PhD

Dr. Sabu Thomas is the Director of the School of Chemical Sciences, Mahatma Gandhi University, Kottayam, India. He is also Professor of polymer science and engineering and the Director of the International and Inter University Centre for Nanoscience and Nanotechnology of the same university. He is a fellow of many professional bodies. Professor Thomas has authored or coauthored many papers in international peer-reviewed journals in the area of polymer processing. He has organized several international conferences and has more than 420 publications, 11 books, and two patents to his credit. He has been involved in a number of books both as author and editor. He is a reviewer to many international journals and has received many awards for his excellent work in polymer processing. His h Index is 42. Professor Thomas is listed as the 5th position in the list of Most Productive Researchers in India, in 2008.

Ali Pourhashemi, PhD

Ali Pourhashemi, PhD, is currently Professor of chemical and biochemical engineering at Christian Brothers University (CBU) in Memphis, Tennessee. He was formerly the Department Chair at CBU and also taught at Howard University in Washington, DC, USA. He taught various courses in chemical engineering, and his main area has been teaching the capstone process design as well as supervising industrial internship projects. He is a member of several professional organiza-

tions, including the *American Institute of Chemical Engineers*. He is on the international editorial review board of the *International Journal of Chemoinformatics and Chemical Engineering* and is an editorial member of the *International of Journal of Advanced Packaging Technology*. He has published many articles and presented at many professional conferences.

Abbas Hamrang, PhD

Abbas Hamrang, PhD, is Professor of polymer science and technology. He is currently a senior Polymer Consultant and Editor and member of the academic board of various international journals. His research interests include degradation studies of historical objects and archival materials, cellulose-based plastics, thermogravimetric analysis, accelerated aging process, and stabilization of polymers by chemical and nonchemical methods. His previous involvement in academic and industry sectors at international level include deputy vice-chancellor of research & development, senior lecturer, manufacturing consultant, science and technology advisor.

Ewa Kłodzińska, PhD

Ewa Kłodzińska holds a PhD from Nicolaus Copernicus University, Faculty of Chemistry in Torun, Poland. For 10 years, she has been doing research on determination and identification of microorganisms using the electromigration techniques for the purposes of medical diagnosis. Currently she is working at the Institute for Engineering of Polymer Materials and Dyes and investigates surface characteristics of biodegradable polymer material on the basis of zeta potential measurements. She has written several original articles, monographs, and chapters in books for graduate students and scientists. She has made valuable contributions to the theory and practice of electromigration techniques, chromatography, sample preparation, and application of separation science in pharmaceutical and medical analysis. Dr. Ewa Kłodzińska is a member of editorial board of *ISRN Analytical Chemistry* and the *International Journal of Chemoinformatics and Chemical Engineering (IJCCE)*.

LIST OF CONTRIBUTORS

M. Arabani

Professor, Faculty of Engineering, University of Guilan, Rasht, Postal code: 3756, I. R. Iran; Tel: +98(131)6690270; Fax: +98 (131) 6690270; E-mail: arabani@guilan.ac.ir

Mona Bakr

The National Institute for Laser Enhanced Sciences, Cairo University, Egypt

Marina V. Bazunova

Scientific Degree: The Candidate of the Chemical Sciences. Post: The Docent of the Department of High-Molecular Connections and General Chemical Technology of the Chemistry Faculty of the Bashkir State University; Official Add: 450076, Ufa, Zaks Validi Street, 32; Tel.: (347) 229-96-86; Mob: 89276388192; E-mail: mbazunova@mail.ru

Samarth Bhatt

Jena University Hospital, Friedrich Schiller University, Institute of Human Genetics, Kollegiengasse 10, D-07743 Jena, Germany

K. S. Dibirova

Dagestan State Pedagogical University, Makhachkala 367003, Yaragskii Street 57, Russian Federation

Tarek A. El-Tayeb

The National Institute for Laser Enhanced Sciences, Cairo University, Egypt

Y. G. Galyametdinov

Doctor of Chemical Sciences, Head of Department of Physical and Colloid Chemistry, KNRTU; E-mail: office@kstu.ru

M. A. Goldshtrakh

Military Institute of Chemistry and Radiometry, 105 Allea of General A. Chrusciela, 00-910 Warsaw, Poland, M. V. Lomonosov State University of Fine Chemical Technology, 119571 Moscow, Vernadskogo prosp 86

