MATERIALS BEHAVIOR

Research Methodology and Mathematical Models

Mihai Ciocoiu, PhD
Editor

AAP APPLE ACADEMIC PRESS

CRC Press
Taylor & Francis Group

MATERIALS BEHAVIOR

Research Methodology and Mathematical Models

Edited by
Mihai Ciocoiu, PhD

A. K. Haghi, PhD, and Gennady E. Zaikov, DSc
Reviewers and Advisory Board Members

AAP APPLE ACADEMIC PRESS

Apple Academic Press Inc.
3333 Mistwell Crescent
Oakville, ON L6L 0A2
Canada

Apple Academic Press Inc.
9 Spinnaker Way
Waretown, NJ 08758
USA

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

International Standard Book Number-13: 978-1-77188-075-6 (Hardcover)

Library and Archives Canada Cataloguing in Publication

Materials behavior : research methodology and mathematical models/edited by Mihai Ciocoiu, PhD; A.K. Haghi, PhD, and Gennady E. Zaikov, DSc, reviewers and advisory board members.

Includes bibliographical references and index.
ISBN 978-1-77188-075-6 (bound)
1. Statistical mechanics. 2. Materials--Testing. 3. Polymers--Testing. 4. Surface chemistry. 5. Molecular dynamics. I. Ciocoiu, Mihai, editor

QC174.8.M38 2015 620.1'10721 C2015-902886-8

Library of Congress Cataloging-in-Publication Data

Materials behavior : research methodology and mathematical models / Mihai Ciocoiu, PhD [editor] ; A.K. Haghi, PhD, and Gennady E. Zaikov, DSc, reviewers and advisory board members.

pages cm
Includes bibliographical references and index.
ISBN 978-1-77188-075-6 (alk. paper)
1. Statistical mechanics. 2. Materials--Testing. 3. Polymers--Testing. 4. Surface chemistry. 5. Molecular dynamics. I. Ciocoiu, Mihai. II. Haghi, A. K. III. Zaikov, G. E. (Gennadii Efremovich), 1935-

QC174.8.M355 2015 620.1'10721--dc23 2015015266

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**

MIX
Paper from responsible sources
FSC www.fsc.org FSC® C013056

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

MATERIALS BEHAVIOR

Research Methodology and Mathematical Models

ABOUT THE EDITOR

Mihai Ciocoiu, PhD

Mihai Ciocoiu, PhD, is a Professor of Textiles-Leather and Industrial Management at Gheorghe Asachi Technical University of Iasi, Romania. He is the founder and Editor-In-Chief of the *Romanian Textile and Leather Journal*. He is currently a senior consultant, editor, and member of the academic board of the *Polymers Research Journal* and the *International Journal of Chemoinformatics and Chemical Engineering*.

REVIEWERS AND ADVISORY BOARD MEMBERS

A. K. Haghi, PhD

A. K. Haghi, PhD, holds a BSc in urban and environmental engineering from 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 65 books as well as 1000 published 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.

Gennady E. Zaikov, DSc

Gennady E. Zaikov, DSc, is Head of the Polymer Division at the N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow, Russia, and Professor at Moscow State Academy of Fine Chemical Technology, Russia, as well as Professor at Kazan National Research Technological University, Kazan, Russia. He is also a prolific author, researcher, and lecturer. He has received several awards for his work, including the Russian Federation Scholarship for Outstanding Scientists. He has been a member of many professional organizations and on the editorial boards of many international science journals.

LIST OF CONTRIBUTORS

Arezo Afzali
University of Guilan, Rasht, Iran

R. M. Akhmetkhanov
Bashkir State University, 32 ZakiValidi Street, 450076 Ufa, Republic of Bashkortostan, Russia, Tel.: (347) 2299686; Fax: (347) 2299707

M. V. Bazunova
Bashkir State University, 32 ZakiValidi Street, 450076 Ufa, Republic of Bashkortostan, Russia, Tel.: (347) 2299686; Fax: (347) 2299707; E-mail: mbazunova@mail.ru

