Ivane Javakhishvili Tbilisi State University

ICSP & AM 8

Eighth International Caucasian Symposium on Polymers and Advanced Materials

Dedicated to the Memory and 75th Birthday
Anniversary of Professor
Omar Mukbaniani

August 1-3, 2023
Tbilisi, Georgia

Welcome

Dear Colleagues,

On behalf of the Organizing Committee, I wish to extend a cordial welcome to all participants of the “8th International Caucasian Symposium on Polymers and Advanced Materials” which is dedicated to the memory and 75th birthday anniversary of its establisher and chairman Professor **Omar Mukbaniani.**

First, in 2007, 16 years ago, this symposium took place at Tbilisi State University, Tbilisi, Georgia. In the 2021 year, our previous symposium was held during the Covid-19 pandemic situation in a hybrid format. Now we conducting the 8th meeting also a hybrid. This will enable many scientists to join and attend the symposium remotely, especially our friends and colleagues from Ukraine.

We are delighted to host you this year in our beautiful Georgia, in Tbilisi. These meetings led to thefact that we cooperate with the Max Planck Institute for Polymer Research (Mainz, Germany), Polish Universities in the Erasmus+ program, as well as with the Kaunas University of Technology.

We hope that this symposium will in the future lead to the strengthening of close scientific relations with other countries.

The conference's purpose is to encourage scientists working in polymer chemistry and advanced materials to present their investigations dedicated to problems and discoveries in the above-mentioned fields. Also “ICSP&AM 8” will help to introduce effectively innovative scientific research of Georgia in Caucasian and neighboring scientific teams, which are less known in world scientific society. We hope that this year’s meeting, gathering almost 100 participants, shall provide a good platform for academic and industrial scientists to discuss recent advances in the area of polymers and advanced materials.

The symposium is conducted with the support of Ivane Javakhishvili Tbilisi State University and Shota Rustaveli National Science Foundation of Georgia (Project № MG-ISE-23-172).

Dr. Tamara Tatrishvili

Assistant Professor

Organizing Committee:
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In Memoriam
Professor Omar Mukbaniani
Ivane Javakhishvili Tbilisi State University, Georgia

Professor Omar Mukbaniani (1948-2022), Doctor of Chemical Sciences, was a Professor at Ivane Javakhishvili Tbilisi State University, Head of the chair of Macromolecular Chemistry, and Head of the Department of Chemistry. He also served as the Director of the Institute of Macromolecular Chemistry and Polymeric Materials at Ivane Javakhishvili Tbilisi State University.

Professor Omar Mukbaniani was a member of the Academy of Natural Sciences of Georgia. For several years he served as a member of the advisory board and the editorial board of the Journal Proceedings of Ivane Javakhishvili Tbilisi State University (Chemical Series) and contributing editor of the journal Polymer News, the Polymers Research Journal, and Chemistry and Chemical Technology journal.

The research interests of Professor Omar Mukbaniani include polymer chemistry, polymeric materials and the chemistry of organosilicon compounds. Methods of precision synthesis to build block, graft and comb-type structures are developed. The mechanisms of reactions leading to these polymers are also studied. Some effort is devoted to synthesizing various functionalized silicon polymers, copolymers, block copolymers, and composites.

Prof. Omar Mukbaniani, with his colleagues Prof. Marc Jean M. Abadie and Dr Vazha Tskhovrebashvili, was the founder of the “Caucasian Symposium on Polymers and Advanced Materials" (ICSP&AM). The first conference started in 2007, and ICSP&AM 7 was held in July 2021.

Prof. Omar Mukbaniani was the main author of the idea to publish the full texts of the conference abstracts in Apple Academic Press. This book is the fifth edition.

Unfortunately, Professor Omar Mukbaniani is not with us now. His absence is a great loss for their colleagues and the entire chemical community. We will pursue Omari's work in both the organization of ICMP&AM and the publication of the Symposium book where Omari will continue to be the editor.

T. Tatrishvili

Dr Tamara Tatrishvili
Assistant Professor, Department of Chemistry at Ivane Javakhishvili Tbilisi State University;
Director of the Institute of Macromolecular Chemistry and Polymeric Materials, (TSU);
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SYMPOSIUM SCHEDULE

AUGUST 1 **TSU, BUILDING I, ROOM 115**		
08.00-16.00	***Registration***	
09.00-09.30	***Opening Ceremony***	
ORAL PRESENTATIONS: PRESENTATION -10 MINUTES; QUESTIONS -5 MINUTES		
Co-chairmen: Dr. Justyna Kozlowska, Dr. Tamara Tatrishvili		
09.30-09.50	***Marc J.M. Abadie***- *Cross-Linked Polymer Structures: Benefits and Drawbacks”* *Institute Charles Gerhardt Montpellier ICGM, University of Montpellier. France.*	1 (Online)
09.50-10.10	***Vladyslav Zhezherya-*** *“The Role of Various Groups of Natural Organic Substances in Complexation in the Ukraine’s Surface Waters”.* *Institute of Hydrobiology of the National Academy of Sciences of Ukraine.*	2 (Online)
10.10-10-30	***Petro Linnik***- *“Natural Organic Substances’ Transformation in the Ukraine’s Surface Waters Under the Solar Radiation”.* *Institute of Hydrobiology of the National Academy of Sciences of Ukraine.*	3 (Online)
10.30-11.00	***Jozef Haponiuk*** *– „Challenges at Thermomechanical Recycling of Car Tires”.* *Polymers Technology Department, Faculty of Chemistry, Gdansk University of Technology, Gdansk, Poland*	4
11.00-11.30	**Coffee Break**	
Co-chairmen: *Prof. Talkibek Jumadilov, Prof. Akaki Peikrishvili*		
11.30-11.45	***Juozas Vidas Gražulevičius-*** *“Organic Electronically Active Materials for Organic Light Emitting Diodesand Sensors”.* *Department of Polymer Chemistry and Technology, Kaunas University of Technology, Kaunas, Lithuania*	5
11.45- 12.00	***Vladimer Tsitsishvili***- *“Adsorption Properties of Natural and Modified Heulandite-Clinoptilolite”. Georgian National Academy of Sciences, Tbilisi, Georgia*	6 (Online)
12.00-12.15	***Nazilya Salmanova***- *Synthesis and Deployment of Carbon Nanotubes for The Water Surface Purification from Oil Products Films* *Institute of Geotechnological Problems of Oil, Gas and Chemistry Azerbaijan.*	7 (Online)
12.15-12.30	***Sergei Kostjuk-*** *Through-Space Charge-Transfer Thermally Activated Delayed Fluorescence Alternating Donor Acceptor Copolymers: Synthesis, Properties and Application* **“.** *Belarusian State University, Minsk, Belarus.*	8
12.30-12.45	***Justyna Kozlowska*** *– “Polymers in Microencapsulation Systems for Active Substance Controlled Release”.* *Faculty of Chemistry, Department of Chemistry of Biomaterials and Cosmetics, Nicolaus Copernicus University in Torun, Torun, Poland*	9

13.00-13.15	***Eldar Zeynalov*** *– „Modification of Cement Composites with Carbon Nanotubes.Nagiyev Institute of Catalysis & Inorganic Chemistry, Azerbaijan*	10
13.15-14.00	***Krzysztof Matyjaszewski-*** *“New Materials by Macromolecular Engineering Using Atom Transfer Radical Polymerization”.*	11 (Online)
14.00-15.00	**Lunch Break**	
Co-chairmen: *Prof. Eldar Zeynalov, Prof. Efkan Çatıker*		
15.00-15.20	***Akaki Peikrishvili- “****Shock assisted high temperature consolidation & synthesis of diamond containing powders”.* *Ferdinand Tavadze Institute of Metallurgy and Materials Science Country Georgia*	12
15.20-15.40	***Laura Garzón-*** *“Applications of Advanced Catalysts in Petroleum Industry” UFPA, Brazil.*	13 (Online)
15.40-16.00	***Aleksandre Vanishvili- “****Synthesis and characterization of pseudo-proteins modified by polyamides – Poly (Ester amide-co-amide) s”.* *Agricultural University of Georgia. Tbilisi*	14
16.00-16.30	***Michael Nazarkovsky-*** *“Morphological and Optical Properties of Manganese-Doped Zinc Oxide/Nanosilica Designed For The Visible Light Photocatalysis* *Pontifical Catholic University of Rio de Janeiro, Brazil.*	15 (Online)
16.30-17.30	***Poster Presentation***	
18.00	***Fourchette***	
AUGUST 2 **TSU, BUILDING I, ROOM 115**		
Co-chairmen: *Prof. Jozef Haponiuk, Prof. Sergei Kostjuk*		
9.00-9.20	***Efkan Çatıker- “****Swelling Behavior of Polyepichlorhydrin Cross-Linked with Polyethylene Glycol Bridges in Solvents of Different Polarity”.* *Ordu University, Faculty of Science &Literature, Department of Chemistry, Ordu, 52200, TURKEY*	1
9.20-9.40	***Dmitrii Roshchin-****„ Free radical polymerization in a microdroplet with initiation at the interface “* *N.N. Semenov Federal Research Center for Chemical Physics, Russia*	2
9.40-10.10	***Marcin Wekwejt- “****Novel Ceramic-Polymer Bone Cement Based on Magnesium Phosphate Modified with Phema Hydrogel”.* *Department of Biomaterials Technology Faculty of Mechanical Engineering & Ship Technology Gdańsk University of Technology Poland*	3
10.10-10.30	***Ana Fonseca-*** *α-Amino Acid Based Poly (Ester Amide) S in the Prevention of Tendon Adhesions. University of Coimbra; Portugal*	4 (Online)
11.00-11.30	**Coffee Break**	
Co-chairmen: ***Dr. Marcin Wekwejt, Prof. Juozas Vidas Gražulevičius***		

11.30-11.45	***Talkybek Jumadilov- “****Sorption behavior of the two-component interpolymer systems at interaction with rhenium and rare earth metal ion”* *Institute of chemical sciences, Kazakhstan.*	5
12.00-12.15	***Ketevan Chubinidze- “****Targeted Multidrug Delivery Micro Containers Based on Gelatin Matrix Incorporated Liquid Crystals”.* *Georgian Technical University Institute of Cybernetics, Tbilisi, Georgia*	6
12.15-12.30	***Zoia Haholkina-*** *“Preparation and Properties of Hemostatic Sponges Based on Chitosan with Microparticles and Water-Soluble Polysaccharides”.* *Grupo de Polímeros, Departamento de Física, Universidade da Coruña, Escuela Universitaria Politécnica, Campus de Ferrol, Spain*	7 (Online)
12.30-12.45	***Ioseb Metskhvarishvili- “****Synthesis of the Tl-based superconducting materials by the sol-gel method iodine vapor pressure”* *Ilia Vekua Sukhumi Institute of Physics and Technology, Tbilisi, Georgia*	8
13.00-13.15	***Tengiz Kantaria*** *– Synthesis of New Degradable Ab-Type Polyesters Through “Click Chemistry” Agricultural University of Georgia, Tbilisi*	9
13.15-13.30	***Temur Kantaria*** *– „ Dexamethasone Loaded Pseudo-Protein Nanoparticles for Ophthalmic Drug Delivery: Evaluation of Drug Encapsulation Efficiency and Drug Release”. Agricultural University of Georgia, Tbilisi*	10
13.30-13.45	***Shio Makatsaria- “****Intercalation of Hexagonal Boron Nitride and Graphene Oxide by Magnetic Clusters”. Georgian Technical University, Tbilisi, Georgia*	11
14.00-15.00	**Lunch Break**	

AUGUST 2
TSU, BUILDING I, ROOM 007

	Co-chairmen: ***Dr. Nino Zavradashvili***	
11.30-11.50	***Nino Zavradashvili*** *– „ Library of Cationic Polymers for Versatile Biomedical Application”* *Agricultural University of Georgia, Tbilisi, Georgia*	12
11.50- 12.10	***Andrii Masiuk****- “Polylactide Starch-Containing Composites: Preparation and Properties”. lviv polytechnic national university, Lviv, Ukraine*	13 (Online)
12.10-12.30	***Kakha Karchkhadze –*** *“Study of Pelettes Obtained from Biomass”* *Petre Melikishvili Institute of Physical and Organic Chemistry TSU, Tbilisi, Georgia.*	14
12.30-12.50	***Gia Daghelashvili- “****Study of Belousov-Zhabotinsky reaction in water droplets of sodium bis (2-ethylhexyl) sulfosuccinate reversed microemulsions”. Ivane Javakhishvili Tbilisi State University, Tbilisi, Georgia*	15
12.50-13.10	***Lali Gurchumelia – “****High Temperature Processing and Recovering of Nanoscale Carbon from Plastic Waste and Its Activation in Overheated Vapor Environment”.* *Ferdinand Tavadze Institute of Metallurgy and Materials Science, Georgia*	16
13.10-13.30	***Zaqaria Melashvili****- “Consolidation and synthesis of Ta-Al-B(B4C) Reactive Blends by Hot Electro Rolling Method.”*	17

	Ferdinand Tavadze Institute of Metallurgy and Materials Science, Tbilisi, Georgia	
14.00-15.00	**Lunch Break**	
16.00	**City Excursion**	

AUGUST 3

08.30- Excursion (Mtskheta, Shato Mukhrani);
19.00 -Gala Dinner: Restaurant “Ethno Tsiskvili”.

Abstract

CROSS-LINKED POLYMER STRUCTURES: BENEFITS AND DRAWBACKS

Marc J.M. Abadie

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The cross-linked polymeric structures, called as thermosets TSs or Duromers, representabout 25% of the total polymers with a preponderance of use of thermoplastics TPs (≈75%) in the industry. This is mainly due to the intrinsic structure of thermosets that form a 3D network and therefore cannot be remolded unlike thermoplastics. However,thermosets have superior properties compared to thermoplastics *vz.* some general properties of TSs include: mechanical strength, thermal stability, chemical resistance, swelling behavior to cite some of them.

After having briefly compared the intrinsic properties of thermosets and thermoplastics,we will study the particularities of thermosets, such as:

Rate coefficient of TSs (step polymerization) *vs.* TPs (chain polymerization)

Calculus of average functionality of multifunctional monomers

Cell size and degree of cross-linking

Determination of gel point by physical methods (DMTA, rheometer,viscosimeter)

Some applications will be presented such as composites structures for marine applications, optimization of epoxy/hardener mixture (Ea), and UV curing for biodegradablehydrogels.

Key points: Thermosets, Cross-linking, Cell size, Gel point, Kinetics

ADSORPTION AND REMOVAL OF PARACETAMOL FROM WATER BY CARBON MATERIAL PRODUCED FROM NUTSHELLS

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Ivane Javakhishvili TSU Institute of Inorganic Chemistry and Electrochemistry, Mindeli 11,Tbilisi, Georgia
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In recent years, a serious environmental problem has been caused by pharmaceuticals in hospital wastewater and water purification systems. The elimination of these pollutants is difficult due to their resistance to biological degradation[1]. Pharmaceuticals originating from humans and feedstock in wastewaters often found their way into surface water sources[2]. Among the drugs frequently used in the world, analgesics and antiinflammatories are the most common, and they are widely consumed with or without a medical prescription. Out of the mentioned drugs paracetamol (acetaminophen) is the most widely used one[3].

Therefore, removing paracetamol from the water is an urgent task that has to be addressed seriously. The removal of paracetamol from wastewater has recently been investigated with a variety of techniques, including biological treatment, coagulation, sedimentation, ozonation, photocatalysis, electrochemical degradation, and adsorption. Due to its attractive advantages, such as low cost, environmental friendliness, and simple operation, adsorption has been considered to be one of the most promising approaches.

The purpose of this work is to study the sorption properties of carbonaceous materials from nutshells by a technology developed[4, 5] at the Institute of Inorganic Chemistry and Electrochemistry of the Ivane Javakhishvili Tbilisi State University and to determine the possibility of their use for purifying water polluted with pharmaceuticals. The produced adsorbent showed a good yield (76%) and relatively high surface area (469.37 $m^2\ g^{-1}$), area and volume of micropore were 314.94 $m^2\ g^{-1}$, 0.15 $cm^3\ g^{-1}$ respectively.

The activated carbon was characterized by various techniques and methodologies such as N_2 adsorption at -196ºC, using a surface area analyzer Micrometrics GEMINI VII 2390T and scanning electron microscope (SEM) HITACHI TM 3030 Plus. In order to assess the adsorptive properties of carbon material, it was applied for paracetamol removal. The effects of adsorbent dose, contact time, pH, and initial paracetamol concentration in the solution on paracetamol adsorption were studied.

The optimum values of adsorbent dose and initial concentration in this experiment were determined to be 0.02 g (particle size 50 µm) and 50 mgL^{-1}, respectively. It was concluded that the maximum amount of paracetamol that can be bound by 0.02 grams of sorbent in a 50 ml solution is 76% (adsorption takes place at a very fast rate, during the first 30 minutes).

An increase in the amount of adsorbent raised the number of active sites which is reciprocated in the value of sorption efficiency (99.3%) by largely improving it. Studies have shown that in the case of low concentrations in the solution complete adsorption of paracetamol occurs. It was found that the adsorption process was well described by the Langmuir isotherm model. It is observed that the adsorption capacity of obtained carbon material reaches the max value when the pH value is set at 5. If the pH value is further adjusted to 10, the adsorption capacity is gradually weakened to a certain extent.

Combining adsorption results, it can be concluded that the produced nutshell carbon material showed to be an efficient adsorbent material for removing organic pollutants in aqueous solutions.

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Abstract

VARIANTS OF THE THERMAL DECOMPOSITION OF CONDENSED PHOSPHATES AS AN OPPORTUNITY TO OBTAIN NEW CYCLIC OR POLYMERIC COMPOUNDS

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A lot of important fundamental research is being carried out on condensed phosphates, so-called inorganic polymers, such as double oligomeric, cyclo- or polymeric phosphates, and/or triple polymeric, and substituted phosphates [1-7].

The current data are the results of our studies – examination,and analysis of the experimental records after the synthesis of new inorganic polymers-double condensedphosphates of Gallium, Indium, Scandium & Aluminiumwith K, Rb, Ag, and the investigation of their thermal behavior at 100-800 °C [6].

We have examined the process of decomposition of synthesized condensed double acidic diphosphates and triphosphates. The phase transition process of acidic oligo-phosphates and the formation of long-chain polymers and/or cyclic phosphates with a higher degree of anions' condensation have been studied [7-10].

The sufficient thermal stability of oligo- and polymeric phosphates has been proven.

Since in the course of thermal conversion experiments of acidic oligo-phosphates, new cyclic compounds with a high degree of anions' condensation, as well as long-chain double polymeric composites and long-chain polyphosphateswere obtained, it can be concluded that this is a kind of solid phase synthesis of new inorganic polymers.

Usually, condensed double diphosphates of trivalent metals during decomposition at temperatures from 370-340 °C, and, between 500-675°C sometimes,form either long-chain poly-, or cyclotetra-, or cyclooctaphosphates. As for the triphosphates: they are most often transformed into either cyclooctaphosphatesand alsonormal diphosphates, or long-chain polyphosphatesand moreover diphosphates.

Acknowledgement: I would like to express my great and special gratitude to Professor Omar Mukbaniani for his encouragement and support of my work in the field of polymer chemistry, as well as for his important advice over the decades.

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Abstract

STUDY OF BIOLOGICAL ACTIVITY OF HERBAL CONCENTRATE RUMIPHOS

***Iamze Beshkenadze*[a], *Nazibrola Klarjeishvili*[a], *Maia Gogaladze*[a,b], *Eter Salukvadze*[a], *Leila Japaridze*[a], *Marina Chikaidze*[c]**

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Improvement of ecological situation and population health is a global problem nowadays. One of the decisive roles in solving this problem can be played by earthworms. This is explained by the fact that with their help a unique, natural, environmentally friendly, organic biohumus is obtained and protein mass of earthworms, used for balancing mixed feed for farm animals and poultry as a vitamin-protein, high-quality, concentrated supplement. [1,2]

For this purpose, we have studied the influence of herbal concentrate "Rumiphos" (first stage) and the same concentrate enriched with zinc (second stage) on the protein mass and reproduction quality of earthworms. The concentrate is obtained by extracting raw materials from endemic cereal crops based on Biotex. (Research Center for Biorational Technologies.)

The experiment was carried out under the same conditions at both stages: Solutions of three different concentrations were prepared: maximum (Max.), Normal (Norm) and minimum (Min.) At both stages, containers were prepared in triplicate each. 200-200gr of the substrate, treated with"Rumifos" solutions of various concentration, were placed in each container. 5-5 worms were placed in each one observation were made to determine the protein mass of worms and the quality of breeding cocoons according to the method developed by us. The experiment lasted three months.

Based on the analysis and calculation of the results of the experiment carried out et the first stage when the substrate only treated with the "Rumiphos'' concentrate, it was found that for the entire experiment, the mass of worms increased on average by 5%, the degree of reproduction of cocoons on average 6-7 times. At the second stage, when the substrate was treated with zinc-enriched concentrate, the weight gain of worms is on average 4%, and the degree of reproduction of cocoons increases 7-8 times.

Thus, balancing the earthworm substrate with Rumiphos has a positive effect on the growth of the mass of earthworms and significantly improves the quality of cocoon reproduction. In air opinion, this is due to the "Rumofos" concentrate, containing the biologically active compounds of different chemical classes and the influence of trace element zinc.

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Abstract

IMPORTANT CONCEPTS IN POLYMER SCIENCE AND ENGINEERING

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Certain concepts in Polymer Science and Engineering have been taken over from Metals Science and Engineering. This applies to concepts such as tensile modulus or compressive strength. All such transferred concepts have a basic inadequacy: metal properties are independent of time – while properties of polymers and also of polymer-based composites (PBCs) strongly depend on time. In this situation, new concepts pertaining to polymers and PBCs have been defined.One of such properties is polymer brittleness, defined [1, 2] as

$$\mathbf{B = 1/(E'\cdot e_b)} \quad (1)$$

Here E' is the storage modulus determined at the temperature of interest by dynamic mechanical analysis (DMA) [2, 3] at the frequency of 1.0 Hz.

Another such property – applicable also to polymer composites – is polymer flexibility Y defined [4] as

$$\mathbf{Y = V_{sp}/(S_i^n U_{bi})} \quad (2)$$

In Eq. (2) V_{sp} is the specific volume in cm^3/g at a given temperature. In the denominator we have$S_i^n U_{bi}$) that is the sum of the strengths of bonds in the monomer of a given polymer. Eq. (2) is based on the ideas of Linus Pauling [5] on the strength of the chemical bonds.

When providing the definition, Y has been related to dynamic friction of polymers – thus connecting volumetry, chemistry and tribology. It has also been demonstrated that B can be related to impact strength [6] and to thermal expansivity of polymers [7].

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SYNTHESIS OF A NEW HYBRID (AZO AND SPIRO) PHOTOCHROMIC COMPOUND

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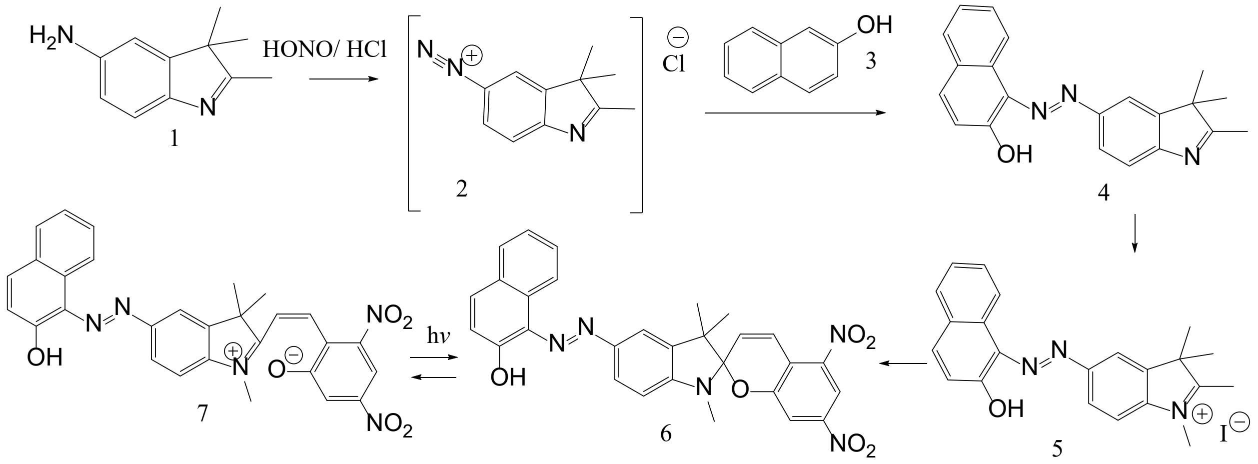
This work describes the synthesis of a hybrid (containing an azo and a spiro group) photochromic compound, which was carried out according to the given scheme:



The azo compound 4 was obtained by N-nitrosation (diazotization) of 2,3,3-trimethyl-3H-indolenine-5-amino (**1**) at low temperatures and by coupling the diazonium ion (2) to 2-naphthol (3) via an electrophilic aromatic substitution reaction [1]. The quaternized salt (5) was obtained by the interaction of (E)-1-((2,3,3-trimethyl-3H-indole-5-yl)diazenyl)naphthalen-2-ol (4) with CH_3I in the shallow ampule and product **5** was obtained. Treating of quaternary salt (5) with an alkaline solution and its condensation with 2-hydroxy-3,5-dinitro benzaldehyde, ensure the formation of compound **6** containing both spiropyran and diazo center. The ultraviolet-visible spectral study has been conducted on the synthesized photochromic compound 6.

The result of the study confirmed the transition of the closed (colored) molecule to the open (7) (merocyanine) form by ultraviolet radiation [2].

The structure of the synthesized compounds (1, 4, 5, and 6) was established by IR, NMR spectroscopy, and Mass spectral analysis [2].

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SYNTHESIS AND PROPERTIES OF NEW BIS AZO DYES

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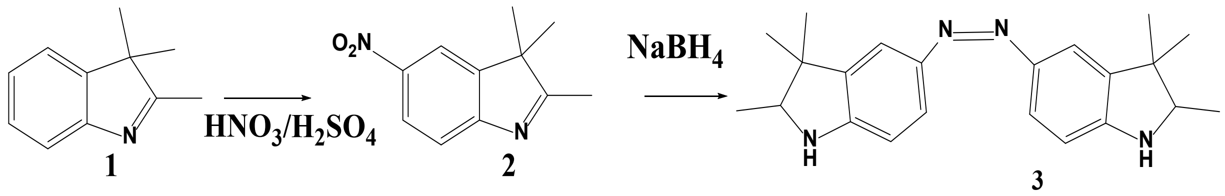
In this research, nitration of 2,3,3-trimethyl-3H-indolenine (1) was conducted and the mononitration product 2 was isolated. Azo Compound 3 with a high yield was obtained by reduction of 2,3,3-trimethyl-5-nitro-3H-indolenine in the presence of $NaBH_4$ in Methanol at room temperature. The analysis shows that during the interaction of $NaBH_4$ with the nitro group the reduction of the pyrrole ring in the indolenine nucleus takes place, while the diazo group remains stable in the molecule. Which is well seen in the infrared (corresponding peak 3200 cm-1) and NMR spectrum. The substance has a yellow color.



The molecular structure of the synthesized compounds (1,2, 3) was established by spectroscopy analysis, including IR, ^1H, ^{13}C NMR, and UV study.

The synthesized azo compound was studied on Gram-positive and Gram-negative bacteria. The implemented antimicrobial research showed interesting results.

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SWELLING BEHAVIOR OF POLYEPICHLORHYDRIN CROSS-LINKED WITH POLYETHYLENE GLYCOL BRIDGES IN SOLVENTS OF DIFFERENT POLARITY

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PEG macromonomers (PEG-400 and PEG-1450) of different lengths to be used as a cross-linking agent (bridge) were converted into propargyl groups (PEG400-diP and PEG1450-diP) [1]. Commercial polyepichlorohydrin (PECH) was cross-linked by a “Click Chemistry” [2,3] reaction after being chemically modified. Thermal analyses of cross-linked products were carried out by differential scanning calorimeter (DSC) and thermogravimetric analysis (TGA) to obtain information about the glass transition temperature of the products and the crosslinking agent ratio in the products. The swelling rates of the obtained polymers with different crosslinking degrees in THF, DMF, methanol, and acetone at 25 and 37°C were determined as a function of time.

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POLYMER WASTE - RAW MATERIALS FOR OBTAINING LIQUID MOTOR FUEL COMPONENTS

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Currently, there are several approaches for polymer and technical rubber wastes (worn car tires) utilization, mainly incineration for thermal energy and grinding to form crumb, used as an additive in construction and to improve petroleum bitumen properties.

Gasification and pyrolysis are thermal methods of polymer and technical rubber waste utilization. Gasification of such wastes produces gaseous products that can be used as fuel gas, synthesis gas, and pyrocarbon as a solid residue.

The pyrolysis of polymer and rubber wastes is carried out in installations of periodic action at 450-500 ºC forming a liquid pyrocondensate product, pyrolysis gases, and a solid pyrocarbon residue. Pyrolysis pyrocondensate is mostly used as furnace fuel. However, this method of its use is economically disadvantageous, considering the relatively low cost of this type of fuel. A detailed study of the composition and properties of pyrocondensate would propose new directions for its use, mainly for obtaining hydrocarbons that can be attributed to gasoline and diesel fractions.

We studied the composition and properties of pyrolysis pyrocondensates of used car tires, polyethylene and polypropylene waste, and narrow hydrocarbon fractions obtained from them.

During the obtained pyrocondensates fractionation on a laboratory installation under atmospheric pressure two fractions were obtained: the fraction with boiling temperature limits of s.b. - 200°C, the fraction of 200-300°C, and the residue.

The fraction of s.b. - 200°C obtained from pyrocondensate is a transparent liquid from light yellow to dark brown with a characteristic smell. Such a fraction is characterized by a weighted fractional composition, low saturated vapor pressure, and relatively high density, as for gasoline. It contains a certain proportion of unsaturated hydrocarbons in its composition and corresponds to the gasoline fraction.

The 200-300°C fraction obtained from the pyrolysis pyrocondensates of the previously mentioned waste is a cloudy liquid from dark yellow to dark brown with a precipitate and a characteristic smell. This fraction meets the requirements for summer diesel fuels by cloud point and pour point. The same as for pyrocondensate and the gasoline fraction obtained from it, the diesel fraction contains unsaturated hydrocarbons.

The pyrocondensate distillation residue is a product that visually resembles plastic lubricant. It also contains many unsaturated hydrocarbons and is characterized by a pour point of 29-42°C.

The content of individual chemical elements in pyrocondensates and narrow fractions extracted from them was determined using X-ray fluorescence spectral analysis. It was found that pyrocondensates and their fractions practically do not contain heavy metals typical of petroleum fractions and residues.

It was found by IR spectroscopy that the composition of the obtained pyrocondensates includes paraffin-naphthenic hydrocarbons, monocyclic and polycyclic aromatic hydrocarbons, olefinic hydrocarbons, and oxygen-containing compounds.

In the future, the determined quality indicators can be the basis for developing an option for the rational use of pyrocondensate and obtaining from it commercial motor fuels.

Abstract

THERMO- AND HEAT-RESISTANT POLYMERS BASED ON BISPHENOLS WITH NORBORNENE-TYPE SUBSTITUENTS

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The influence of the structure of phenols on the properties of epoxy polymers is investigated. In works [1-3], epoxy polymers obtained on the basis of diglycidal esters of various bisphenols are described. The purpose of this work was to study the effect of the chemical structure of the hardener on the properties of epoxy polymers and the synthesis of polymers with enhanced physical, mechanical, and chemical properties.

Since the thermal and heat resistance and other properties of polymers, in addition to the structure of bisphenols, also depend on the structure and nature of the hardener used, amine hardeners of different chemical structures were used to improve both thermal and other parameters of polymers.

The influence of the chemical structure of these hardeners on the properties of epoxy polymers has been studied. We used aromatic diamines of various chemical structures as hardeners. 4.4′ - diaminodiphenylsulfone was used to cure diglycidal esters. The heat and heat resistance of the synthesized polymers were investigated by thermomechanical and thermogravimetric analysis. The resulting epoxy polymers are characterized by high thermal and heat resistance.

The presence of a substituted methyl group in bisphenol reduces the heat resistance. The weight reduction by 10% is reduced from 400 to 320^{0}C. The 5% deformation of the epoxy polymer obtained on the basis of 4,4′- diaminodiphenylsulfone is 235^{0}C (while the deformation of epoxy polymers based on 2,2-bis-(4-oxyphenyl) propane, bis-(4-oxyphenyl)phenylmethane, bis-(4-oxyphenyl) diphenylmethane, phenolphthalein and other bisphenols, it is equal to 80, 103, 100 and 120^{0}C, respectively.

4.4′– diaminodiphenylsulfone gives a particularly high result in heat resistance. Polymers obtained by curing glycide esters with this hardener begin to deform in the temperature range 220-310^{0}C.

At temperatures above 600^{0}C, polymers completely decompose without the formation of a coke residue, which is generally characteristic of other classes of polymers based on polycyclic bisphenols of the Norbornane type.

Of particular interest was the use of aliphatic silicon-containing diamine as a hardener. Diglycidal ether 4,4′-(hexahydro-4,7-methylenindane-5-ylidene)diphenol with α,ω-bis-(aminopropylsiloxy)-methylphenylsiloxane. When silicon-containing diamine is used as a hardener, the decrease in polymer mass by 10% is 320^{0}C, and by 50% - 480^{0}C.

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CHEMICAL EPOXIDATION OF PETROLEUM BITUMEN

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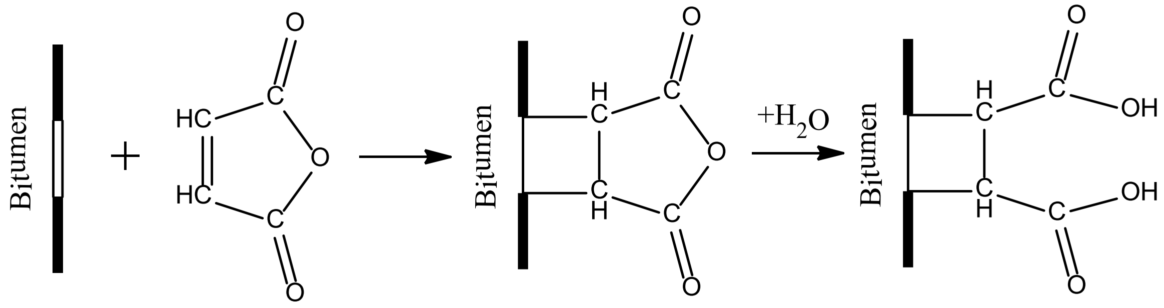
Chemical modification using epoxy resins is one of the ways to preserve road petroleum bitumen with improved properties. Although the process has not yet been used in industry, it is quite often possible to obtain modified bitumen with better properties than when using physical modifiers.

In the work, several substances were used to carry out the process of chemical modification of oxidized bitumen (OB), in particular, maleic anhydride (MAH), which was added to the unmodified bitumen sample, and epoxy resins - DEG-1 and Epidian-5, which were added into already maleinized bitumen (oxidized bitumen modified with maleic anhydride). The modification process was carried out as follows: oxidized petroleum bitumen was loaded into a round-bottomed three-necked flask, which was heated to a liquid state, after which mixing was turned on and the raw materials were heated to the working temperature of the process (110-170 °C). Next, the first stage of modification was carried out in a nitrogen atmosphere according to reaction equation 1 (4.0 wt % MAH, 170 °C, 1 h).

After the first stage, the second stage was carried out according to the reaction equation 2 (one of the indicated epoxies was introduced in the amount of 2.0-6.0 wt %, 180 °C, 3 h). A two-stage modification process was proposed: the first stage is the interaction of bitumen with MAH; the second is the interaction of maleinized bitumen with an epoxy compound. It was found that an increase in the amount of DEG-1 from 2.0 to 6.0 wt % added to maleinized bitumen leads to an increase in penetration at 25 °C from 29 to 47 dmm; a decrease in the softening point from 56 to 50 °C and an increase in adhesion to crushed stone to a maximum value (5 points).

The introduction of Epidian-5 epoxy resin in the amount of 2.0 to 6.0 wt % leads to an increase in penetration at 25 °C from 32 to 39 dmm; a slight decrease in the softening point from 55 to 52 °C and an increase in adhesion to crushed stone up to 5.0 points.

Thus, it can be argued that the use of epoxy resins in the modification of MAN bitumen allows to obtain binders with better performance properties than without them. In particular, this is due to the fact that epoxy resins DEG-1 and Epidian-5 contain free epoxy groups in their structure.



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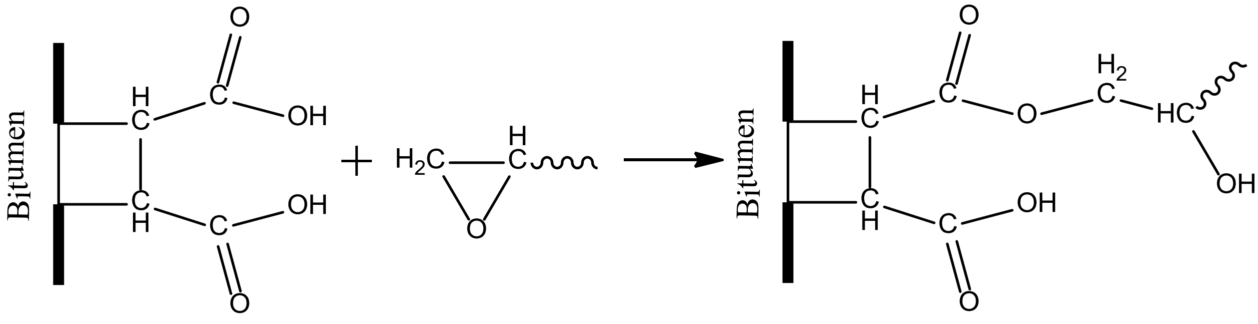

(2)

Abstract

ELECTROCHEMICAL SYNTHESIS AND CORROSION RESISTANCE OF Zn@Al_2O_3 COMPOSITE COATINGS

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A thin layer of metal, alloy or composite coating protects the product surface from damage. Coatings containing zinc, zinc alloys and various composites are used in various aggressive environments due to their good corrosion resistance and low cost [1-3].