Iman E. Gomaa

German University in Cairo, Egypt, Main Entrance of Al-Tagamoa Al-Khames; E-mail: iman.gomaa@guc.edu.eg; Tel: +20-0100 2155053; Fax: +20-2-27590772

A. K. Haghi

Professor, Faculty of Engineering, University of Guilan, Rasht, Postal code: 3756, I. R. Iran; Tel: +98(131)6690270; Fax: +98 (131) 6690270; E-mail: Haghi@guilan.ac.ir

V. I. Kodolov

Basic Research High Educational Centre of Chemical Physics & Mesoscopy, Udmurt Scientific Centre, Ural Division; Russian Academy of Sciences, M. T. Kalashnikov Izhevsk State Technical University

Sergei V. Kolesov

Scientific Degree: The Doctor of the Chemical Sciences. Post: The Professor of the Department of High-Molecular Connections and General Chemical Technology of the Chemistry Faculty of the Bashkir State University; Official add: 450076 Ufa, Zaks Validi Street, 32; Tel.: (347) 229-96-86; E-mail: Kolesovser-vic@mail.Ru

G. V. Kozlov

Dagestan State Pedagogical University, Makhachkala 367003, Yaragskii Street 57, Russian Federation

Elena I. Kulish

Scientific Degree: The Doctor of the Chemical Sciences. Post: The Professor of the Department of High-Molecular Connections and General Chemical Technology of the Chemistry Faculty of the Bashkir State University. Official add: 450076, Ufa, Zaks Validi Street 32; Tel.: (347) 229-96-86; E-mail: Onlyalena@mail.Ru

N. G. Lebedev

Volgograd State University, Volgograd, Russia; E-mail: lebedev.ng@mail.ru

Thomas Liehr

Jena University Hospital, Friedrich Schiller University, Institute of Human Genetics, Kollegiengasse 10, D-07743 Jena, Germany

A. M. Lipanov

Institute of Mechanics, Ural Branch of the Russian Academy of Sciences, T. Baramsinoy 34, Izhevsk, Russia; E-mail: postmaster@ntm.udm.ru

G. M. Magomedov

Dagestan State Pedagogical University, Makhachkala 367003, Yaragskii Street 57, Russian Federation

K. Majewski

Military Institute of Chemistry and Radiometry, 105 Allea of General A. Chrusciela, 00-910 Warsaw, Poland; E-mail: K.Majewski@wichir.waw.pl

M. Mehdipour

Textile Engineering Department, Guilan University, Rasht, Iran

A. I. Nigmatullina

Chemistry and Processing Technology of Elastomers Department, Kazan National Research Technological University, 68 K Marks street, Kazan, Russia; E-mail: Chembio@sky.chph.ras.ru

A. A. Nikiforov

Chemistry and Processing Technology of Elastomers Department, Kazan National Research Technological University, 68K Marks street Kazan, Russia; E-mail: Chembio@sky.chph.ras.ru

Babak Noroozi

Department of Textile Engineering, University of Guilan, P. O. Box 41635-3756, Rasht, Iran

G. Nyszko

Military Institute of Chemistry and Radiometry, 105 Allea of General A. Chrusciela, 00-910 Warsaw, Poland, E-mail: Grzegorz.Nyszko@wichir.waw.pl

N. A. Okhotina

Chemistry and Processing Technology of Elastomers Department, Kazan National Research Technological University, 68 K Marks street Kazan, Russia; E-mail: Chembio@sky.chph.ras.ru

A. A. Olkhov

N. N. Semenov Institute of Chemical physics Russian Academy of Sciences, 119991 Moscow, street Kosygina, 4; E-mail: aolkhov72@yandex.ru

V. V. Osipova

Ph. D. Department of Physical and Colloid Chemistry, KNRTU

O. A. Panfilova

Chemistry and Processing Technology of Elastomers Department, Kazan National Research Technological University, 68K Marks street, Kazan, Russia, E-mail: Chembio@sky.chph.ras.ru

J. Pielichowski

Cracow University of Technology, Department of Polymer Science and Technology, Warszawska street, 31-155 Krakow, Poland, E-mail: Pielich@pk.edu.pl

Saeedeh Rafiei

Department of Textile Engineering, University of Guilan, P.O. Box 41635-3756, Rasht, Iran

S. A. Sudorjin

Volgograd State University, Volgograd, Russia, Volgograd State Technical University, Volgograd, Russia; E-mail: sergsud@mail.ru

