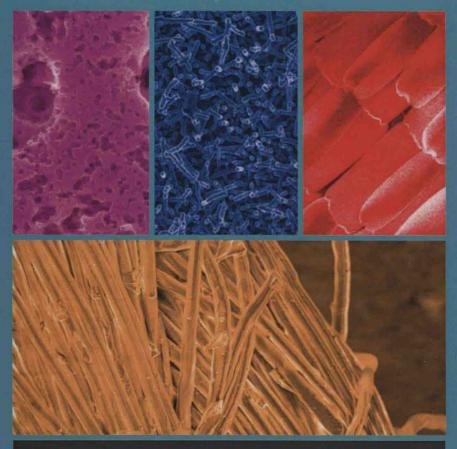
The Chemistry and Physics of Engineering Materials

Limitations, Properties, and Models



Editors

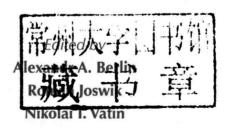
Alexandr A. Berlin, DSc Roman Joswik, PhD Nikolai I. Vatin, DSc





THE CHEMISTRY AND PHYSICS OF ENGINEERING MATERIALS

Volume 2 Limitations, Properties, and Models



Reviewers and Advisory Members

A. K. Haghi

Gennady E. Zaikov



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

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

©2016 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: 978-1-77188-080-0 (Hardcover)

International Standard Book Number-13: 978-1-4987-0607-0 (ebook)

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 and Archives Canada Cataloguing in Publication

The chemistry and physics of engineering materials / edited by Alexandr A. Berlin, Roman Joswik, Nikolai I. Vatin; reviewers and advisory members, A.K. Haghi, Gennady E. Zaikov.

Includes bibliographical references and index.

Contents: Volume 2. Limitations, properties, and models.

ISBN 978-1-77188-080-0 (volume 2: bound)

1. Materials. 2. Chemistry, Physical and theoretical. I. Berlin, Alexandr A., editor

II. Joswik, Roman, editor III. Vatin, Nikolai I., editor

TA403.C54 2015

620.1'1

C2015-904265-8

Library of Congress Cataloging-in-Publication Data

The chemistry and physics of engineering materials / [edited by] Alexandr A. Berlin, Roman Joswik, Nikolai I. Vatin; reviewers and advisory members, A.K. Haghi, Gennady E. Zaikov.

volumes cm

Includes bibliographical references and index.

Contents: volume 2. Limitations, properties, and models

ISBN 978-1-77188-080-0 (alk. paper)

1. Materials—Mechanical properties. 2. Strength of materials. 3. Metallurgical analysis. 4. Polymers—Structure. 5. Chemistry, Technical. I. Berlin, Al. Al., 1940-II. Joswik, Roman. III. Vatin, Nikolai I. (Nikolai Ivanovich) IV. Haghi, A. K. V. Zaikov, G. E. (Gennadii Efremovich), 1935-

TA405 .C4155

620.1'1292--dc23

2015023971

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



THE CHEMISTRY AND PHYSICS OF ENGINEERING MATERIALS

Volume 2 Limitations, Properties, and Models

LIST OF CONTRIBUTORS

I. B. Abdrakhmanov

Establishment of Russian Science Academy, Institute of Organic Chemistry of Ufa Science Center of RSA, 450054, 71 Prospect Octyabrya str, Ufa, Russia, Tel.: +(347)235-38-15; E-mail: Chemhet@anrb.ru

Arezo Afzali

University of Guilan, Rasht, Iran

V. A. Babkin

Sebryakov Department, Volgograd State Architect-Build University, 400074, Russia

O. A. Baulin

Ufa State Petroleum Technical University, 1 Kosmonavtov St. Ufa, 45006, Russia

D. A. Chuvashov

Bashkir State University, 32, Validy Str., Ufa, 450076, Ufa, Russia

R. Ya. Deberdeev

Kazan National Research Technological University, Kazan, Tatarstan, Russia

Mandana Dilamian

University of Guilan, Rasht, Iran

V. Yu. Dmitriev

Sebryakov Department, Volgograd State Architect-Build University, 400074, Russia

A. K. Haghi

University of Guilan, Rasht, Iran

B. A. Howell

Central Michigan University, Mount Pleasent, Michigan, USA

A. V. Ignatov

Sebryakov Department, Volgograd State Architect-Build University, 400074, Russia

V. F. Kablov

Volzhsky Polytechnical Institute (branch), Volgograd State Technical University, Russia; E-mail: kablov@volpi.ru

S. L. Khursan

Establishment of Russian Science Academy, Institute of Organic Chemistry of Ufa Science Center of RSA, 450054, 71 Prospect Octyabrya str, Ufa, Russia, Tel.: +(347)235-38-15; E-mail: chemhet@anrb.ru