To obtain a galvanic coating, an electrolysis process is used, during which the anode is a source of ions of the coating metal, and the cathode is a coating detail on the surface of which the metal is precipitated (recovered) from the electrolyte solution.

γAl_2O_3 is added to the zinc matrix as a filler to increase the corrosion resistance of the coating. A composite coating of Zn@γAl_2O_3 is obtained from ammonia and sulfate electrolyte solutions. The stability characteristics of the γAl_2O_3 suspension are established through the zeta potential. The effect of γAl_2O_3 content in the electrolyte on zinc current output and corrosion stability at different current densities is determined. Corrosion potential, corrosion current density and corrosion rate are determined from the polarization curves of coatings obtained in sulfate and ammonia solutions containing different concentrations of γAl_2O_3. Impedance spectroscopy is additionally used to study the corrosion processes, which provides a lot of information about the processes taking place at the electrode/electrolyte boundary. It allows studying the kinetics and mechanism of corrosion processes without interfering with the process.

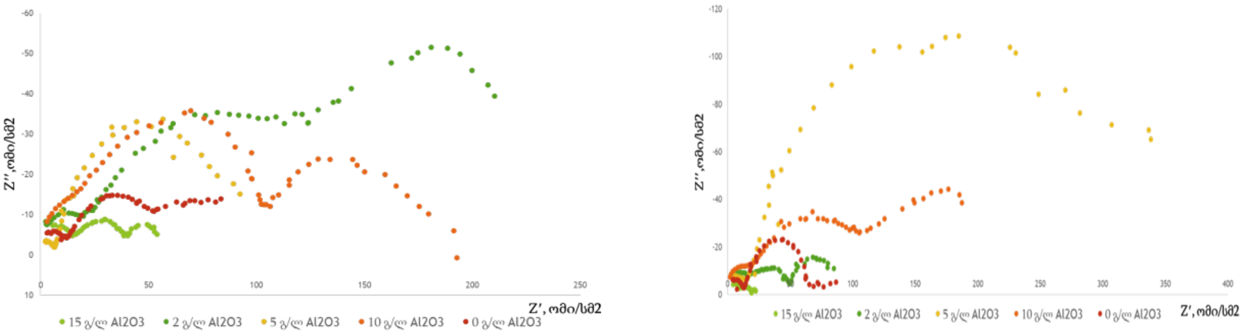

Figure 1. The impedance spectroscopy of the coatings a) sulfate electrolyte
b) Ammoniacal electrolyte

Based on the total impedance determined from the impedance spectroscopy of the coatings obtained in sulfate and ammonia solutions, the optimal content of γAl_2O_3 in the case of ammonia electrolyte is 2-10 g/l, and for sulfate electrolyte it is 5-10 g/l.

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Abstract

BIODEGRADABLE POLYLACTIDE FILMS WITH FUNGIBACTERIC PROPERTIES FOR PACKAGING FOOD PRODUCTS AND MEDICINES

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The development of polymer composites for special purposes is one of the main scientific and technical directions that are intensively developing and which are associated with the use of such materials in a wide variety of fields. Among the promising biodegradable polymers, polylactides have found wide application in many spheres, especially in the packaging industry, in agriculture, in many areas of health care, such as tissue engineering, cardiovascular implants, dental niches, drug carriers, orthopedic interventions, cancer therapy, skin and tendon healing, medical instruments and equipment [1].

However, more efforts are needed to enhance to improve the technological and operational properties of such composites, in particular, fungicidal and bactericidal ones. Nanoparticles of noble metals, especially the silver nanoparticles, have been widely used as antimicrobial agents in food and drug packaging materials, conductive materials and electronic components. Their unique properties in many cases depend upon size and shape of the nanoparticles. Silver nanoparticles are effective against fungi and a wide range of gram-negative and gram-positive bacteria [2]. It is this property that determines the superiority of silver over many modern chemotherapeutic agents.

The regularities of obtaining polylactide film composite materials by the method of watering from a solution with the simultaneous formation of silver nanoparticles in their structure were reserched. The influence of the nature of polylactide and its structure (amorphous and amorphous-crystalline), of the polyvinylpyrrolidone modifier, glycerin plasticizer on the solvent evaporation kinetics was determined. To give polylactide composites fungicidal properties, the silver reduction reaction by the interaction of argentum salts with polyvinylpyrrolidone was applied. The formation of silver nanoparticles is confirmed by the method of energy dispersive analysis of the composite.

The surface morphology of the films was researched. Films plasticized with glycerin without nanoparticles are relatively smooth, strong and uniform. Films with silver nanoparticles have a color from light to dark brown depending on the content of nanoparticles. The obtained polylactide composite materials were tested for fungicidal and bactericidal activity against various groups of bacteria and fungi, namely Escherichia coli HB 101 (E. coli), Staphylococcus aureus (S. aureus) and the mold fungus Aspergillus niger (A. niger).

It has been determined that the silver-containing composites exhibit good bactericidal and fungicidal activity evidencing inhibition zones appearance in the range of 60...100% for bacteria and 80% for fungi. Composites that did not contain silver nanoparticles did not show fungicidal properties.

The biodegradability of the composites depending on the temperature, air oxygen and pH of the medium was reserched**.** A main technological scheme for obtaining films based on polylactide with fungicidal properties is proposed. Above mentioned includes the stages of dissolving polymers and silver salt, mixing solutions, applying the composition to a moving fluoroplastic tape, evaporating the solvent and packing the film. It provides effective practical usage of the films fungicidal properties as packaging materials for food products and medicines.

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Abstract

STUDY OF SORPTION POTENTIAL OF CARBON MATERIAL FROM POLYMER WASTE (FOR EXAMPLE OF SOME POLLUTANTS OF LEACHATE OF TBILISI LANDFILL)

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Today, the harmonization of waste management process by Georgian government with European waste management policy is one of the priority issues, which should be focused on reduction of waste generation and reuse. This in turn is directly related to transition from linear economy to circular economic development and the use of new economic management models. The introduction of circular economy principles in Georgia is unthinkable in the conditions of irrational management of one of difficult to decompose waste - the polymer waste.

Our preliminary studies have shown, that the share of one the most difficult to decompose fractions of municipal solid waste in Georgia - plastic is 14%, namely 126 thousand tons/year [1]. Our research includes the minimization of the amount of the most harmful and hard degradable organic fractions (polymers) of municipal solid waste by obtaining sorbents and the study of their sorption potential for treatment of leachate of Tbilisi landfill (Norio) from some chemical indicators [2-4].

The result of our research shows the high sorbtion potential for main pollutants - heavy metals, biogenic substances, microbiological indicators and organic impurities, and is on average 80%.

Acknowledgement: This research [FR-21-12546] has been supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG)

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OBTAINING THE NEW CARBON MATERIAL THROUGH ANAEROBIC THERMOCHEMICAL PROCESSING OF THE POLYMER WASTE WITH THE USE THE HORIZONTAL AND VERTICAL REACTORS

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Waste utilization or else, the process of converting waste materials into new, harmless materials is one of the main trends of waste management. The most of the municipal, agricultural and other wastes generated in the country is recyclable.

Our study includes use the rational and environmentally beneficial minimization of municipal solid waste method, which developed at R. Agladze Institute of Inorganic Chemistry and Electrochemistry, in particular, low-temperature thermochemical processing of such hardly decomposable fractions of solid waste as polymeric waste, in order to obtain carbon and study the possibility of its use as a sorbent of pollutants from wastewater.

The first stage of the research was thermochemical treatment of polymer waste samples (polypropylene) through horizontal type reactor, constructed as part of research. The yield of carbon materials was only 20% and 80% was a liquid by-product [1,2]. The next stage was thermochemical treatment of polymer waste samples (polypropylene) through vertical type reactor, which was also constructed as part of research.

A study shows that use of a horizontal reactor, the optimal temperature for the formation of carbonaceous material is 390-410ºC, with a product yield of about 20%, and the use a vertical reactor, the temperature for receiving carbonaceous material is 530-600ºC (polypropylene/polyethylene).

Acknowledgement: This research [PHDF-21-268] has been supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG)

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SUPRAMOLECULAR MECHANISMS OF SIMULTANEOUSLY HIGH STRENGTH AND TOUGHNESS IN BIOMIMETIC CONTINUOUS NANOFIBERS

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Classical manufacturing techniques of advanced polymer fibers rely on a combination of high polymer crystallinity and high degree of macromolecular alignment to achieve superior mechanical properties. As a consequence, advanced polymer fibers such as Kevlar and Spectra possess extraordinary strength, but low strains to failure and toughness.

Our recent analysis of electrospun nanofibers (NFs) in the ultrafine (below 200 nm) diameter range showed extraordinary simultaneous size effects in strength, modulus, AND toughness. Finest nanofilaments exhibited strength approaching that of advanced structural fibers, while exceeding their toughness by more than an order of magnitude. Structural investigations showed that this unique and highly desirable nonlinear mechanical behavior may be due to high degree of macromolecular alignment in conjunction with low crystallinity.

Here, we demonstrate that it is possible to further improve NF mechanical properties by changing nanomanufacturing parameters. Reduction in crystallinity of nanofibers achieved through processing resulted in further increases in strain to failure and toughness. Several recent examples of biomimetic nanofibers and their applications will be presented and discussed.

The proposed new structural explanation of the unusual NF mechanical behavior can lead to a new class of fibers with ultrahigh toughness in addition to strength.

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ZEOLITE-COAL NANOCOMPOSITE AND SOIL STRUCTURE

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Soil is one of the main natural resources of mankind. Restoring the productivity of degraded and contaminated soils and soil conservation is an urgent problem of modernity.

Natural zeolites are unconventional mineral fertilizers capable of increasing crop yields. This minerals – crystalline hydrated aluminosilicates – are nanoporous materials with a pore size in the range of 1.5-10 nm [1,2] and are of interest for nanotechnology [3]. The main and important feature of zeolite structure is the system of intracrystalline pores and channels, where ion-exchange, occlusion and release of small molecules can easily take place, resulting in a great ability of zeolite adsorption and desorption.

Brown coal is rich in biologically active complex humic substances, which containing humic acids and humates and acting on a complex "soil-plant" system like zeolites. Humates are easily soluble salts that, after entering the nanoporous space of zeolites, form such biomineral composites that have the ability to increase and accelerate physiological and biochemical processes. During their systematic use, the buffer and ion-exchange properties of the soil are improved, the phosphorus and organo-mineral balance in the soil and the plant, as well as the mineral elements are transformed into a form available to the plant, the plant's root system is strengthened and the vegetation period is shortened [4,5].

The goal of the work is to study the effect of organoceolite fertilizer (zeolite - brown coal), prepared on the basis of local raw materials, on the bioproductivity of the agrolandschaft. Such fertilizer will help to manage brown coal waste and will contribute to the long-term enrichment of the soil with humic components using zeolite and increase fertility.

The research was be carried out under laboratory conditions. The structure and properties of the obtained nanomaterial were studied by chemical, IR-spectroscopy and X-ray diffractometric analysis methods. X-ray diffractometric analysis was carried out on a Dron-4 device (Russia); infrared spectrometric analysis was carried out on an Agilent Cary 630 FTIR Spectrometer in the range of 350-5000cm^{-1} (USA); chemical analysis was carried out on a Spectroscout XEP-04 (Germany); The optimal ratio of zeolite and lignite was be established; Current changes in soil and plants was be studied.

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PREVENTING EXTRA PRODUCED WATER FROM AN OIL RESERVOIR BY INJECTING POLYMER GEL INTO THIS RESERVOIR

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After a period of production, the pressure of the reservoir will drop, and it should not be allowed to produce oil until the natural energies of the reservoir are exhausted, because this action may cause irreparable damage to the reservoir [2]. To compensate for the pressure drop in the reservoir, there are many methods. In fact, optimal oil recovery is different processes that seek to overcome those natural forces that prevent the extraction and exploitation of all the oil in place [6]. One of these methods is polymer gel injection. Production of excess and unusable water is one of the major problems of hydrocarbon reservoirs especially reservoirs with water drive mechanism. Due to the creation of a channel between the water zone and the reservoir, a large volume of water enters the well because of water conning due to the pressure drop of the reservoir. This amount of water is produced together with hydrocarbon as associated water. Polymer gels blocks the passage of this water, so decreases extra produced water from a hydrocarbon reservoir [4].

Polymer can cause a decrease in the mobility ratio of water to oil and an increase in the viscosity of water. Polymers used to increase oil recovery are generally based on acryl amide, which is a synthetic polymer that is soluble in water [1]. Due to its reasonable price, solubility in water under various conditions, and the ability to prepare it in non-ionic, anionic and cationic forms, as well as the ability to achieve high and different molecular weights, this polymer has received much attention to be used for increasing oil recovery [3].

In this paper, according to actual condition of an oil field, while familiarizing with polymer gels, various factors affecting the structure of polymer gel, gelation time and gel kinetics are discussed and analyzed and a solution is presented to stop or reduce water production from oil production wells by using polymer gel and optimize and specify making the most suitable gel according to the condition of the purposed oil field. The most suitable composition will be specified and the percentage of the desired polymer gel will be obtained.

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α-AMINO ACID BASED POLY (ESTER AMIDE) S IN THE PREVENTION OF TENDON ADHESIONS

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In recent years, poly(ester amide)s based on α-amino acids (AAA-PEAs) have gained renewed interest for applications in the biomedical field. This is due to the fact that these materials combine the good biodegradability of polyesters with the good mechanical properties of polyamides. These materials can be obtained with a wide variety of structures, which allows fine-tuning of their physicochemical properties (e.g., hydrophilicity, stiffness, degradability). In addition, the presence of α-amino acids enables the enhancement of cell-material interactions, thereby increasing cell adhesion and proliferation.

This presentation will make an overview about the developments in the field of AAA-PEAs in the PolySyc Group, at the University of Coimbra, with particular emphasis on the design of new materials to prevent tendon adhesions.

The tendon is a complex tissue whose function is to convert muscle contraction into joint movement. Tendon injuries are quite common and occur due to from accidents, sports activities, tumours or degenerative pathologies. Tendons are surrounded by a thin layer, the tendon sheath, which is responsible for their nutrition and gliding. When an injury occurs, the tendon sheath is disrupted and the intrinsic and extrinsic healing processes are activated. Extrinsic healing involves the migration of exogenous fibroblasts into the injury site, and when this outweighs intrinsic healing, tendon adhesions form. Despite all efforts, the occurrence of tendon adhesions remains a major problem, contributing to a loss of tendon range of motion and adversely affecting patient mobility and comfort.

There are already some strategies to prevent adhesions, but the best results are provided by the use of physical barriers. Membranes seem to be the most reliable material for this purpose. These are usually made of synthetic or natural polymers or a mixture of both. Among the most commonly used synthetic polymers are the polyesters, which, when degraded, release acidic byproducts that can cause a drop in the pH of the surrounding tissue and induce an inflammatory response. To overcome this drawback, we proposed the use of AAA-PEAs for the development of the membranes. The obtained results show that the AAA-PEAs are indeed promising materials for the application.

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Abstract

APPLICATIONS OF ADVANCED CATALYSTS IN PETROLEUM INDUSTRY

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A catalyst is a substance which speeds up a reaction, but is chemically unchanged at the end of the reaction. Most of all commercially produced chemical products involve catalysts at some stage in the process of their manufacture. Petroleum refining makes intensive use of catalysis for alkylation, catalytic cracking, naphtha reforming and steam reforming [3].

Even the exhaust from the burning of fossil fuels is treated via catalysis: Catalytic converters, typically composed of platinum and rhodium, break down some of the more harmful byproducts of automobile exhaust. Some of the largest-scale chemicals are produced via catalytic oxidation, often using oxygen. Many other chemical products are generated by large-scale reduction, often via hydrogenation. Bulk polymers derived from ethylene and propylene and polyesters and polyamides are often prepared via catalysis [1]. Catalytic processes are one of the most important operations of oil, gas, and petrochemical industries in developed countries, and due to the fact that catalysts are needed in the production of various types of fuels, their importance is increasing day by day. Platinum catalysts are activated on acid base.

These catalysts are two factors, that is, both the metal and the acid base play an effective role in activating the reactions. In the reforming operation, platinum activates dehydrogenation and hydrogenation reactions, and the acid agent is effective in isomerization and hydrocracking reactions [4]. Catalytic cracking is one of the most important refining processes used to convert heavy cuttings into lighter and more valuable materials, especially gasoline. In this process, the relevant feed is usually primary distillation diesel, but it can also use diesel produced in other refinery units as feed. Its final product is saturated and unsaturated light gases, gasoline, light and heavy (unconverted) diesels.

Alkylation means adding an alkyl group to an organic compound, but in oil refining terms, alkylation is the term. From the reaction of a light olefin with an isoparaffin at high temperature and pressure, the alkylation reaction can take place without a catalyst, but in industrial processes, alkylation is done at a low temperature and in the presence of a catalyst. Catalytic processes, in this case, occupy a much smaller volume than the processes of the oil industry, but they produce extremely important and very diverse products, such as the production of polyethylene and ethylene, the production of propene, the dehydrogenation of linear paraffins, and the production of cyclohexane. In this paper, we discuss about uses of catalysts in oil and gas industry [2].

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oRGANIC ELECTRONICALLY ACTIVE MATERIALS FOR ORGANIC LIGHT EMITTING DIODES AND SENSORS

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Growing interest has been in recent decades focused on organic glass-forming electronically active materials. They are used as emitters and hosts in organic light emitting diodes, as charge transporting materials (HTMs) in rapidly developing organic and hybrid sol cells. Organic emitters exhibiting long-lived emission such as thermally activated delayed fluorescence or room-temperature phosphorescence are recently widely studied as active materials of the different sensors. The examples of organic semiconductors recently synthesized, studied in the laboratories of the author are reviewed.

Asymmetric multiple donor-acceptor type derivatives of *tert*-butyl carbazole and trifluoromethyl benzene were designed and synthesized exploiting different electron-accepting anchoring groups [1]. Sky blue emitting OLED with the emitting layer of one compound dispersed in host 1,3-bis(N-carbazolyl)benzene displayed emission peak at 477 nm, brightness over 39 000 cd/m^2, and external quantum efficiency (EQE) up to 15.9%.

Compounds containing triphenylamine or 9-phenylcarbazole as donor moieties and pyrimidine-5-carbonitrile as electron-withdrawing unit were synthesized and studied [2.] Pure blue and greenish-blue fluorescent OLEDs with EQE reaching 7% and 6%, correspondingly, were obtained using the newly synthesized compounds as emitters. EQE of more than 20% and the operation time exceeding 20000 h were recorded for electroluminescent devices with pyrimidine-5-carbonitriles as the hosts.

Sky-blue emitting derivatives of pyrimidine-5-carbonitrile and electron-donating carbazole, tert-butylcarbazole or methoxy carbazole showed good performance both as emitters of OLEDs and as active materials of oxygen sensors [3]. Sky-blue OLED with EQE of 12.8% was fabricated using the newly synthesized emitter. The emitters were also used as xygen probes with fast response, high sensitivity and good stability.

Derivatives of thianthrene and phenothiazine were synthesized as emitters for oxygen sensing [4]. Room temperature phosphorescence (RTP) of the different intensity was detected for the compounds being in crystalline or amorphous phase and for their dispersions in different polymeric matrices. Fast oxygen response (ca. 0.1 s) of RTP was observed for only 1 wt.% of the dispersion in polymeric host.

Very sensitive probes for quantitative and organoleptic detection of oxygen based on conformer-induced RTP enhancement of the derivative of triazatruxene and phenothiazine were developed [5]. For 1% solid solution of the compound in Zeonex, the ratio of intensity of RTP observed under vacuum and fluorescence intensity recorded in air reached the value of 19.

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Abstract

INFLUENCE OF THE CHEMICAL STRUCTURE OF THE HARDENER ON THE THERMAL PROPERTIES OF EPOXY POLYMERS

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Works [1-4] describe epoxy polymers based on bisphenols.The influence of the chemical structure of bisphenols on the properties of epoxy polymers based on polycyclic bisphenols of the norbornane type has also been investigated.

Since the thermal and heat resistance of epoxy polymers, in addition to the chemical structure of bisphenols, also depend on the structure of the hardener, acid hardeners of different chemical structure were used to improve the thermal properties of polymers as heat and heat resistance. The influence of the chemical structure of these hardeners on the properties of epoxy polymers has been studied. Diglycidal esters of polycmulic bisphenols of the norbornane type were used as diols, and acid anhydrides of various chemical structures were used as hardeners.

The following hardeners give high results in heat resistance: pyromellite and methyltetrahydrophthalic anhydrides. Polymers obtained by curing these anhydrides of diglycidal ephmers of bisphenols with norbornane-type substituents they are deformed in the temperature range 220-245^{0}C. The use of these hardeners gives high results in terms of heat resistance. They decrease in mass by 10% in the temperature range 340-400^{0}C.

At temperatures above 600^{0}C, polymers completely decompose without the formation of a coke residue, which is typical for other classes of polymers based on polycyclic bisphenols of the norbornane type.

The properties of epoxy polymers are greatly influenced by the chemical structure of the hardener. In addition to the above hardeners, anhydrides of acids of the norbornane type were tested, namely, anhydrides of 2,3-dicarboxynorbornane, 1,4, 5, 8-dimethylene-2,3-carboxy-naphthalene and polyarylate 4,4′ -(hexahydro- 4,7–methylenindane-5-ylidene) diphenol. The glycide ester of 4,4′- (hexahydro-4,7–methylenindane-5-ylidene) diphenol was used as a curable component. When using acid anhydrides of norbornane thyl and polyarylate as hardeners, the resulting polymers are characterized by high heat and heat resistance, which can be explained by the high content of norbornane cyclic groupings in the structured polymer, which cause the rigid structure of the polymer.

Epoxy polymer is characterized by good adhesion and hardness; high physico – mechanical and dielectric properties, water and chemical resistance, resistance to UV rays of coatings. The impact strength for varnishes after thermal aging at 150^{0}C practically does not change.

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Abstract

COMPOSITE SORBENT BASED ON HUMIC ACIDS AND ALUMINOSILICATES

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A method has been developed for the introduction of humic acids into the composition of aluminosilicate porous materials. It is known that various natural materials have pronounced sorption properties, however, due to the fact that they do not have rigid structures, their sorption properties are not fully manifested. This statement is especially relevant for peat as a carrier of humic acids. It is known that peat as a source of humic acids in reality has a very developed porous structure (in particular, specific surface area), but they are not fully manifested during sorption processes. For the full involvement of humic compound in sorption processes, it is necessary to isolate humic acids from peat and apply them to the surface of inorganic carrier.

For this purpose, sodium humate is obtained from peat (Vardenis deposit of the Gegharkunik region of Armenia), which is pre-treated with 5% hydrochloric acid. The purpose of acid treatment is to remove adsorbed metals from the peat surface. Then, washing with water is carried out until a neutral reaction and removal of chlorine ions.

Firstly, a stable solution of sodium aluminate and sodium liquid glass is obtained (which is stable for 10-15 minutes) to introduce humic compounds into the aluminosilicate frame. Then, sodium humate (8 wt.% humic compounds) is introduced into this solution with stirring. The gel is washed with acidified water (pH1.5-2.0) after gelling this system and aging it for 2-3 hours. In this case, sodium humate passes into insoluble humic acid and is fixed in the pores of the aluminosilicate framework. Then, drying and fractionation is carried out (at 120°C).

ELECTRICAL PROPERTIES OF GRAPHENE/PDMS NANOCOMPOSITE

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Carbon nanostructures has attracted electronic industrial interest due to its exceptional electrical properties [1]. One of the most promising applications of this material is in polymer nanocomposites to develop the most technologically promising devices. This work presents the synthesis of graphene/ polymer nanocomposites and discusses the effect of various factors on their electrical conductivity. The widely found graphene are used to manufacture graphene/polymer nanocomposites have many defects, which affect electrical conductivity of the final product. Hence, one of the principal tasks is the synthesis of graphene by simple and cheap methods, where defects will be minimized [2]. Also necessary is the polymers' design and synthesis in order to produce novel graphene-based functional nanocomposites. The graphene/polymer nanocomposites' production methods play a significant part in the structure/morphology determination[[3].

Graphene was synthesized by the intercalation method and a stable suspension of graphene was obtained. Commercial polydimethylsiloxane was used as the polymer matrix. Graphene/polymer nanocomposite was prepared by solution mixing method. The synthesized materials were gradually studied and identified by different optical methods. What about electrical properties of graphene/polymer nanocomposites, The Hall-effect measurements were carried out in the prepared nanocomposites to understand the electronic properties at room temperature.

Table 1. Electrical properties of PDMS/GNP nanocomposites

№	**Name**	**Specific resistivity ρ Ohm, cm**	**Electric conductivity σ Ohm^{-1}, cm^{-1}**
1	PDMS	$1.05 X 10^{11}$	$9.4 X 10^{-12}$
2	PDMS/GNP 0.5%	$1.6 X 10^{8}$	$6.25 X 10^{-9}$
3	PDMS /GNP 1%	$2.89 X 10^{7}$	$3.46 X 10^{-8}$
4	PDMS/GNP 5%	$1.2 X 10^{7}$	$8.4 X 10^{-8}$
5	PDMS/GNP 10%	$3.3 X 10^{7}$	$3.01 X 10^{-8}$
6	PDMS/GNP 12%	$1.1 X 10^{7}$	$9 X 10^{-8}$

Research has shown that the electric conductivity of synthesized polymer nanocomposites increases with increasing filler concentration. The electrical conductivity is maximum at 10% graphene nanoplates concentration, and was found to be $3.01 X 10^{-8}$ Ohm^{-1}, cm^{-1}.

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INVESTIGATING THE INFLUENCE OF CONDUCTIVE CARBON BLACK ON THE EMI SHIELDING PERFORMANCE OF NATURAL RUBBER-BASED COMPOSITES

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The proliferation of electronic devices and wireless communication systems has led to a growing demand for effective electromagnetic interference (EMI) shielding materials. This study investigates the effect of conductive carbon black on the EMI shielding performance of natural rubber-based composites. By incorporating conductive filler, such as carbon black, into the rubber matrix, the electrical conductivity and EMI shielding effectiveness of the composites were evaluated.

The study examines the impact of filler type, concentration, and dispersion on the electrical and EMI shielding properties of the composites. The results highlight the importance of filler characteristics and dispersion in achieving enhanced EMI shielding efficiency.

The findings contribute to the development of highly efficient EMI shielding materials for applications in electronic and communication systems, addressing the growing need for electromagnetic compatibility.

Keywords: EMI shielding, natural rubber, conductive carbon black, composites, electromagnetic interference, EMI shielding effectiveness.

SORPTION BEHAVIOR OF THE TWO-COMPONENT LEWATITCNPLP(H+)-POLY-2-METHYL-5-VINYLPYRIDINE SYSTEM IN INTERACTION WITH RHENIUM IONS

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The interpolymer system showed the greatest sorption activity with respect to rhenium ions at a molar ratio of Lewatit CNP LF(H+):P2M5VP equal to 6:0, and according to the results of the residual concentration of salts in the solution, the highest degree of sorption (55.0%) was observed after 48 hours of the sorption process. The maximum sorption of rhenium occurs at 48 hours of remote interaction of ion exchangers at a ratio of 6:0, the initial concentration of rhenium in saline solution decreases from 100 mg/l to 44.93 mg/l. Whereas for an interpolymer system for different ratios, the residual concentration readings are relatively small. For example, at ratios of 3:3 and 2:4, the residual concentration readings decrease from 100 mg/l to 53.09 mg/l and 55.05 mg/l, respectively

The degree of binding increases with time, and the most significant increase in the parameter is observed at the Lewatit CNP LF(H+)- P2M5VP molar ratios of 6:0 and 5:1. The degree of binding is 0.54% and 0.37% for these ratios after 0.5 hours of remote interaction. And for the remaining ratios, the degree of binding in this case is relatively low 0.20% and 0.18%, etc., respectively. After 48 hours of interaction, the degree of binding of the polymer chain increases in the ratios of 6:0 and 5:1 to 4.63% and 4.46%, respectively.

The sorption of rhenium ions is accompanied by a strong increase in the effective dynamic sorption capacity for Lewatit CNP LF(H+) with a ratio of - 6:0 from the beginning of sorption (0.5 h) — it is 0.00029 mmol/g; while the capacity is 0.00012 mmol/g for a pair of Lewatit CNP LF(H+): P2M5VP in a ratio of 1:5 and 0.00008 mmol/g for P2M5VP. A strong increase in the sorption parameter is observed after 48 hours; for Lewatit CNP LF(H+) with a ratio = 6:0 is equal to 0.00246 mmol/ g and for a pair of interpolymers in a ratio of 1:5 it is 0.00177 mmol/g; for P2M5VP — 0.00151 mmol /g after 48 hours of sorption.

Also, during the experiments, desorption was carried out in an aqueous solution of 2% nitric acid for 72 hours. From the data obtained, it can be seen that the main part of rhenium is extracted within 72 hours of desorption, at a ratio of 6:0 Lewatit CNP LF(H+) - P2M5VP.

The results obtained indicate the possibility of using the Lewatit CNP LF(H+) polymer and an interpolymer system for a highly efficient sorption technology for the extraction of rhenium ions from industrial solutions.

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DEXAMETHASONE LOADED PSEUDO-PROTEIN NANOPARTICLES FOR OPHTHALMIC DRUG DELIVERY: EVALUATION OF DRUG ENCAPSULATION EFFICIENCY AND DRUG RELEASE

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Ophthalmic drug delivery for treating various eye diseases still remains a challenge in ophthalmology. One promising way of overcoming this problem is to use the nanoscale biodegradable drug carriers that are able to safely deliver pharmaceuticals directly to the locus of disease and maintain a therapeutic concentration of drug for a long time. The goal of the present study was the preparation of drug (dexamethasone, DEX) loaded pseudo-protein nanoparticles (NPs) and investigation of drug encapsulation efficiency and drug release kinetics. DEX-loaded NPs based on the pseudo-protein 8L6 (DEX-NPs) were successfully prepared by nanoprecipitation method under the optimal conditions that were established previously [1,2]. DEX-NPs were characterized by size (average diameter), particle size distribution (polydispersity index), and surface charge (zeta-potential) using DLS. The incorporation characteristics of DEX were determined using the UV-spectrophotometric method and the kinetics of DEX release from the DEX-NPs was studied according to the dialysis method in PBS at 37°C.

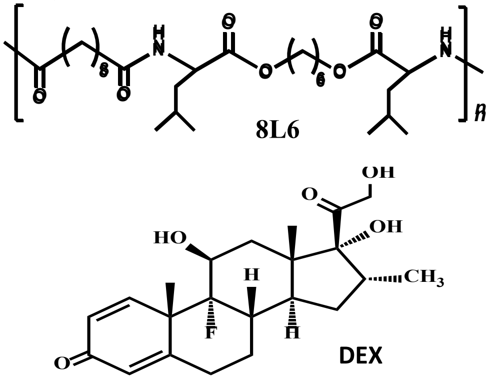

Figure 1. Chemical structures of the pseudo-protein 8L6 and drug DEX

The obtained results showed that the size of DEX-NPs varies within 143.6 – 164.1 nm depending on the DEX content during the preparation. DEX incorporation characteristics – encapsulation efficiency and actual drug loading were high enough and reached 55.1 and 10.2%, respectively.

The kinetics of DEX release from the DEX-NPs showed a typical biphasic release pattern - an initial burst release and further much more continuous slow release. Based on the obtained data we can conclude that the elaborated DEX-NPs have potential for the application in ophthalmology as ocular drug delivery nanocarriers.

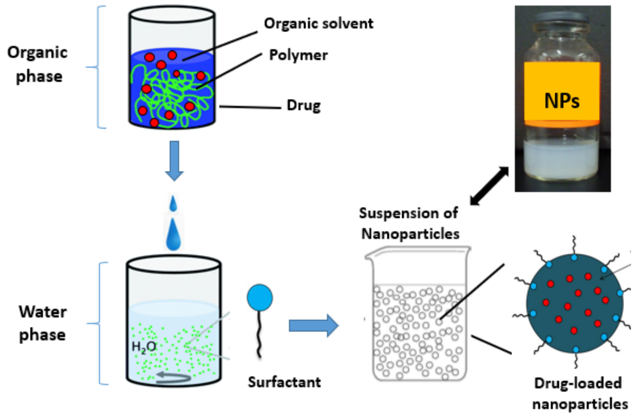

Figure 2. Scheme of the nanoprecipitation method

Acknowledgements: This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [YS-21-2215].

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SYNTHESIS OF NEW DEGRADABLE AB-TYPE POLYESTERS THROUGH “CLICK CHEMISTRY”

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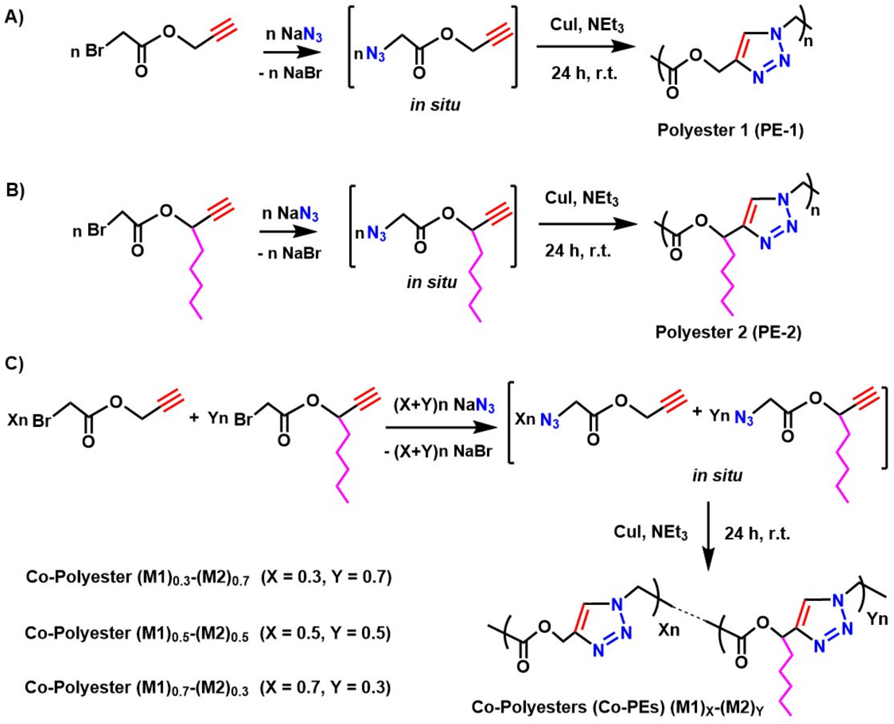
New aliphatic AB-type polyesters (PEs) and co-polyesters (co-PEs) bearing 1,4-disubstituted 1,2,3-triazole rings in the main chain were successfully synthesized via Cu(I)-catalyzed click step-growth polymerization (SGP) *via* hetero-bifunctional monomers according to one pot two step synthetic strategy we have previously elaborated [1]. The structure of the click polymers was confirmed by FT-IR and NMR analysis. According to GPC, the obtained PEs and co-PEs had average molecular weights (Mw) within 11,500 – 21,500 g/mol. These MWs correspond to rather high degree of polymerization (DP = 33-53) that is quite enough to give elastic films by casting from HFIP solutions. The polyesters are prone to hydrolytic degradability that was proved by measuring total organic carbon (TOC) concentration produced after hydrolysis of a co-polyester in PBS at r.t. The new AB-type polymers enrich a library of available degradable click polymers with functionally interesting 1,2,3-triazole moieties in the backbone. They can be considered as having a potential for various biomedical application. As a case study, first the click PEs reported in this work will be used as precursor polymers for designing 1,2,3-triazolium containing degradable cationic systems with tunable hydrophilicity/hydrophobicity for potential application as potent antimicrobial agents with optimal antimicrobial activity and minimal toxicity. This study is in progress now.



Scheme 1. Synthesis of AB-type click PEs and Co-PEs

Acknowledgements: This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [YS-21-2522].

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Abstract

POLYMERIC BIOMIMETICS

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Nowadays, great efforts are focused on the design of biodegradable materials for applications in the biomedical field such as tissue engineering and organ regeneration, drug delivering constructs, etc.

It is important the rate of degradation must be adjustable and the corresponding degradation products must not be toxic, the devices produced from the selected material must retain their mechanical integrity before regeneration, the material should guarantee zero to low immunogenicity, and even should have capacity to tune cell adhesion, proliferation, and differentiation.

With all these in mind one of the most promising look artificial polymers made of physiological building blocks, mimicking naturally occurring polymers – so called polymeric biomimetics. There are two the most important biomimetics which most closely meet the requirements for biomaterials. Those are polymers composed of phosphoric acid mimicking nucleic acids, and polymers made of α-amino acids mimiking proteins [1,2].

Among these two the α-amino acids' based polymers possess by far more wide spectrum of structure and properties. Among four basic families of artificial polymers made of α-amino acids such as poly(α-amino acid)s, polydepsipeptides, pseudo-(poly-α-amino acids), and pseudo-proteins the latter two are more important from view point of synthetic diversity and materials' versatility.

