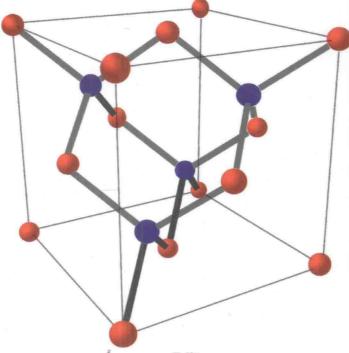
## Chemical and Applied Engineering Materials

Interdisciplinary Research and Methodologies



Editor Maria Rajkiewicz, DSc





## CHEMICAL AND APPLIED ENGINEERING MATERIALS

Interdisciplinary Research and Methodologies

Edited by
Maria Rajkiewicz, DSc

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



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#### LIST OF ABBREVIATIONS

AG acrylate guanidine

BMEP brake mean effective pressure

CNTs carbon nanotubes

DAGA N,N-Diallylguanidine acetate

DAGTFA N,N-Diallylguanidine trifluoroacetate

HOMO highest occupied state

LUMO lowest free state

MAG methacrylate guanidine MAO methylalumi- noxane MCC microcrystalline cellulose

PEDA phosphorus-boron-nitrogen-containing oligomer

PFT polymerization-filling technique

PVP polyvinyl pyrrolidone SDS sodium dodecyl- sulfate

SWCNTs single-walled carbon nanotubes

TBP tetrabenzoporphyrin
TEG thermal expanded graphite
TPC tetrapyrrole compounds
TPP tetraphenyl porphyrin

#### LIST OF SYMBOLS

h Planck constant  $I_{\rm ph}$  photocurrent in Ma W absorbed light power  $\lambda$  wavelength m C speed of light in m/s.

 $PR_{\infty}$  pressure ratio at surge line

PR... pressure ratio at surge control line

 $E_i$  orbital energy

W, bond energy of an electron

n<sub>i</sub> number of elements of the given orbital
 K maxing or hybridization coefficient

 $egin{array}{ll} N_0 & & \text{number of particles} \\ r & & \text{radius of rotating bodies} \end{array}$ 

h film thickness

N number changing depending on the nanostructure shape

υ crystallinity degree

τ duration

k value corresponding to specific process rate

a nanoreactor activity

 $\varepsilon_{_{S}}$  surface energy reflecting the energy

 $\epsilon_{_{
m V}}$  nanoreactor volume energy

 $\varepsilon_{\rm S}^0$ d multiplication of surface layer energy by its thickness

 $\epsilon^0_{\ v}$  energy of nanoreactor volume unit S surface of nanoreactor walls

V nanoreactor volume

#### **PREFACE**

This new research book explores and discusses a range of topics on the physical and mechanical properties of chemical engineering materials. Chapters from prominent researchers in the fields of physics, chemistry and engineering science present new research on composite materials, blends, carbon nanotubes, and nanocomposites along with their applications in technology. Discussing the processing, morphology, structure, properties, performance, and applications, the book highlights the diverse and multidisciplinary nature of the field.

In the first chapter a study on highly filled composite materials with regulated physical and mechanical properties based on synthetic polymers and organic and inorganic fillers is presented. For predication of photoelectrochemical properties of selected molecules by their structure, chapter 2 could be used as an advanced review. In chapter 3 performance of turbocharged spark ignition engine equipped with anti-surge valve and bypass flow control mechanism at various working conditions is presented in detail. Chapter 4 describes the dependence of some thermodynamic characteristics upon initial spatial-energy parameters of free atoms. Fire retardant coatings based on perchlorovinyl resin with improved adhesive properties to protect fiberglass plastics are presented in chapter 5. As an multidisciplinary engineering subject, of course, the modification of peculiarities of microcrystalline cellulose and its oxidized form Guanidine-containing monomers and polymers of vinyl and Diallyl series in chapter 6 could be very interesting for the readers. Research progress on carbon nanotube-polymer composites as well as CNT/polymer composites from the chemistry, mechanics and physics aspects are well developed in chapters 7 and 8. In the next two chapters trends in nanochemistry for metal-carbon nanocomposites as well as production technology of carbon-metal containing nanoproducts in nanoreactors of polymeric matrix are described in detail. In chapter 11 a note on Redox processes in polymeric matrix nanoreactors and in chapter 12 conditions for carbon black accumulation at the interface in heterogeneous binary polymer blends are well presented. Performance analysis of multilayer insulations in cryogenic applications is presented in chapter 13. The effect of particle size of microheterogenous catalyst TiCl4-Al(iso-C4H9)3 on the basic patterns of isoprene polymerization is shown in chapter 14. Internal structure and the equilibrium configuration of separate non-interacting nanoparticles by the molecular mechanics and dynamics methods is another multidisciplinary subject that is

xx Preface

presented in chapter 15. A very detailed review on membrane filtration technology is selected for chapter 16. In this chapter theory and application presented step-by-step for readers in science and engineering.