R. Tanzadeh

Department of Civil Engineering University of Guilan, Rasht, Iran. Tel: +98(131)3229883; Fax: +98 (131) 3231116; E-mail: rashidanzadeh@yahoo.com

V. V. Trineeva

Basic Research High Educational Centre of Chemical Physics & Mesoscopy, Udmurt Scientific Centre, Ural Division; Russian Academy of Sciences, Institute of Mechanics, Ural Division, Russian Academy of Sciences

Rustam Tukhvatullin

Bashkir State University, 32 Zaki Validi Street, 450076 Ufa, Republic of Bashkortostan, Russia

A. V. Vakhrushev

Institute of Mechanics, Ural Branch of the Russian Academy of Sciences, T. Baramsinoy 34, Izhevsk, Russia; E-mail: postmaster@ntm.udm.ru

Denis R. Valiev

Scientific Degree:-Post: The Student of the Department of High-Molecular Connections and General Chemical Technology of the Chemistry Faculty of the Bashkir State University Official add: 450076, Ufa, Zaks Validi Street, 32; Tel. Official: (347) 229-96-86; E-mail: valief@mail.ru

S. I. Volfson

Chemistry and Processing Technology of Elastomers Department, Kazan National Research Technological University, 68K Marks street, Kazan, Russia; E-mail: Chembio@sky.chph.ras.ru

Gennady E. Zaikov

Institute of Biochemical Physics named N. M. Emanuel of Russian Academy of Sciences Scientific Degree: The Doctor of the Chemical Sciences; Official add: 4 Kosygina Street, 119334, Moscow, Russia; E-mail: chembio@sky.chph.ras.ru

L. O. Zaskokina

Master of Department of Physical and Colloid Chemistry, KNRTU

LIST OF ABBREVIATIONS

AC	Activated Carbon
ACF	Activated Carbon Fibers
ACHF	Activated Carbon Hollow Fibers
ACNF	Activated Carbon Nanofiber
AFM	Atomic Force Microscope
AN	Acrylonitrile
BEM	Boundary Element Method
BET	Brunner-Emmett1-Teller
BGK	Bhatnagar-Gross-Krook
BJH	Barrett Joiner Halenda
BSA	Bovine Serum Albumin
CF	Carbon Fiber
CFD	Computational Fluid Dynamics
CH	Calcium Hydroxide
CNT	Carbon Nanotubes
CS	Cellulose
CVD	Chemical Vapor Deposition
DAAD	Deutsche Akademische Austausch Dienst
DDT	Dichlorodiphenyltrichloroethane
DMF	Dimethylformamide
DSB	Double Strand Breaks
EDLCs	Electrochemical Double-Layer Capacitors
EDXS	Energy Dispersive X-Ray Spectrometry
EELS	Electron Energy Loss Spectroscopy
EMEM	Eagle's Minimal Essential Medium
ERKs	Extracellular Signal-Regulated Kinases
FEM	Finite Element Methods
FRC	Fiber-Reinforced Concrete
FTIR	Fourier Transform Infrared
GUC	German University in Cairo
HDPE	High Density Polyethylene
HTS	High Temperature Shearing
HTT	Heat-Treatment Temperature
ISCN	International System for human Cytogenetic Nomenclature
ITZ	Interfacial Transition Zone

LBM	Lattice Boltzmann methods
LDPE	Low Density Polyethylene
LED	Light Emitting Diode
LERT	Large Electrical Relaxation Time Limit
LIBs	Lithium-Ion Batteries
MA	Maleine Anhydride
MD	Molecular Dynamics
MFCs	Microbial Fuel Cells
MMA	Methyl Methacrylate
MWNTs	Multiwall Carbon Nanotubes
NDT	Nottingham Device Test
NEMs	Nano-Electro-Mechanical Systems
NF	Nanofiltration
NILES	National Institute of Laser Enhanced Sciences
NPs	Nanoparticles
NS	Nano-SiO ₂
NT	Nano-TiO ₂
ODE's	Ordinary Differential Equations
PAA	Poly (Acrylic Acid)
PAN	Polyacrylonitrile
PBS	Phosphate Buffer Saline
PCN	Polymer Clay Nanocomposites
PDEs	Partial Differential Equations
PEM	Proton Exchange Mat
PGA	Poly(Glycolic Acid)
PHEV	Plug-In Hybrid Electric Vehicles
PLLA	Poly (L-Lactic Acid)
PMMA	Poly(Methyl Methacrylate)
POM	Polarization Optical Microscopy
PP	Polypropylene
PPX	Poly (P-Xylylene)
PTT	Photo Thermal Therapy
PVDC	Polyvinylidene Chloride
PZT	Plumbum Zirconate Titanate
RF	Radio-Frequency
RNP	Responsive Nanoparticle
RSM	Response Surface Methodology
RVE	Representative Volume Element
SAN	Styrene-Co-Acrylonitrile
SBS	Styrene-Butadiene-Styrene
SEI	Solid Electrolyte Interphase
SEM	Scanning Electron Microscope