These biomimetics having a non-proteinaceous molecular architecture fit well for biomedical applications - they, along with NH-CO bonds providing a high compatibility with tissues, contain in the backbones additional hetero-bonds such as ester, urea, urethane, etc. providing a wide range of properties along with low or zero immunogenicity of biomaterials. Besides, the biomimetics release physiological products upon biodegradation - α-amino acids thus showing the nutritional properties inherent in proteins.

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POLY (-CYCLODEXTRIN-CO-CITRIC ACID) FUNCTIONALIZED NATURAL NANOZEOLITE: AN ECO-FRIENDLY PLATFORM FOR IB DELIVERY

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Zeolites, due to their porous nature and inherent pH-sensitive properties, are widely studied as drug delivery systems. However, natural zeolite pores are usually larger than drug molecules, which can cause rapid drug release. Consequently, to solve this problem, the zeolite structure must be modified to achieve controlled drug release. On the other hand, the preparation of nanoscale zeolites enables them to enter the living cell. [1-3]

To achieve these objectives, a natural nanozeolite was modified by poly (β-cyclodextrin-co-citric acid) (PCD-zeolite), and used for the loading and release of IB (IB).(figure 1)

Due to the presence of hydroxyl and carboxyl groups in the PCD-zeolite structure, pH plays a vital role in the adsorbed IB; thus, the maximum adsorbed IB was observed at pH = 7. The in vitro release of IB from PCD-zeolite-IB in a phosphate buffer was examined; the PCD-zeolite containing IB (30 wt%) showed the highest release at pH = 3.6 within the first 3–48 h. As a result, the PCD-zeolite, by trapping IB, can improve its solubility and bioavailability. Moreover, the decrease in the dissolution rate of the polymer matrix in an acidic medium may also lower the toxicity of IB.

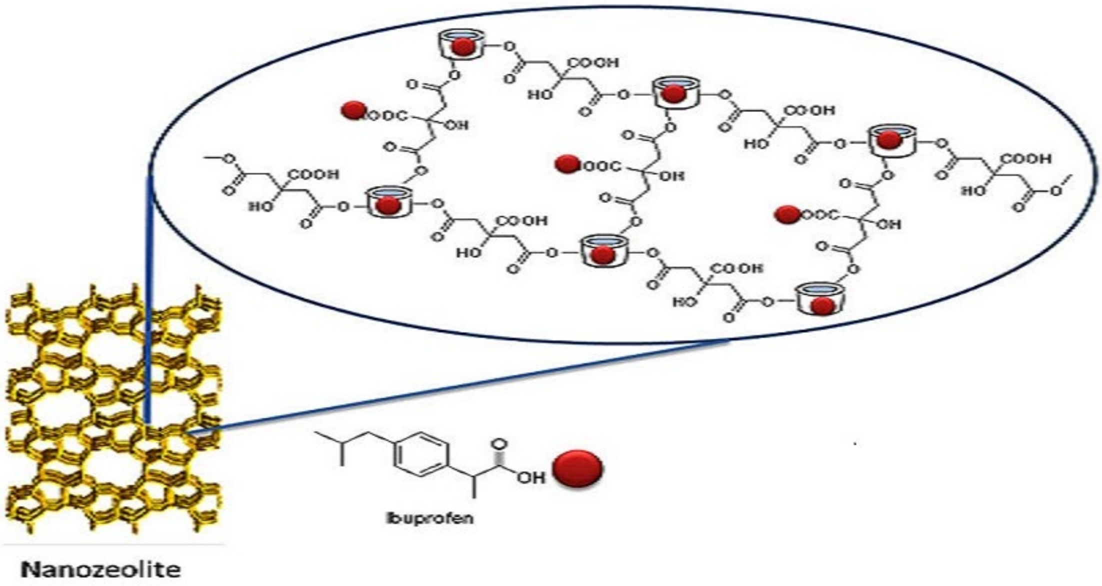

Figure 1

Acknowledgement: We would like to thank the University of Georgia (Tbilisi) for the financial support of this work.

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THROUGH-SPACE CHARGE-TRANSFER THERMALLY ACTIVATED DELAYED FLUORESCENCE ALTERNATING DONOR ACCEPTOR COPOLYMERS: SYNTHESIS, PROPERTIES AND APPLICATION

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Organic light-emitting diodes (OLEDs) are widely used for the fabrication of flat panel displays and different lightening devices. Basically, emitters largely determine the performance of devices and their selection is critical for the fabrication of highly efficient OLEDs. Thermally activated delayed fluorescent (TADF) emitters, following prompt fluorescent and phosphorescent ones, represent the third generation of electroluminescent materials for OLEDs. TADF materials which contain no any heavy metals are capable of harvesting both triplet and singlet excitons and, therefore, theoretically can reach 100% of internal quantum efficiency. Up to date, many TADF organic emitters covering from deep-blue to red emission spectra were synthesized and used for the fabrication of efficient OLEDs. However, an expensive vacuum deposition technique is typically used for the fabrication of devices based on small molecules TADF emitters. Therefore, polymeric TADF emitters, which are suitable for simple, low-cost and easily scalable solution (wet) processing methods represent significant interest. In addition, polymeric emitters are characterized by much higher morphological and thermal stability than organic TADF materials [1].

In this presentation, the synthesis of a series of donor-acceptor alternating copolymers with M_n $\leq$12,000 g mol^{-1} and moderate polydispersity (Đ=1.5 - 2.5) via RAFT copolymerization of styrene-based donor monomers and maleimide-type acceptor monomers in the presence of S-dodecyl-S′-(α,α′-dimethyl-α′′-acetic acid)trithiocarbonate as a chain transfer agent will be presented. Importantly, all synthesized alternating copolymers were characterized by high thermal stability (T_{d5}>375 ºC) and most of them exhibited exciplex emission via the through-space charge-transfer (TSCT) mechanism and displayed of aggregation-induced emission enhancement. The color of emission of synthesized copolymers is largely depended on the nature of acceptor monomer and could be changed from blue to orange.

These copolymers in solid state demonstrated delayed fluorescence in the range between 0.35 and 6.2 μs and moderate photoluminescence quantum yield (2.12 - 6.32%) in air. Multicolor host-free solution-processable TADF OLEDs using synthesized alternating copolymers as emitters were fabricated, which showed good stability of electroluminescence spectra at the different voltages. The highest external quantum efficiency of 7.84 % was reached for green emitting device [2].

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Abstract

POLYMERS IN MICROENCAPSULATION SYSTEMS FOR ACTIVE SUBSTANCE CONTROLLED RELEASE

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Encapsulation technology includes enclosing active agents (core materials) within a polymer matrix (wall material) at the micro/nano-scale. In recent years encapsulation has become very popular in many fields, such as the food industry, textile industry, drug delivery, agriculture, cosmetics, coatings, adhesives, dyes, and paints. This method develops a physical barrier between the core materials and the environment. It is very useful because it can prevent the active ingredient from degradation, facilitates its handling and transportation, and allows controlled release.

Encapsulation can also increase the stability of the active agent and, thus, its bioavailability [1, 2]. Many polymers, such as sodium alginate, gelatin, chitosan, carrageenan, gums, whey protein, or starch, may be used to trap the active substance inside the micro/nano-capsules. There are also known a few chemical or physical techniques available for encapsulation, such as coextrusion, emulsion-solvent evaporation/extraction methods, spray drying, coacervation-phase separation interfacial, and in situ polymerization [3-5].

Microcapsules are mainly used in oral, intramuscular, subcutaneous, and nasal controlled-release drugs. The main challenge in using them in skin preparations is the difficulty of penetrating many substances through the epidermal barrier due to the specific structure of the stratum corneum [6].

This study aims to obtain new materials for cosmetic or dermatological applications by incorporating polymer microparticles (containing plant extract) in the polymer matrix with. Because materials used in dermatology, pharmacy, and cosmetology should be characterized by biocompatibility and non-toxicity, the different biopolymers, which are known for their unique properties suitable for medical applications, were used in this study.

The project's main goal was to develop an innovative class of polymeric materials that would increase the efficiency of the penetration of biologically active substances through the skin, contributing to a better therapeutic effect. These materials can become the basis for developing new forms of cosmetic and dermatological preparations.

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THE CONTRIBUTION OF THERMAL DEFECTS TO THE SEMICONDUCTING PROPERTIES OF P-TYPE SIGE ALLOY

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Recently, p-n structures of extremely small sizes are widely used in micro- and nanoelectronics devices, the lifetime of which significantly depends on the structural state of the surface layers of semiconductor monocrystalline substrates[1]. Special attention is paid to monocrystalline SiGe alloys. The distribution quality of Ge atoms contributes to the structure of their surface layers, which can be characterized by inhomogeneity in the case of high concentrations [2]. Under such conditions, a subsystem of defects formed by thermo-mechanical processing with variable electrical, optical and structural characteristics is created.

Determining their composition, stability and activity management capabilities is a necessary prerequisite for the development of new generation highly efficient semiconductor devices and systems based on SiGe alloys.

The paper presents the results of an experimental study of the electrophysical characteristics of the (111) oriented p-type Si+2at.%Ge:B alloy annelaed at high temperatures.

Nonmonotonic changes in the characteristics of the electrophysical properties and absorption spectra of infrared radiation in p-Si+2at.%Ge:B alloy with (111) orientation have been revealed under the influence of thermal vacuum annealing at high temperatures.

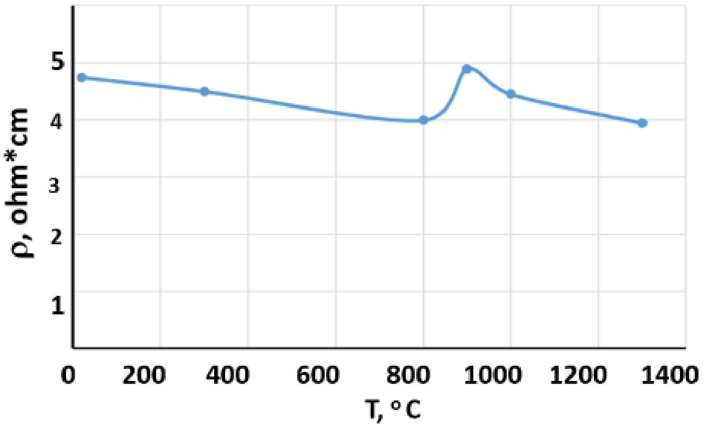

Figure 1. Dependence of electrical resistivity of Si+2at.%Ge:B on thermal annealing temperature

The redistribution of oxygen and carbon atoms from optically active positions of interstitial and substitution into thermal origin defects has been shown. A significant part of thermal defects are dissociated during high-temperature annealing, which results in an increase in the oxygen and carbon content in optically active positions. The results obtained are interesting for the problem of creating semiconductor materials and devices with specified characteristics based on SiGe alloys.

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Abstract

MODELING OF THERMO-MECHANICAL PROPERTIES AND WEAR BEHAVIOR OF HYBRID COMPOSITE MATERIALS

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Development of functionalized polymeric hybrid binder systems with different structures has become one of the most attractive topics for scientists in composite materials and in materials science during the last years because of their progressive and wide-range applications [1,2]. Polyfunctional polymers with linear macrochains and regular structure, including heterochain organic polymers, carbofunctional silicon-organic and other polyfunctional heterochain polymers have the prospect in modern technologies developed to obtain advanced composites with specific properties.

Among them fluorinated polymers and copolymers have been attracting much attention as they display high thermal stability, excellent mechanical properties at extreme temperatures, resistance to oxidation and hydrolytic decompositions, unique inertness to solvents, hydrocarbons, acids, and alkalis, weatherability, low flammability, high optical transparency, low dielectric constant and low surface energy.

Due to such unique combination of exceptional properties fluoropolymers are widely used in advanced technology areas: architectural, optoelectronic, automotive, aerospace and aeronautic industries, microelectronics, and chemical engineering as well as in medicine, such as dental materials and artificial joint [3, 4].

Multifunctional hybrid materials based on functionalized perfluoropolymers and selected bio-additives have been elaborated. Based on preliminary investigations co-monomers by molar ratio of 1:1, 7:3 have been taken. Thermo-mechanical characteristics − the glass and phase transition temperatures, decomposition behavior and thermal stability parameters, scratch resistance, wear, dynamic friction, surface morphology, optical stabillity of the obtained composites and materials have been studied.

The investigation of tested transparent hybrid composites has been shown: good adhesion on various surfaces (plastic, wood etc.); high viscoelastic recovery; lower values of wear rate; an improvement with an increase in glass transition temperatures and thermal stability for high temperature application;

Namely, by increasing of fluoroalkyl chain length the resistance to thermal degradation of corresponding hybrids mainly has been improved and the range of weight loss has been shifted to the higher temperatures; these effects have been enhanced further by addition of bioactive component and by increasing of curing agent content.

Based on the obtained data of sliding wear determination improvement of the resistance to instantaneous deformation of targeted materials as a result of the proper modeling of the structure of basic perfluoropolymers and composition of hybrid composites have been shown. No phase separation in SEM micrographs of modified systems has been displayed. Enhanced mechanical strength of obtained hybrid composite materials is useful for abrasion resistance necessary as a function for protective and corrosion-resistant coatings.

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NATURAL ORGANIC SUBSTANCES' TRANSFORMATION IN THE UKRAINE'S SURFACE WATERS UNDER THE SOLAR RADIATION

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Natural organic matter of surface water bodies is the main source of organic carbon and some nutrients, including nitrogen, phosphorus, silicon, iron, etc. They significantly affect the surface waters' chemical composition and determine the aquatic environment's quality as a habitat for aquatic organisms. The most common group of dissolved organic matter (DOM) is humic substances (HS), which belong mainly to terrigenous organic compounds by their origin. A certain part of HS can be formed in the reservoirs themselves (the so-called "water humus"), but their share in the overall balance is much lower than that which enters with surface runoff. An important place is also occupied by exometabolites – organic substances, which released by phytoplankton and higher aquatic vegetation at development and dying. First of all, these are carbohydrates and protein-like compounds (PLC).

The HS, carbohydrates and PLC concentration in the water bodies of Ukraine, located in different physical and geographical zones, varies widely 1.2–120.5, 0.4–4.9 and 0.03–1.41 mg/L, respectively (Figure 1). HS predominate in the overall balance of DOM. Thus, their share in the Dnipro cascade's reservoirs is 52.8–76.5%, while the share of carbohydrates does not exceed 7.2–9.8%, and PLC – 1.1–3.2%.

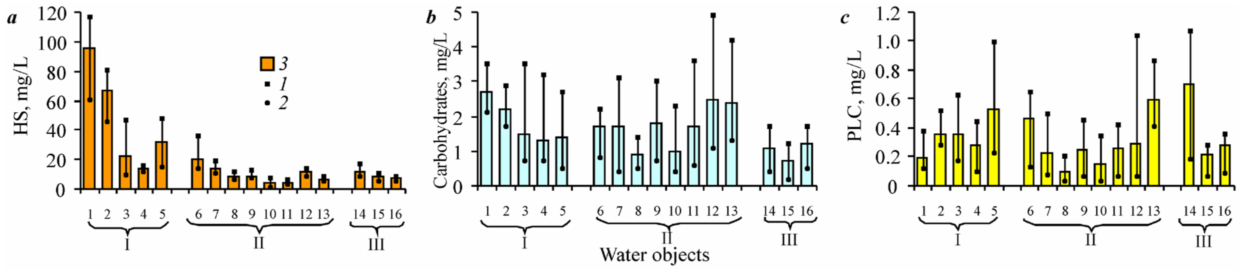

Figure 1. Limit (1, 2) and averaged (3) concentrations of HS (a), carbohydrates (b) and PLC (c) in the water bodies from different physical and geographical zones of Ukraine: I – mixed forests zone (1, 2 –the Stvyga and Pripyat' rivers, 3, 4 –the Lyutsymir and Velike Chorne lakes, 5 – the Kyiv Reservoir); II – forest-steppe zone (6 – the Kaniv Reservoir, 7–10 –the Desna, Pivdenny Bug, Ros', and Seret rivers, 11 – the Ternopil Reservoir, 12 – the upper Kytaivsky Pond, Kyiv City, 13 – Tel'bin Lake, Kyiv City); III – steppe zone (14 – the Kakhovka Reservoir, 15 – the Kiliya Danube delta, 16 – the Sasyk Reservoir, the Danube basin).

The mentioned natural organic substances are characterized as high weight molecular compounds, which have a wide range of molecular weight values. Thus, the weight average (M_w) molecular weight of humic acids is 6.9–12.2 kDa, and fulvic acids – 2.5–7.3 kDa. The molecular weight of dissolved carbohydrates varies over a wide range – from < 1.0 to > 70.0 kDa. However, polysaccharides dominate. Their relative content in the total balance of carbohydrates is on the average 67.7–83.7%. The weight average (M_w) molecular weight of PLC ranges from 11.6 to 43.0 kDa. The share of the fraction with molecular weight < 5.0 kDa is on the average 39.3–57.9% the total PLC concentration.

HS belong to stable organic compounds of natural waters, as they experience little bacterial degradation in contrast to other organic substances, such as carbohydrates, PLC etc. However, it is known that HS strongly absorb ultraviolet (UV) radiation from the sunlight and undergo photochemical changes. The HS ability to absorb ultraviolet light decreases when their concentration decreases.

As a result of photochemical oxidation, the transformation of high-molecular fractions of HS into compounds with a lower molecular weight occurs. The results of our studies have shown that HS undergo the greatest transformation in the spring and summer period when the photochemical processes' intensity reaches its maximum. There is an increase in the share of the HS fraction with a molecular weight not exceeding 5 kDa in general and < 1 kDa in particular during this period.

Carbohydrates and PLC belong to easily oxidized DOM. They undergo bacterial destruction at increased water temperature and activation of microbiological activity. However, there is evidence that carbohydrates are also photodegraded in the presence of HS. The largest share of carbohydrates with a molecular weight ≤ 5 kDa is observed in autumn (38–48%), when biological processes and bioaccumulation of their low molecular weight fractions gradually decrease.

Abstract

THE ROLE OF VARIOUS GROUPS OF NATURAL ORGANIC SUBSTANCES IN COMPLEXATION IN THE UKRAINE'S SURFACE WATERS

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An important existence form of metals in natural surface waters is complex compounds with various groups of dissolved organic matter (DOM) and different molecular weight. It's the complexation that contributes to the increase in the metals' migration mobility, their preferential presence in a dissolved state. It significantly affects metal toxicity and potential bioavailability.

To study the metals distribution between different groups of DOM with which they formed appropriate complex compounds, chromatographic methods were used to extract individual groups of DOM from water, subsequently analyzing them for metal content. In our study, ion exchange columns were used, which were filled with cellulose exchangers DEAE (diethylaminoethyl cellulose) and CM (carboxymethyl cellulose).

Consecutive passage of natural water filtrates through such columns allows the separation of DOM into acidic (anionic), basic (cationic) and neutral groups with the dominance in their composition of humic substances (HS), protein-like compounds and carbohydrates, respectively. It turned out that HS play a primary role in complexation.

This is due to the fact that they dominate among other groups of DOM in most surface water bodies of Ukraine. However, in water bodies with a relatively low content of HS and high bioproductivity, the metal ions' binding into complexes also occurs with other DOM groups, in particular carbohydrates and, to a much lesser extent, protein-like compounds. This situation is typical for small water bodies in Kyiv City.

In particular, the share of Al, Cu, Fe, Zn, and Pb anionic complexes in the Dnipro cascade's reservoirs and the Stvyga, Prypyat', Desna, and Ros' rivers was of 55.7–85.6% (on average 67.6%), 34.5–78.2% (on average 62.3%), 23.5–83.5% (on average 54.6%), 45.7–65.8 (on average 57.8%), and 57.5–73.6% (on average 67.3%), respectively. The share of dissolved Cd in the form of the anionic complexes reached 56.0–75.0% in the water of the Dnipro cascade's reservoirs (on average 61.8%). Remarkably, even the metals with the variable oxidation state (molybdenum and vanadium) were found predominantly in the anionic fraction of DOM, pointing at the significant role of HS in metal migration.

The share of the investigated metals in neutral complexes with carbohydrates is on average in the range of: 23.8–66.1% $Fe_{dissolved}$; 4.6–53.4% $Al_{dissolved}$; 9.2–56.9% $Cu_{dissolved}$; 12.3–53.5% $Cr_{dissolved}$; 11.7–47.6% $Zn_{dissolved}$; 14.5–33.3% $Pb_{dissolved}$; 17.5–53.3% $Cd_{dissolved}$; and 30.5–34.6% $V_{dissolved}$. The highest share of the neutral complexes is observed in small water bodies which are characterized by a high bioproductivity and relatively low HS concentrations. First of all, such water bodies include small lakes within the Kyiv City, in particular the lakes of the Opechen' system, Verbne, Jordan and some other lakes.

The major fraction of the studied metals was detected in the HS fractions with the relatively low molecular weight (<1 and 1–5 kDa): 51.6–65.3% of $Al_{anionic}$, 55.6–72.9% of $Fe_{anionic}$, and 41.8–57.8% of $Cu_{anionic}$ ($Al_{anionic}$, $Fe_{anionic}$, and $Cu_{anionic}$ – total metal concentration in complexes with HS). For example, data are given on the distribution of the mentioned metals among anionic complexes with HS in the water of the Desna River (Figure 1).

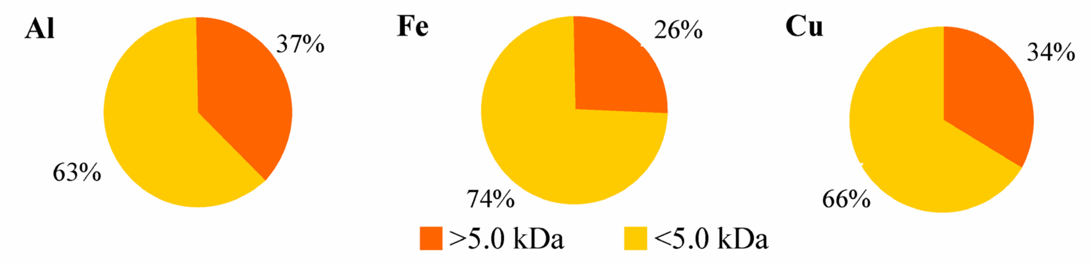

Figure 1. Relative content of various metals' anionic complexes with HS in water of the Desna River (in % to the total concentration of each of the metals in the mentioned complexes' composition).

The molecular weight distribution of metals' neutral complexes with carbohydrates has a slightly different character. Most of the specified complex compounds are high molecular weight, and the share of complexes with a molecular weight ≤ 5.0 kDa does not exceed 50% of their total content in the neutral complexes' composition.

Abstract

CALCULATION METHODOLOGY OF STABILITY CONSTANTS OF FULVATE COMPLEXES

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Macromolecular organic substances - fulvic acids (FA) are natural organic complex formation agents, found in natural objects. FA have functional groups and that's why they form stable complexes with heavy metals and radionuclides. Theoretically, in water solutions according to pH in complex formation process take part the ionic form of metals and hydroxo complexes of metal.

The concentration of fulvate complexe equals to the difference between final concentration of metal $[M(II)_{total}]$ received after formation of complex and initial concentration of metal $[M(II)_{free}]$. In solution, in the hydrolysis zone, initial concentration of ionic form of metal $[M^{2+}]$ is expressed by means of hydrolysis constants (K_1K_2). By simple transformations will be got the formula of calculation of stability constants of fulvate complexes (1:1):

$$\beta=([M(II)_{total}]-[M(II)_{free}])/([M(II)_{free}])/(1+K_1/[H]+K_2/[H^+]^2)[FA]) \qquad (1)$$

where $[M(II)_{free})]/(1+K_1/[H]+K_2/[H^+]^2)=[M^{2+}]$, **[FA]**- the concentration of free ligand, which equals to the difference of total concentration of fulvic acids and the concentration of fulvate complex in solution.

(1) equation is a universal formula by which is calculated stability constants of fulvate and hydroxo fulvate complexes in wide range of pH. At first glance, the formula is flawless and involves hydrolysis processes.

But if you look closely, it is easy to see that (1) indicates that only one form of metal can take part in the complex formation process. Whereas fulvic acids can react with true metal ionic (M^{2+}) form and its hydroxo complexes. In addition, when using equation (1), in the case of two metals with the same complex formation abilit, the stability constants of fulvate complexes may differ from each other by several ranges. The difference will be greater, the more hydrolysable the metal ion will be.The main drawback is that even in the case of the same metal, during $[M_{total}]$-$[M(II)_{free}]$ difference and constant concentration of ligand, taking into account hydrolysis in solution, stability constants of the complex will be different at different pH values. This will be especially noticeable in the case of easily hydrolysable metals.

To put it simply, as paradoxical as it sounds, if during complex formation occurs the formation of ML, MOHL, $M(OH)_2L$ etc types of complexes calculation of stability constants by using of hydrolysis constants in the case of fulvic acids and any other ligand is incorrect. Because, if hydroxo complexes take part in complex formation reaction ,the calculation of the concentration of the ionic form using the hydrolysis or hydroxo complex constants will willy-nilly lead to the same result, the value of the stability constant is artificially increased and cannot be used to calculate the migration forms of elements and assess the ecological and chemical condition of water reservoirs.

The optimal method for calculation of stability constants of fulvate complexes is using Leden function:

$$F(L)=F(FA)=([M(II)_{total}]-[M(II)_{free}])]/([M(II)_{free}].[FA_{free}])=\beta_1+\beta_2[FA_{free}] \qquad (2)$$

By using of Leden function, by the graphical method can be found stability constant of complex. When the concentration of free ligand aspires to zero, section which is cut on the ordinate by the straight-line built-in coordinates F(FA)— $[FA_{free}]$ equals to the stability constant.

OPTOELECTRONIC PROPERTIES OF BIPOLAR THIOXANTHONE DERIVATIVES SUBSTITUTED WITH DIFFERENT ELECTRON DONATING MOIETIES

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Materials exhibiting thermally activated delay fluorescence (TADF) which are considered as the emitters of the third generation of organic light emitting diodes (OLEDs) are promising for the enhancement of the efficiency of OLEDs. TADF emitters can theoretically allow to reach 100% internal quantum efficiency of the devices through the efficient reverse intersystem crossing without involvement of noble-metal complexes [1].

To realize efficient OLEDs, emitters are usually molecularly dispersed in an appropriate host matrix. Even though many host materials are either electron-transporting or hole-transporting materials, a balanced transport of positive and negative charges in the emissive layer is crucial for efficient recombination and high external quantum efficiency of OLEDs. Bipolar materials usually combine both electron donor and acceptor moieties in a single molecule to facilitate the injection and transport of both holes and electrons [2,3].

In this work, four newly synthesized derivatives of thioxanthone substituted with the different donors were studied and the effects of different electron-donating strengths on the optoelectronic properties were investigated. Two derivatives containing phenoxazine and *tert*-butyl-dimethylacridine donor moieties were characterized by small singlet-triplet energy gap (ΔE_{ST}), which is necessary for TADF effect. Time-of-flight technique was used for the investigation of charge-transporting properties of the compounds.

The compounds were characterized by relatively good hole and electron injecting properties. Bipolar charge-transporting properties were observed for two compounds with *tert*-butyl-carbazole and *tert*-butyl-dimethylacridine donors. The highest hole mobility of 3.1×10^{-4} cm^2 V^{-1} s^{-1} was recorded at 4.1×10^5 V/cm for the derivative of thioxanthone and phenoxazine. However, electron-transporting properties were not observed for this compound. The PLQY values of neat films of the compound were found to be higher than those of the solutions because of the decrease of non-emissive energy losses due to the restriction of molecular rotations or vibrations.

This observation can prove that the compounds were characterized by aggregation-induced emission enhancement (AIEE) properties [4]. The ionization potentials values of compounds which were estimated by photoelectron emission spectrometry ranged from 5.42 to 5.74 eV while the the ionization potentials extracted from CV measurements ranged from 5.38 to 5.95 eV.

The thermal stability and transitions of the synthesized compounds were studied by thermogravimetric analysis and differential scanning calorimetry. The compounds showed 5% weight loss temperatures higher than 323 °C.

In order to investigate the influence of the host matrices on the electroluminescent characteristics of the thioxanthone derivatives, OLEDs with the similar structures were fabricated using two different hosts. OLEDs containing the synthesized compounds as emitters showed very different power efficiencies (1-

21.2 lmW^{-1}), current efficiencies (2.5-29.3 cdA^{-1}), external quantum efficiencies (0.9-10.3%) and blue, sky-blue, green, or yellow electroluminescence colours.

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Abstract

POLYLACTIDE STARCH-CONTAINING COMPOSITES: PREPARATION AND PROPERTIES

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The development of all industries and human activities requires new materials, especially polymers. At the same time, in the technology of polymer and composite materials the direction of biodegradable polymers and polymers obtained from renewable raw materials has been developing most intensively in recent years. The most promising are those that are not only capable of biodegradation in environment conditions in a short time, but can be also synthesized from renewable sources of raw materials, in particular raw materials of the agro-industrial complex.

Polylactide (poly lactic acid, PLA) has the most researched and practical used among such materials. Among the methods of obtaining the polymer material with the required properties, the most common are the creation of polymer composite materials as result of modifying the original polymer with additives of different nature: plasticizers, compatibilizers, active and inert fillers.

Promising for the production of biodegradable polymer composites are starch - as an active filler, a regulator of biodegradability and the ability of PLA to hydrolyze in the environment. Epoxidized soybean oil is a plasticizer, impact modifier and compatibilizer. Dispersed calcium carbonate - as a filler to increase the manufacturability of blends, improve the strength and thermophysical properties of polylactide and reduce the cost of the final material.

Ingeo 2500 HP polylactide (NatureWorks) and disperse industrial filler - calcium carbonate, which are treated with stearic acid, were used to obtain polylactide composite materials. Potato starch and epoxidized soybean oil were also used to modify the PLA.

According to value of the deformation modulus, the developed polylactide composite materials can be attributed to low-deformability, which are mainly characterized by reverse deformations and strong elastic aftereffect. Filled with nano $CaCO_3$ and modified by 10% wt. ESO polylactide is characterized by a reduced value of the modulus of deformation and elasticity compared to pure PLA.

Such patterns are primarily related to the plasticizing effect of ESO, which significantly increases the free volume in the system and promotes the relaxation of polylactide macromolecules after stress relief. In this case, the introduction of starch into the system leads to an increase in the modulus of deformation and elasticity, in particular the highest values of 2767 MPa and 7796 MPa, respectively, are characteristic of the material with the highest starch content of 25% wt. Also, we can conclude that the presence in the system ESO eliminates the negative impact of $CaCO_3$ as an inert filler on the structure of the polylactide, in particular the reduction fragility of the material.

For polylactide composites there is a decrease in the modulus of high elasticity, which is characterized by changes in the conformations of macromolecules and rearrangement of the spatial fluctuation network, which leads to increased elasticity of the material, apparently due to the plasticizing effect of ESO and modifying effect of starch. However, with some critical filling of the PLA, the modulus of high elasticity is already growing.

One of the significant disadvantages of polylactide as a polymer material is low resistance to thermal deformation (Vicat softening point = 60 ºC), which significantly limits its use in many industries, including packaging and food. Obviously, in multicomponent polymer systems, the value of heat resistance of the material primarily depends on the presence and content of additives, in particular, inorganic fillers and plasticizers.

The introduction of ESO and $CaCO_3$ significantly increases the Vicat softening point of developed materials, there is an increase of 10-15 ºC. The effect of the filler is primarily due to the low deformability of the filler particles under the action of temperature and load, and as a consequence, the increase in heat resistance. At the same time, ESO as a plasticizer increases the free volume of the system, which promotes the crystallization of polylactide. The highest values of heat resistance - 133.3 ºC are characteristic of the material with the maximum content of all components. In this case, we can predict that in the process of analyst there is a partial crystallization of the PLA under the action of temperature, resulting in a significant increase in the crystallinity of the polymer, with $CaCO_3$ and starch particles acting as nucleation centers.

A slight increase in the hardness of highly filled PLA materials was established. At the same time, an increase in the ESO content by more than 10% by wt. leads to a decrease in surface hardness by 10-15%, apparently due to the plasticizing effect of ESO in PLA.

With the help of thermomechanical analysis, it was found that the addition of starch almost does not affect the nature of the thermomechanical curves, at the same time, the introduction of ESO leads to a stepped appearance of the thermomechanical curves, which indicates the process of PLA transition into a viscous state in two stages and a shift in its melting temperature in region of higher temperatures.

The effective use of the developed materials for 3D printing, the packaging industry and for the manufacture of disposable products is expected.

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NEW MATERIALS BY MACROMOLECULAR ENGINEERING USING ATOM TRANSFER RADICAL POLYMERIZATION

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Macromolecular Engineering (ME) is a process comprising rational design of (co)polymers with specific architecture and functionality, followed by precise and efficient polymer synthesis and processing to prepare advanced materials with target properties.

Many advanced nanostructured functional materials were recently designed and prepared by reversible deactivation radical polymerization. Copper-based ATRP (atom transfer radical polymerization) catalytic systems with polydentate nitrogen ligands are among most efficient reversible deactivation radical polymerization systems.

Recently, by applying new initiating/catalytic systems, Cu level in ATRP was reduced to a few ppm. ATRP of acrylates, methacrylates, styrenes, acrylamides, acrylonitrile and other vinyl monomers was controlled by various external stimuli, including electrical current, light, mechanical forces and ultrasound, also in the presence of air.

Various copolymers, molecular brushes, hybrid materials and bioconjugates were prepared with high precision. Special emphasis will be on nanostructured multifunctional hybrid materials for application related to biology, environment, and energy.

Abstract

SYNTHESIS OF THE Tl-BASED SUPERCONDUCTING MATERIALS BY THE SOL-GEL METHOD IODINE VAPOR PRESSURE

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Among the members of Tl-based series, Tl-1223 is one of the preferable candidate superconductors for fundamental and applied research because it's very high T_c and its efficient flux pinning properties. The high-temperature superconductors Tl-1223 show a superconducting transition temperature T_c above 118 K, and when synthesized under high pressure, the critical temperature can reach 133.5 K.

A review of numerous reports shows that the solid-state reaction route commonly used in the synthesis of the precursor severely limits the ability to control stoichiometry and makes it impossible to obtain a homogeneous superconductor with the desired phase composition.

Comparative of these methods wet chemistry are an advanced method, because the high-temperature superconducting materials have several constituent ions, three for Y-123 superconductors, four for Bi-1223 and Tl-1223 superconductors, and sometimes more than four. Therefore, in solid solutions, amplify the problems solid-state reaction and co-precipitation methods.

Therefore, polycrystalline superconductors with the same overall composition often exhibit different properties, reflecting small phase purity and compositional homogeneity differences. The sol-gel process has an advantage over the other methods to achieve homogeneous mixing of the component cations on the atomic scale and form bulk superconducting materials from gels.

The novelty of the research is that, as dopants, we use Iodine pentoxide, whose transition temperature to steam is lower than Tl_2O_3 oxide. Using this approach, we controlled Tl vapor pressure in the sealed quartz tube and make sintering at high ambient pressures.

As far as we know, such methods in synthesizing Tl-based superconductor materials and their influence on phase formation, transport, and magnetic properties were investigated first.

In summary, we could conclude that Iodine pentoxide enhancement phase purity and superconductivity properties of the Tl-1223 phases

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ANALYSIS OF ENGINEERING PROPERTIES AND APPLICATIONS OF POLYMER COMPOSITES USING DEEP LEARNING WITH REFERENCES

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Polymer composites have emerged as an important class of materials with unique combinations of properties that make them suitable for various applications. However, the optimization of their properties and their applications is still a challenging task. Deep learning has emerged as a powerful tool in materials science, offering a way to extract insights from vast amounts of data and to make predictions of properties and applications [1,2].

This paper provides a comprehensive review of the use of deep learning in the analysis of engineering properties and applications of polymer composites. The review covers various aspects of the use of deep learning, including data preparation, model development, and validation. It also provides examples of applications of deep learning in the analysis of various properties of polymer composites, including mechanical, thermal, and electrical properties [3-6].

The paper highlights the advantages of deep learning in materials science, including its ability to handle high-dimensional data, learn complex relationships between different variables, and make predictions with high accuracy. The review also identifies the challenges in the use of deep learning in materials science, such as the need for large amounts of high-quality data and the potential limitations of the models.

Overall, this review provides a valuable resource for researchers and engineers working in the field of polymer composites. It summarizes the current state of the art in the use of deep learning in materials science and identifies areas for future research. The paper also provides references to recent studies that have applied deep learning to the analysis of engineering properties and applications of polymer composites, which can help guide further research in this area.

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OBTAINING OF HIGHLY ABSORBENT MATERIALS USING NATURAL SORBENTS

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The important task of the present day is protection of the environment and mainly of water basins (rivers, lakes, oceans, seas, etc.) from pollution with petroleum and petroleum products and other toxic organic compounds.

Today for purification of water surface an adsorption method is widely used. For sorption of spilled petroleum and petroleum products more than 200 different types of sorbents are produced and used.

Quality of sorbent is characterized by volume of absorbed petroleum and its products, and by its ability of regeneration, utilization and floatation [1-3].

Porous sorbents are effectively used as heat and sound insulation materials. We carried out studies in the sphere of natural mineral sorbents usage in polymer compositions to obtain porous materials on their basis.

Perlite, zeolite and diatomite were chosen as natural sorbents. With the aim of activation of sorbents their thermal and chemical modification was carried out.Optimal conditions of thermal modification of natural sorbents were determined: for perlite – heating at 420-660°C for 3.5 hours; for zeolite – heating at 350–780°C for 6 hours; and for diatomite – heating at 1040°C for 3 hours.

With the aim of widening of zeolite pore size and activation its chemical modification was carried out. The optimal conditions of chemical modification of zeolite were determined: temperature, time, concentration of solutions and ratio of components.

Optimal conditions of hydrophobization of diatomite, perlite and zeolite were studied-260°C for 5.5 hours in silicon area.