M. Dilamian
University of Guilan, Rasht, Iran

I. V. Dolbin
Kabardino-Balkarian State University, Nal'chik – 360004, Chernyshevsky st., 173, Russian Federation, E-mail: I_dolbin@mail.ru

Walter W. Focke
Institute of Applied Materials, Department of Chemical Engineering, University of Pretoria, Pretoria 0002, South Africa, Tel.: (+27) 12 420 3728, Fax: (+27) 12 420 2516

Dhorali Gnanasekaran
Institute of Applied Materials, Department of Chemical Engineering, University of Pretoria, Pretoria 0002, South Africa, Tel.: (+27) 12 420 3728, Fax: (+27) 12 420 2516

Mahdi Hasanzadeh
Department of Textile Engineering, University of Guilan, Rasht, Iran; E-mail: hasanzadeh_mahdi@yahoo.com

V. A. Ilatovsky
N.N. Semenov Institufe of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., 119991 Moscow, Russia

M. Kanafchian
University of Guilan, Rasht, Iran

G. G. Komissarov
N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., 119991 Moscow, Russia; E-mail: gkomiss@yandex.ru; komiss@chph.ras.ru

G. V. Kozlov
Kabardino-Balkarian State University, Nal'chik – 360004, Chernyshevsky st., 173, Russian Federation

E. T. Kruts'ko
Doctor of Technical Sciences, Professor (BSTU), Sverdlova Str.13a, Minsk, Republic of Belarus

Shima Maghsoodlou
University of Guilan, Rasht, Iran

Pedro H. Massinga Jr.
Universidade Eduardo Mondlane, Faculdade de Ciências, Campus Universitário Principal, Av. Julius Nyerere, PO Box 257, Maputo, Moçambique

F. V. Morev
Postgraduate, Belarusian State Technological University, Sverdlova Str.13a, Minsk, Republic of Belarus

N. R. Prokopchuk
Corresponding Member of National Academy of Sciences of Belarus, Doctor of Chemical Sciences, Professor, Head of Department (BSTU), Sverdlova Str.13a, Minsk, Republic of Belarus, E-mail: prok_nr@mail.by

G. A. Ptitsyn
N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., 119991 Moscow, Russia

Jozef Richert
Institut Inzynierii Materialow Polimerowych I Barwnikow, 55 M. Sklodowskiej-Curie str., 87-100 Torun, Poland, E-mail: j.richert@impib.pl

G. V. Sinko
N.N. Semenov Institute of Chemical Physics, Russian Academy of Sciences, 4 Kosygin str., 119991 Moscow, Russia

O. V. Stoyanov
Kazan National Research Technological University, Kazan, Tatarstan, Russia, E-mail: OV_Stoyanov@mail.ru

G. E. Zaikov
N.M. Emanuel Institute of Biochemical Physics of Russian Academy of Sciences, Moscow 119334, Kosygin st., 4, Russian Federation, E-mail: Chembio@sky.chph.ras.ru

LIST OF ABBREVIATIONS

ABS	Acrylonitrile–Butadiene–Styrene
ANOVA	Analysis of Variance
BPE	Branched Polyethylenes
CCD	Central Composite Design
CD	Cross-Direction
CNT	Classical Nucleation Theory
CV	Coefficient of Variation
CSC	Crystallites with Stretched Chains
DSC	Differential Scanning Calorimetry
EDANA	European Disposables and Nonwovens Association
EP	Epoxy Polymer
EVA	Ethylene-co-Vinyl Acetate
FH	Fluorohectorite
FOD	Fiber Orientation Distribution
FT	Fourier Transform
HBP	Hyper Branched Polymer
HRR	Heat Release Rate
HRTEM	High Resolution Transmission Electron Microscopy
HT	Hectorite
HT	Hough Transform
I(e)	Informational Entropy
IP	Inclined Plates
IRDP	Institutional Research Development Programme
LDHs	Layered Double Hydroxides
LDPE	Low Density Polyethylene
LOI	Loss on Ignition
MC	Monte Carlo
MD	Machine Direction
MD	Molecular Dynamics
MFI	Melt Flow Index
MMT	Montmorillonite
NRF	National Research Foundation
NSMs	Nano Structured Materials
PA	Polyurethane
PAr	Polyarylate
Pc	Phthalo Cyanines