K. R. Khusnitdinov

Establishment of Russian Science Academy, Institute of Organic Chemistry of Ufa Science Center of RSA, 450054,71 Prospect Octyabrya str, Ufa, Russia, Tel.: +(347)235-38-15; E-mail: chemhet@anrb.ru

R. N. Khusnitdinov

Establishment of Russian Science Academy, Institute of Organic Chemistry of Ufa Science Center of RSA, 450054, 71 Prospect Octyabrya str, Ufa, Russia

V. I. Kodolov

Kalashnikov Izhevsk State Technical University, Russian Federation

Gennady G. Komissarov

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

G. A. Korablev

Izhevsk State Agricultural Academy, Izhevsk 426000, Russia; E-mail: korablev@udm.net

R. G. Korablev

Izhevsk State Agricultural Academy, Izhevsk 426000, Russia

G. V. Kozlov

FSBEI HPE "Kh.M. Berbekov Kabardino-Balkarian State University," Chernyshevsky st., 173, Nal'chik-360004, Russian Federation

Shima Maghsoodlou

University of Guilan, Rasht, Iran

G. M. Magomedov

FSBEI HPE "Daghestan State Pedagogical University," M. Yaragskii st., 57, Makhachkala-367003, Russian Federation

A. K. Mikitaev

Kh.M. Berbekov Kabardino-Balkarian State University, Chernyshevsky st., 173, Nal'chik-360004, Russian Federation

A. G. Moustafin

Establishment of Russian Science Academy, Institute of Organic Chemistry of Ufa Science Center of RSA, 450054, 71 Prospect Octyabrya str, Ufa, Russia, Tel.: +(347)235-38-15; E-mail: chemhet@anrb.ru

A. K. Osipov

Izhevsk State Agricultural Academy, Izhevsk 426000, Russia

N. G. Petrova

Ministry of Informatization and Communication of the Udmurt Republic, Russian Federation

A. I. Rakhimov

Volgograd State Technical University, Lenin Avenue, 28, Volgograd, 400005, Russia

N. A. Rakhimova

Volgograd State Technical University, Lenin Avenue, 28, Volgograd, 400005, Russia

F. B. Shevlyakov

Ufa State Petroleum Technical University, 1 Kosmonavtov St. Ufa, 45006, Russia

E. S. Titova

Volgograd State Technical University, Lenin Avenue, 28, Volgograd, 400005, Russia

V. V. Trifonov

Sebryakov Department, Volgograd State Architect-Build University, Russian Federation

List of Contributors ix

T. G. Umergalin

Ufa State Petroleum Technical University, 1 Kosmonavtov St. Ufa, 45006, Russia

N. I. Vatin

Civil Engineering Institute, Saint-Petersburg State Polytechnical University, 29 Polytechnicheskaya Street, Saint-Petersburg, 195251, Russia; E-mail: vatin@mail.ru

Kh. Sh. Yakh'vaeva

FSBEI HPE "M.M. Dzhambulatov Daghestan State Agrarian University," M. Gadzhiev st, 180, Makhachkala, 367032, Russian Federation

G. E. Zaikov

Institute of Biochemical Physics, Russian Academy of Sciences, 4 Kosygin str., Moscow 119334, Russian Federation; E-mail: chembio@sky.chph.ras.ru

V. P. Zakharov

Bashkir State University, 32, Validy Str., Ufa, 450076, Ufa, Russia; E-mail: Zaharov VP@mail.ru



LIST OF ABBREVIATIONS

ADH adipic dihydrazide

ART activation-relaxation technique

ATNMRI Advanced Technologies and New Materials Research

Institute

BET Brunauer–Emmett–Teller BGK Bhatnagar-Gross-Krook

BKS van Beest, Kramer and van Santen

BMH Born–Mayer–Huggins BSA bovine serum albumin

CA chitosan

CNT classical nucleation theory

DLCA diffusion-limited cluster-cluster aggregation

DMC dynamic Monte Carlo
ECM extracellular matrix
EDP electric desalting plant

FENE finitely extensible nonlinear elastic

FSSE first shell substitution effect

GAG glycosaminoglycan
GNC globular nanocarbon
HA hyaluronic acid
HCl hydrochloridric acid
HMDS hexamethyldisilazane