Thermally modified diatomite after hydrophobization does not get wet and does not sink, effectively absorbs petroleum and its products from the surface of polluted water.

The perlite heated at 420–660 °C is used when the concentration of petroleum does not exceed 6·103 mg/L. If the concentration of petroleum product is high, the modified at 700°C perlite is used.

To obtain polymeric compositions on the base of perlite the second main component – carbamide-formaldehyde, melamine-formaldehide and carbamide-melamine-formaldehyde complex oligomers were synthesized, that were perspective materials for usage as matrix in compositions [4-5].

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Abstract

ELASTIC PETROLEUM SORBENTS WITH WIDE RANGE OF PROPERTIES

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Nowadays protection of the environment from pollution with petroleum and petroleum products is very actual.

Decontamination of oceans, rivers, water basins and other surfaces polluted with petroleum and its products by way of development and usage of new effective methods, usage of plastic foam materials and especially of polyurethane foams as insulation (heat, vibration, electric, hydro- and sound) materials and for other constructional purposes contributes to partial solution of this global problem [1-3].

Our goal is to provide obtaining of new type of ecologically friendly, cheap, ultra light, flexible, hybrid polymer compositions on the base of homogenous olygoesthers, aromatic polyisocyanates and local natural sorbents with high sorption activity, enhanced physical and chemical properties, and a high heat, sound, vibration, electrical and hydro-insulation properties. Instead of expensive silicone and paraffin oils the waste oils will be used in the polymer composition [4-6].

The objective can be achieved according to the following scheme: 1) Addition of activators and natural excipients to improve properties; 2) Thermal and chemical modification of natural sorbents. This gives a possibility to widen the pore sizes and to enhance effectiveness of sorption; 3) Hydrophobization of sorbent that specifies its selectivity and floatability; 4) Selection of aromatic polyisocyanates to obtain composition of light foam polyurethanes; 4) Investigation of light composition obtaining process on the base of aromatic polyisocyanate and polyester in case of water excess; 6) Obtaining of organic-mineral elastic hybrid porous polymeric compositions that are characterized by high sorption ability and floatability, as well as high thermal, electrical, vibration, sound and heat insulation properties;

Perlite, zeolite and diatomite were chosen in the capacity of natural sorbents. Optimal conditions of thermal modification of natural sorbents were determined: for perlite – heating at 500–700°C for 2 hours; for zeolite – heating at 300–750°C for 5 hours; and for diatomite – heating at 1200°C for 2 hours.

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Abstract

METALIZATION OF LARGE TONNAGE POLYMER GRANULES

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Polymer composites as a basis for creating modern structural materials have significant prospects. This is caused by the possibility of combining in one material high strength, low weight and a number of unique and specific properties, which creates conditions for their possible use and implementation in various and very wide areas of application. In particular, for the time being, such materials are used in medicine, space, aviation and defense industries. Polymer composite materials with dielectric fillers have good heat-conducting properties, which allows them to be used in heat removal and dissipation systems. The use of new types of fillers makes it possible to obtain composite materials characterized by higher mechanical properties compared to conventional materials and new properties which are not typical for polymers.

Among composite materials, metal-filled polymer composites also have significant prospects. Such materials combine the low mass of the polymer matrix with the plastic and strength properties of metals, which allows their use as a light and highly efficient material for industrial use. However, obtaining metal-filled composites with predictable mechanical properties using traditional production methods is a complex technological task. This is caused by the difficulty of controlling the distribution of the filler in the polymer matrix and the low interphase interaction between the system components. Accordingly, the development of new methods of introducing a metal filler into a polymer matrix with the possibility of a predictable effect on the final mechanical properties of the material is an urgent task.

We are developing a technology for the production of metal-filled polymer composites, the basis of which is the production of metallized polymer granules and their subsequent processing into products [1-3]. At the same time, the introduction and uniform distribution of metal in the polymer matrix is ensured as a result of processes that are not used in traditional industrial methods.

In order to obtain metallized polymer raw materials, the classical technology of polymer metallization was used. This technology has long and successfully been used to apply a metal layer on a polymer surface, however, the number of polymers that are used for metallization on an industrial scale is insignificant and does not include a number of high-tonnage polymers.

According to the classic technology of metallization, at the first stage, the polymer surface was cleaned and degreased with ethyl alcohol. After degreasing, the polymer granules were dried and used for etching in order to change the structure of the polymer surface. CCl_4, chromium mixture and boiling concentrated HNO_3 were used as etching agents. The next stages of sensitization are processing of granules in an acidic tin chloride solution and activation in an ammonia solution of silver nitrate. Metallization of activated polymer granules was carried out in a solution of chemical precipitation, which consisted of $CuSO_4 \cdot 5H_2O$, EDTA-Na_2, NaOH and formalin.

The obtained results of metallization of the surface of polyethylene, polypropylene, rigid and plastic polyvinyl chloride granules according to the classical technology showed its low efficiency, as well as the fundamental unsuitability for forming a metal (copper) coating on the granules. In addition, the classic technology of metallization is characterized by multi-stage, the need to use precious metals, volatile and aggressive environments, and also requires repeated washing and drying of polymer granules. Thus, the proposed technology for obtaining metal-filled composites as a result of the processing of metallized granules cannot be based on the use of classical metallization technology and requires the development and implementation of new technological solutions [4].

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Abstract

POLYMER AND LIQUID CRYSTAL FILM LASERS: SPATIAL PROPERTIES OF PUMPING

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The light emission properties of the dye doped film lasers depending on the spatial distribution of energy in the pump spot have been studied. It was shown that at a constant density of pumping the emission from the dye doped film strongly depends on the dimensions of the pump spot. Namely, at the same density of pumping the lasing can be observed only with a small pump spot. For each specific laser film there is a threshold diameter of the pump spot above which the laser emission is impossible. Usually, in practice, this value is 0.5…2 mm.

Since the size of the film laser can be much larger than the indicated values, the question arises: is it possible to obtain laser emission from a larger film area? We pumped the dye doped film with a uniform spot of 8 mm in diameter.

Only fluorescence was emitted from the film. But if we violate the spatial homogeneity of the pump spot, for example, by overlapping the pump beam with a mask in the form of a two-dimensional grating, laser emission appears. In this case, the luminescent area turns into an array consisting of tens of micro-lasers.

Two types of dye doped film lasers have been studied: a polymer laser with a resonator formed by the film surfaces and a cholesteric liquid crystal laser with a photonic band gap. Second harmonic of Q-switched Nd:YAG laser (532 nm) was used for pumping.

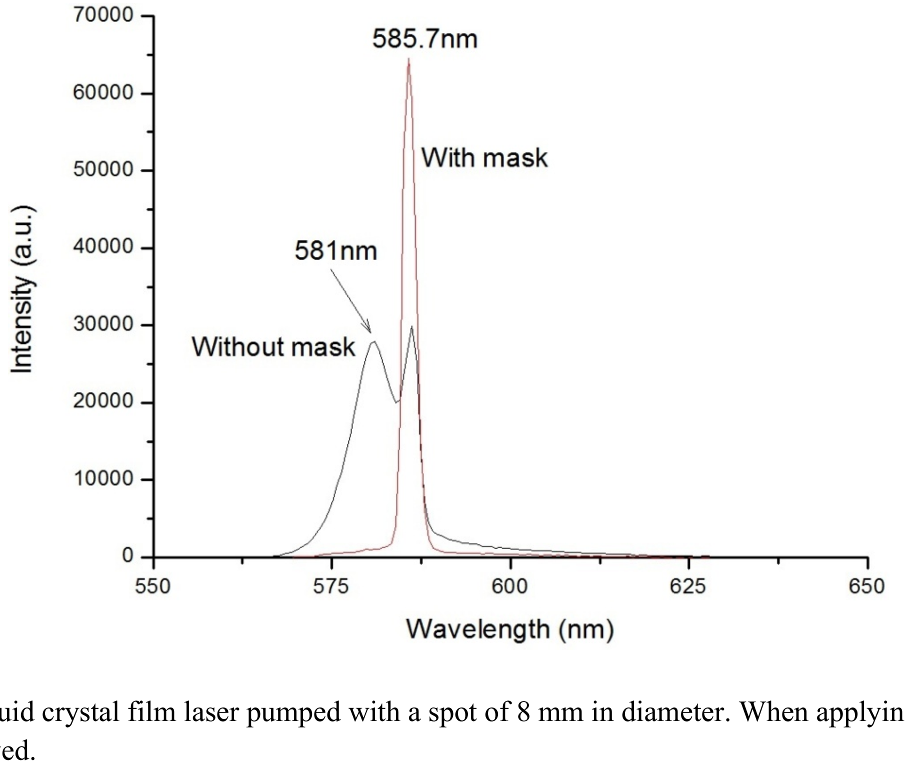

Figure 1. A liquid crystal film laser pumped with a spot of 8 mm in diameter. When applying the mask, lasing is observed.

SMECTIC LIQUID CRYSTAL-G PHASE RETARDER

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Phase retarders or wave-plates are the birefringent optical devices used to modulate the phase of polarized light in bulk optical systems. The most common polarization modulators act as converters between linear and circular polarization states and between linear polarization states with different directions of linear polarization. Due to their low cost, no moving parts, low driving voltage, and small sizes, the liquid crystals (LCs) are outstanding candidates for use in phase modulators as they exhibit a broadband birefringence (□n), a giant optical nonlinearity and a transparent spectral region from 400 nm to 20 □m. LC-based polarization modulation is used in various optical devices for beam steering, spatial light modulation, imaging Stokes polarimetry, optical switching, and display applications. This technology provides important benefits for other typical retarders or phase shifters [1, 2].

We prepared and investigated a smectic liquid crystal-G (SmLC-G) phase and have shown for the first time that it can use as an optical phase retarder. Mixing two nematic liquid crystals, an SmLC-G phase was obtained, and its temperature-dependent phase transitions had studied. The prepared mixture exhibits a wide temperature interval of the SmLC-G phase, which presents a multidomain, polycrystalline structure (figure 1), where each domain acts as a uniaxial crystal.

Over time the domains merged, and a uniaxial, monodomain crystal with 3D symmetry formed, which is transparent in the ultraviolet, visible, and near-infrared ranges of the optical spectrum. Since to its high birefringence, the SmLC-G -based phase retarder is much thinner than the most commonly used phase retarder, such as the quartz–based one. In addition, we have shown several examples of the possibility of using SmLC-G phase retarders, such as spatial-temporal modulation of two collinear laser beams, solar spectral radiation division, and aerospace applications. Besides, the proposed SmLC-G phase retarder can be used in many directions as medicine, environmental monitoring, astronomy, and polarimetry.

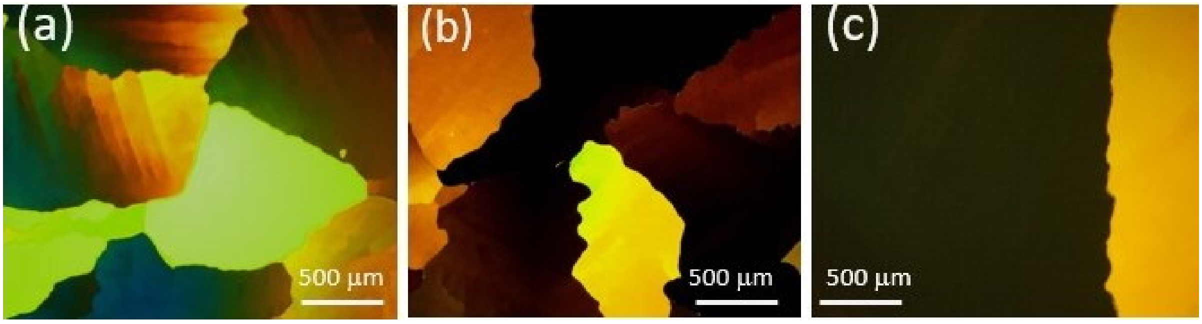

Figure 1. Time-dependent transformation of the SmLC-G phase from the initial mosaic multi-domain textures (a, b) into the final single-domain uniaxial one (c).

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DEVELOPMENT OF DIABETES MELLITUS TREATMENT ALTERNATIVE MODALITY BASED ON PHOTOCHROMIC DRUG DELIVERY MICROCAPSULES

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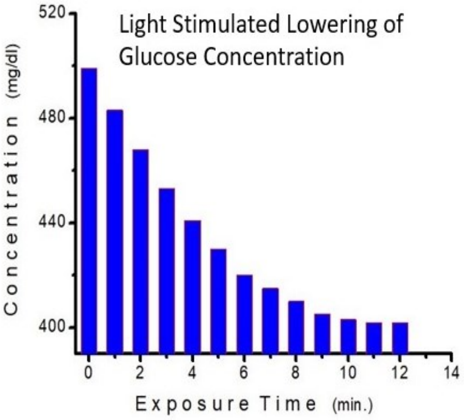

Diabetes has become a global health problem since it is the most common clinical disorder, affecting nearly 10% of the world's population and constantly increasing day by day. The World Health Organization (WHO) reported that about 1.1 million people die of diabetic complications annually, and the death rate is expected to increase up to 50% in 2030 [1]. Despite the insulin represents a lifesaving therapeutic aid for people suffering from diabetes, at present, it is no longer considered the first choice for type 2 diabetes, and an expanding range of new therapeutic possibilities is emerging.

While these may lack the potency of insulin, at a minimum, they allow a major reduction in the intensity of insulin use. Therefore, the search for new glucose-lowering drugs with minimal or no side effects is undoubtedly an active challenging area for research and development worldwide [2]. In this regard, controlling the glucose level in blood by external stimuli such as light offers a new route to governing blood glucose concentration with the required dose and at the appropriate time.

Light-activated and light-controlled drug delivery systems offer distinct advantages over other stimuli because the light is a fascinating and green stimulus with a micron-or submicron-sized focusing area with controllable wavelength and energy, non-invasiveness and non-destructive nature, precisely controlled direction, and availability that can release a drug at a desired time and place, so it only targets cells and not surrounding healthy tissues [3].

One of the unique examples of light-controlled molecular switches is the spiropyrans (SPs), whose closed ring, hydrophobic isomer transforms into a highly polar, open-ring merocyanine (MC) isoform upon exposure to UV light, whereas the reverse reaction can be induced by visible light or by heat. In this work, we prepared SP doped liquid crystal (LC) microspheres, emulsified in a 5% Dextrose (D-Glucose) solution, and showed that upon exposure to the light-emitting diode (LED) with violet (405nm) light, the SP isoforms are converting into their MS isoforms, which in turn stimulates MC isoforms to translocate across the interface of LC-Dextrose solution and interact with the glucose molecules leading to a lowering of the total glucose concentration in a solution by 20%.

We envisage that the proposed modality could give a possibility to dynamically regulate the concentration of glucose in the blood with the required dose and at the appropriate time to manage and treat type 2 diabetes noninvasively.

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Abstract

THERMO AND PHOTOCHROMIC LIQUID CRYSTAL POLYMER COMPOSITES FOR THE DISPLAYING OF OPTICAL INFORMATION

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Integrating thermochromic liquid crystal (LC) and photochromic LC systems with polymer enables the creation of new multifunctional polymer materials, which is very promising for using such systems in modern thermo- and photo-optically controlled devices to record, display, and store information. Qualitatively new polymer films - as polymer composites, consisting of thermochromic nemato-chiral LC mixture or photochromic Spiropyran (SP) doped in the nemato-chiral LC matrix compositions, have been obtained using the technological process of the innovative microencapsulation method [1, 2].

The microencapsulation method was improved by the authors by choosing the ice acetic acid as a suitable emulsifier, which provides encapsulated emulsion in the dispersion system composition – polymer solution. The initial properties of the composition are fixed in microcapsules and ensure the production of technologically perfect polymer composites. Elastic and homogeneous LC and SPLC polymer films of various shapes and sizes are made following the practical requirements by controlling the microencapsulation technological process.

At all stages of the process regulation of technological characteristics – sizes of microcapsules in film, the thickness of the film, non-stretched and stretched film – influence the thermo- and photo-optical parameters of polymer composites. Spectral and microscopic research has shown: a) reducing the size of microcapsules in films significantly increases the intensity of reflection of LC and the photosensitivity of SPLC polymer films; b) change in the thickness does not affect the intensity of selective reflection of the LC polymer films, but an increase in thickness significantly increases the photosensitivity of the SPLC polymer films; c) film stretching significantly increases the selective reflection intensity of color temperature parameters of LC polymer films and improves the photosensitivity of SPLC polymer films.

The received nemato-chiral thermochromic LC and photochromic SPLC polymer films are photochemically stable-over time, multiple uses of polymer films are possible, technological characteristics determine the engineering properties of thermo- and photo-optical parameters of polymer composites, which is very important for practical use of LC and SPLC polymer films.

Practically application of LC polymer films as rewritable thermoindicator polymer materials is promising for visualizing the distribution of thermal fields in various areas of thermal indication, such as medical thermographic diagnostics, liquid crystal thermometry, and flaw detection. SPLC polymer films with improved photosensitivity as photosensitive rewritable materials are very important for developing high-performing optically photonic devices, such as UV irradiation dosimeters, holograms light-controlled molecular and fluorescent switches [3, 4].

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DEVELOPMENT OF TITANIUM DIOXIDE NANOPARTICLES DOPED FILMS FOR PHOTOTHERAPEUTIC APPLICATIONS

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Novel methods based on combination photodynamic therapy (PDT) with nanotechnology have shown great promise in anticancer treatment in recent years. Nanoparticles (NPs) can be used to treat cancer due to their specific advantages, such as biocompatibility, reduced toxicity, excellent stability, enhanced permeability, retention effect, and precise targeting [1]. Another promising application of NPs is their use in the decomposition of bacteria, viruses, and fungi as an alternative to antibiotics. Among the NPs, titanium dioxide (TiO_2) NPs exhibit unique medicinal properties. TiO_2 has been considered an attractive antimicrobial compound due to its photocatalytic nature and because it is chemically stable, non-toxic, inexpensive, and recognized as a safe substance.

Several studies have revealed that this metal oxide demonstrates excellent antifungal and antibacterial properties against a broad range of both gram-positive and gram-negative bacteria [2]. Under ultraviolet (UV)-light irradiation, the valence band electrons of TiO_2 are excited to the conduction band (CB), and the resulting electron holes have the capability of generating various cellular ROS, including hydroxyl radical ($OH\cdot$), hydrogen peroxide (H_2O_2), and superoxide (O_2^-). The $O_2^{\bullet -}$ molecules can quickly penetrate and influence subcellular organelles (nuclei, mitochondria, and others), ultimately governing cellular function and resulting in the decomposition of organic pollutants, bacteria, viruses, and cancer cells.

However, the biggest obstacle in the clinical application of TiO_2-based NPs for PDT is the TiO_2 high band gap. We prepared a polyvinyl alcohol (PVA)-based elastic polymer film with a thickness of 50 microns, in which the TiO_2 NPs and various organic luminescent dyes have been incorporated. The size of TiO_2 NPs was 80-100 nanometers, and the dyes used have based on rhodamines, coumarins, and stilbene derivatives. The percentage of the weight of TiO_2 NPs in the polymer nanocomposite compared to the polymer matrix was 10^{-4}, and that of the organic luminescent dyes was 10^{-5}. It has shown that upon irradiation of a polymer film with ultraviolet light, a rapid decomposition-degradation of organic luminescent dyes have caused, which was stimulated by the photocatalytic effect of TiO_2 NPs.

These proposed nanocomposite films can be used to accelerate wound healing and tissue regeneration, as well as to break down bacteria, viruses, and air, water, and soil pollutants.

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CHOLESTERIC LIQUID CRYSTAL BASED PHOTOCHROMIC SMART WINDOWS

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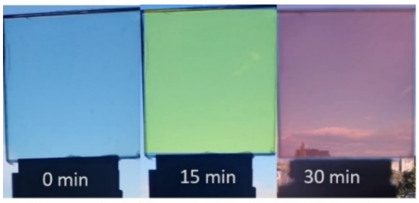

Exposure-time Dependent Tuning of SRB of PSW

The high energy use has caught people's attention and sparked an interest in new energy sources, energy conservation, and methods to reduce energy demand. About 30-40 % of the energy in the world is used in buildings due to heating, cooling, lighting, and ventilation [1,2]. Considering varying climates during the day or season, building energy savings can be achieved by using windows that control incoming visible light and solar energy.

Thus, it can be possible to allow solar energy to pass into a building if heating is required, and it can be likely not enable solar energy to pass into a building if cooling is needed. Controlling incoming light and solar energy can be provided by materials having variable optical properties. These materials are called chromogenic materials or chromic materials. The smart window is a system that can sense and respond to external stimuli such as light, heat, or electricity. It controls light passage through its glass, promising the advantages of reversible control of indoor light and temperature in applications to next-generation household or industrial windows for multiple purposes. The materials used in these systems are generally classified into the following three categories, as mentioned above: electrochromic, thermo-chromic, and photo-chromic. In this work, we fabricated a photochromic smart window (PSW) based on the cholesteric liquid crystal (CLC) mirror. The CLCs are formed by chiral elongated organic molecules and are among the best materials capable of selective reflection of light. The proposed window can reflect visible or infrared light without needing an external power source. Moreover, the CLC mirror-based PSW can respond to the environmental light intensity to independently rearrange a light reflection, which easily can be adjusted, to daylight time and climate regions. In this experiment, the photosensitive material was used nematic liquid crystal ZhK-440 which is a mixture of two-thirds p-n-butyl-p-methoxyazoxybenzene and one-third p-n-butylp-heptanoylazoxybenzene [3]. As the optically active dopant MLC-6247 was used. By mixing the initial materials with the following percentage in weight 75% wt. Zhk-440 + 25% wt MLC-6247 a CLC mixture with desired selective reflection band (SRB), was obtained.

To assemble a photochromic smart window, we used two glass plates with dimensions 120x120x1 mm. The alignment layers are composed of 99.4 % Water + 0.6 % Polyvinyl Alcohol (PVA) solution deposited on the glass substrates by spin-coating and then rubbed to obtain planar alignment of the CLC material.

The smart window was sealed using polyacrylic glue. The fabricated PSW was placed under direct solar irradiation and using a spectrometer the exposure time-dependent spectral tuning of SRBs was recorded. The maximum spectral shift of SRB was 220 nanometers over 30 minutes of exposure time. The proposed smart windows can be used to regulate the amount of light entering buildings, which will reduce energy consumption.

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THE INFLUENCE OF THE SORPTION EFFECT ON THE POLYMER'S CREEPING

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The polymer's creeping is due to intermolecular connection breaking, that causes macromolecule structure transformation and conformational changes. It's natural to think that, polymer creeping will increase more when it's weak connections and will be as big as it's systems free volume, that's necessary for macromolecule changes. Polymers features are determined by not only groups in the molecules, but also with distances, that makes the energy between molecules and structure elements mobility. Space between moleculars causes that polymer volume's part is not connected with it's mass. This part was given name – free volume.

Different autors put different ideas in this term. For example: Frenkel [1] thinks behind the free volume body's excess volume on the given temperature compane with it's volume on the absolute zero V_0:

$$V_f = V_T - V_0 \qquad (1)$$

Gildebrand and Bond called the magnitude V_f - the expansion volume V_E according to the following equation [2]

$$V_E = V_T - V_W \qquad (2)$$

Our first conducted tries show that, polymer creeping drew in the liquid environment. Compare with the same polymer in the air creepimg, as happened liquid sorption in the polymer's free volume.

Where V_T and V_W are body volumes on the given temperature and there molecules own volume.

Free volume and arrangement coefficients are connected with easy dependence.

$$1 - k = \frac{V_E}{V_T} \qquad (3)$$

It shows that, in their atoms and molecules the most tight arrangement, there is free or spare volume, that's body volume's 20-32 %.

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PETROLEUM RESINS WITH CARBOXYLIC GROUPS OBTAINED IN THE PRESENCE OF A PEROXIDE INITIATOR

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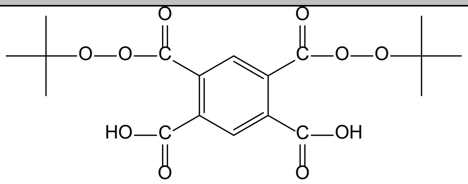
Petroleum resins (PR), oligomerization products of unsaturated compounds, are characterized by good physicochemical properties and are used as substitutes for food and other products of natural origin.

The functional groups' presence in the PR structure, particularly carboxyl ones, makes it possible to improve their physical and mechanical properties, and chemical resistance to aggressive environments of products based on them, as well as significantly expand the application scope in various industries.

Petroleum resins with carboxyl groups (PRC) were obtained by the method of initiated oligomerization of unsaturated hydrocarbons, which are part of the C_9 fraction of the pyrolysis pyrocondensate of diesel fuel, in the presence of a peroxide initiator with carboxyl groups - ditret-butyldiperpyromellitate (Table 1).

Table 1

Characteristics of reaction mixture components

Properties	Value
Raw material	
Density (d_4^{20})	0.908
Molecular weight (M_n), g/mol	125
Bromine number, g Br_2/100 g	112
Xylenes content, wt%	19.84
Styrene content, wt%	16.93
Vinyltoluenes content, wt%	9.13
Dicyclopentadiene content, wt%	17.78
Initiator	
Formula	
Molecular weight (M_n), g/mol	398
Carboxylic group content, %	22.6
Active oxygen (O)act., %	8.0

As a result of the experimental studies, it was found that with an increase in the initiator content in the reaction mixture, the PRC yield (from 13.2 to 19.8 wt%) and acid number (from 34 to 118 mg KOH/g) increases, and its molecular weight decreases (from 1390 to 905). This is explained by the fact that with the increase in the initiator concentration, the number of formed functional radicals in the reaction mixture increases, which accelerates recombination. As a result, an oligomeric product with a lower molecular weight and a higher content of carboxyl groups is formed. The bromine number of PRC, which characterizes the content of unsaturated bonds, decreases (from 32 to 9 g of Br_2/100 g) when the initiator content in the reaction mixture increases. An increase in temperature leads to the same consequences as an increase in the initiator content in the reaction mixture.

The initiator content in the reaction mixture of 2.5 wt% per raw material is optimal in terms of yield, quality, and economic considerations. Other established optimal conditions for PRC synthesis are as follows: temperature – 393 K; oligomerization - 50 hours.

REE RADICAL POLYMERIZATION IN A MICRODROPLET WITH INITIATION AT THE INTERFACE

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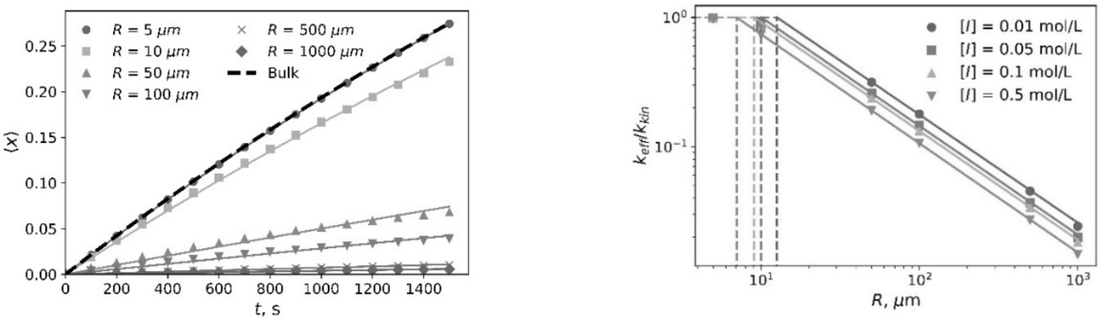
Production of polymeric particles and capsules via microfluidic devices became an important topic in recent decades due to rapid development of microfluidic technologies. To date there are many studies, where microdroplets were successfully used as microreactors for polymer synthesis. Initiator in such a microfluidic realization might be distributed inside droplet or in the outer phase. In the latter case polymerization process is affected by diffusion of the radicals that are generated at the droplet interface, leading to the dependence of polymerization kinetics, as well as molecular weight of obtained product, on droplet radius. This work is devoted to modelling of radical polymerization in monomer droplet, surrounded by the ambient medium containing initiator.

To solve the problem under consideration, we use a generalized method of moments. In this method, we solve a set of diffusion-reaction equations on moments of living radicals and polymer chains with source terms corresponding to kinetics of free radical polymerization. This approach allows, after averaging over droplet volume, to obtain dependencies of monomer conversion, average chain length and dispersity on reaction time. Fig. 1a shows kinetic curves for droplets of different radius R. It can be seen, that, while the smallest droplet (R = 5 μm) coincide with bulk kinetics (dashed line), increasing droplet radius slows down the reaction rate sufficiently, which is due to increasing role of radical diffusion. Fig. 1b shows the corresponding effective kinetic constants for different initiator concentration outside the droplet. One can see, that there is two regimes of polymerization: 1) kinetic regime, when $k_{eff} = k_{kin}$ (k_{kin} is kinetic constant for quasi-stationary approximation), and 2) diffusion regime, when effective constant k_{eff} depends on droplet radius as $\frac{k_{eff}}{k_{kin}} = \alpha R^{-\beta}$. The critical radius R_c, corresponding to transition between these two regimes, was shown to be a power-law function of initiator concentration in the ambient phase.



(a) (b)

Figure 1. Kinetic curves for different droplet radii (a) and reaction rate constants for different initiator concentration in the ambient phase (b)

Beyond polymerization kinetics, molecular weight characteristics were also studied. We have shown, that increasing droplet radius leads to increasing both average chain length and polydispersity index. It was also found, that for small droplets average chain length may be as low as five monomer units, which means, that microfluidic technology may be seen as a possible route for oligomer synthesis.

Acknowledgements: This work was supported by the State Assignments of Federal Research Center for Chemical Physics of Russian Academy of Sciences (n. FFZE-2022-0010) and Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry (n. AAAA-A19–119071190040–5).

SYNTHESIS AND DEPLOYMENT OF CARBON NANOTUBES FOR THE WATER SURFACE PURIFICATION FROM OIL PRODUCTS FILMS

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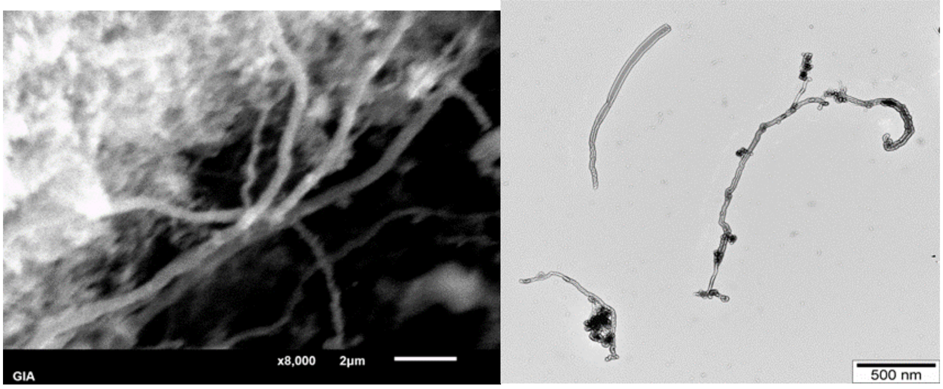
The surface area of water reservoirs purification from spilled oil products as a result of offshore oil production and maritime transportation activities continues to be one of the top priorities for environmental preservation.

However, even though adequately efficient techniques for water surface purification from heavy layers of oil and petroleum products, for instance, installation of floating booms or pumping out, have been developed, these methods do not work for removing thin oil films. Nonetheless, even extremely thin layers of hydrocarbons may seriously harm the ecosystem of reservoirs because they block sunlight and air oxygen from reaching the water column, destroying fish and plankton. Carbon nanotubes are considered one of the most promising adsorbents for capturing thin oil films. They have buoyant characteristics because of their low density and strong sorption capacity for petroleum compounds.

Furthermore, carbon nanotubes are adsorbents that can be used multiple times since they can resist numerous regeneration cycles. Nevertheless, the comparatively exorbitant price of carbon nanotubes caused by the high cost of the chemical reagents used in their production prevents their widespread application.

We utilized an accessible and reasonably priced propane gas as a crude for the production of Multi-Wall Carbon Nanotubes (MWCNT) to decrease the cost of the nanocarbon adsorbent. Specifically enhanced and expressly built for this objective laboratory setup was used for the synthesis. As a catalytic precursor, ferrocene was deployed. The synthesis was conducted at the temperature of 900C and the atmospheric pressure. SEM – see Fig.1a and TEM - see Fig.1b methods were applied to identify and determine the morphology of the synthesized MWCNT. These microphotographs demonstrate the presence of a small number of non-tubular entities (presumably coke or soot) in carbon nanotubes synthesized from propane gas. Oil sorption capacity of synthesized carbon nanotubes research revealed that, depending on the oil-specific density, the numerical values of this parameter vary between 3 and 4 ml / g.



a) b)

Fig.1. MWCNT produced from propane gas SEM (a) and TEM (b) micrographs

The targeted and purposeful modification of the MWCNT for petroleum products has significant potential in increasing the absorption capacity; however, this will be the focus of our future study.

Results:

1. Based on the results of SEM and TEM analysis, it was revealed that the synthesized from propane MWCNTs are well structured and contain a small number of impurities.
2. The synthesized MWCNTs were studied as floating sorbents for cleaning the water surface from oil pollution; as a result, it was found that their sorption capacity for oil products is 3–4 ml/g.

LUMINESCENCE COMPLEXES AND METALOPOLYMERS OF GD(III) AND THE INFLUENCE OF THE NATURE OF SUBSTITUTES ON THEIR EMISSION

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Coordination compounds of lanthanides cause not only fundamental but also applied interest. This is due to their high luminescent properties, the possibility of various practical applications, in particular, in biosensors and telecommunication devices, LEDs, lasers, etc. [1-3].

One of the main factors affecting the properties is the influence of the nature of the ligand systems, which can prevent or significantly reduce non-radiative energy losses. It is known that maximum luminescence intensities can be achieved only at minimum energies of phosphorescence and fluorescence. The difference in energies between the triplet level of the ligand and the resonant level of the lanthanide ion, as well as the structure of the ligand, which will prevent shielding of the radiating centers of lanthanide ions, are important [4].

The use of β-diketones with unsaturated substituents in chelate rings as starting ligand systems makes it possible to further synthesize metallopolymers and copolymers based on them. This aspect will significantly expand the areas of their practical application, as it will increase the chemical and thermal stability of such systems.

The new complexes of Gd(III) □-diketones containing unsaturated, alkyl- and aryl- substituents were obtainted. Their heteroligand complexes with phenanthroline and biphenyl were synthesized. Quantum-chemical calculations of ligand molecules and metal complexes were performed. The main energy characteristics of ligand molecules were calculated: enthalpy of formation, total energy of the molecule and bond lengths, electronic population parameters of ligands. Metal polymers based on synthesized complexes were obtained by the method of radical polymerization. The composition and structure of synthesized complexes and metal polymers are established. It is shown that during polymerization the coordination environment of the central ion remains unchanged.

The spectral-luminescent characteristics of the synthesized compounds were studied. The peculiarities of the influence of substituents in the diketonate fragment on the luminescent properties of metal complexes have been established. It is shown that the emission intensity of powdered samples depends on their morphology and dispersion.

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RECOVERY OF METALLIC LEAD FROM LEAD OXIDE RESIDUES BY POLYETYLENTEREPHTHALATE

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The present article offers a new technology with the use of secondary polymer-polyethylenterephtalate (PET**)** for removing metallic lead from lead oxide residues instead of expensive traditional reducers (coke, natural gas, etc.). For this purpose, waste alcoholic and non-alcoholic beverage package bottles are used, their main component is PET. Polymer waste does not degrade for many years and, if exposed to nature, creates major environmental problems. Because of this, their disposal is of great importance for improving the ecological condition of the environment. That's why their utilization is of great importance for improving the ecological condition of the environment.

One of the aspects of our innovative technology is the use of potassium and sodium carbonate melt as a reaction medium in the lead oxidation recovery process instead of the traditional chloride system, after its melting harmful products are released. Based on our research, it has been established that carbonate alloys, which perform the function of flux, at the same time shield lead ions from oxygen and promote the adsorption of lead vapor droplets, thereby reducing the evaporation of lead and its compounds into the environment.

Based on our research, it has been established that carbonate alloys, which perform the function of flux, at the same time, it shields lead ions from oxygen and promotes the adsorption of lead vapor into droplets, thereby reducing the evaporation of lead and its compounds and scattering in the environment, which is important for ecological system. In lead oxide recovery processes using PET as the reducing agent, the recovery reactions take place at relatively lower temperatures (750 - 800^{0}C), than in traditional technologies, resulting in increased metal lead yield. The quality of lead recovered during the experiments was checked by spectral analysis - Atomic Absorption Spectroscopy Method, according to which it can be said that high quality (98%) metal bullets are obtained.

Thus, with the new technological method proposed by us, by joint processing of polymer tare and lead rust industrial and household waste it is possible to obtain low cost and high quality metal lead. It is much safer in terms of environmental pollution and is more economical compared to traditional technologies.