PC	Polycarbonate
PET	Poly(ethylene terephthalate)
PGD	Pores Geometry Distribution
PHRR	Peak of Heat Release
PMMA	Poly(methyl methacrylate)
POSS	Polyhedral Oligomeric Silse Squioxaneo
PP	Polypropylene
PVD	Pore Volume Distributions
REP	Rarely Cross-Linked Epoxy Polymer
RSM	Response Surface Methodology
SEM	Scanning Electron Microscope
SR	Smoke Release
TBP	Tetrabenzoporphyrin
TEM	Transmission Electron Microscopy
TGA	Thermogravimetric Analysis
THR	Total Heat Release
TPC	Tetra Pyrrole Compounds
TPP	Tetraphenyl Porphyrin
TTI	Time to Ignition
VA	Vinyl Acetate
WL	Weight Loss
0DNSM	Zero-Dimensional Nanostructured Materials
1DNSM	One-Dimensional Nanostructured Materials
2DNSM	Two-Dimensional Nanostructured Materials

LIST OF SYMBOLS

a	the acceleration
a and b	integers
a_{i}	the acceleration of particle i
b	Burgers vector
c	speed of light in m/s
C_{∞}	characteristic ratio
d	dimension of Euclidean space
D_{p}	nanofiller particles diameter in nm
d_{surf}	nanocluster surface fractal dimension
d_{u}	fractal dimension of accessible for contact ("nonscreened") indicated particle surface
d_{w}	dimension of random walk
E	the potential energy of the system
E_a	the distance from the surface acceptor level to the E_v
E_{n} and E_{m}	elasticity moduli of nanocomposites and matrix polymer, respectively
F	the force exerted on the particle
F_{i}	the force exerted on particle i
F_s	the distance from the Fermi level at the surface to E_v
G	shear modulus
G_{∞}	equilibrium shear modulus
G_{c}, G_{m} and G_{f}	shear moduli of composite, polymer matrix and filler, respectively
G_{cl}	the shear modulus
h	Planck constant
I	the scattering intensity
I_0	a reference value of intensity
I_{ph}	photocurrent in μ A
k	Boltzmann constant
K_{s}	stress concentration coefficient
K_{T}	bulk modulus
L	filler particle size
l_0	main chain skeletal length
l_k	specific spatial scale of structural changes
l_{st}	statistical segment length
m	the mass
M	the total sampling number

m and n	exponents in the Mie equation
$m_{absorbed\ water}$	weight of the saturated condensed vapors of volatile liquid, g
M_{cl}	molecular weight of the chain part between cluster
M_e	molecular weight of chain part between entanglements
m_i	the mass of particle i
m_{sample}	weight of dry sample, g
N	the number of atoms in the system
N_A	Avogadro number
n_{cl}	statistical segments number per one nanocluster
N_α and N_β	the numbers of particles of the entities of type α and β, respectively
p	solid-state component volume fraction
p_c	percolation threshold
q	the parameter
q	the wave number
Q_1 and Q_2	the charges
R	a hydrogen atom or an organic group
r	the position
R	universal gas constant
r_{ij}	the distance between a pair of atoms *i* and *j*
r^N	the complete set of 3N atomic coordinates
S	macromolecule cross-sectional area
T, T_g and T_m	testing, glass transition and melting temperatures, respectively
$u(r)$	an externally applied potential field
v	the velocity
V	the volume of the system
W	absorbed light power W
w	activation energy of the transition to the charged form
W_n	nanofiller mass contents in mas.%,
Z_i	the effective charge of the i-th ion

Greek Symbols

$f_\infty^{(0)}$	the equilibrium distribution
$\langle\rangle$	ensemble average
σ_f^n	nominal (engineering) fracture stress
σ_f^c and σ_f^m	fracture stress of composite and polymer matrix, respectively
a	the efficiency constant
α_i	the electric polarizability of the i-th ion
β	coefficient
β_p and ν_p	critical exponents (indices) in percolation theory
ΔS	entropy change in this process course
ε	misfit strain arising from the difference in lattice parameters