HRTEM high resolution transmission electron microscopy

HYAL hyaluronidase

LAAO limited access of atmospheric oxygen

LDPE low density polyethylene
MBA 1-methyl-2-butenyl-aniline

MC Monte Carlo

MD molecular dynamics
MFI melt flow index

xii List of Abbreviations

PCCM polycondensation capable monomers PCT physical and chemical transformations

PDF pair distribution function

PEI polyethyleneimine

PLL poly-L-lysine PP polypropylene

RCP random close packing ROS reactive oxygen species

SAIA Slovak Academic Information Agency SANS small-angle neutron scattering data

SEM scanning electron microscopy

SF synovial fluid SR sustained release

THz terahertz

TM technical materials
TMOS tetramethoxysilane

UHMPE ultrahigh molecular polyethylene VACF velocity autocorrelation function

LIST OF SYMBOLS

	A analomation of montials
a	Acceleration of particle
A	Atom-type dependent constants
В	Strength of the three-body interaction
b_0	Ideal bond length
C_{ik}	Constants
D	Effective dielectric function
d_f	Fractal dimension, df, of porous systems
E	Potential energy
$E_{ m kin}$	Kinetic energy
F	Force
H	Hamiltonian
H	Strength
H_{ij}	Strength
$k_{_{ m B}}$	Boltzmann constant, 1.3806 × 10-23 J/K
K _b	Force constant for bound atoms
K_{θ}	Force constant for bond angels theta
m	Mass of particle
M	Total sampling number
N	Number of atoms
P	Momentum
q	Atomic charges
r	Distance between two atoms
S	Entropy
T	Temperature
t	Time
$u(r^N)$	Potential energy
V	Potential
v	Velocity
x	Direction
Zi	Formal ionic charges

Time interval

 Δt

Greek Symbols

\mathcal{O}_{ijkl}	Torsion angles
$ heta_{ijk}$	Band angel
φ_{IJ}	Lennard-Jones potential
α	Electric polarizability
3	Energy
ϵ_0	Permittivity of free space
η	Exponent of steric repulsion
η_{ij}	Exponent of steric repulsion
θ	Angle between the vector position of the atoms
ρ	Density
σ	Length parameters
τ	Relaxation time

PREFACE

The collection of topics in the two-volume publication reflects the diversity of recent advances in this field with a broad perspective which may be useful for scientists as well as for graduate students and engineers. This new book presents leading-edge research from around the world in this dynamic field.

Diverse topics published in this book are the original works of some of the brightest and most well-known international scientists in two separate volumes.

In the first volume, modern analytical methodologies are presented here.

The first volume offers scope for academics, researchers, and engineering professionals to present their research and development works that have potential for applications in several disciplines of engineering and science. Contributions range from new methods to novel applications of existing methods to provide an understanding of the material and/or structural behavior of new and advanced systems.

In the second volume, limitations, properties and models are presented. These two volumes:

- are collections of articles that highlight some important areas of current interest in recent advances in chemistry and physics of engineering materials
- give an up-to-date and thorough exposition of the present state-ofthe-art of chemical physics
- describe the types of techniques now available to the chemist and technician, and discuss their capabilities, limitations and applications.
- provide a balance between chemical and material engineering, basic and applied research.

We would like to express our deep appreciation to all the authors for their outstanding contributions to this book and to express our sincere gratitude for their generosity. All the authors eagerly shared their experiences and expertise in this new book. Special thanks go to the referees for their valuable work.

ABOUT THE EDITORS

Alexandr A. Berlin, DSc

Director, Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia

Professor Alexandr A. Berlin, DSc, is the Director of the N. N. Semenov Institute of Chemical Physics at the Russian Academy of Sciences, Moscow, Russia. He is a member of the Russian Academy of Sciences and many national and international associations. Dr. Berlin is world-renowned scientist in the field of chemical kinetics (combustion and flame), chemical physics (thermodynamics), chemistry and physics of oligomers, polymers, and composites and nanocomposites. He is a contributor to 100 books and volumes and has authored over 1000 original papers and reviews.

Roman Joswik, PhD

Director, Military Institute of Chemistry and Radiometry, Warsaw, Poland Roman Joswik, PhD, is the Director of the Military Institute of Chemistry and Radiometry in Warsaw, Poland. He is a specialist in the field of physical chemistry, chemical physics, radiochemistry, organic chemistry, and applied chemistry. He has published several hundred original scientific papers as well as reviews in the field of radiochemistry and applied chemistry.

Nikolai I. Vatin, DSc

Director of Civil Engineering Institute, Saint-Petersburg State Polytechnical University, Chief of Construction of Unique Buildings and Structures Department

Nikolai I. Vatin, DSc, is the Chief scientific editor of *Magazine of Civil Engineering* and Editor of *Construction of Unique Buildings and Structures*. He is a specialist in the field of chemistry and chemical technology. He published several hundred scientific papers (original and review) and several volumes and books.

xviii About the Editors

A. K. Haghi, PhD

Member of the Canadian Research and Development Center of Sciences and Cultures (CRDCSC), Montreal, Quebec, Canada; Editor-in-Chief, International Journal of Chemoinformatics and Chemical Engineering; Editor-in-Chief, Polymers Research Journal

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 165 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

Head of the Polymer Division, N. M. Emanuel Institute of Biochemical Physics, Russian Academy of Sciences, Moscow; Professor, Moscow State Academy of Fine Chemical Technology and Kazan National Research Technological University, Russia

Gennady E. Zaikov, DSc, is the 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.