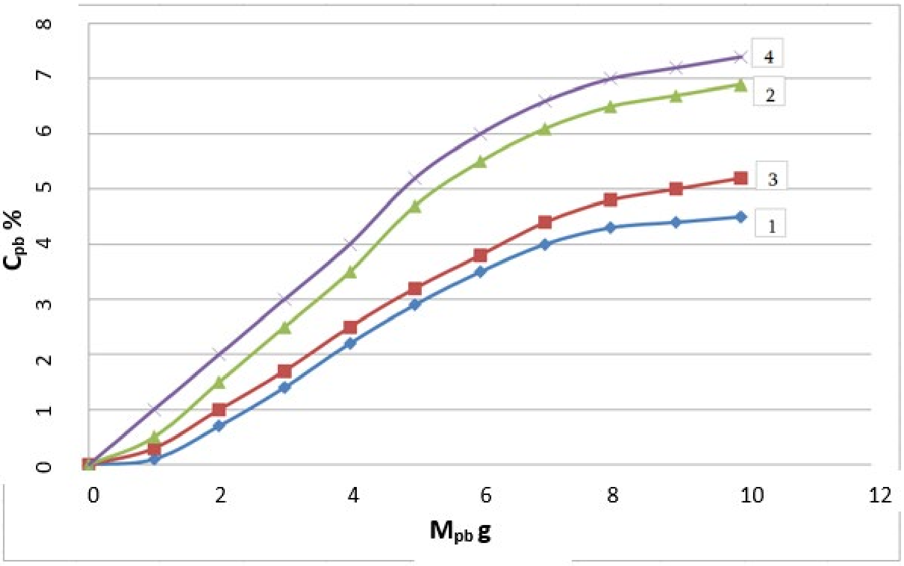

Fig. 1. Dependence of lead oxide solubility on temperature and fracture composition (fracture weight MPbO = 100 g).

K_2CO_3-Na_2CO_3 -$CaCO_3$ (1- 750^{0}C 3-800^{0}C)
K_2CO_3-$NaCO_3$ (2-750^{0}C 4-800^{0}C)

Table 1
Recovering of the lead oxide by PET. The weight of briquette M=200 gr; T=750^0 C

Sample N	Contentof PETP. %	Content of Lead in the oxidebriquette. %	Contentof Lead in the briquette. %	Weightof metallic lead. gr.	Output of the lead. %
1	10	90	25,06	21,18	87,8
2	15	85	23,67	21,35	90,2
3	20	80	22,27	21,54	94,9
4	25	75	20,88	19,85	95,1
5	30	70	19,49	18,51	95,0
6	35	65	18,09	17,18	95,0
7	40	60	16,70	15,41	92,3
8	45	55	15,30	13,94	91,1
9	50	50	13,92	12,53	90,0

Table 2
Lead oxide content in lead slag after recovery of the oxide with polyethylene PET in the melt K_2CO_3 - Na_2CO_3, M = 200 g, T = 750^{0}C

Sample №	Content of Lead oxide in the briquette. %	Content of PETP. %	Content of Lead oxide in the briquette. %.	Weigh of slag. gr.
1	10	90	3,41	190
2	15	85	3,18	189
3	20	80	2,25	192
4	25	75	1,98	191
5	30	70	2,00	188
6	35	65	1,95	185
7	40	60	1,95	186
8	45	55	1,8	185
9	50	50	1,7	183

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STUDY OF THE STABILITY OF GEOPOLYMER MATERIALS IN AN AGGRESSIVE ENVIRONMENT

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In recent years, environmental problems have become more and more acute all over the world. This is especially true for reducing CO_2 emissions into the atmosphere. Since the cement industry is one of the strongest air pollutants with carbon dioxide, the worldwide efforts of scientists have led society to search for new substitutes for Ordinary Portland Cement (OPC). Replacing OPC with geopolymer material (GPM) is one of the most realistic strategies to reduce environmental impact [1].

For the development of the production of geopolymer materials, it is necessary, along with other properties, to study their durability, as well as their behavior in aggressive environments, i.e., corrosion resistance.

On the basis of our laboratory studies, technologies for obtaining geopolymer materials based on thermally modified clay rocks of Georgia were developed [2-4].

The GPM synthesized by us have high mechanical strength and are characterized by durability and higher stability in aggressive solutions compared to OPC [5].

It was found that the indicators of corrosion resistance of geopolymer materials (changes in mass and strength) correspond to changes in their phase compositions after immersion in various aggressive solutions (Table.1).

Table 1. Corrosion resistance of GPM and OPC

Name	Weight loss of samples (%) after 180 days immersion in solution					Strength before testing, MPa	Loss of strength of samples (%) after 180 days immersion in solution				
	H_2SO_4		HCl		Na_2SO_4		H_2SO_4		HCl		Na_2SO_4
	2%	5%	2%	5%	5%		2%	5%	2%	5%	5%
GPM	0.25	1.32	0.15	3.91	0.63	92.5	7	11	10	15	1.9
OPC	18.11	*	27.7	*	32.8	73.0	62	*	70	*	80

* Samples collapsed.

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REACTION CONDENSATION OF 4,4′-DIAMINODIPHENYL OXIDES WITH D-GLUCOSE AND D-GALACTOSE

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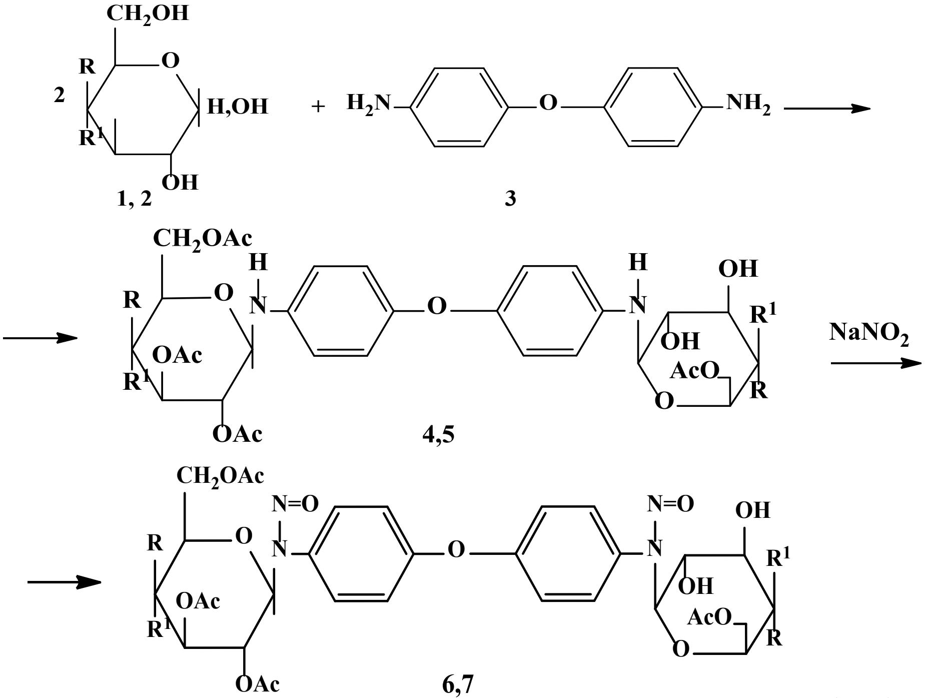
Synthesis of carbohydrate derivatives and the study of their biological activity is an important process for disease prevention.

Especially, carbohydrates containing nitroso group, because they have the effect of vasodilator; They play an important role in the process of apoptosis and cell proliferation. Also, carbohydrate derivatives containing nitroso group participate in the functioning of the immune system and nervous system.

The goal of the present investigation consists of the synthesis of N-glycosilamines contained in a molecule nitrosogroup (N=O). Asan initial substance in the given work has been used the products of condensation of D-glucose (1) and D-galactose (2) from 4,4-diaminodiphenyloxydes (3) - N-β-bis(2,3,4,6-tetra-O-acetyl-D-glycopyranosyl)-4,4′-diaminodiphenyloxydes (4) and N-β-bis(2,3,4,6-tetra-O-acetyl-D-galactopyranosyl)-4,4′- diaminodiphenyloxydes (5). By interaction of compounds (4,5) with sodium nitrite corresponding nitroso derivatives (6,7) has been received. Reaction proceeds according to the following scheme:



D-glucosa R = H; R^1 = OH (1,4,6); D-galactosa R = OH; R^1 = H (2 5,7)

The structures of obtained compounds were established by physical-chemical methods of analysis.

The IR spectra were obtained on a UR-20 spectrometer in KBr disks. The ^{1}H NMR spectrum was recorded in $CDCl_3$ on a Bruker WM-250 spectrometer (250 MHz) with TMS internal standard; the ^{13}C NMR spectrum was taken on Bruker AM-300 spectrometer (75 MHz) in $CDCl_3$. The purity of the compounds obtained and the R_f values were determined on Silufol UV-254 using solvent systems C_6H_6: C_2H_5OH (9:1 system a); C_2H_5OH: H_2O (3:2 system b); 1,4-dioxan: C_6H_6 (3:1 system c). The optical rotation was measured on a SU-3 general-purpose saccharimeter at 20 ± 2^0C.

DERIVATIVES OF (TRIFLUOROMETHYL)QUINOXALINE WITH DIFFERENT DONOR MOIETIES EXHIBITING THERMALLY ACTIVATED DELAYED FLUORESCENCE

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The molecular design strategy is crucial to develop high-efficiency and long-wavelength thermally-activated-delayed-fluorescent (TADF) emitters. The inherent limitations of energy gap laws degrade the efficiency of red or orange TADF emitters. To solve the low-efficiency problem, we designed and synthesized several TADF emitters. TADF materials have attracted much attention as they can achieve 100% theoretical internal quantum efficiency (IQE) in organic light emitting diodes (OLEDs) by harvesting all singlet and triplet excitons to emit prompt and delayed fluorescence by thermal activation of the triplet excitons. The key factor for TADF molecules is an extremely small singlet–triplet energy splitting (DEST), which is in favor of electron-generated non-radiative triplet excitons up-converting to radiative singlet ones via an effective reverse intersystem crossing (RISC) process[1].

Compounds containing CF_3 groups are particularly interested in TADF research because of the unique electronic and thermal properties which can be induced by this functional group. The CF_3 group is electron withdrawal moiety, which reduces the energy of the lowest unoccupied molecular orbital (LUMO) and reduces the energy gap between single and triplet excited states. Furthermore, CF_3 groups are relatively bulky, affecting molecular packing and leading to enhanced intersystem crossing and emission efficiency [2].

Two derivatives of quinoxaline substituted by 9,9-dimethyl-9,10-dihydroacridine and 5H-dibenzo[b,f]azepine donor moieties are characterized by small singlet-triplet energy gap, which is necessary for the TADF effect. Thermogravimetric analysis and differential scanning calorimetry were used to investigate the thermal stability and transitions of the synthesized compounds. The compounds demonstrated 5% weight loss temperatures higher than 360 °C.

Acknowledgement: This research was funded by the European Union's Horizon 2020 Research and Innovation Programme under the Marie Skłodowska-Curie grant agreement No. 823720.

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Abstract

SYNTHESIS AND INVESTIGATION OF ORGANOSILICON POLYMERS WITH PHOTOSWITCHABLE FRAGMENTS IN THE SIDE CHAIN

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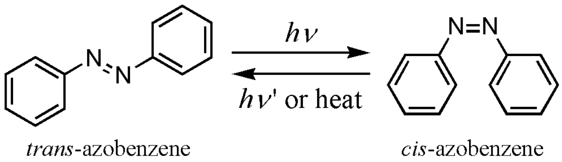
Azobenzene, with two phenyl rings separated by an azo (–N=N–) bond, serves as the parent molecule for a broad class of aromatic azo compounds. Azobenzenes' photochromic trans-cis isomerization has been used extensively in molecular switches, often taking advantage of its shape change upon isomerization to produce a supramolecular result. In particular, azobenzenes incorporated into polymer backbone give switchable receptors, and azobenzenes in monolayers can provide light-controlled changes in surface properties.



These chromophores are versatile molecules and have received much attention in fundamental and applied research areas. The strong electronic absorption band can be tailored by ring substitution to fall anywhere from the ultraviolet to red visible regions, allowing chemical fine-tuning of color.

This, combined with the fact that the azo groups are relatively robust and chemically stable, has prompted an extensive study of azobenzene-based structures as dyes and colorants.

One of the most interesting properties of these chromophores, however, is the readily induced and reversible trans–cis photoisomerization of the azo bond and the geometric changes that result when azo chromophores are incorporated into polymers and other materials.[1,2]

Examples of azobenzene-based photo-control have been demonstrated in photoswitchable phase changes[3], phase separation (or reversal of phase separation), [4,5] solubility changes [6,7], and crystallization [8, 9].

This work aims to synthesize new comb-type organosilicon polymers with azobenzene side groups in the chain. By inserting azobenzene chromophore groups in the siloxane matrix, the flexibility, hydrophobicity, and thermal stability of obtained polymers and films will increase compared to organic analogues.

The obtained monomers, polymers, and polymer films were carefully characterized at all stages of preparation using various experimental techniques.

We used FTIR and NMR spectroscopy to study the synthesized materials at different stages of the synthesis and confirm their chemical structures and compositions.

Gel permeation chromatography (GPC) was used to estimate the molecular weight of the prepared polymers. Also, differential scanning calorimetry (DSC) studies of the temperature characteristics of the polymers were provided. In particular, we investigated the correlation between the polymer structure and the glass transition, crystallization, and melting temperatures.

We also studied the viscoelastic properties of the prepared polymer films. Temperature and frequency dependencies of the real (G') and imaginary (G'') parts of the complex shear modulus were measured. Such studies provide important information not only about the mechanical properties of these systems but also about the glass transition temperature and eventual melting and crystallization processes. These results are compared to the DSC studies to obtain a more comprehensive picture.

These studies revealed important information about the static elastic properties of the films. Stress vs. draw ratio dependencies were recorded and used to evaluate the elastic modulus, elongation at break, and stress at break of the samples. Furthermore, the performance of the materials was examined at large deformations by performing quasi-static stress-strain cycles with successively increasing maximum strain.

These types of studies may reveal important information for plastic deformation resulting from changes in the internal structure of the materials.

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THE THEORETICAL DESCRIPTION FOR MANGANATE AND HYPOMANGANATE PYRROLIC MONOMER ASSISTED CATHODIC ELECTROPOLYMERIZATION

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Under the term “indirect electropolymerization” we understand the process of electricity-driven conducting polymer deposition, in which the monomer molecule does not interact directly with the electrode. In other words, the monomer doesn’t participate in the electrochemical reaction. In this case, the electrochemical reaction produces the chain initiator.

$$I^0 + ne^- \rightarrow I \qquad (1)$$
$$I + M \rightarrow I^* + P \qquad (2)$$

Herein I^0 stands for the initiator precursor, I, for initiator, M for the monomer, P for the polymer, n is the number of electrons transferred (which may be positive or negative) and P for the product.

Contrarily to the direct electropolymerization, the indirect electropolymerization yields somehow more tunable polymers with more developed and flexible properties. Moreover, it is very interesting from the mechanistic point of view, as it provides the alternative path to electrochemical conducting polymer deposition. For example, it provides the cathodic deposition of the polymer, based on a monomer uncapable to form anion-radicals on cathode, which becomes important for corrosion protection and energy storage.

The indirect electropolymerization may be realized for different monomers, and the redox pair used to initiate the polymerization is chosen according to the monomer properties. Also, the electrochemical instabilities, typical for the direct electropolymerization, may also occur in the indirect electropolymerization, depending on the monomer and initiator nature.

Abstract

In this work, we analyze the electropolymerization of a substituted pyrrolic derivative, assisted by manganate and hypomanganate-ions (1 – 3):

$$MnO_4^- + e^- \rightarrow MnO_4^{2-} \qquad (1)$$

$$MnO_4^{2-} + Py \rightarrow MnO_4^{3-} + Py^{*+} \qquad (2)$$

$$MnO_4^{3-} + Py + 4H_2O \rightarrow Py^{*+} + MnO_2 + 4OH^- \qquad (3)$$

The stages (2) and (3) generate cation-radical, providing, thereby, the chain growth. The electropolymerization yields a composite, capable to be used in energy storage.

The correspondent mathematical model has been developed and analyzed by means of linear stability theory and bifurcation analysis. The analysis of the model shows that the electrochemical oscillations frequency and amplitude will be highly dependent on the substituent in the pyrrole ring, as the ionic form transformation on the chemical stage depends on it. Either way, it will me far less probable than for the direct anodic electropolymerization of analogous system.

THE THEORETICAL DESCRIPTION FOR THE GALVANOSTATIC ELECTROPOLYMERIZATION OF A NATURAL DYE FROM AGARICUS XANTHODERMUS

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Agaricus is one of the most cultivated mushroom genus in Europe. Two of them (Agaricus bisporus and Agaricus campestris), correspondent to button and field mushroom, are edible and are known as the common name champignon. There are so popular that in some languages the name champignon corresponds to the meaning "edible mushroom".

Nevertheless, one of the Agaricus species is a toxic mushroom Agaricus xanthodermus, popularly known as yellow stainer. It is toxic, when consumed and it may be readily grown among the edible Agaricus mushrooms, sharing the same mycelium. Its toxicity and color are caused by the presence of the phenolic compounds (Fig. 1), including 4-4'-dihydroxyazobenzene, a unique endogenous natural azo-dye. In the mushroom pulp, the phenols act as antioxidants.

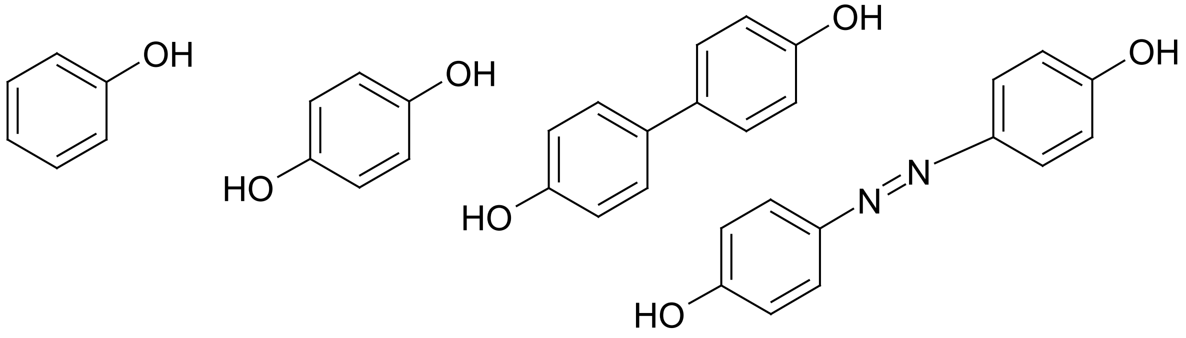

Fig. 1. *Agaricus xanthodermus* phenols

Taking into account the toxicity of the mushroom and its component, it cannot be eaten cooked. Nevertheless, the phenolic compounds from *Agaricus xanthodermus* may be interesting as monomers for conducting polymers, and the proper mushroom – as economic and green renewable natural source for the conducting materials, which needs a theoretical *a priori* investigation. Therefore, the goal of this work is the theoretical description for 4-4'-dihydroxyazobenzene electrochemical polymerization over cobalt (III)-oxyhydroxide modified electrode. This leads to the economic and environmentally friendly composite, capable to be used in sensors, energy storage and material science. Also, this synthesis is compared with the similar systems.

Both direct and indirect electropolymerization may be used to polymerize 4-4'-dihydroxyazobenzene. Indirect electropolymerization, in the case, is initiated by *in situ* formed cobalt dioxide, a product of cobalt (III) oxyhydroxide electrooxidation (1 - 2):

$$\mathbf{CoO(OH) + OH^- - e^- \rightarrow CoO_2 + H_2O} \qquad (1)$$

or

$$\mathbf{CoO(OH) - e^- \rightarrow CoO_2 + H^+} \qquad (2)$$

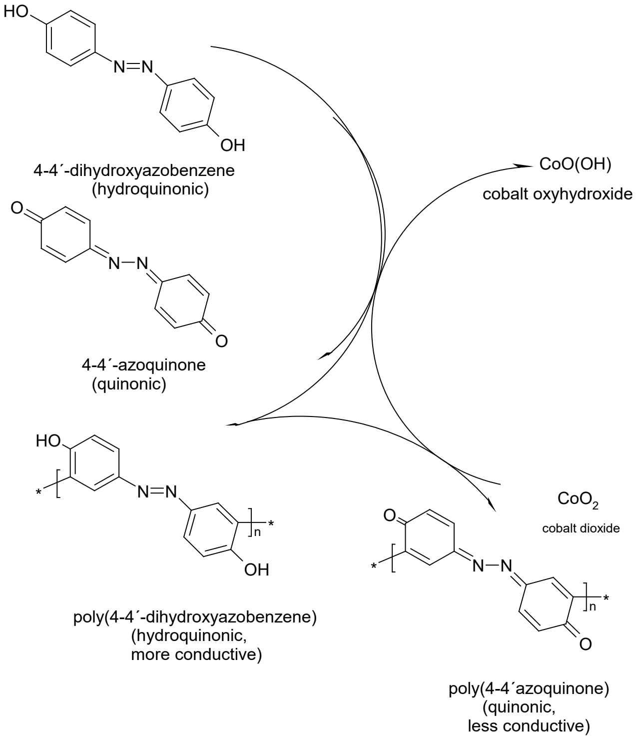

Fig. 2 Schematical description for $CoO(OH)/CoO_2$ – assisted 4-4'-dihydroxyazobenzene and its polymer electrooxidation.

The behavior of the system in galvanostatic mode will be described by a trivariant equation-set:

$$\begin{cases} \frac{dp}{dt} = \frac{2}{\delta}\left(\frac{P}{\delta}(p_0 - p) - r_1 - r_p\right) \\ \frac{dc}{dt} = \frac{1}{C}\left(r_p - r_{O1} - r_{O2}\right) \\ \frac{dq}{dt} = i - i_F \end{cases} \qquad (3)$$

The behavior of the system will be more dynamic than in the potentiostatic mode. Nonetheless, the galvanostatic mode may be efficient for the dye electrochemical determination and polymer composite synthesis.

Abstract

THE THEORETICAL DESCRIPTION FOR THE ELECTROCHEMICAL DETERMINATION OF SESAMOL OVER EXCITING CONDUCTING POLYMER

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Sesamol (Fig. 1) is a hydroxyquinol ether, responsible for the taste of Turkish delights including lokum, tahini halva and baklava. It also may be found in ayran, tan and doug milk drinks and traditional Inebolu simit from the region of Kastamonu. For this and other reasons, the development of a rapid and efficient method for both hydroxyquinol and pyrogallol determination is really actual.

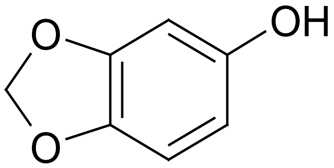

Fig. 1. Sesamol

Sesamol is biosynthetized from hydroxyquinol, which is a fructose fermentation product. Like all the phenolic compounds, it is electroactive, reason why the electroanalytical methods may be applied to it. Moreover, sesamol may be seen as a monomer for conducting polymer, reason why its determination may be valuable.

In this work, we analyze the case of sesamol determination and assisted electropolymerization over an exciting conducting polymer. On the first stage, the polymer is oxidized to the excited state:

$$CP - ne^- \rightarrow CP^* \qquad (1)$$

The excited polymer will thereby attack sesamol molecule, transferring the chain to sesamol, provoking the electropolymerization. Other oxidation mechanism includes the phenolization of *ortho-*

positions of sesamol with the appearance of a new hydroxyquinole fragment and subsequent oxidation to α- or γ-quinone (Fig. 2):

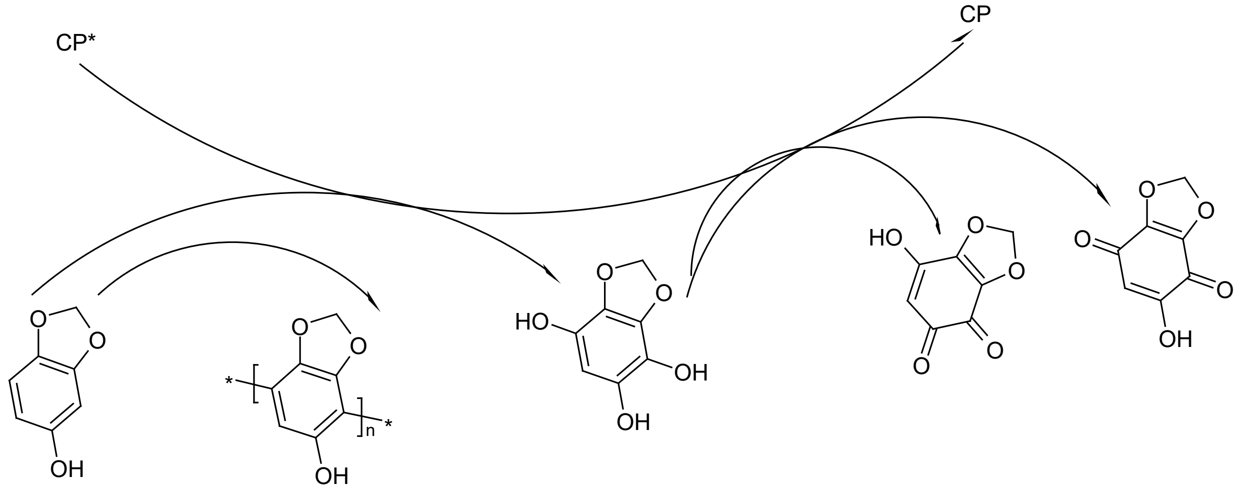

Fig. 2. The scheme of electroanalytical system

By this, the system's behavior will be described by a trivariant equation-set (2):

$$\begin{cases} \dfrac{ds}{dt} = \dfrac{2}{\delta}\left(\dfrac{\Sigma}{\delta}(s_0 - s) - r_p - r_h\right) \\ \dfrac{dh}{dt} = \dfrac{2}{\delta}\left(r_h - r_{q1} - r_{q2}\right) \\ \dfrac{dp*}{dt} = \dfrac{1}{P*}\left(r_1 - r_p - r_h - r_{q1} - r_{q2}\right) \end{cases} \qquad (2)$$

And analysis of the model confirms the efficiency of the model from both electroanalytical and electrosynthetical point of view.

THE THEORETICAL DESCRIPTION FOR NICOTIN AND NORNICOTIN CoO(OH)-ASSISTED ELECTROCHEMICAL DETERMINATION

Volodymyr V. Tkach* [*a,b], ***Marta V. Kushnir*** [a], ***Galyna M. Pochenchuk*** [a], ***Sílvio C. De Oliveira*** [b], ***Vitalii V. Lystvan*** [c], ***Adriano O. Da Silva*** [d], ***Yüksel Akınay*** [e], ***Necdet Karakoyun*** [e], ***Olga V. Luganska*** [f], ***Petro I. Yagodynets*** [a], ***Zholt O. Kormosh*** [g], ***Yana G. Ivanushko*** [h], ***José Inácio Ferrão da Paiva Martins*** [i], ***Jarem R. Garcia*** [j], ***Karina V. Palamarek*** [k], ***Valentyna A. Chychun*** [k], ***Olga G. Vdovichena*** [k], ***Anatolii A. Vdovichen*** [k]

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Nicotin and Nornicotin are the main alkaloids of *Nicotiana tabaccum*. Both of them are responsible for smoking dependence and tobacco toxicity. As for nornicotin, it slowers the nicotin metabolism due to its more expressed aromatic properties (Fig. 1). For this and other reason, the nicotin and nornicotin determination is actual task.

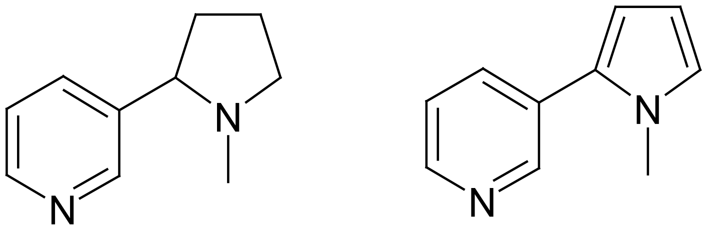

Fig. 1. Nicotin and Nornicotin

In this work, the possibility for nicotin and nornicotin electrochemical determination is theoretically analyzed. The same process may also lead to the efficient tobacco waste and cigarette-end utilization by economic and green conducting (co)polymer synthesis (Fig. 2):

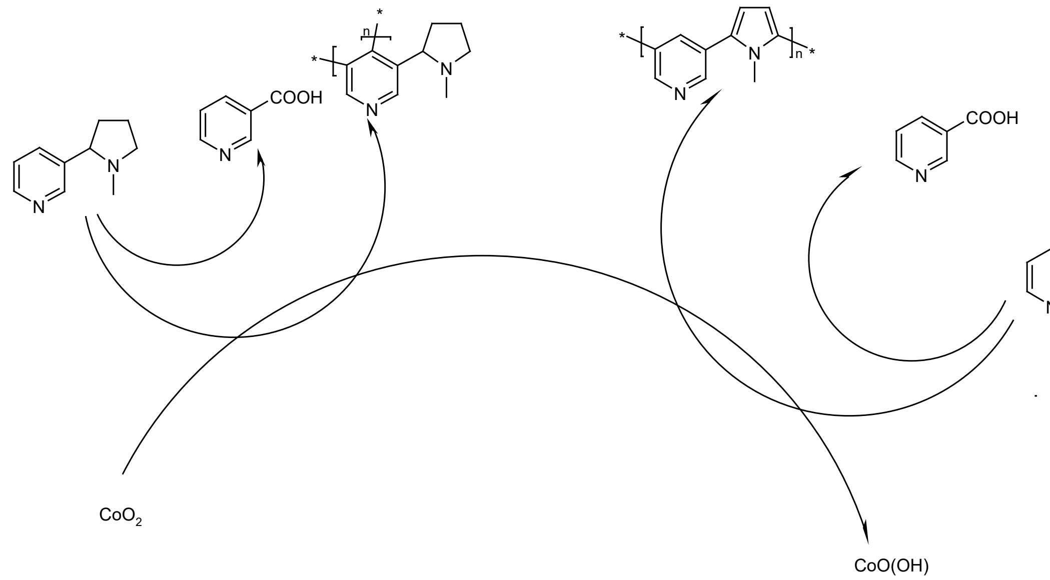

Fig. 2. The scheme of electroanalytical process

The behavior of the system is foreseen to be relatively dynamic. Nonetheless it is efficient from both electroanalytical and electrosynthetical point of view.

ADSORPTION PROPERTIES OF NATURAL AND MODIFIED HEULANDITE-CLINOPTILOLITES

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Adsorption and other properties of natural zeolites widely used in various industries can be improved by acid and heat treatment. The aim of our study was to identify the effect of acid and heattreatment on the adsorption properties of heulandite-containing tuff from the Rkoni plot of theTedzami deposit (Eastern Georgia), zeolitic rock from the Chankanay deposit (Kazakhstan) containing mixture of heulandite and chabazite, and clinoptilolite-containing tuff from the NorKokhb deposit (Armenia), selected for the creation of new zeolite filter materials for purification and desinfection of water[1].

Acid-induced dealumination [2] and the processes of amorphizationand structural changes under the influence of heat [3] have been previously studied. In the presentstudy, it was found that the micropores of heulandite and clinoptilolite are accessible to watermolecules; in Kazakh zeolite, they become available only after acid treatment, which for all samplesalso leads to a slight increase in surface hydrophobicity and, accordingly, to the ability to adsorbnonpolar benzene molecules.

Nitrogen adsorption-desorption isotherms show an acid-mediatedsharp increase in micropore adsorption and BET surface area, as well as changes in mesoporoussystems leading to the predominance of small pores up to 4 nm in diameter in Georgian and Kazakhsamples; in the Armenian clinoptilolite, the action of acid also leads to the “opening” of microporesand an increase in the surface area, but not to the same extent, and the distribution curve ofmesopores with a maximum of about 10 nm broadens, indicating the formation of larger pores.Thermal treatment of Georgian heulandite leads to a decrease in the micropore adsorption capacityand in the surface area due to amorphization, while average size of mesopores slightly increases withan increase in the calcination temperature; in Armenian clinoptilolite, this process does not causeany particular changes in either microporous or mesoporous systems. Samples of Kazakh zeolite,calcined at 400 and 800 °C, have a high adsorption capacity for water and benzene, with regard tonitrogen adsorption, the surface area increases, the mesopore diameter reaches a maximum afterannealing at 700 °C, but sharply decreases with an increase in the calcination temperature.

Acknowledgement: This work was supported by the International Science and Technology Center (ISTC) under the project GE-2506 “Scientific substantiation of the possibility of creating new bactericidal zeolite filtermaterials for purification-decontamination of water from various sources”

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Abstract

NEW COMPOSITES ON THE BASIS OF ECOLOGICALLY PURE BINDERS

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Wood is one of the natural products that human has consumed throughout history without changing its properties. In order to save wood, composite materials were prepared on the basis of renewable plant raw materials [1,2]. Wood sawdust boards are a composite material obtained by hot pressing (120-140^{0}C) from sawdust and glue. Carbamide, melamine, or phenol-formaldehyde resins are used as a binder for the composite.

Such a composition is characteristic of high-grade fiberboard of low, and medium density, which includes phenol-formaldehyde resin, which should be noted in the class of carcinogens due to the release of formaldehyde[3].

Nowadays, this material has a number of disadvantages, among which it is very important that formaldehyde released from resins containing this material is harmful to the human body. Headaches, shortness of breath, depression, adverse effects on the central nervous system, and others. Prolonged exposure to formaldehyde negatively affects human genetic activity, reproduction, eyes, and skin.

One of the technical disadvantages of wood veneer tiles is their instability to moisture (moisture absorption of 16-20%), and poor adhesion to the nail, nail, especially during the second cut. Many countries have adopted appropriate standards for the removal of formaldehyde when using these composite materials.

Interesting works have been proposed in the direction of obtaining environmentally friendly composites, based on renewable plant raw materials, from which phenol-formaldehyde resins are completely removed and replaced with new binders with alkoxysilanes.

The work effort was to obtain new formaldehyde-free environmentally safe compositions on the basis of the renewable plant raw materials[4], more precisely fallen Plane tree leaves, where for the first time as a binder and reinforcing agent styrene and vinyltriethoxysilane will be used.

Also, the aim is to obtain composites with increased physical and mechanical properties, environmental friendliness, easy-making technology, and resistance to microorganisms to meet all the modern requirements[5].

The use of wood composite materials will be safe for the human body.

The work will implement the copolymerization reaction of styrene and Vinyltriethoxysilane 1:1 ratio, with dicumyl peroxide and their applicability for in-situ copolymerization of leaf-based composite materials. The work has been carried out in the field of polymer chemistry, as well as in the field of obtaining new composite materials.

Physical research methods such as Fourier transform infrared spectroscopy, ^{1}H, ^{13}C, Cozy nuclear magnetic resonance spectroscopy, differential scanning calorimetry, thermogravimetric analysis, and optical microscopy were used[6].

Investigations were an interdisciplinary study, the solution of which requires knowledge of several disciplines: organic chemistry, macromolecule chemistry, physical and analytical chemistry, and fundamental and specialized knowledge of polymeric materials.

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LIBRARY OF CATIONIC POLYMERS FOR VERSATILE BIOMEDICAL APPLICATION

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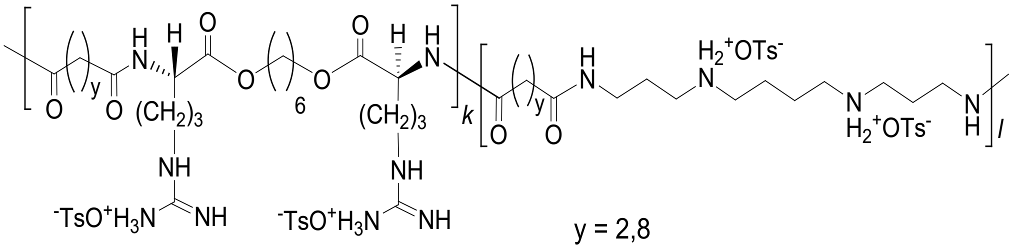
Combinatorially synthesized materials, especially cationic polymers (CPs), with gene transfection function hold great promise in nanotechnology. In adittion, inherent bioactive properties such as antimicrobial, antioxidant, antitumor and anti-inflammatory stimuli response make CPs more promising for enhanced therapeutic potential [1].

CPs that can be cleared from the body following executing their function, i.e. biodegradable ones, look especially valuable. A library of new biodegradable CPs were designed, synthesized and studied on the basis of naturally occurring building blocks such as amino acid arginine (R) [2,3] and endogeneous tetraamine – spermine (Spm) [4].

Highly water-soluble CPs formed nano-sized polyplexes with pDNA, showed less cytotoxicity and higher transfection ability compared to widely-used PEI as well as commercially available transfection agents. Furthermore, new CPs showed selective transfection activity towards certain cell lines, which is important for their potential applications in gene therapy [4].

Recently, hybrid-CPs (containing both R and Spm building blocks) with general formula depicted below in Scheme 1 were synthesized as *p*-toluenesulfonic acid salts by solution active polycondensation (SAP) [5] and their physicochemical properties were studied.



Scheme 1. R and/or Spm based CPs synthesized by SAP

According to the study performed hybrid-CPs appeared as a new class of chiral polymer which consists of cationic units separated by flexible, neutral linkers. They may be applicable to a wider variety of polymer structures and will widen the scope of optically active polymers with helical conformation [5].

Acknowledgement: This work was supported in part by SRNSF (#04/41) and GRDF/CRDF Global (#A6069) joint grant and in part by Hokkaido University (postdoctoral fellowship)

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Abstract

MODIFICATION OF CEMENT COMPOSITES WITH CARBON NANOTUBES

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Cement is the main structural material in concrete construction. Reducing the commissioning time for the construction of residential buildings, as well as industrial facilities, is of great importance, as it directly affects the level of cost and profitability. One of its few drawbacks is slow curing, which can be accelerated by adding chemical modifiers to the concrete mix or by heating it.

After the discovery of carbon nanotubes and the development of nanotechnology, the accelerating effect of small additives of carbon nanotubes on the rate of hardening of cement concrete structures was found in almost all areas of science and technology. In the scientific literature, a concept is expressed that explains this effect by the formation of a large number of new crystallization centers in the sample under study. However, there are practically no systematic studies on the study of this effect when using Azerbaijani-made cements.

For this purpose, research and applied work was carried out in the direction of obtaining composite materials based on cement, reinforced with additives of multilayer carbon nanotubes (MWNTs).