ε_0	the permittivity of free space
ε_f	strain at fracture
ε_Y	the yield strain
η	exponent
J	total concentration of adsorbed molecules
l	wavelength m
λ_b	the smallest length of acoustic irradiation sequence
λ_k	length of irradiation sequence
n	Poisson's ratio
ν_{cl}	cluster network density
ν_p	correlation length index in percolation theory
r	nanofiller (nanoclusters) density
ρ	polymer density
ρ_{cl}	the nanocluster density
ρ_d	the density if linear defects
ρ_α and ρ_β	the corresponding densities of α and β subsystems
τ	the relaxation time (dimensionless)
τ_{in}	the initial internal stress
t_{IP}	the shear stress in IP (cluster)
φ_n	nanofiller volume contents
c	the relative fraction of elastically deformed polymer
Γ	Eiler gamma-function

PREFACE

This book covers a wide variety of recent research on advanced materials and their applications. It provides valuable engineering insights into the developments that have lead to many technological and commercial developments.

This book also covers many important aspects of applied research and evaluation methods in chemical engineering and materials science that are important in chemical technology and in the design of chemical and polymeric products. This book gives readers a deeper understanding of physical and chemical phenomena that occur at surfaces and interfaces. Important is the link between interfacial behavior and the performance of products and chemical processes. Helping to fill the gap between theory and practice, this book explains the major concepts of new advances in high performance materials and their applications.

This book has an important role in advanced materials in macro and nanoscale. Its aim is to provide original, theoretical, and important experimental results that use nonroutine methodologies often unfamiliar to the usual readers. It also includes chapters on novel applications of more familiar experimental techniques and analyzes of composite problems that indicate the need for new experimental approaches.

CONTENTS

List of Contributors ix
List of Abbreviations xi
List of Symbols xvii
Preface xix

1. **Understanding Modeling and Simulation of Aerogels Behavior: From Theory to Application**
M. Dilamian

2. **Biodegradable Polymer Films on Low Density Polyethylene and Chitosan Basis: A Research Note** 00
M. V. Bazunova and R. M. Akhmetkhanov

3. **A Detailed Review on Behavior of Ethylene-Vinyl Acetate Copolymer Nanocomposite Materials** 00
Dhorali Gnanasekaran, Pedro H. Massinga Jr., and Walter W. Focke

4. **The Influence of the Electron Density Distribution in the Molecules of (N)-Aza-Tetrabenzoporphyrins on the Photocatalytic Properties of Their Films** 00
V. A. Ilatovsky, G. V. Sinko, G. A. Ptitsyn, and G. G. Komissarov

5. **On Fractal Analysis and Polymeric Cluster Medium Model** 00
G. V. Kozlov, I. V. Dolbin, Jozef Richert, O. V. Stoyanov, and G. E. Zaikov

6. **Polymers as Natural Composites: An Engineering Insight** 00
G. V. Kozlov, I. V. Dolbin, Jozef Richert, O. V. Stoyanov, and G. E. Zaikov

7. **A Cluster Model of Polymers Amorphous: An Engineering Insight** 00
G. V. Kozlov, I. V. Dolbin, Jozef Richert, O. V. Stoyanov, and G. E. Zaikov

8. **A Note On Modification of Epoxy Resins by Polyisocyanates** 00
N. R. Prokopchuk, E. T. Kruts'ko, and F. V. Morev

9. **Atomistic Simulations Investigation in Nanoscience: A detailed Review** 00
Arezo Afzali, and Shima Maghsoodlou

10. Trends in Application of Hyperbranched Polymers (HBPs) in Textile Industry 00

Mahdi Hasanzadeh

11. A Comprehensive Review on Characterization and Modeling of Nonwoven Structures 00

M. Kanafchian

Index 00

CHAPTER 1

UNDERSTANDING MODELING AND SIMULATION OF AEROGELS BEHAVIOR: FROM THEORY TO APPLICATION

M. DILAMIAN

University of Guilan, Rasht, Iran

CONTENTS

Abstract 2
1.1 Theory 2
1.2 Applications 35
1.3 Conclusion 75
Keywords 77
References 77