SERT	Small Electrical Relaxation Time Limit
SMPE	Sulfophenyl Methallyl Ether
SSB	Single Strand Breaks
SSS	Sodium P-Styrene Sulfonate
SWNTs	Single Wall Carbon Nanotubes
TEM	Transmission Electron Microscopy
TFOT	Thin Film Oven Test
TG	Thermogravimetric Method
THF	Tetrahydrofuran
TLBM	Thermal Lattice Boltzmann methods
VA	Vinyl Acetate
VOCs	Volatile Organic Compounds

LIST OF SYMBOLS

A_m	amplitude of nanocomposite vibration
A_{ms}	coefficients of Fourier expansion
b	width of the Specimen
c	velocity of light
d	density of the adsorbate, g/cm ³
$\langle d \rangle_v$	average arithmetic size
d_f	fractal dimension
F_{max}	maximal force
\vec{F}_c	principal vector of forces
$f_s(p,r)$	Fermi distribution function
$ \vec{F}_{bi} $	force magnitude of the nanoparticle interaction
$\vec{F}_i(t)$	random set of forces at a given temperature
L	span length
\bar{l}	mean segment length
M	mass of the dried sample
\vec{M}_c	principal moment
Me (d)	median of distribution defining the size d
Mo (d)	position of maximum (a distribution mode)
m_i	mass of the i^{th} atom
m	mass of adsorbed benzene
$m_{\text{absorbed water}}$	mass of the water
m_{av}	average mass of medium
m_{cl}	mass of metal containing phase
m_{sample}	mass of the sample
N	number of carbon atoms in lattice
N_{imp}	number of adsorbed hydrogen atoms
N_k	number of atoms forming each nanoparticle
n	number of interatomic interaction types
P	maximum indicated load
p_x	parallel component of the graphene sheet
q	charge of ion
R	flexural strength
S'	modulus of elasticity
S''	loss modulus
s	quasimomentum of the electrons in grapheme

$T(r)$	constant in the linear approximation in magnitude
U	constant of Coulomb repulsion of impurity
U_{trans}	electromagnetic wave transmission velocity
V	hybridization potential
\bar{V}_{i0}, \bar{V}_i	initial and current velocities
V_{lj}	matrix element of hybridization

GREEK CHARACTERS

α_{am}	amorphous phase relative fraction
α_i	friction coefficient in atomic structure
$c_{j\sigma}$	Fermi annihilation
$c_{j\sigma}^+$	creation operators of electrons
ϵ_{ab}	absolute dielectric constant for medium
ϵ_{prog}	nanocomposite surface energy portion
ϵ_s^{NC}	surface energy of nanocomposite
$\epsilon_{l\sigma}$	energy of electron by impurity
Ω_k	area occupied by nanoelement
Φ_{cb}	chemical bonds
Φ_{es}	electrostatics
Φ_{fg}	flat groups
Φ_{hb}	hydrogen bonds
$\Phi(\bar{\rho}_{ij})$	potential depending on mutual positions of all atoms
$\bar{\rho}_{ij}$	radius vector determining the position of the i^{th} atom relative to the j^{th} atom
Φ_{ta}	torsion angles
Φ_{va}	valence angles
Φ_{vv}	Vander Waals contacts
λ	wave length
$n_{l\sigma}^d$	number of electrons on impurities
ρ	medium density
$\bar{\rho}_{cj}$	vector connecting points c and j
g	axial viscous normal stress
χ	relative fraction of elastically deformed polymer
$y(j,l)$	length distribution
t_{Δ}	electron hopping integral
U_{ζ}	velocity vector of the interface
μ_{ab}	absolute magnetic penetrability of medium
φ_m	maximum potential of electromagnetic radiation of nanocomposite
\bar{x}_{i0}, \bar{x}_i	original and current coordinates