Work was carried out in the direction of using MWCNTs synthesized by Chemical Vapor Deposition (CVD) method from propane as a concrete hardening accelerator. On the basis of MWCNTs and superplasticizers, a number of mixtures were prepared, which were used as hardening accelerators for cement composites.

It is known that the use of MWCNTs in this process is associated with their uniform distribution in the volume of concrete, the tendency of nanomaterials to agglomerate, the formation of flakes and clots, which is considered as a defect in the cement matrix, thereby deteriorating the mechanical properties of cement composites. There is an optimal dosage of 0.05 wt.% for the introduction of MWCNTs into the cement matrix, above which undesirable processes can occur, leading to a weakening of the mechanical properties of the cement stone. Methods for introducing multiwalled carbon nanotubes into the composition of cement mixtures, ways of studying and eliminating problems arising in these processes have also been studied.

Appropriate combinations and concentrations of mixtures of MWCNTs in solvents used in the industry and offered for this purpose were prepared, processed by special methods, and then presented for addition to cement-based materials.

When the prepared additives are treated with ultrasound for a certain time, a uniform distribution of MWCNTs in the prepared additive is ensured.

Study of the effect of MWCNTs on the properties of the cement paste showed that the addition of the latter in an amount of 0.0002-0.0004% by weight of cement prolongs the setting time of the cement paste by about 2 times compared to the content without additives.

Studies of the effect of MWCNTs on the properties of the cement paste showed that the addition of the latter in an amount of 0.0002-0.0004% by weight of cement prolongs the setting time of the cement paste by about 2 times compared to the content without additives.

Experimental studies have shown that carbon nanotubes reduce the size of pores and associated channels (densely packed micropores) in cement stone to form a stronger concrete matrix, which prevents he movement of water through micropores due to clogging of channels and, accordingly, improves the strength of the cement stone framework.

PETROLEUM POLYMER RESINS WITH EPOXY GROUPS OBTAINED IN THE PRESENCE OF A PEROXIDE INITIATOR

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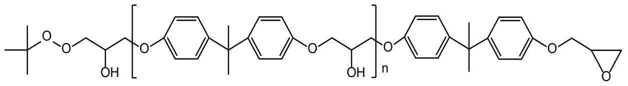
To expand the assortment of petroleum polymer resins (PPR), improve their operational characteristics and expand the field of practical application, a method of obtaining PPR with functional groups, particularly with epoxy ones, has been developed.

Petroleum polymer resins with epoxy groups (PPRE) were obtained by the initiated oligomerization of unsaturated hydrocarbons contained in the C9 fraction of the pyrolysis pyrocondensate of diesel fuel, using as an initiator the peroxide derivative of the epoxy resin Epidian 5 (Ep5P resin) (Table 1).

Table 1

Characteristics of reaction mixture components

Properties	Value
Raw material	
Density (d_4^{20})	0.920
Molecular weight (M_n), g/mol	126
Bromine number, g Br_2/100 g	120
Toluene content, wt %	11.419
p+m-Xylene content, wt %	10.841
Styrene content, wt%.	21.698
Vinyltoluenes content, wt%	12.700
Indene content, wt%	10.206
Initiator	
Formula	
Molecular weight (M_n), g/mol	700
Epoxy number (e.n.), %	5.2
Active oxygen (O)act., %	2.3

The research results showed that increasing the initiator content in the reaction mixture increases the PPRE yield, and the maximum resin yield (28.1 wt% on raw material) is observed at 403 K. A further increase in the oligomerization temperature causes a decrease in the yield due to an increase in the rate of side reactions, particularly the recombination of the initial functional radicals.

When the initiator content increases, the molecular weight of PPRE also increases, which is explained by the high molecular weight of functional radicals that initiate the oligomerization process. A characteristic feature of PPRE is its high molecular weight - up to 6000 and even higher.

It was established that an increase in the initiator content in the reaction mixture increases the PPRE epoxy number (from 0.2 to 1.35%). This is a consequence of an increase in the concentration of functional radicals in the reaction mixture and an increase in the number of epoxy groups in the PPRE structure.

The initiator content (Ep5P resin) of 5.0 wt% per raw material in the reaction mixture is optimal for yield, quality, and economic considerations. Other established optimal conditions for PPRE synthesis are as follows: temperature - 403 K; oligomerization - 40 hours.

ANTIMICROBIAL ACTIVITY OF NATURAL BIOPOLYETHERS FROM DIFFERENT SPECIES OF BORAGINACEAE FAMILY

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Antimicrobial activity of biopolymers poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDHPGA) (**1**) and poly[2-methoxycarbonyl-3-(3,4-dihydroxyphenyl)oxirane] (PMDHPO) (**2**) (Fig.1), extracted from the six plants of Boraginaceae family: *Symphytum asperum* (***SA***), *S.caucasicum* (***SC***), *S.grandiflorum* (***SG***), *Anchusa italica* (***AI***), *Cynoglosum officinale* (***CO***) and *Borago officinalis* (***BO***) collected in the various parts of Georgia was examined.

The study revealed that the antibacterial activity was moderate and only biopolymers from three plants showed activity against all tested bacteria. Biopolymers from ***CO*** stems as well as ***SC*** and ***AI*** did not show any activity except low activity against a resistant *P.aeruginosa* strain, which was the most resistant among all three resistant strains. On the other hand, the antifungal activity was better compared to antibacterial.

Biopolymers from ***BO*** stems exhibited the best activity with MIC/MFC at 0.37-1.00 mg/mL and 0.75-1.5 mg/L respectively, followed by those from ***SG*** stems. Biopolymers from ***SC*** and ***AI*** roots showed antifungal activity against all six fungi in contrast to antibacterial activity, while biopolymers from ***CO*** stems and ***SA*** roots had activities against four fungi and one fungus, respectively.

The sugar-based catechol-containing biopolymer from ***BO*** stems demonstrated the best activity among all tested biopolymers against *T.viride, P.funiculosum, P.cyclpoium var verucosum* and *C.albicans* (MIC 0.37 mg/mL). In addition, biopolymer from ***SG*** stems was twice less active against *A.fumigatus* and *T.viride* than ketoconazole.

Biopolymers from all plant materials except for ***CO*** stems showed higher potency than ketoconazole against *T.viride.* For the first time it was shown that all plant materials exhibit better activity against *C.albicans,* one of the most dreadful fungal compared to other fungal species.

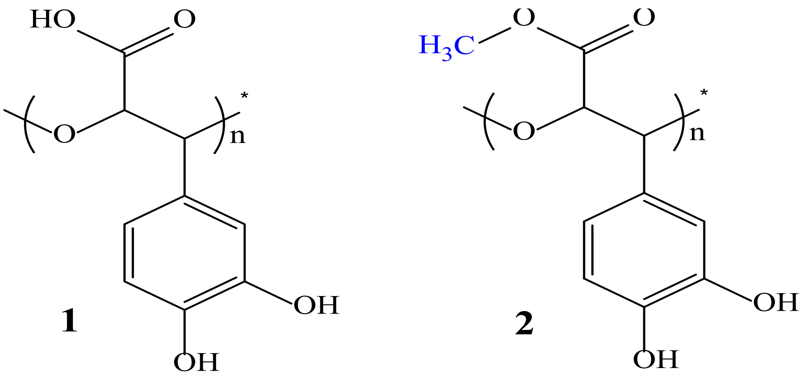

Figure.1. Poly[3-(3,4-dihydroxyphenyl)glyceric acid] (PDHPGA) (**1**) and poly[2-methoxycarbonyl-3-(3,4-dihydroxyphenyl)oxirane] (PMDHPO) (**2**).

DESIGN, SYNTHESIS, AND BIOLOGICAL EVALUATION OF AMANTADINE CONTAINING NEW DERIVATIVES

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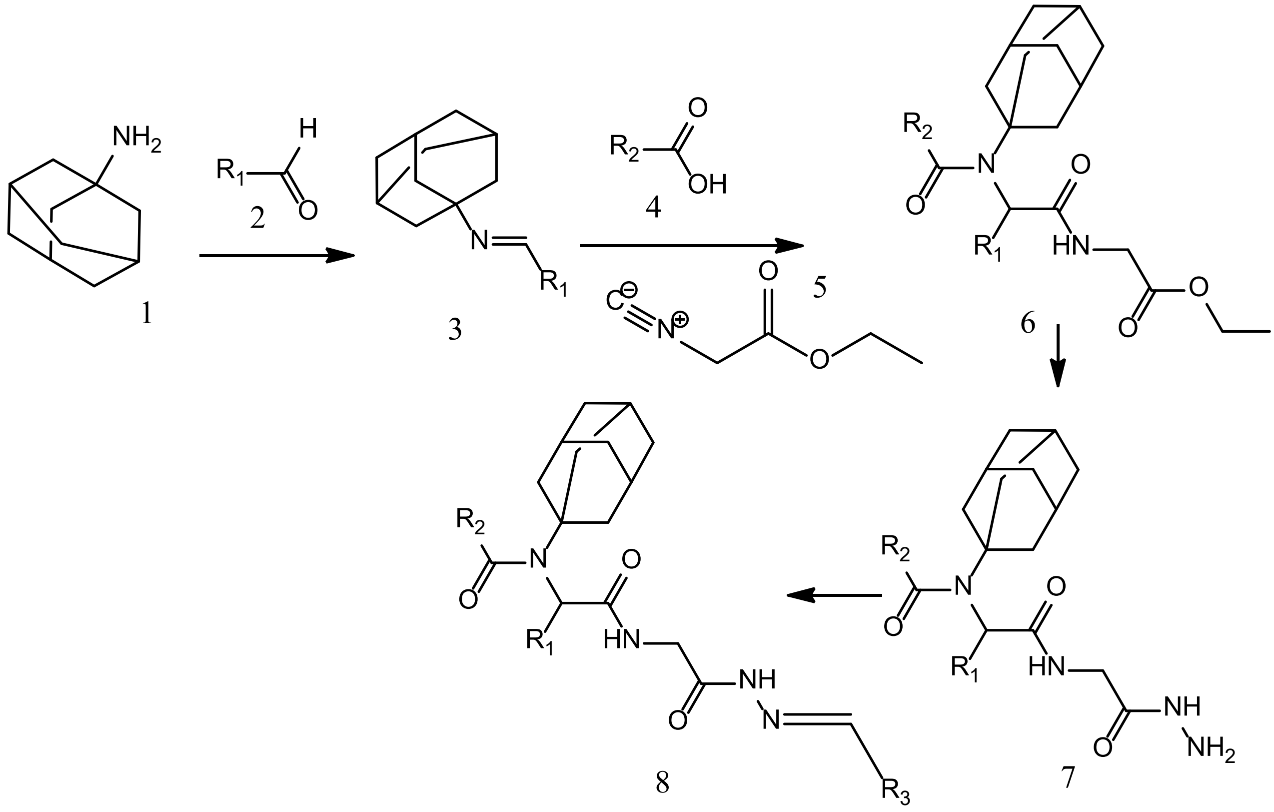
Multicomponent Ugi reactions are an effective method of synthesis to produce a huge variety of products by the interaction of four starting compounds. This work focuses on the synthesis of adamantane containing pseudopeptides via Ugi reaction. In this research 1-amino-adamantane, ethyl isocyanoacetate, some aldehydes, and carboxylic acids were used to synthesize some pseudopeptides.

The Ugi reaction was carried out in alcohol area with constant stirring (72 hours) and heating at 40˚C. The obtained product was worked up with saturated $NaHCO_3$, then with 1M $KHSO_3$, and washed with brine. The organic phase was concentrated and chromatically purified on the column chromatography by the standard method (SiO_2, petroleum/ethyl acetate), accordingly, the corresponding dipeptide (6) was isolated.

The reaction of some dipeptides with hydrazine hydrate gives the hydrazides (7). By reacting them with some aldehydes the corresponding imines **8** were obtained. The structure of synthesized compounds 7,8 were established by IR, NMR, and LC-MS analysis.



R_1 = $CH(CH_3)_2$, C_3H_5; **R_2** = CF_3-CH_2, 4-CH_3O-C_6H_4, **R_3** =C_6H_4OH, 4-NO_2-C_6H_4,

The synthesized dipeptides were studied on Gram-positive and Gram-negative bacteria. The implemented antimicrobial research showed interesting results.

Acknowledgment: This project was funded by Shota Rustaveli National Science Foundation (Grant N YS-21-1340)

DESIGN AND SYNTHESIS OF NEW α-ACYLOXYCARBOXAMIDES VIA PASSERINI REACTION

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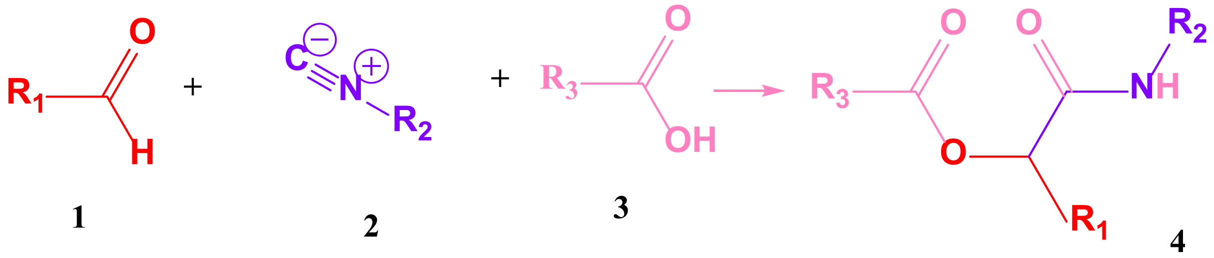
In modern synthetic chemistry, multicomponent reactions (MCR) are considered diversity-oriented syntheses that provide the opportunity to create structurally diverse molecules. Among these multicomponent reactions, the Passerini three-component reaction is worth mentioning, where aldehydes, isonitriles, and carboxylic acids are used as reactive components, which ensure the synthesis of polyfunctionalized α-acyloxyamides (depsipeptides). In this study, we used 1-adamantanecarboxylic acid as one of the reactants along with aldehydes and ethyl isocyanoacetate.

The passerine reaction was performed in an aprotic solvent at room temperature. The obtained product was purified using column chromatography (ethyl acetate/hexane 1/9 reaction mixture) and the structure of the synthesized compounds was proved by IR and NMR spectroscopy.



The synthesized azo compound was studied on Gram-positive and Gram-negative bacteria. The implemented antimicrobial research showed interesting results

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SUSTAINABLE FILLERS BASED ON AGRO WASTE FOR ECO-FRIENDLY COMPOSITE MATERIALS BASED ON POLYOLEFINS

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Agro waste produced in large amounts is a common problem encountered in different agricultural processes, including harvesting [1]. The advantages of using agro waste materials in polymer composites include low cost and reduction the amount of burned materials, resulting in lower CO_2 emissions [2]. For example, a large amount of various nut shells that are generated as waste are usually used as burning feedstock.

Consequently, the use of nut shells for polymer composites manufacturing is highly regarded as an environmentally friendly approach. Therefore, the utilization of nut shells should be encouraged, and their role in various applications, including as a filler in polymer composites, should be studied in detail.

Nut shells are one of the major components of various lignocellulosic wastes [3]. Nut shells are widely investigated agro wastes because of their low cost and abundant nature. Among the nuts should be noted hazelnuts, walnuts, almonds, peanuts and etc., which produce a huge amount of waste in the form of shells (Figure 1).

Figure 1. Various nuts and nut shell powders as filler for eco-friendly composite materials: a – hazelnut; b - walnut; c – almond; d – peanut

The main purpose of this study was to investigate the feasibility of using various nut shells (hazelnut, peanut and almond shell) for producing eco-friendly composite materials based on polyolefin matrix.

The nut shells used as sustainable fillers were purchased from a local market. Nut shells were milled and sieved for obtaining shell powder. The polymer matrix used in this study was a thermoplastic polypropylene random copolymer. The nut shells powder was used in different weight fractions: 5, 10, 15, 20 and 30 wt.%.

The physical and mechanical properties of the composite samples were investigated. The results of physical and mechanical studies showed that with an increase in the filler content, the tensile strength of the samples slightly decreased compared to the values of these indicators of the original polymer, but at 15 wt% filling, this indicator increased by 6%.

The decrease in the tensile strength of the samples in other contents of filler is insignificant and can be eliminated by surface treatment of the nut shells by various methods. Based on this, it can be assumed that the shells of various nuts can be used as a filler to obtain eco-friendly composites.

Acknowledgement: The authors would like to thank the staff of the Department of Investigation of Physical and Mechanical Properties of Polymer Materials, Institute of Polymer Materials of Ministry of Science and Education Republic of Azerbaijan, for their contribution to the preparation of test specimens.

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BIOLOGICALLY ACTIVE POLY[3-(3,4-DIHYDROXYPHENYL) GLYCERIC ACID] FROM THE ROOTS OF *PARACYNOGLOSSUM IMERETINUM* (KUSN.) M.POP. (BORAGENACEAE)

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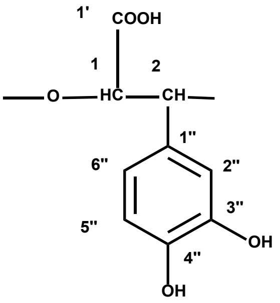
The main chemical constituent of high-molecular water-soluble mucilage preparations from *Symphytum asperum, S.caucasicum, S.officinale, S.grandiflorum, Anchusa italica, Cynoglossum officinale* and *Borago officinalis* (Boraginaceae) was found to be a biologically active caffeic acid-derived polymer poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] or poly[3-(3,4-dihydroxyphenyl)glyceric acid] **(PDPGA)** [1-3].

Within our ongoing search for biologically active caffeic acid-derived polymers in plant species belonging to different genera of the Boraginaceae family, the isolation and structure elucidation of a main chemical constituent of water-soluble high-molecular mucilage fraction (Mr>500 kDa) from *Paracynoglossum imeretinum* roots (**HMP-PR)** was carried out.

According to data of UV, IR, liquid-state ^{1}H, ^{13}C NMR, gCOSY and 2D heteronuclear ^{1}H/^{13}C gHSQCED experiments, the main structural element of HMP-PR by analogy of HMFs from *S.asperum, S.caucasicum, S.officinale, S.grandiflorum*, *A.italica, B.officinallis and C.officinale* was found to be a regularly substituted polyoxyethylene, poly[3-(3,4-dihydroxyphenyl)glyceric acid] or poly[oxy-1-carboxy-2-(3,4-dihydroxyphenyl)ethylene] **(PDPGA)** (TABLE 1, Fig. 1).

TABLE 1. The signal assignment in the ^{13}C and ^{1}H NMR spectra of **PDPGA** from the roots of *P.imeretinum*

	C atom no.	^{13}C chemical shift, δ_C, ppm	^{1}H chemical shift, δ_H, ppm
 **Fig. 1. The repeating unit of PDPGA**	1'	175.0	
	1	77.5	5.7
	2	79.6	5.1
	1"	130.7	
	2"	116.6	7.6
	3"	143.9	
	4"	143.0	
	5"	117.8	7.5
	6"	121.5	7.4

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Abstract

MANGANESE-CONTAINING BIONANOCOMPOSITE BASED ON κ-CARRAGEENAN AS MULTIFUNCTIONAL AGENT FOR BIOMEDICINE APPLICATIONS

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Within the framework of the project, a series of manganese-containing nanocomposites based on the natural polysaccharide κ-carrageenan with different manganese content was obtained. κ-carrageenan itself is a biopolymer with a number of attractive properties such as biocompatibility, non-toxicity, hydrogelation and hydrotropism, and others [1]. At the same time, manganese oxides have a number of properties – high oxidizing ability, magnetism and electrical conductivity, antibacterial and even antioxidant activity [2]. Manganese-containing nanoparticles in the matrix, most likely formed in the form of $Mn(OH)_2 \times nH_2O$, occupy spatially vacant regions during the formation of the composite due to various interactions of the polysaccharide with the surface of the nanoparticles. Due to the numerous hydroxyl and other oxygen-containing groups of κ-carrageenan, a stable nanosystem is created with the synergy of the properties of biomacromolecules and manganese-containing nanocrystals.

During the synthesis κ-carrageenan was kept under stirring in water while was heating at 50 °C until a homogeneous medium, then $MnSO_4 \times nH_2O$ and NH_4OH were added. After 24 h, the reaction product was precipitated into ethanol. The product was thoroughly washed with ethanol to obtain a nanocomposite with a mass content (wt%) of manganese of 4-20%, depending on the amount of manganese sulfate salt used. According to the data of transmission electron microscopy, the spread in the size of nanoparticles in the composite is 2–11 nm with a predominant size of 5–6 nm.

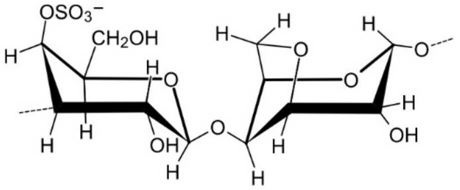

Figure 1. Molecular structure of κ-carrageenan

Natural sulfated polysaccharide κ-carrageenan is a system of intricately twisted interwoven fibers in the form of double helixes, in which the chains are intertwined coaxially, the structure of which is well described in reviews [3]. The additional presence in the structure of the polysaccharide of a highly ionizable sulfo group in the natural sulfated polysaccharide κ-carrageenan imparts increased water solubility, additional polyprotonic and polyanionic properties, potential antiviral activity, immunomodulatory and heparin-like anticoagulant, antiatherogenic, as well as stimulating beneficial microbiota properties [4]. The presence of highly acidic sulfo $-OSO_3H$ groups opens up the possibility of hydrophilic immobilization by polyprotonic groups of various hydrophobic basic pharmacons, for example, piroxicam [5]. Including manganese-containing bionanocomposites are also widely used in agriculture as non-toxic universal trophic low-dose fertilizers [1].

Acknowledgement: The reported study has been funded by Shota Rustaveli National Science Foundation of Georgia (SRNSFG), project number STEM-22-1751. The authors are grateful to the Center of Instrumental Analysis (R. Agladze Institute of Inorganic Chemistry and Electrochemistry, Georgia) for spectral and analytical measurements.

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POLYMER ELECTROLYTE MEMBRANES ON THE BASIS OF COMB-TYPE FLUORORGANOSILOXANES

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Polymer electrolytes (PE) play an important role in electrochemical devices such as batteries and fuel cells. To achieve optimal performance, the PE must maintain a high ionic conductivity and mechanical stability at both high and low relative humidity. The polymer electrolyte also needs to have excellent chemical stability for long product life and robustness [1-3].

According to the prevailing theory, ionic conduction in polymer electrolytes is facilitated by the large-scale segmental motion of the polymer backbone and primarily occurs in the amorphous regions of the polymer electrolyte. Crystallinity restricts polymer backbone segmental motion and significantly reduces conductivity. Consequently, polymer electrolytes with high conductivity at room temperature have been sought through polymers which have highly flexible backbones and have largely amorphous morphology.

The interest to polymer electrolyte was increased also by potential applications of solid polymer electrolytes in high energy density solid-state batteries, gas sensors and electrochromic windows [4].

The hydrosilylation reaction of 2.4.6.8-tetrahydro-2.4.6.8-tetramethylcyclotetrasiloxane (D_4^H) with allyl trifluoroacetate in the presence of platinum catalysts (platinum hydrochloric acid, Karstedt's catalysts and Pt/C (10%) at 50^0C have been carried and corresponding addition adduct ($D_4^{R`}$) have been obtained.

The synthesized product D_4^R was analyzed by FTIR, ^{1}H, ^{13}C, and ^{29}Si NMR spectroscopy. Polymerization reaction of D_4^Rtype fluororganocyclotetrasiloxane in the presence of catalyst tetramethylammonium fluoride have been carried and comb-type fluororganosiloxanes have been obtained.

Sol-gel reactions of this comb-type fluororganosiloxanes doped with Lithium trifluoromethylsulfonate (triflate) or Lithium bis (trifluormethanesulfonyl) imide and tetraethoxysilane have been studied and solid polymer electrolyte membranes have been obtained. Via electrical impedance spectroscopy ion-conductivity of solid polymer electrolyte membranes have been determined.

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Abstract

PREPARATION OF REDUCED GRAPHENE OXIDE-METAL OXIDE (TiO_2, Fe_2O_3) COMPOSITES BY VACUUM EXFOLIATION

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Graphene oxides and materials obtained from them have a number of unique properties. Currently, much attention is paid to the creation of new types of biologically active composites and their use both for solving environmental problems. The purpose of our work is to obtain preparation of reduced graphene oxide (rGO)-metal oxide (TiO_2, Fe_2O_3) composites by vacuum exfoliation technique. The method is based on the property of graphene oxide (GO) to undergo vacuum exfoliation at 200-250ºC, resulting in the formation of large volumes of reduced graphene oxide, the thickness of each layer is several nanometers.

We obtained complexes GO-$Fe(NO_3)_3$ and GO-Ti(OH)x. Their vacuum exfoliation takes place at a relatively low temperature of 120-140°C, as a result fluffy powders are formed with a bulk density of 20-27 mg/ml. The non-magnetic rGO-Fe_2O_3 composite was obtained in a vacuum at 120-135°C. According the EDX analysis, the rGO-Fe_2O_3 composite contained 9.7zavradadhvili% Fe(mas).

Thermal exfoliation of GO-Ti(OH)x produces rGO-TiO_2 (anatase) composite. Expanded peaks of rGO-TiO_2 (anatase) composite prove that the particle size of nano titanium oxide is small and is in the range of 5-20 nanometers. At the same time the diffraction maximum GO ($2\theta = 10.62°$) disappears and a new peak $2\theta = 25.1°$ is formed, which corresponds to rGO. Peak $2\theta = 25.3°$ corresponds to titanium oxide (crystalline modification - anatase). The distance between the two layers of rGO-TiO_2 composite is 171 nm, although it consists of several layers.

Thus the thickness of each layer is clearly less than 171 nm, so we can conclude that the rGO-TiO_2 composite consists of nano-sized components, while wide diffraction peaks of TiO_2 indicate the small size of its particles. The structural-morphological structure of the rGO-Fe_2O_3 composites is clearly different from that of the rGO-TiO_2 composite (Fig.1. a, b). During the decomposition of GO-$Fe(NO_3)_3$ complex nitrogen oxides, oxygen and water are released. As a result of the thermal exfoliation of GO-Ti (OH)x, only water is released. In the case of nitrate complexes, the pressure between the layers of graphene oxide is higher and their decomposition proceeds more qualitatively than in the case of GO-Ti(OH)x.

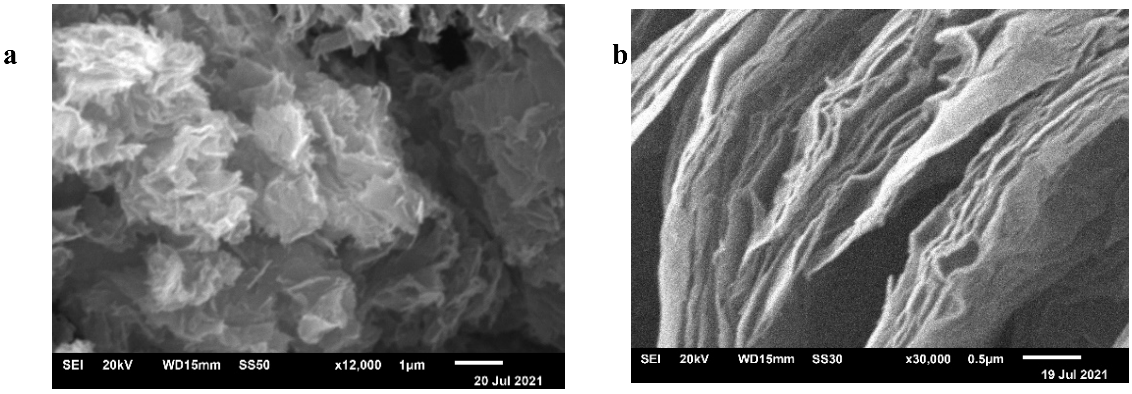

Figure 1. (a) SEM images of rGO-Fe_2O_3 and (b) rGO-TiO_2 composites

SHOCK ASSISTED HIGH TEMPERATURE CONSOLIDATION & SYNTHESIS OF DIAMOND CONTAINING POWDERS

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The WC-Co -Diamond and Cu-Diamond powder mixtures were formed into cylindrical rods or tubes using a hot shock-wave consolidation process. The aims of investigation were to fabricate composites and to obtain rigid coating onto the cylindrical surface of steel tubes as well as to investigate morphology of reminder diamond particles behind of shock wave front.

The cylindrical geometry of shock wave loading to consolidate and to synthesize composites in hot condition. The processing temperature were changed up to 1000^0C. The intensity of loading was under the 10GPa.

The investigation showed that the combination of high temperature and shock wave loading was beneficial to the consolidation of the WC-Co-Diamond composites, resulting in near theoretical densities, high hardness values, and the formation of transient layer between the coating and the steel tube's wall. The structure and property of the samples obtained, and the formation of the transient layer depended on the shock loading conditions and the phase content of precursor powders.

As for Cu-Diamond precursors there was observed depending on value of temperature there takes place perfection of diamond crystals and under 1000^0C practically its have ideal morphology.

The above mentioned as well as other features of the structure/property relationship of the consolidated and synthesized The WC-Co -Diamond and Cu-Diamond powder as a function of the loading conditions (experimental set-up, intensity of loading, or preloading temperature) are discussed too.

Abstract

HIGH TEMPERATURE PROCESSING AND RECOVERING OF NANOSCALE CARBON FROM PLASTIC WASTE AND ITS ACTIVATION IN OVERHEATED VAPOR ENVIRONMENT

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The ecologically safe and economically profitable method of obtaining recovered activated carbon from plastic (PET) waste, that includes low-temperature pyrolysis of waste at the initial stage, and then high-temperature thermo-chemical treatment in overheated water vapor environment will be presented.

The vapor treatment at low temperatures (up to 700^0C) activates the pyrolysis process and increases the primary reactions of hydrocarbon decomposition. Accordingly, the release of gases increases and the main part of which during the pyrolysis process is extracted as a liquid fraction - pyrolytic oil and reminder amorphous coal containing different organic/inorganic impurities.

After increasing of the temperature (above 700^0C) and simultaneously feeding of vapor, the overheated water vapor increases the rates of side reactions and full decomposition pyrolytic reminders takes place. As a result, the loosening of the formed carbon aggregates occurs and formation of the highly dispersed, nanoscale carbons take place.

As investigation showed the characteristics of obtained nanoscale activated carbon structure and physical characteristics depends from treatment conditions (vapor temperature, feeding rate, treatment period etc.), changes wide range and can be reach to 920 m2/g (BET surface area) and 98.7% (purity) respectively.

The mentioned, as well as other features of the structure/characteristics of recovered nanoscale carbon as a function of the processing conditions (temperature, vapor amount, time) will be presented and discussed too.

Acknowledgements: This work was supported by Shota Rustaveli National Science Foundation of Georgia –SRNSFG (Grant number STEM 1113).

CONSOLIDATION AND SYNTHESIS OF TA-AL-B(B4C) REACTIVE BLENDS BY HOT ELECTRO ROLLING METHOD

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The Ta-Al-B(B4C) blend of powder were formed into plates using combined self- propagating high temperature synthesis and hot electrical rolling processes. The aims of investigation were to synthesized and to fabricate near to theoretical density different Ta_xAl_y-TaB_x(B4C) composites in the forms of sheets having perfect structure and high value of strength properties.

The preliminary investigation showed that the combination of high temperature electrical rolling method with combination of SHS processes between the Ta-Al-B reactive blends of powders just at the beginning of rolling was beneficial to the consolidation/syntheses of the Ta_xAl_y-TaB_x composites, resulting in near theoretical densities, high hardness values, and the formation of different intermetallic compounds of Ta_xAl_y The structure and property of the samples obtained depended on the loading conditions and the phase content of precursor powders.

The processing temperature at the beginning of rolling were changed up to 1000^0C. The intensity of loading was under the 60MPa.

The mentioned as well as other features of the structure/property relationship of the consolidated and Synthesized plates of Ta_xAl_y- TaB_x(B4C) composites as a function of the loading conditions (experimental set-up, intensity of loading, preheating temperature, pre-density) will be presented and discussed too.

Acknowledgements: This work was supported by Shota Rustaveli National Science Foundation of Georgia –SRNSFG (Grant number STEM 1113).

EXTERNAL STIMULI ACTIVATED SINGLE AND MULTI-DRUG DELIVERY SYSTEMS BASED ON LIQUID CRYSTAL MICRO CONTAINERS

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We demonstrate novel, light, pH, and temperature-controlled drug delivery systems based on photochromic, pH-sensitive dye-doped liquid crystal (LC) microspheres and temperature-dependent phase transition in liquid crystals.

Experimental results have shown that upon exposure to UV light, pH, and temperature, the photo and thermo-chromic and pH-responsive molecules located inside the LC microspheres experience an interconversion from the hydrophobic, oil-soluble, non-polar state to the hydrophilic, water-soluble, highly polar condition. Light, pH, and temperature-induced isomerization destabilizes the LC water interface, stimulates its translocation across the LC-water barrier, and result in their homogeneous distribution throughout an aqueous environment. The proposed strategy can consider as a new platform for the photo-stimulated, pH, and temperature-sensitive drug delivery systems that offer the possibilities of the controlled delivery and release of a wide variety of drugs into the body at a suitable time and desired sites, fight different kinds of diseases including cancer diseases.

Despite the clinical breakthroughs emerging in cancer therapy, drug resistance inevitably appears in cancer treatments. The concept of multi-drug therapy by mixing individual drugs based on conventional drug delivery administration has proven to be a simple and efficient approach to providing systematic therapy to treat complex health conditions [1]. We propose a new concept of a multi-drug delivery system with sequential release based on nanoparticle-doped liquid crystal microspheres as drug carriers, figure 1.

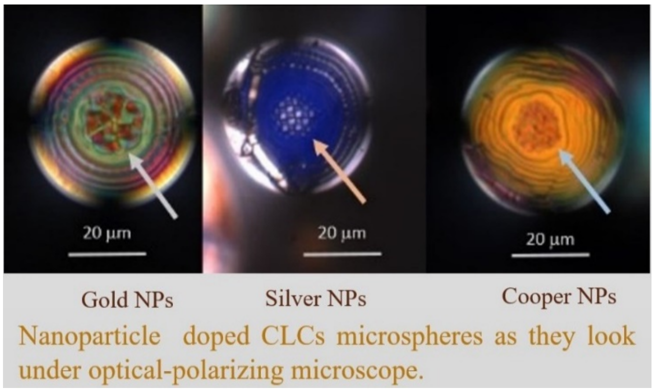

Figure 1. LC microspheres are loaded with Gold, Silver, and copper nanoparticles

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Abstract

CHALLENGES AT THERMOMECHANICAL RECYCLING OF CAR TIRES

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Low-temperature devulcanization is a promising technique for the recycling and reprocessing waste tyres. Here is a characterization of this process:

Environmentally Friendly: The low-temperature devulcanization process is an environmentally friendly solution for waste tyre management. It reduces the need for the incineration or landfilling of used tyres, both of which have significant environmental impacts.

Energy Efficient: As the name suggests, low-temperature devulcanization operates at lower temperatures than traditional devulcanization processes, thereby saving energy.

Preservation of Material Properties: One significant advantage of low-temperature devulcanization is that it retains more of the original material properties of the rubber. This is because the lower temperatures reduce the degradation of the rubber's structure, leading to a higher-quality recycled material.

Application of Devulcanized Rubber: The resulting devulcanized rubber can be reused in various applications, including producing new tyres, rubber mats, asphalt additives, and other rubber products.

Process Overview: The process involves breaking the sulfur bonds in the vulcanized rubber. This is usually achieved through certain chemicals, ultrasonic waves, or microwaves. In low-temperature devulcanization, this process is done at temperatures significantly lower than in traditional methods, typically below 200°C.

Limitations: Despite its benefits, low-temperature devulcanization does face challenges. It often requires specialized equipment and can be slower than traditional methods. Furthermore, it may not be as effective in breaking down all types of vulcanized rubber.

In conclusion, low-temperature devulcanization is a vital technique that could help improve the recycling of waste tyres, ultimately contributing to a more sustainable economy.

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ANTIBACTERIAL PAA-OLYHEXAMETHYLENEGUANIDINE IPN HYDROGELS AS WOUND DRESSING

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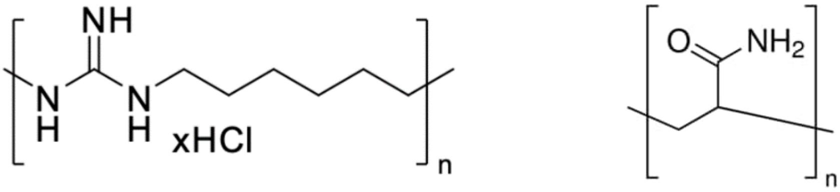
Hydrogels are 3D hydrophilic polymer networks that can absorb and conserve significant amounts of aqueous fluids. Hydrogel wound dressings play an important role in wound healing promoting hemostasis, tissue regeneration, re-epithelialization, and forming physical barriers to keep the wound away from microbial invasion, and sustaining an ideal moisture environment at the wound site.

For over half a century, cationic biocides have been prominent among other agents used to combat of infection in veterinary, dental, domestic and hospitalsettings. Polyhexamethylene guanidine hydrochloride (PHMG) is a cationic colourless, odourless, non-corrosive and non-irritating antimicrobial biocide of the guanidine family (Fig.1.). PHMG has broad-spectrum activity against Gram-positive and Gram-negative bacteria, fungi, yeasts and viruses, including human immunodeficiency virus [1]. It has been widely used for many years as an antiseptic in medicine and the food industry, as a disinfectant for a variety of solid surfaces and also in water treatment.