#### CONTENTS

	List of Contributorsxi
	List of Abbreviationsxv
	List of Symbolsxvii
	Prefacexix
1.	Investigation on Highly Filled Composite Materials with Regulated Physical and Mechanical Properties Based on Synthetic Polymers and Organic and Inorganic Fillers
2.	Predication of Photoelectrochemical Properties of Selected Molecules by Their Structure
3.	Investigation on Performance of Turbocharged Spark Ignition Engine Equipped with Anti-Surge Valve and Bypass Flow Control Mechanism at Various Working Conditions
4.	The Dependence of Some Thermodynamic Characteristics Upon Initial Spatial-Energy Parameters of Free Atoms
5.	Fire Retardant Coatings Based on Perchlorovinyl Resin with Improved Adhesive Properties to Protect Fiberglass Plastics
6.	Modification of Peculiarities of Microcrystalline Cellulose (MCC) and Its Oxidized Form (dialdehyde cellulose DAC) Guanidine-Containing Monomers and Polymers of Vinyl and Diallyl Series87  Azamat A. Khashirov, Azamat A. Zhansitov, G. E. Zaikov, and Svetlana Yu. Khashirova
7.	Research Progress on Carbon Nanotube–Polymer Composites93 Shima Maghsoodlou and Arezoo Afzali
8.	CNT/Polymer Composites from Chemistry, Mechanics and Physics Aspects

9,	Trends in Nanochemistry for Metal/Carbon Nanocomposites
10.	A Research Note on Production Technology of Carbon-Metal Containing Nanoproducts in Nanoreactors of Polymeric Matrixes193 V. I. Kodolov, V. V. Trineeva, O. A. Kovyazina, and A. Yu. Bondar
11.	Redox Processes in Polymeric Matrixes Nanoreactors:  A Research Note
12.	Conditions for Carbon Black Accumulation at the Interface in Heterogeneous Binary Polymer Blends
13.	Performance Analysis of Multilayer Insulations in Cryogenic Applications
14.	The Effect Particle Size of Microheterogenous Catalyst TiCl4-Al(iso-C4H9)3 on the Basic Patterns of Soprene Polymerization
15.	Internal Structure and the Equilibrium Configuration (Shape) of Separate Non-Interacting Nanoparticles by the Molecular Mechanics and Dynamics Methods
16.	Trends in Membrane Filtration Technology: Theory and Application
	Index

# INVESTIGATION ON HIGHLY FILLED COMPOSITE MATERIALS WITH REGULATED PHYSICAL AND MECHANICAL PROPERTIES BASED ON SYNTHETIC POLYMERS AND ORGANIC AND INORGANIC FILLERS

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#### **CONTENTS**

1.1	Aims and Backgrounds	2
1.2	Introduction	2
1.3	Experimental	2
1.4	Results and discussions	3
1.5	Conclusions	8
Кеуч	vords	9
Refer	ences	9

#### 1.1 AIMS AND BACKGROUNDS

The aim of the carried out work was to elaborate the highly filled composite materials with regulated physical and mechanical properties based on synthetic polymers and organic and inorganic fillers that can be used in creation of biodegradable in the environment goods of different purposes. Aspects, essential for technology, such as physical and chemical, structural, rheological properties, were investigated. Methods of electron paramagnetic probe, IR-spectrometry were used to prove that inorganic filler plays the role of plasticizer in creation of hybrid composites. Microbiological aspects will be the subject of another article.

#### 1.2 INTRODUCTION

One of the promising trends from the viewpoint of ecology is the development of biodegradable polymer composites. These materials, along with the polymer base more resistant to biodegradation, comprise fillers, which are not only accessible for microbial degraders but are also agro-industrial wastes to be utilized [1]. Search for cheap fillers and development of polymer composites makes it possible not only to reduce the cost of product, but also contributes to the solution of ecological problems.

#### 1.3 EXPERIMENTAL

Third-grade threshed grain wastes (size of particles, 63–240 µm; bulk density, 350 kg/m³; humidity, 4%) were used as organic filler. As inorganic filler, we took a Rastvorin-A water-soluble mineral fertilizer (OST 10-193-96, produced by the Buysk Mineral Fertilizer Plant) of the following composition (in %): (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>, 35; NH<sub>4</sub>H<sub>2</sub>PO<sub>4</sub>, 6; KNO<sub>3</sub>, 32; MgSO<sub>4</sub>·7H<sub>2</sub>O, 27.

The physicomechanical properties of specimens within a broad range of ingredient ratios were determined according to GOST 14236-82; the rheological characteristics of filled compositions, by the method of capillary viscosimetry.

In the work, use was made of the method of electron paramagnetic probe, which was stable nitroxyl radical 2,2,6,6-tetramethylpiperidine-1-oxyl. The radical was introduced into films from vapors at  $T=25^{\circ}\mathrm{C}$  up to a concentration of  $10^{-3}$  mol/l. A reference solution of the radical in  $\mathrm{CCl_4}$  with a known number of spins was used in the determination of the concentration of radicals in films. The number of spins in a specimen was determined by comparing the areas under the absorption curves of the specimen studied and the reference. The rotational

mobility of the probe was characterized by the correlation time  $\tau$ . The values of  $\tau$  were assessed from the EPR spectra by the method outlined in [2].

#### 1.4 RESULTS AND DISCUSSIONS

At the introduction of fillers into SEVA irrespective of its grade, we found that the strength and relative elongation decrease with an increase of the content both of organic and inorganic filler in two-component polymer—filler systems (see Figures 1.1 and 1.2). In the case of filling with organic filler specimens become more rigid; at the introduction of inorganic filler even at a high concentration (60 wt. %) specimens preserve a high plasticity (the breaking strain is 400%).

Considering three-component systems (SEVA/inorganic filler/organic filler, Figure 1.3), it should be noted that in this case too an increase in the content of inorganic filler leads to more plastic specimens.

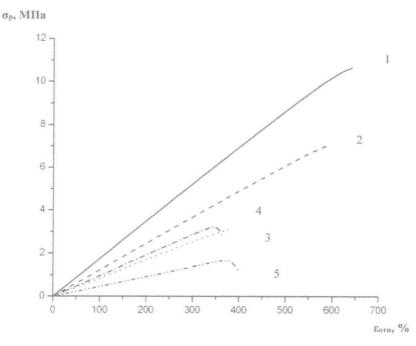


FIGURE 1.1 Change of the physicomechanical properties of a two-component system (SEVA/inorganic filler, wt. %): 1, 100/0; 2, 80/20; 3, 60/40; 4, 50/50; 5, 40/60.