PHMG PAA

Figure 1. Chemical structure of polymers

A combination of polymers in a hybrid architecture is expected to induce a synergy in the gel properties and enhance the performances of hydrogels. Semi-interpenetrated polymer network (semi-IPNs) hydrogels are usually synthesized by polymerizing a monomer in the presence of preexisting polymer chains.

Composite semi-IPNs hydrogels were synthesized by free-radical polymerization using polyhexamethyleneguanidehydrochloride as an ionic physical entrapped polymer, acrylamide monomer and N,N′-methylene-bis(acrylamide) as cross-linking agent. Their swelling and absorption/desorbtion properties were evaluated as a function of gel composition.

The antibacterial properties of hydrogels *in vitro* against strains of *Staphylococcus aureus*, *Escherichia coli*, *Klebsiella quasipneumoniae*, and *Pseudomonas aeruginosa* were studied. It was found that the synthesized hydrogels inhibit the growth of bacteria *in vitro* and can potentially be used for the treatment of bacterial wound infections.

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ACTIVE FILLER OF POLYMERS FROM NATURAL ALUMINOSILICATE

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A highly dispersed and polymerophilic polymer filler was obtained from natural aluminosilicate (zeolite-containing tuff - "clinoptilolite", Tedzami deposit, Georgia) by wet grinding. Since the efficiency of the resulting filler was tested for organosilicon varnishes, the dispersion of clinoptilolite was carried out in a toluene medium. To facilitate the process of dispersion of clinoptilolite in the treated medium, a surfactant, octadecylamine (ODA), was added. In the process of dispersion, in a toluene medium, on the active centers of freshly formed clinoptilolite particles (at the sites of rupture of Si-O-Si and Si-O-Me valence bonds), chemisorption fixation of octadecylamine occurs (organophilization surfaces of particles).

The sizes and nature of the distribution of the obtained organophilized particles of clinoptilolite were studied, with the content of octadecylamine in the dispersion medium, in the range of 0.025 - 1.5% (relative to the mass of air-dry clinoptilolite). It has been established that with an increase in the ODA content in the dispersible system, a decrease in the proportion of large particles (over 10 μm) is observed. With a content of 1.0% ODA in the dispersant, there are virtually no particles larger than 10 microns. A further increase in the content of octadecylamine in the system does not significantly change the nature of the distribution of particles by dispersion.

The degree of organophilization of the surface of clinoptilolite particles was determined by studying powders from suspensions (after removal of toluene) obtained in dispersant of clinoprilolite at various ODA contents. The IR spectra of powders from suspensions, which were obtained with a content of no more than 1.0% ODA in the dispersant, showed the practical invariance of the intensity of the bands at 2940 and 2865 cm^{-1} (corresponding to the vibrations of the hydrocarbon chains of octadecylamine) before and after extraction. Along with this, the presence of octadecylamine was found in the toluene extracts of organophilized powders, which were obtained from a suspension with a content of more than 1,0% ODA in the dispersant. On the basis of the data obtained, it can be assumed that at a degree of organophilization of no more than 1,0% ODA, chemisorption fixation of octadecylamine occurs on the surface of clinoptilolite particles. At a higher degree of organophilization, multilayer adsorption apparently occurs, since only physically adsorbed octadecylamine can be present in toluene extracts of powders.

The degree of organophilization of the surface area of particles of clinoptilolite powders can be judged by the effect of their wetting with water (according to the method of fixing the change in the amount and rate of capillary impregnation of liquid into powder during their direct contact). From the data on the rate of impregnation of organophilized powders with water, it follows that the more organophilic sites on the surface of powder particles, the lower the rate of their impregnation. Wetting of the powders stops when they are obtained from a suspension containing 1.0% ODA during dispersion, which ensures a hollow organophilization of the particle surface.

It has been established that the content of 1.0% ODA (from the mass of the air-dry mineral) during the dispersion of clinoptilolite in a toluene medium determines the production of a filler with the highest possible dispersion and optimal organophilicity of the particle surface.

The effectiveness of the developed filler was tested by studying the physical and mechanical properties of the coating (adhesion strength, internal stress, impact strength, hardness) of the KO-921 siliconorganic lacquer. Concentrated suspensions, obtained by dispersion cleroptilolite in a toluene medium, in an amount of 50% (by weight of the silicon-polymer) were added to the lacquer. Spersions were charged both with and without the addition of the optimal amount of octadecylamine (1.0% by weight of the air-dry mineral). The tests showed that the composite coating containing clinoptilolite with an optimally organophilized surface in all physical and mechanical parameters is superior to the coatings, both from pure varnish and containing clinoptilolite with a non-organophilized surface.

NUANCES OF THE SYNTHESIS OF POLYACRYLAMIDE HYDROGELS BY THE METHOD OF FRONTAL POLYMERIZATION IN THE CONTINUOUS MODE

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Frontal polymerization, proceeding in the mode of propagation of a thermal wave, began to be studied in the 70s of the last century. Based on the accumulated experience, scientific foundations have been developed and prerequisites have been created for the Practical implementation of the Synthesis of Polymethyl Methacrylate in Continuous Cylindrical Frontal Action Reactors with the regulation of both kinetic and macrokinetic parameters. It should be noted that at present Frontal Polymerization is being practiced in many large Research Institutes and Universities of the world.

Studies are carried out under periodic conditions and on different monomers; they are of scientific interest, but are insufficient for practical implementation. To implement the method of Frontal Polymerization in industry, proceeding in the mode of propagation of a thermal wave, it is necessary to carry out the process under continuous conditions, when the initial mixture is supplied from one side and the finished product is removed from the other end in continuous frontal conditions, taking into account the elementary reactions occurring in the synthesis process. and macrokinetic nuances affecting the stability of the process.

To this end, we studied both the influence of the flow rate, the kinetics and adiabaticity of the environment, and macrokinetic parameters that can disrupt the linearity and stationarity of the process both in the direction of the radius and along the reactor. To this end, it is necessary, in addition to the basic initial parameters for the kinetics and macrokinetics of the process, to take into account the nuances of the system exiting the stationary state as a result of a violation of the stability of the kinetics of elementary reactions. In this case, it turned out to be especially important to study the kinetic and macrokinetic parameters during the process in continuous reactors, when even a slight change in elementary reactions along the length or radius of the reactor during the continuous process of supplying the monomer and removing the resulting polymer, deviations from the front stability are possible, which can affect the properties the resulting gel with a violation of the reproducibility of the synthesis. Calculations in this direction were carried out in the 2D dimension (52-54), and after the installation of the reactor also in the 3D dimension in the process of a continuous front, where a clear visual opportunity is created to follow the nuances of the process, the data on these calculations will be presented in the article of the same name. Since in this case, for the process of Frontal Polymerization in a flat tubular geometry, the establishment of a stable (stable) stationary front is necessary not only in the direction of front propagation along the length of the reactor, but also along the radius of the reactor, when autowave propagation transitions from one state to another are possible depending on various kinetic parameters of the reaction and macrokinetic impact on the process of Frontal Polymerization as a result, such a change in the nature of the wave until the optimum propagation velocity is also reflected in the properties of the resulting product.

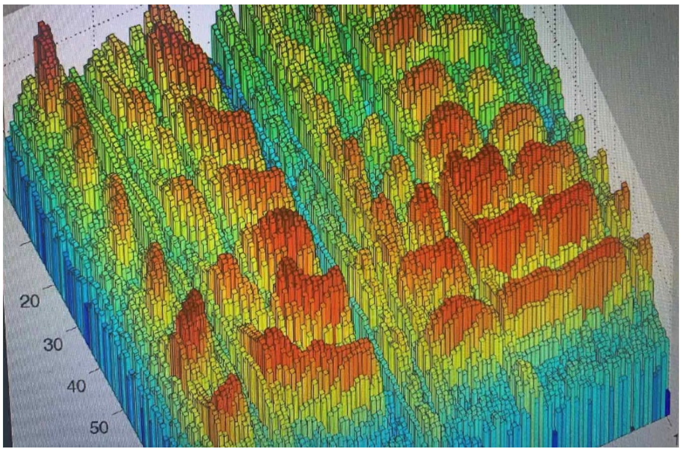

Figure 1. Distribution of the FP in continuous conditions due to the flow of the initial mixture and the output of the final product in a continuous mode.

As can be seen from Figure 1, in some places, both along the length of the tubular reactor and in the radial direction of the front, there are violations of the stationarity of the polymerization wave. Accordingly, the average value of the given parameters for the resulting hydrogel may fluctuate with some deviation from the given value.

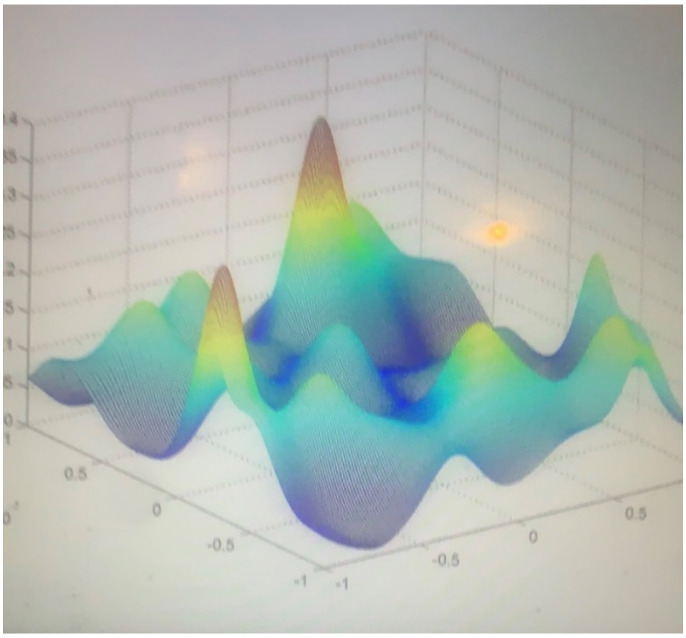

Figure 2. Loss of stability of the front as a result of a violation of the adiabaticity of the reactor walls with an increase in ambient temperature by 20 degrees

Figure 2 shows that during hydrogel synthesis, depending on the rate of propagation of the process in a continuous frontal mode, after a certain period of time, a jet of flow can form, which violates the uniformity of propagation of auto-waves in the radial direction.

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Abstract

MORPHOLOGICAL INVESTIGATION AND FRACTAL PROPERTIES OF NEW INORGANIC-BASED NANO MATERIALS AND NANOCARRIERS

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By combining nano and fractal, many of the surrounding events can be justified. Regarding nanotechnology, drugs can with improved physical and chemical properties, such as high reactivity and the ability to select a cell membrane from pathogenic bacteria, can be produced [1]. Many fields are exciting at the start of this journey to improve the basic quality of human life.

Nanoparticles have the potential to overcome many drugs design and delivery problems. Inorganic nanoparticles have different applications in drug delivery mechanisms and have drawn a lot of attention owing to their various features such as wide accessibility, proper biocompatibility, and excellent surface functionality.

Employing nanomaterials as carriers is a heated debate in drug molecule release and delivery. Moreover, the gradual release of drugs as nanoparticle carriers can correspond to the drug delivery systems, having advantages like extended release time and accurate drug delivery to locations. For a practical usage of LDH (layered double hydroxide) as a drug delivery carrier, it is very important to control the release rate of drug molecules, and thereby characterize the maintenance time of drug molecules in vivo [2-3].

In this research, some of the new nano compounds were synthesized. These new compounds were characterized by spectroscopic methods such as FT-IR and UV spectra, X-ray diffraction, SEM techniques and some physical properties.

The biological activities such as antitumor activities of these nano compounds against a different kinds of tumor cells such as panel of human tumor cell lines have been studied. Fractal Geometry has recently been recognized as an analytical tool suitable for describing nanostructures. Also, fractals are infinitely complex models that are self-similar across different scales.

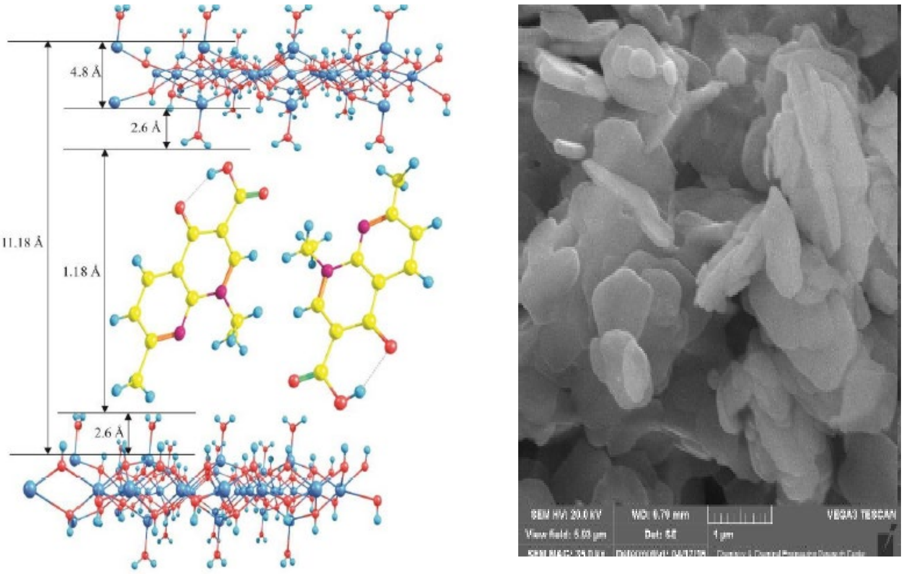

Figure 1. Schematic picture and SEM of nano carrier

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INFLUENCE OF CARBON AND METAL-CONTAINING NANOPARTICLES ON PROPERTIES OF COMPOSITIONS BASED ON POLYPROPYLENE

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In the modern world, various types of polymer composite materials based on nanofillers are actively replacing traditional materials. Modification of polyolefins in the presence of metal-containing and carbon nanoparticles is a promising approach to obtaining functionalized polymeric materials with high thermal and electrical resistance [1, 2].

The presented work is devoted to obtaining and studying the properties of composites based on isotactic polypropylene (PP): 1 - PP, fullerene soot (FS), maleized high-pressure polyethylene (MPE); 2 - PP, a mixture of C60/70 fullerenes and nickel oxide nanoparticles - (NPNiO); 3 - PP, multi-walled carbon nanotubes (MWCNTs) and nickel oxide nanoparticles - (NPNiO);

Compositions were prepared by mixing in a polymer melt at a temperature of 160-165 °C. To determine the physico-mechanical properties of the obtained compositions, the mixtures were pressed for 10 minutes at a temperature of 190 °C and a pressure of 10 MPa.

It has been shown that the introduction of FS together with MPE into the composition of the PP composition at a ratio of components (mass%): 100/0.2/1.0 leads to a significant increase in the tensile strength, relative elongation, and thermal-oxidative stability of the obtained nanocomposites. The activation energy (Ea) of the thermal-oxidative destruction of the obtained nanocomposite increases from 145.45 to 210.52 kJ/mol, which is associated with the synergistic effect of the interfacial interaction of fullerene-containing nanoparticles in the PP matrix with the components of the polymer composition - MPE maleic groups.

Compositions based on PP, mixtures of C60/70 fullerenes (MWCNT) together with NiO NPs at a ratio of components (mass%): 100/0.04/0.5; (100/0.05/0.5) leads to a significant increase in strength and thermal properties. The activation energy of thermal-oxidative degradation of the resulting nanocomposites: PP/ C60/70/NPNiO increases from 145.45 to 220.72 kJ/mol, and for PP/MWCNT/NPNiO from 145.45 to 260.62 kJ/mol.

The obtained results are confirmed by SEM analysis data, which indicate that small amounts of nanofillers introduced into the polymer play the role of structure formers - artificial crystallization nuclei that promote the formation of a fine spherulite structure in the polymer, which is characterized by improved physicomechanical and thermal properties of the resulting nanocomposites.

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PROPERTIES OF NANOCOMPOSITES BASED ON HIGH DENSITY POLYETHYLENE AND HOUSEHOLD WASTE THERMOASH

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In this work, the main attention is paid to the study of a complex of physical-mechanical and technological characteristics of nanocomposite materials based on high density polyethylene and household waste thermoash. When evaluating the physical-mechanical characteristics of polymer composites, it was important to identify which properties are most sensitive to changes depending on the concentration of thermoash. Considering that nanodispersed thermoash is used as a filler for the first time, it should be clear how important it is to clarify the role of the size factor in changing properties [1].

Table-1 shows the study results of the influence of thermoash concentration and the size of their particles on the nature of the change in properties. Comparing the data presented in this table, it can be established that the size of the filler particles has a significant effect on the physical-mechanical properties. From a comparative analysis of the presented data, it can be seen that samples obtained on the basis of thermoash nanoparticles with a size of 75–110 nm are characterized by relatively high values of strength and Vicat softening temperature. Characteristically, with an increase in the size of the filler particles, there is a general trend towards deterioration of the properties of the composites. At the same time, the most sensitive to changes in the concentration and particle size of thermoash are such indicators as elongation at break, ultimate tensile stress and Vicat softening temperature. As can be seen from Table 1, if the highest value of the ultimate tensile stress for nanocomposites is manifested at a concentration of 5.0 wt%, then for composites with relatively large particle sizes, the maximum strength is formed in samples with a thermoash content of up to 10 wt % inclusive. 1 g of nanoscale thermoash contains a significantly larger number of particles than 1 g of a conventional dispersed filler. That is why the loading of a minimum amount (5.0 wt %) of nanosized thermoash is sufficient for a significant increase in the strength of the nanocomposite. Thus, it can be stated that among composites filled with thermoash, nanocomposites have relatively better physical-mechanical and technological characteristics. Even at high filler concentrations, composites retain their ability to be processed on standard equipment

Table 1. Influence of the concentration and particle size of thermoash on the main physical-mechanical properties of composite materials based on HDPE.

№	Formulation of the composites based on HDPE + thermoash (ta), wt %.	Thermoashparticle size, nm	Ultimate tensile stress, MPa	Elongation at break, %	Melt Flow Rate, g/10min	Vicat softening temperature, C°
1	HDPE	-	31.4	475	1.25	124
2	95HDPE+5ta	75-110	36.7	125	1.54	125
3	90HDPE+10ta		33.2	85	1.46	128
4	80HDPE+20ta		26.3	45	1.33	130
5	70HDPE+30ta		23.5	35	1.01	130
6	60HDPE+40ta		21.7	30	0.82	135
7	95HDPE+5ta	300-500	31.3	95	1.42	125
8	90HDPE+10ta		32.7	65	1.05	126
9	80HDPE+20ta		25.1	30	0.93	128

10	70HDPE+30ta		22.0	25	0.97	129
11	60HDPE+40ta		19.1	20	0.68	131
12	95HDPE+5ta	1200-2000	28.8	55	1.45	125
13	90HDPE+10ta		28.4	35	0.94	126
14	80HDPE+20ta		23.3	20	0.88	126
15	70HDPE+30ta		19.6	20	0.87	127
16	60HDPE+40ta		17.2	15	0.55	128

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S-(ACYLOXY)BUTYL-N,N-DIETHYLDITHIOCARBAMATES – PLASTICIZERS-THERMOSTABILIZERS OF POLYVINYL CHLORIDE COMPOSITION

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It is known that the combination of derivatives of dialkyldithiocarbamic acids of heteroatoms of various nature (N, S, O) with ester group in the molecule essentially expands the area of their application as insectofungicides, potentially biologically active substances, protectors for radiation protection, accelerators of rubbers vulcanization in the rubber industry and it is no coincidence that they attract increasing attention of researchers of various scientific profile. However, the works devoted to the use of derivatives of dialkyldithiocarbamic acid and in particular diethyldithiocarbamic acid as plasticizing-modifying additives to the polymer compositions are extremely limited.

In this paper the information on the synthesis of s-(acyloxy)butyl-N,N-diethyldithiocarbamates (V-VII) by the interaction of the corresponding 4-chlorobutyl carboxylate (II-IV) with trihydrate of N,N- sodium diethyldithiocarbamate in an aqueous medium, proposed as new plasticizers-thermostabilizers of polyvinyl chloride plasticate are presented. The reaction has been carried out in an aqueous medium according to the scheme:

$$(C_2H_5)_2N - C(=S)SNa + RCOO(CH_2)_4Cl \xrightarrow[-NaCl]{H_2O} (C_2H_5)_2N - C(=S)S(CH_2)_4OC(=O)R$$

$$R=n.C_5H_{11}\ (V);\ n.C_6H_{13}\ (VI);\ n.C_7H_{15}\ (VII).$$

The composition of the compounds (V-VII) has been confirmed by elemental analysis, the structure – by data of IR and NMR ^1H spectra .

The synthesized s-(hexanoiloxy)- (V), s-(heptanoiloxy)- (VI) and s-(octanoiloxy)-butyl-N,N-diethyldithiocarbamate (VII) are the transparent liquids (weakly straw-color), almost odorless. They are insoluble in water, well soluble in organic compounds (ether, CCl_4, $CHCl_3$ etc.).

It has been shown that the unique solvating (hydrating) ability of the used solvent (H_2O) and the tendency of the sodium cation in a molecule (I) to solvation together provide the penetration of the anion into the organic phase of the reaction system $[\geq N\text{-}C(=S)S^-]$ and stipulate the substitution of the chlorine atom in a molecule of the corresponding alkylating agent (II-IV) under comparatively mild conditions and the selectivity of the process.

It has been established that dithiocarbamates (V-VII) are well combined with PVC resin and, as a result of the combination of an ester group in their molecule with dithiocarbamate fragment containing a tertiary nitrogen atom, they have both plasticizing and thermostabilizing properties of PVC plasticate and, moreover, the availability of dithiocarbamate group can play an important role in the protection of materials from bio-damage and action of mold fungi. Thus, the tensile strength and specific elongation of the plasticate obtained with the participation of the tested compound (VI), taken in the range of 30,40,50 mass p. to 100 mass p. of PVC, are at the level of indices of plasticate made using a standard plasticizer (DOPh) at the same ratios. However, *the thermal stability of the tested samples is almost 1.4-1.5 times higher than the corresponding standard index.

Thus, the reveal of plasticizing-thermostabilizing properties of dithiocarbamates (V-VII) allows to expand the assortment of the chemical compositions of effectively plasticizing-thermostabilizing PVC plasticate. The obtained results indicate that these materials can be recommended for practical use in various branches of industry.

*It has been determined on the derivatograph of "Paulik-Paulik-Erdei" system (Hungary).

Abstract

THE ROLE OF ANTIBACTERIAL MATERIALS IN HUMAN LIFE

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Using copolymers containing biologically active monomers (morpholine, salicyl, benzamide, etc.) as antibacterial additives, the composite materials based on olefins have been obtained, their physical-mechanical properties have been studied. The resistance of the obtained materials to the action of fungi has been studied. It has been established that the studied polymers have high bactericidal and fungicidal properties.

Besides, the physical-mechanical properties of polymer materials used in the household, it is also important that they have antibacterial properties[1], since the bacteria posing a threat to human life are accumulated on polymer materials widely used in everyday life. In this connection, there is a need for polymers with sterile, bactericidal and fungicidal properties, and this need is increasing every day.

For preparation of the antibacterial polymers, bactericidal additives must be introduced into their composition, or antibacterial compounds and monomers must be included in polymer materials at the processing stage. Such monomers include morpholine, salicylic acid, styrene, benzamide, etc.

Also, one of the problems is the rapid washing of additives from the surface of antibacterial composite materials made from simple molecular additives, which reduces their service life and negatively affects some of their properties. The introduction of biologically active groups into polymers with the aim of extending their service life and retention of the necessary properties is an actual problem and a perspective direction [2].

The antibacterial polymer additives allow to obtain materials with various compositions and characteristics which can be used for food packaging, and can be used in agriculture.

The main purpose of the this work is the preparation of composition materials based on olefins containing salicylic group, which serves as a continuation of the previously carried out investigations connected with the study of their physical-mechanical and antibacterial properties

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INFLUENCE OF TIO_2 ON THE DEPENDENCE OF SHEAR RATE ON SHEAR STRESS OF POLYMER COMPOSITE BASED ON LDPE / HDPE MIXTURE

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The base polymers produced in the polymer industry are not always able to meet the increased requirements of modern technology in terms of their characteristics. In this regard, the modification methods undertaken in the direction of improving the structure and complex of properties of polymers make it possible, to one degree or another, to approach the implementation of the task. One of the most common methods of polymer modification is the mixing of polymer with polymer, as a result of which it seems possible to predict the possibility of forming composite materials with predetermined properties [1-3].

The rheology of composites plays an important role in evaluating their processability by injection molding and extrusion. In this regard, the task of this study was to find out how the process of mixing an LDPE/HDPE (50/50) polymer mixture with titanium dioxide (1 wt%) can affect the pattern of change in their rheological characteristics. Rheological studies of polymeric materials were carried out on a MELT FLOW TESTER, CEAST MF50 capillary rheometer (INSTRON, Italy).

For comparison, the flow curves of the initial LDPE/HDPE mixture and the LDPE/HDPE composite with 1wt% TiO_2 were presented simultaneously. Figure 1 shows the flow curves of these polymer composites. When considering the dependences of the shear rate on the shear stress, some differences are observed in the patterns of change in the flow curves. Since, if for a mixture of LDPE/HDPE at 190°C there is a linear dependence of $\lg\gamma$ on $\lg\tau$ close to the Newtonian regularity of the melt flow, then for samples of LDPE / HDPE with 1 wt% TiO_2 there is a break in all investigated temperature ranges. Mixing the polymer mixture with finely dispersed titanium dioxide leads to the appearance of a non-Newtonian region. At the same time, a comparative analysis of the curves shows that the composite with LDPE/HDPE + 1 wt % TiO_2 composition has a higher shear rate at 5 different shear stress values. This is due to the fact that, with the inclusion of a structure forming agent (TiO_2) in the composition of the LDPE/HDPE mixture, an increase in melt fluidity is observed, which contributes to the movement of associates of macrosegments relative to each other.

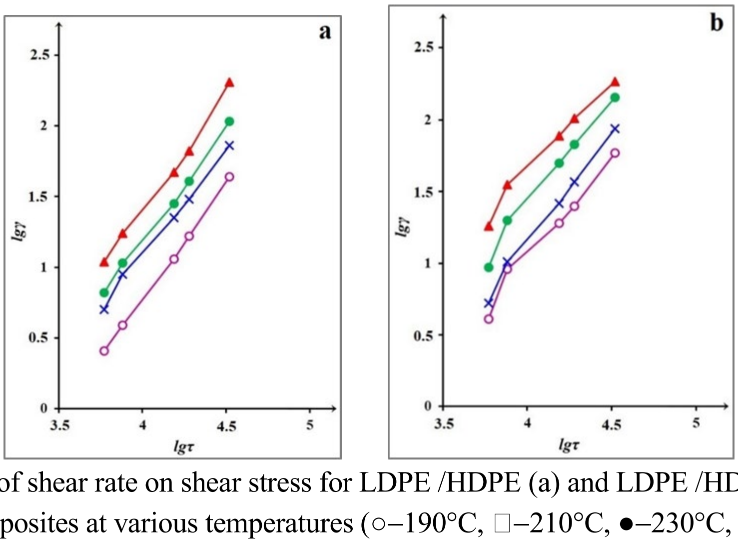

Figure 1. Dependence of shear rate on shear stress for LDPE /HDPE (a) and LDPE /HDPE + 1 wt % TiO_2 (b) polymer composites at various temperatures (○–190°C, □–210°C, ●–230°C, ▲–250°C).

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INVESTIGATION OF THE REGULARITIES AND PROPERTIES OF THE OXIDATIVE COPOLYCONDENSATION REACTION PRODUCTS OF 1-NAPHTHYLAMINE WITH 1-NAPHTHOL

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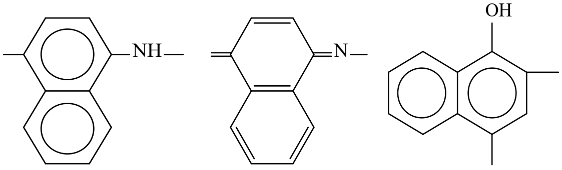
The oxidative polycondensation reaction of 1-naphthylamine with 1-naphthol in the presence of an aqueous solution of hydrogen peroxide has been carried out. The results of the investigation showed that the temperature rise in the range of 343 ÷ 368 K, the molar ratio of H_2O_2:(NA+NPh) in the range of 1:1÷3:1, and also the quantity of naphthylamine in the reaction mixture leads to an increase of yield of the oligomer products of the oxidative copolycondensation reaction of 1-NA with 1-NPh in the presence of H_2O_2.. For this process, the optimal value of the carrying out of reaction is 8 h and the addition of ethanol to the reaction medium leads to an increase of yield of cooligomers. On the basis of gel-chromatogram of the samples of cooligomers synthesized in the various conditions, their molecular-weight indices have been found. It should be noted that the curves of the molecular-weight distribution of the products of oxidative copolycondensation of NA and NPh have a bimodal character. The reaction products consist of fractions of low-molecular $\overline{M}_n$ =330÷580 =330÷580 and high-molecular $\overline{M}_w$ =5230÷6480. The content growth of the oxidizer and reaction temperature is accompanied by an increase of molecular-weight indices and simultaneously by polydispersity of the reaction products. The obtained results indicate that the synthesized copolymers as a result of the oxidative copolycondensation of the monomer pair NA and NPh consist of the following structural fragments:



It is seen that the obtained cooligomers include the reactive structural fragments and have the ability for dissolution and melt. They interact intensively with the oxirane ring of epichlorohydrin and epoxy diane resins, and also molecular oxygen in an alkaline medium. These peculiarities allow to synthesize the stable macroradicals, characterized by high paramagnetic and electrically conductive properties by oxidation on their basis.

As a result, the obtained cooligomers can be used as antistatic additives to thermoplastics and an elastomer. The introduction of these cooligomers into the composition of polyethylene, polystyrene and polypropylene in a quantity of ~ 5-10% allows to reduce the values to ~ 10 ~10^7-10^8 $Om^{-1}\cdot cm^{-1}$

The synthesized samples of NA+NPh cooligomers have been also used as an active additive on the basis of rubbers, for example, butyl rubber (BR).

In this case, the rubber mixtures on the basis of BC have been made according to the standard recipe of ingredients with the only difference that instead of carbon black (partially or completely), cooligonaphthylamine naphthols are used (from 5.0 to 45 m.p. per 100 m.p. of rubber). It has been established that the introduction of the synthesized oligomer into the composition of the rubber mixtures instead of carbon black leads to an increase of the specific elongation, tensile strength and a decrease of the modulus of elasticity of the obtained rubbers. Along with this, the thermal stability and service life of the obtained rubbers are increased, which has been connected with the structural peculiarity of NA + NPh cooligomer, the naphthalene rings in the aromatic polyconjugation chain stipulate the high temperature resistance, and the availability of amine and hydroxyl groups in naphthalene rings and chain – antioxidant activity. The samples of NA+NPh cooligomer exhibit the high electrical conductivity, their joint use with electrically conductive carbon black allows to obtain the rubbers with σ_v ~10^{-8}÷10^{-6} $Om^{-1}\cdot cm^{-1}$. Moreover, the content growth of the cooligomer from 22.5 to 45.0 m.p. (from mass of BR) instead of carbon black, leads to an increase of the specific electrical conductivity of the obtained rubbers. The percolation effect is reached at a content of ~ 23.5 m.p. of cooligomer for rubbers obtained from BR. The accumulation of static electric charges on the surface of rubber-technical products on the basis of the developed rubbers during their exploitation is minimized.

DEVELOPMENT OF COMPOSITION MATERIALS ON THE BASIS OF HIGH- AND LOW-DENSITY POLYETHYLENE, NANOCLAY AND SYNTHETIC LUBRICATING OIL

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In this paper the results of investigations on the development of polymer composition materials with improved strength and antifriction properties on the basis of high-density polyethylene (HDPE), as well as low-density polyethylene (LDPE) and modifying additives – Azerbaijani clays and synthetic lubricating oil are presented. It has been established that the introduction of 5-25% nano-sized clays and 1-3% of the above-mentioned oil into the composition allows to obtain the thermoplastic materials with sufficiently high antifriction and other properties. In addition, the influence of the temperature regime and the pressure of melt extrusion in a material cylinder on the physical-mechanical properties of composites on the basis of propylene were investigated.

The optimal conditions of processing of multicomponent composites have been shown. It has been established that with the temperature rise regime of the material cylinder within the established limits and an increase in the casting pressure is accompanied by a slight increase in the breaking shear stress and a noticeable decrease in the wear of the composite samples. The most optimal conditions for holding time under pressure is 10 sec. Also, modifying the properties of the industrial polyethylenes with cheap inorganic additives, one can create the composition materials with high strength and antifriction properties.

So, for example, at the lowest pressure and lower temperature regime of casting, the wear after the first cycle is 26.53 mg. At the highest values of the pressure and temperature regime of casting, the wear was 21.48 mg, i.e. decreased by 4.05 mg, i.e. in1.2 times.

In estimation of the quantitative change in the composite wear from the above-mentioned processing factors, we have proceeded from the notion that in all other equal conditions, this index value depends mainly on their density and hardness. In other words, the higher the density of the same material, the greater its wear resistance should be. Indeed, it has been established at a relatively low temperature (150-160-170-180 ºC) and low pressure (50 MPa) that the density of the composite is 953 kg/m^3 and, conversely, at a high pressure (150 MPa) and at processing temperature 150-170-190-210ºC, its density becomes equal to 961 kg/m^3.

SYNTHESIS OF NEW PHOTOSENSITIVE POLYMER MATERIALS

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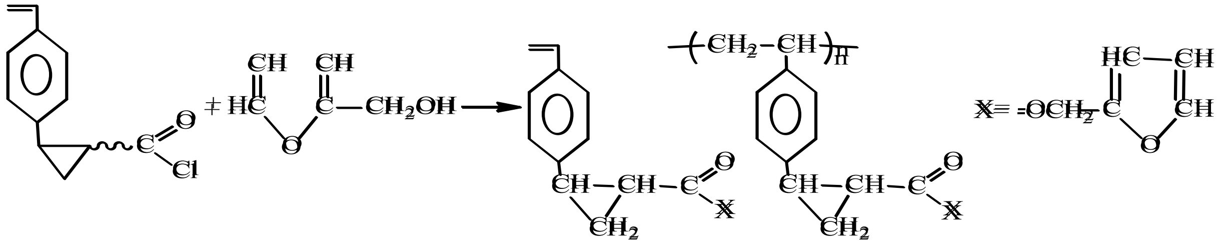
New photoreactive homopolymer containing suspended reactive fragments has been synthesized with homopolymerization on the basis of new monomer. The various structures have been established by methods of spectroscopy (IR, NMR, etc).

The synthesis of a new monomer – furanoxycarbonylparacyclopropyl styrene (FCCS) and its copolymerization were carried out as follows:



The structure of the obtained monomer and polymer is confirmed by data of IR and NMR spectroscopy, and the composition of the obtained polymer – by elemental analysis. The synthesized polymer has high light sensitivity, film-forming ability, good solubility before irradiation, resistance to solvents, plasma etchants after cross-linking and good thermal stability, which is very important for a photoresist. The availability of the synthesized polymer, reactive groupings of various chemical nature in the macromolecule links is of great interest for the preparation of photoresist polymer materials for microelectronics.

In this connection, the photochemical investigations of the synthesized polymer have been carried out. The structuring of photochemical processes was controlled by a method of IR spectroscopy.

It has been revealed that with an increase in the irradiation duration (2-3 min.), the intensity of the maxima of the absorption bands characteristic for the cyclopropane ring (1030-1035 cm^{-1}) of the double bond of the furan ring and the carbonyl group (1720 cm^{-1}) is decreased.

Under the influence of UV irradiation, the polymer on the basis of FCCS easily undergoes the structuring, as a result of which the film obtained on its basis becomes insoluble and with a small defect.

The synthesized polymer is a perspective class of high-molecular compounds with a wide range of practically valuable properties.

In the side chain, the macromolecules of chromophore groups such as phenyl, cyclopropane, furan and carbonyl groups favor their structuring at action of UV irradiation. Due to the availability of fragments strongly absorbing light energy in the polymer macromolecule, the polymer is a high-quality photosensitive material (55cm^2/J).

The synthesized polyfunctional polymer containing groups highly sensitive to UV irradiation is a valuable object of the photochemical investigations and can serve as a basis for the creation of negative photosensitive materials.

THERMAL DEFORMATION PROPERTIES OF METAL-POLYMER COMPOSITES BASED ON LOW DENSITY POLYETHYLENE AND COPPER

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Polyolefins are one of the most widely used polymers in the industry. This is due to their valuable complex of physical-mechanical and technological characteristics. But even these advantages are not always sufficient to expand the areas of their practical use [1, 2]. This is explained by the fact that one of the main disadvantages of non-polar polyolefins is their poor compatibility with foreign components, which include polar natural minerals or metals. The lack of good technological compatibility, as a rule, is reflected in the agglomeration of filler particles, accompanied by some decrease in the strength characteristics of composite materials obtained on their basis [3]. In this regard, much attention has been paid to the use of compatibilizers that can improve their miscibility and technological compatibility with fillers.

Taking into account that such studies of metal-polymer systems have practically not been carried out, it seemed interesting, using the example of low-density polyethylene (LDPE), to consider the selective effect of dispersed metal particles on the thermomechanical curves of the dependence of deformation on temperature. The results of the study of thermomechanical curves for composites based on LDPE and copper, presented in Fig.1. As can be seen from this figure, the first-order phase transition occurs in a narrow temperature range. So, for example, the softening temperature of composites was changed in the following sequence: initial LDPE – 107°C, in copper-containing- 0.5 wt %-110°C; 1.0 wt %-114°C; 5.0 wt% - 118°C; 10 wt % – 115°C; 20 wt % – 111°C и 30 wt % – 109°C. From a comparative analysis of the curves in this figure, it can be established that the copper concentration has a significant effect on the first-order phase transition or the softening temperature of the composites.

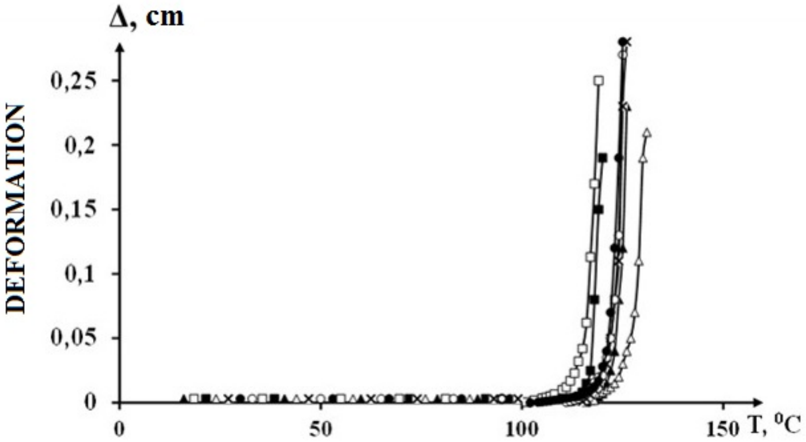

Figure1. Thermomechanical curves of temperature dependence of deformation of composites based on LDPE and copper, wt %: □-initial LDPE; ■-0.5; ▲-1.0; Δ-5.0; x- 10; o- 20 and ●- 30.

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PREPARATION OF ECOLOGICALLY PURE COMPOSITES ON THE BASIS OF LOW-PRESSURE POLYETHYLENE, NEW INORGANIC MINERAL AND ORGANIC FILLERS AND THE INVESTIGATION OF SOME PHYSICAL-MECHANICAL PROPERTIES

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LPPE, occupying a unique place among industrial polymers, has many excellent properties, as well as some disadvantages. The high elongation at break, high MFI, low modulus of bending elasticity, low Vicat temperature resistance, etc. can be shown as an example. For adjustment of these properties of the polymer, the new composites can be obtained using various inorganic mineral and organic fillers. In this regard, it is possible to obtain composites with high physical-mechanical properties with use of hazelnut shell bran found in the Absheron region of the Republic of Azerbaijan as mineral and organic filler.

The advantage of the found new mineral over other known minerals can be explained by its rich composition of various oxides, ions and anions of metals and non-metals. Al_2O_3, BaO, Bi_2O_3, CaO, CdO, Fe_2O_3, K_2O, Na_2O, MnO, P_2O_5, PbO, SO_3, SiO_2 and other heavy metal oxides are also present in the known mineral in various percentages. The chemical composition and IR spectrum of the mineral have been investigated. It has been established that its composition consists of various metal and non-metal oxides, anions and hydrates.

The new mineral can be widely used as filler in the production of composite materials on the basis of various industrial polymers. The various compositions based on mineral filler and hazelnut shell bran have been obtained from LPPE and some of their physical-mechanical properties have been studied. With the aim of determination of the physical-mechanical properties of the obtained composites with maintenance of a constant mass fraction of the organic filler, the mineral filler was included in the composition of the LPPE in various mass fractions.

The problems of reduction of the cost of composites obtained due to organic and inorganic fillers included in the composition of low-pressure polyethylene (LPPE) have been successfully implemented. Both fillers are considered very inexpensive fillers. Even with 60% mineral filler, they are easily processed and show high physical-mechanical properties.

In the obtained composite materials, the hazelnut shell bran, being organic filler, is 10%, and the quantity of mineral filler is taken at ratio 30%; 40; 50; 60 mass %. Some physical-mechanical properties of these composites, which can be used in various fields of industry and agriculture, are as follows: tensile strength (σ) – 22; 20.34; 18.96; 18.49 MPa, specific elongation (ε) – 8; 4: 2 and 1%. The melting flow index of the obtained composite (MFI, g/10 min) was respectively characterized by values 1.50; 1.35; 1.05 and 0.90. The Vicat heat resistance corresponds to the following values 155°C; 157°C, 158°C and 159°C.

The analysis of these values shows that as the quantity of fillers added to the composition increases, the specific volume value is naturally decreased. At the same time, with an increase in the quantity of filler in the composition, the tensile strength is increased, and the specific elongation is decreased. The organic fillers increase strength by increasing the pores between the molecules and creating a reticular structure. With the increase of the quantity of filler MFI is naturally decreased, and Vicat heat resistance is increased.

POLYMER COMPOSITES BASED ON COPOLYMER OF ALLYL ETHER OF SALICYLIC ACID WITH METHYL METHACRYLATE AND ABS

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ABS (acrylonitrile-butadiene-styrene copolymer) based antibacterial composition materials (CM) were obtained and their properties were studied using the copolymer of allyl ester of salicylic acid with methyl methacrylate as an antibacterial additive.

It was determined that the addition of 4, 12, 20 wt % salicylic acid allyl ester copolymer with methyl methacrylate to the composition of the ABS composite material practically does not affect its physical-mechanical properties, but the thermal resistance properties increase by increasing the amount of the additive.

When 4, 12, 20 wt% salicylic acid allyl ether and methyl methacrylate co-polymer are added to the composition of ABS-based CM, their physical-mechanical properties practically do not change or change very little. The results obtained from the studies are presented in table 1.

Table 1. Physical-mechanical parameters of ABS-based antibacterial CM

Samples	Formulation of composition, wt %	Elongation at break	Ultimate tensile strength	MFI (200ºC/2.160 kg)
		%	MPa	g/10 min.
CM_1	ABS CM	40	38	0.5
CM_2	ABS CM + CPAESAMM (4%)	38	38	0.7
CM_3	ABS CM + CPAESAMM (12%)	34	39	0.92
CM_4	ABS CM + CPAESAMM (20%)	29	38	1.01

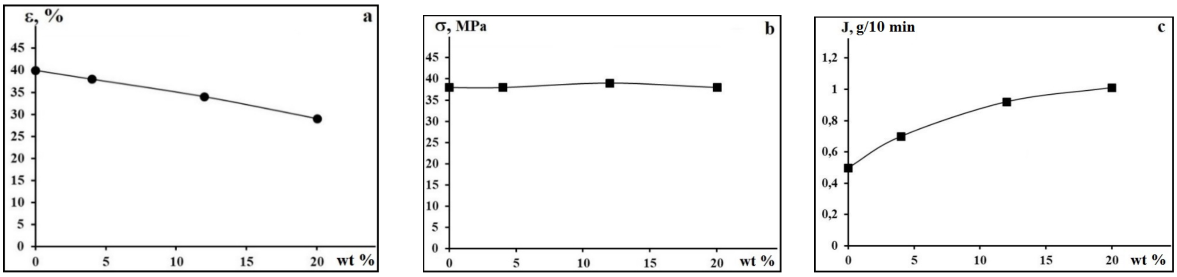

Figure 1. Dependencies of elongation at break (a), tensile strength (b) and MFI (c) in ABS CM+ CPAESAMM composite on CPAESAMM amount.

Physical-mechanical properties of polymer composite samples are characterized by ultimate tensile strength (σ, MPa) and elongation at break (ε, %), which are more sensitive to the structure and composition of composite materials. Based on the data in Table 1 and Figure 1(b), it can be noted that there is no significant change in the value of the ultimate tensile strength of the polymer composition samples. In the elongation at break of the polymer composition samples, a downward tendency is noticeable with the increase of the amount of antibacterial additive (table 1 and figure 1(a)).

PREPARATION OF COPOLYMER ON THE BASIS OF MALEIC ANHYDRIDE AND N-VINYLPYRAZOLINES

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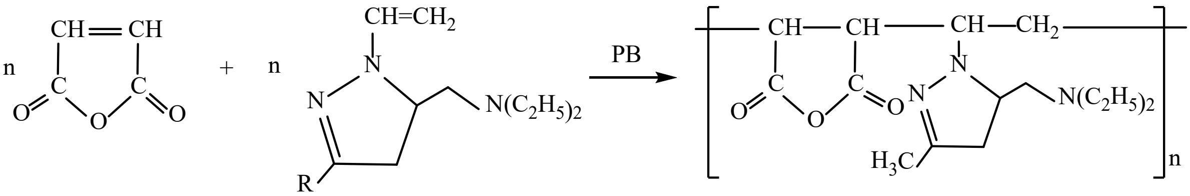
The copolymers of maleic anhydride (MA) with various monomers are widely used in medicine and pharmaceuticals due to their well-defined structure, solubility in water and their further chemical conversions [1-3]. The biologically active polymers are unique opportunity for creation a certain, almost ideal type of drugs of the future. Among such polymers, the polymers or composition materials with biologically active heterocyclic fragments occupy a special place. The finding of a pyrazoline (PZ) fragment in the copolymer molecule expands their areas of application, since these copolymers can be used as bearers of drugs for transportation in the human body. Moreover, such copolymers have their own biological and physiological activity [4, 5].

These properties of these copolymers are of interest in study of the copolymerization process of N-vinylpyrazolines (VPZ) and maleic anhydride (MA).



(I-III)

R= $-CH_3$(I), $-C_2H_5$(II), -Ph(III)

This mixture is poured into a reactor equipped with a stirrer and a refrigerator and heated in a water bath at definite temperature in the presence of the initiator. The various solvents (methyl ethyl ketone, 1,4-dioxane, benzene, etc.) have been used during the process. The copolymerization was carried out at 60ºC in the presence of the initiator of benzoyl peroxide (BP, 1 mass% $=8.0\cdot10^{-3}$mol / l) and the molar ratio of monomers MA:VPZ = 1:1 in benzene solution. Under the selected conditions, N-vinylpyrazoline fragment is untouched and the chain structure is not disturbed. In this case, the best results have been obtained in benzene. For preparation copolymers, we have used a monomer pair of N-vinylpyrazolines (VPZ) and maleic anhydride (MA), in which maleic anhydride is more active (gMA = 1.22, gVPA= 1.14). The monomers, initiator and solvents were purified to basic substance content 99.8%. As a result of study of the copolymerization process of maleic anhydride and N-vinylpyrazolines for 3-6 h, the alternating copolymers with molecular weight of 23000-30000 Da are formed. Such samples are perspective for their further modification with the aim of preparation of new bearers of drugs.

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OBTAINING AND STUDYING THE PROPERTIES OF NANOCOMPOSITES BASED ON A MIXTURE OF HIGH- AND LOW-PRESSURE POLYETHYLENE WITH METAL-CONTAINING NANOFILLERS

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The addition of nanoparticles to polymer composites has led to a new generation of composite materials with improved and new properties. The use of nanoparticles of metals with variable valence in polymers allows obtaining fundamentally new materials that are widely used in radio and optoelectronics, such as magnetic, electrical conductors, and optical media. Metal-polymer composite materials are mainly used in the electronic and radio engineering industry, as well as in aircraft and rocket construction [1, 2].

This work has been devoted to the preparation and investigation of the properties of nanocomposites on the basis of HPPE and LPPE with use of the metal-containing nanoparticles stabilized by the polymer matrix as nanofillers.In the work used: –high pressure polyethylene of 15803-020, $\rho = 0.917 - 0.921$, MFI 1.5-2.5 g·10-1min (T=190ºC,load -2,16 kg);– low pressure polyethylene of mark HM0349PE, $\rho = 0.949$, MFI 8.3 г·10-1min (T=190ºC, load- 21.6 kg). The zinc-containing nanoparticles stabilized by the polymer matrix were used as nanofillers. The ratio of the components of the composition (mass%): HPPE/LPPE/NF =50/50/ (0; 0.5; 1.0). The nanocomposite polymer materials have been obtained by mixing HPPE and LPPE with the metal-containing nanofiller on laboratory rollers at temperature 150°C for 15 min. For carrying out of the mechanical testing, the obtained mixtures were pressed as plates with thickness 1 mm at 190°C and pressure 10 MPa for 10 min. The physical-mechanical, heat-physical and thermal properties of the obtained nanocomposites have been investigated.

It was determined that the physical-mechanical and thermal properties of the obtained nanocomposite improved as a result of the introduction of the nanofiller containing HPPE/ LPPE /ZnO (1%) nanoparticles into the initial mixture. The introduction of 0.3 – 0.5 mass% of NF into the composition leads to an increase in the strength index from 16.69 to 19.93MPa. The increase in the concentration of NF more than 0.5 mass% leads to the decrease in the strength of the composite (17.78 MPa), which has been probably stipulated by the aggregation of nanoparticles, leading to the formation of microdefects in the volume of the polymer matrix. The investigation of Vicat heat resistance of the obtained compositions showed that the introduction of nanofiller into the composition of the polymer mixture leads to the decrease in the heat resistance index from 155ºC to 110 ºC. It is due to brittleness of Zn metal. The study of the thermal properties of the sample showed that the addition of nanofillers containing Zn oxide to the polyolefin mixture contributes to a significant increase in the decomposition temperature of the sample (423-430°C). The obtained results indicate that small quantities of nanofiller (0.3-0.5 mass%) introduced into the polymer, evidently, play the role of structure-forming agents– artificial crystallization nuclei, which favors the appearance of fine spherulite structure in the polymer, characterized by improved physical-mechanical and thermal properties of the obtained nanocomposite.It has been shown the perspectivity of use of nanofillers containing NP of the zinc oxide, stabilized by the matrix of high-pressure polyethylene obtained by a mechanical-chemical method to a mixture of polyolefins on the basis of HPPE/LPPE, which favors the creation of a fine-crystalline structure of the composition, and as a result of which its properties are improved, and thereby the areas of application of the obtained nanocomposite are expanded.

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Abstract

POLYMERIZATION OF 2-[N-ALLYL-N-(β-CHLOR)ALLYL]AMINO-PROPANOIC ACID

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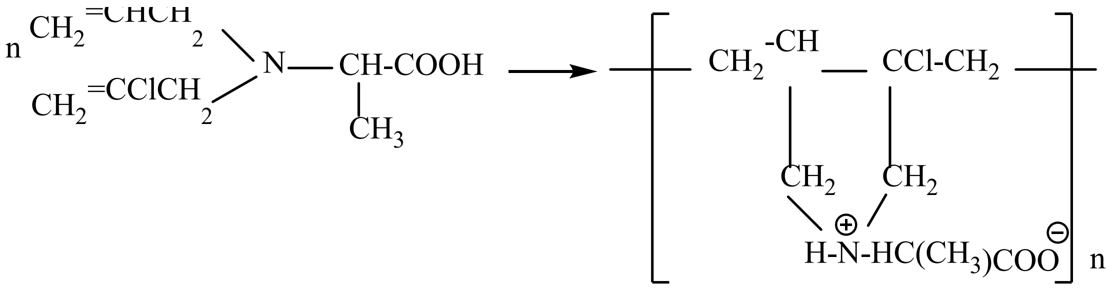
Radical polymerization of 2-[N-allyl-N-(β-chlor)allyl]aminopropanoic acid (ABPA) was carried out in aqueous solutions in the presence of ammonium persulfate (AP). Carrying out the polymerization reaction without radical initiators has shown that the reaction practically does not procced. The reaction of radical polymerization of ABPA proceeds according to the following scheme:



The results of polymerization are shown in the table.

Table. Results of the reaction of radical polymerization of ABPA

Monomer, [M]=2 mol/l	Initiator, [I]=5x10^{-3} mol/l	Polymerization medium	Temperature, °C	Yield, %	Reduced viscosity ($\eta_{red.}$), dl/g
ABPA	AP	Water	60	40	0.15
	AP	Water	70	45	0.17
	AP	Water–alcohol	60	25	0.04
	AP	Water–alcohol	70	30	0.06

As can be seen from the table, the highest values of the reduced viscosity were obtained in an aqueous solution as a AP initiator at a temperature of 70°C.

To establish the structure of the monomer (ABPA) and polymer, they were investigated by physical and chemical methods.

By the bromide – bromated method (Knopp method), it was found that the resulting ABPA – based polymer does not contain unsaturated allyl groups. Thus, the polymerization of ABPA proceeds according to the known cyclolinear mechanism via double bonds of diallyl groups with the formation of a polymer with a pyrrolidine structure.

Polymers of the diallyl series, in agriculture they serve to improve soil structure.

The synthesized polymer based on ABPA was tested as a soil structure. It has been shown that this polymer significantiy enhances the structuring effect even with small amounts (using a 2% aqueous solution) of its introduction into the soil. When it is used for alkaline soils, a strong lumpy structure is formed, and the cation exchange capacity is also enhanced.

Abstract

DYNAMICLY VULCANIZED THERMOPLASTIC ELASTOMERS

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In recent years, much attention has been paid to research in the field of obtaining and processing multicomponent polymer systems based on polyolefins [1, 2]. This practice makes it possible to use the advantageous features of the properties of each of the components of the mixture in one composite material. The main disadvantage of such composite materials, as a rule, is the poor compatibility of the mixed components of the mixture, accompanied by a deterioration in their final properties. In this regard, the purpose of this work was to conduct a set of studies to systematize the properties of polymer mixtures based on thermoplastic polyolefins and synthetic rubber, which make it possible to obtain various types of thermoplastic elastomers with an improved set of physical-mechanical characteristics.

Low-density polyethylene (LDPE), high-density polyethylene (HDPE), isotactic polypropylene (PP), butyl rubber (BR) were used as polymer components. The components were mixed on rollers at a temperature of 150-180°C. To obtain samples for testing, pressing was carried out at a temperature of 170-190°C. Physical-mechanical characteristics were determined according to standard methods: ultimate tensile stress and elongation at break in accordance with GOST 11262-80, bending strength in accordance with GOST 4648-71, the melt flow index was determined on a MELT FLOW TESTER, CEAST MF50 device (INSTRON, Italy) at a temperature 190°C and load - 5 kg.

Before proceeding to the study of the properties of multicomponent polymer mixtures, it seemed interesting, using the example of a number of polyolefins, to consider the effect of BR concentration on the change in such properties of compositions as ultimate tensile stress (σ_{ts}) and tensile yield strength (σ_{ys}). It was found that with an increase in the concentration of BR in the composition of a thermoplastic polyolefin, a regular decrease in the ultimate tensile stress and tensile yield strength is observed, accompanied by a decrease in the difference between them. The existence of σ_{ts} and σ_{ys} indicates the plasticity of the polymer material. At the moment when σ_{ts} becomes equal to σ_{ys}, the polymer composition loses its plasticity and, like a thermoplastic elastomer, it acquires rubber-like properties. For example, for compositions based on LDPE, the loading of BR leads to a sharp deterioration in their strength properties. At 20 wt % BR content σ_{ts} and σ_{ys} are aligned. In the case of PP and HDPE, the equality of σ_{ts} and σ_{ys} manifests itself with the loading of 40 wt % BR. The effect of chemical cross-linking of polyolefin mixtures of thermoplastic + BR with dicumyl peroxide on the main physical-mechanical properties of the compositions was studied. with an increase in the concentration of dicumyl peroxide (DP) from 0.5 to 2.0 wt %, an ambiguous change in properties is observed. According to the experimental data obtained, chemical crosslinking of polymer mixtures in all compositions improves their strength properties. And in the case of the original thermoplastic polymers, crosslinking, on the contrary, leads to a deterioration in their properties.

Thus, on the basis of the foregoing, it can be concluded that in the process of studying polymer mixtures based on polyolefins, it seems possible to change their physical-mechanical characteristics in a fairly wide range. The additional use of a crosslinking agent makes it possible to bring the properties of polymer composite materials to a level at which it is possible to significantly improve their performance, provided that satisfactory processability is maintained by injection molding and extrusion.

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POLYETHYLENE BASED METAL-CARBON NANOCOMPOSITES

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Due to the unique properties of modern nanomaterials, many companies design complex electronic devices that are used in the aviation and space spheres to assemble powerful computers, video equipment, help diagnose various diseases, as well as quickly transmit information. Such nanostructured materials are obtained by embedding nanoparticles into various polymer matrices [1].

The presented work is devoted to the obtaining and study of the properties of nanocomposites based on high-pressure polyethylene (LDPE) and low-pressure polyethylene (HDPE) using metal-containing nanoparticles (CoO, NiO) stabilized by a polymer matrix and multi-walled carbon nanotubes (MWCNT) as nanofillers (NF). Nanocomposite polymeric materials are obtained by mixing LDPE (HDPE) with metal-containing nanofillers and MWCNTs on laboratory rollers at a temperature of 130-135ºC for 15 minutes. To carry out mechanical tests, the obtained mixtures were pressed in the form of plates 1 mm thick at 170°C and a pressure of 10 MPa for 10 minutes. The physico-mechanical, thermophysical and thermal properties of the obtained nanocomposites were studied. The optimal ratio of components for obtaining improved physical-mechanical and thermal properties of the studied nanocomposites was found (wt.%): HDPE(HDPE)/NPCoO(NiO)/MWCNT (100/1.0/0.05). An improvement in the strength and deformation parameters, as well as in the thermal-oxidative stability of the obtained nanocomposites, was revealed, which can be attributed to the effects of structural and chemical stabilization of the polymer matrix. The activation energy (E_a) of the thermal oxidative degradation of LDPE/NPNiO/MWCNT increases from 191.45 to 267.91 kJ/mol (HDPE/NPNiO/MWCNT increases from 201 to 275.28 kJ/mol), and LDPE/NPCoO/MWCNT increases from 191.45 to 291.38 kJ/mol (HDPE/NPCoO/MWCNT increases from 201 to 298.55 kJ/mol). Numerous experimental data on the mechanical, strength, relaxation, and other properties of polymer-polymer, polymer-filler mixtures are explained in terms of the concept of the presence of an interfacial layer. A necessary condition for obtaining the best properties of carbon nanomaterials in a polymer composite is to achieve the maximum degree of dispersion of the filler and its optimal orientation in the polymer matrix.

The results of physical-mechanical and thermal properties are confirmed by the data of SEM and AFM analyses. SEM - analysis of the obtained nanocomposites showed that the combined use of metal-carbon nanoparticles leads to an improvement in the dispersion of nanofillers in the polyethylene matrix and the formation of a new three-dimensional fine-crystalline supramolecular structure, which positively affects the physical- mechanical and thermal properties of nanocomposites. AFM micrographs show a complex interweaving of nanoparticles with each other, which indicates an increase in the linkage between them and, thereby, an improvement in all properties of the obtained nanocomposites. The metal-containing nanoparticles and MWCNTs used in the work, located in the interfacial layer of the structural elements of LDPE (HDPE), contribute to the formation of heterogeneous nucleation centers in the composition melt, which, in the process of stepwise cooling of the nanocomposite, contribute to an increase in crystallization centers, leading in general to an improvement in the crystallization process and the formation of a relatively fine spherulitic structure. The results obtained indicate that small amounts of nanofillers introduced into the polymer obviously play the role of structure formers - artificial crystallization nuclei, which contributes to the formation of a fine spherulite structure in the polymer, which is characterized by improved physical, mechanical and thermal properties of the obtained nanocomposite.

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SYNTHESIS AND PROPERTIES OF HETEROCYCLIC GLYCIDYLMETHACRYLATE ESTER-ALCOHOLS

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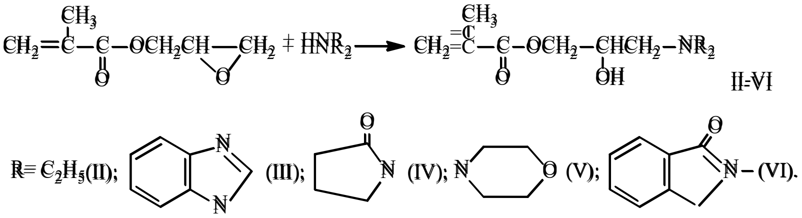
The opening of the oxirane ring of glycidylmethacrylate esters in their interaction with heterocyclic nitrogen-containing compounds has been studied insignificantly. Glycidylmethacrylate esters as monomers, and also as initial products undergo the chemical conversions and occupy an important place in organic and pharmaceutical chemistry [1].

The study of methods of the synthesis of heterocyclic glycidylmethacrylate ester-alcohols is an actual task, which has been stipulated by the perspectivity of use of these compounds in biological and pharmaceutical chemistry [2].

By the interaction of diethylamine, phthalimide, pyrrolidone, morpholine, benzimidazole with glycidylmethacrylate according to the following reaction, the corresponding ester-alcohols have been obtained:



The characteristics of the synthesized heterocyclic glycidylmethacrylate propropyl diethylamine (II), 2-hydroxy-3-glycidylmethacrylate propropyl benzimidazole (III), 2-hydroxy-3-glycidylmethacrylate propropyl pyrrolidone (IV), 2-hydroxy-3-glycidylmethacrylate propropyl morpholine (V), 2-hydroxy-3-glycidylmethacrylate propyl phthalimide (VI), which can be used in preparative and organic chemistry, are given in Table.

Table 1. Characteristics of the synthesized ester-alcohols

Compound	B.p., °C (mm merc.c.)	n_D^{20}	Brutto formula	$\frac{\text{Found}}{\text{Calculated}}$,%			Yield, %
				C	H	N	
II	167-168 (1)	1.4603	$C_{11}H_{21}O_3N$	61.39 61.48	9.76 9.45	6.51 5.96	80
III	164-166 (1)	1.5160	$C_{13}H_{16}N_2O_2$	66.95 67.00	6.90 7.00	11.92 12.00	82
IV	142-143 (1.5)	1.1650	$C_{10}H_{19}NO_4$	55.90 56.00	7.95 8.00	6.96 7.00	55
V	124-126 (1.5)	1.4744	$C_{10}H_{19}NO_3$	57.90 58.00	7.94 8.00	5.96 6.00	59
VI	180-182 (1.5)	1.5560	$C_{15}H_{15}NO_5$	62.92 63.00	4.96 5.00	4.98 5.00	68

The structure of ester-alcohols (II-VI) has been determined by modern physical-chemical methods of analysis.

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SYNTHESIS AND HYDOSILYLATION OF 2-METHYL(ETHYL)-1-PROPARGYL PYRROLE

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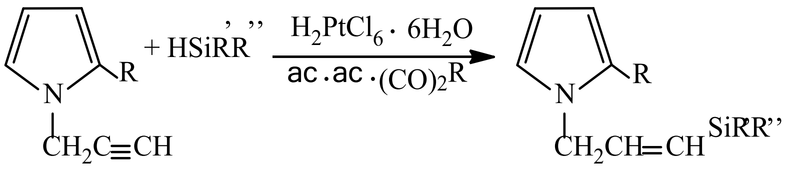
It is known from the analysis of native and foreign literature that the pyrrole and its derivatives occur in nature in a free state, and also as fragments in the composition of the complex natural compounds. In the body they participate in the performance of the most important physiological functions [1].

Considering the above-mentioned one and in the continuation of investigation in the field of synthesis of organosilicon 2-methyl(ethyl)-1-propargyl pyrrole-containing compounds [1] the study of the hydrosilylation reaction of trialkyl (aryl)hydridsilanes with 2-methyl(ethyl)-1-propargyl pyrrole in the presence of 0.1n platinohydrochloric acid or rhodium acetylacetonate bicarbonyl and thereby elucidation of the influence of the nature of substituents in the multiple bond of the propargyl radical on the yield and structure of the reaction products is of scientific interest.

We have developed the method of the synthesis of pyrrole-containing organosilicon compounds by the hydrosilylation reaction of trialkyl(aryl)hydride silanes with 2-methyl(ethyl)-1-propargyl pyrrole in the presence of catalyst (0.1n platinohydrochloric acid) according to the following scheme:



(I, II) (III - XIV)

R=CH_3 (I); R'=CH_3 , R"=C_2H_5 (III); C_3H_7 (IV); C_4H_9 (V); C_5H_{11} (VI); C_6H_5 (VII); $(CH_2)_4$ (VIII);

R=C_2H_5 (II); R'=CH_3, R'=C_2H_5(IX); C_3H_7(X); C_4H_9 (XI); C_5H_{11} (XII); C_6H_5 (XIII); $(CH_2)_4$ (XIV)

The study of spectra of the compounds (III-XIV) showed that the absorption peak at 3400-3440cm^{-1} belongs to the vibration of pyrrole ring. Also in the spectrum there are absorption bands in the field of 1251-1231 cm^{-1} referring to the valence vibrations of C-N bond, and the absorption band in the field of 1620 cm^{-1} belongs to the deformation vibration of Si-C- alkyl bond. There are also deformation (1358, 1421, 1458 cm^{-1}) and valence (2873, 2911, 2951 cm^{-1}) vibrations of bond referring to the vibration of C-H-bond in CH_2–group [2].

Thus, under the conditions accepted by us, the addition reaction of trialkyl(aryl)silanes with 2-methyl(ethyl)-1-propargyl pyrrole catalyzed by platinohydrochloric acid or rhodium acetylacetonate dicarbonyl proceeds via C-C bond of propargyl radical with the formation of unsaturated organosilicon pyrrole compounds, and trialkyl(aryl)silanes are fixed at the peripheral carbon atom.

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SYNTHESIS AND COPOLYMERIZATION OF GLYCIDYL ETHER OF 2-METHYL-4-VINYLPHENOL WITH CYCLOPROPYLMETHYL ACRYLATES

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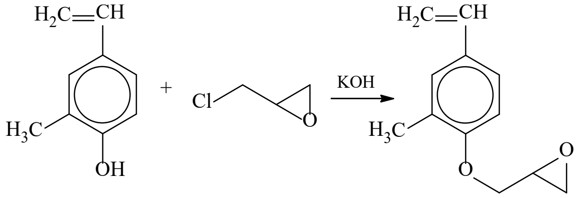
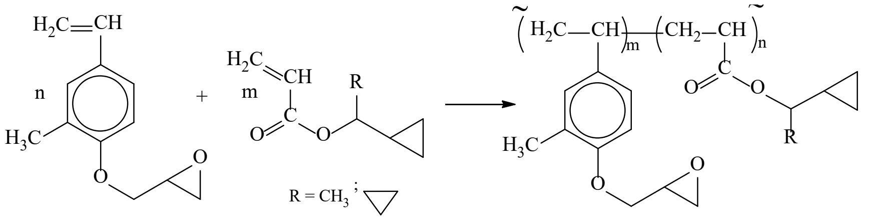
It is known that the high-molecular compounds containing active functional groups in macromolecules exhibit the high sensitivity to various sources of radiation and are widely used in microelectronics as a light-sensitive basis for photo- and electronoresists. The increased sensitivity of such polymers to light energy has been connected with the tendency of functional groups or fragments to photochemical reactions. Considering the above-mentioned one, in this report the results of the synthesis of glycidyl ether of 2-methyl-4-vinylphenol and its copolymerization with the cyclopropylmethyl acrylates synthesized by us are presented [1]. The availability of epoxide and three-membered cycles in the macromolecules of the obtained copolymers, which can be crosslinked under the influence of irradiation, would allow to obtain negative-type resistive materials on their basis.

The synthesis of glycidyl ether of vinylphenol was carried out by the interaction of 2-methyl-4-vinylphenol with epichlorohydrin in the presence of powdered ptassium hydroxide:



The copolymerization of the synthesized glycidyl ether of vinylphenol with cyclopropyl-substituted methyl acrylates was carried out at 70°C in the presence of azo-*bis*-isobutyronitrile in benzene solution according to the scheme presented below:



The influence of the ratio of comonomers in the initial mixture on the structure and composition of the obtained copolymers has been investigated. The polymerization constants of the initial monomers and *Q-e* parameters characterizing the specific activity of the initial monomers and the polarity of the radicals formed from them have been calculated. The investigated process proceeds with the participation of donor-acceptor-type complexes with the formation of copolymers of alternating structure. The obtained copolymers are white powdery substances dissolving well in polar organic solvents.

Some properties, including thermal and lithographic characteristics of the obtained copolymers, have been studied.

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SYNTHESIS OF POLYAMIDOIMIDE FROM ROSIN ADDUCT AND ANHYDRIDE OF 4-CYCLOHEXENE-1,2-DICARBOXYLIC ACID

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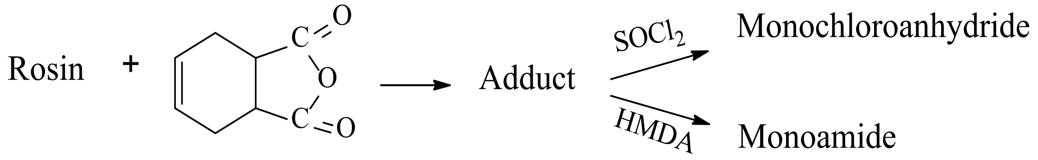
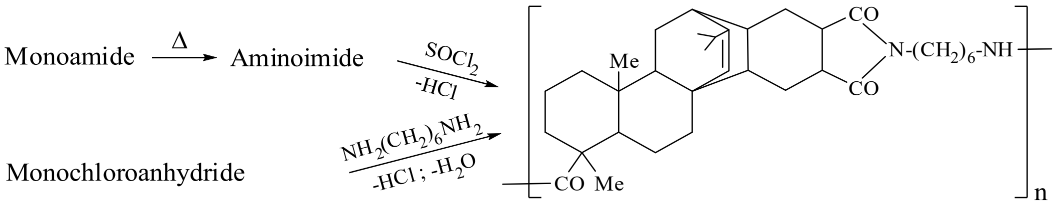
The polyamidoimides are an important class of thermostable polymers, which have exceptional mechanical, thermal and chemical resistance. The polyamidimides are widely used as anti-corrosion coatings for creation of the strong materials, withstanding high pressure, etc [1, 2].

In this work the polyamidoimide (PAI) from rosin adduct with anhydride of 4-cyclohexene-1,2-dicarboxylic acid (RCHA) and hexamethylene diamine (HMDA) has been synthesized. For this purpose, the obtained adduct has been converted by its reaction with thionyl chloride into monochloroanhydride or by its reaction with HMDA into monoamide on the following scheme:



It has been shown that as a result of the interaction of RCHA with $SOCl_2$, the obtained monochloroanhydride is well soluble in many polar solvents – cyclohexanone, dichloroethane, methyl ethyl ketone, chloroform, dichlorobenzene, but is not dissolved in alkanes, cycloalkanes, aliphatic alcohols, etc. The preparation of monoimide has been carried out as follows: a solution of HMDA in DMF was added to a solution of RCHA in DMF at room temperature with stirring. Then the reaction temperature was raised to 150°C and at this temperature the reaction was carried out for 2.5 h. Upon completion of condensation, the reaction mixture was poured into water; the obtained product was filtered and dried in vacuum.

Both monochloroanhydride and monoimide have been used for preparation of PAI. These reactions have been carried out at higher temperatures:



The similar reactions have been repeated with the participation of other diamines.

The structures of the obtained polymers have been confirmed by data of spectral and elemental analyses. The characteristic viscosities of the synthesized polymers were corresponded to 0,20-0,88 dl/g. The obtained amorphous PAI are thermostable to 250ºC, 5% of losses of their weights were observed at temperature ~300ºC.

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SYNTHESIS OF MATERIALS OF RETICULAR STRUCTURE ON THE BASIS OF COPOLYMERS OF MALEIC ANHYDRIDE AND CYCLOPROPANE-CONTAINING ALLYL ETHERS

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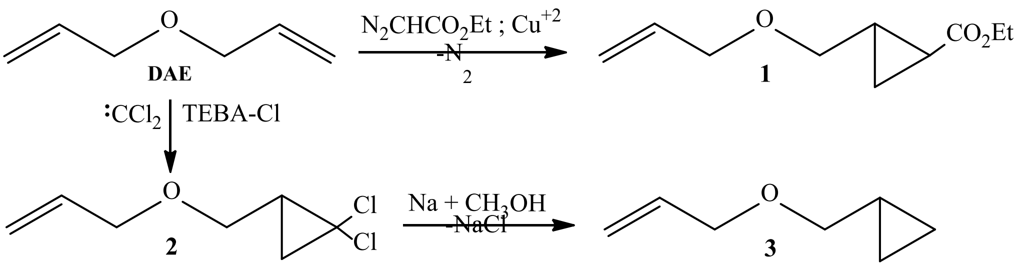
The copolymerization is one of the spread methods of synthesis of polymers of various composition and structure. Monomers such as maleic anhydride (MA) have a lack of electron density of double bond and form alternating copolymers with electron-donor vinyl monomers possessing excess of electron density of double bond. The copolymerization of vinyl ethers with maleic anhydride is accompanied by a decrease in the polarity of the double bond of the ether and the appearance of donor-acceptor complexes, the polymerization of which leads to a strict alternation of the links of both comonomers [1]. MA copolymers are of interest primarily because they are multifunctional: the structure of the macromolecule includes anhydride links and other functional groups which are reaction centers for post-polymerization conversions [2]. The materials on the basis of MA are used in the development of biomedical devices and drug delivery systems.

In this work, previously synthesized compounds were used for preparation of MA copolymers: **1-3** according to the scheme:



The synthesis of copolymers was carried out under the conditions of a free radical initiation reaction in a benzene medium with an equimolar ratio of comonomers. The copolymers were weakly colored crystalline products, insoluble in aromatic hydrocarbons, well soluble in polar organic solvents. The characteristic viscosities and MW of copolymers were 0,47-0,60 dl/g and 2800-3600 g·mol^{-1}, respectively. The results of IR spectroscopy showed that the copolymerization of compounds **1-3** with MA proceeded with the participation of a double bond with the formation of copolymers of linear structure and alternating structure. For preparation of the materials of the reticular structure, the copolymers were esterified with di- and triethylene glycol at various ratios. After thermal treatment, the modifications esterified to varying degrees lost solubility, but acquired the swelling capacity, which allows them to be used as bearers of physiologically active compounds [3].

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SYNTHESIS AND POLYMERIZATION OF 2-METHYL-4-(2-METHACRYLOYLOXY)-3-OXO-7-ETHYL-1,2-DIHYDROPYRROLO[3,4-C]PYRIDINE

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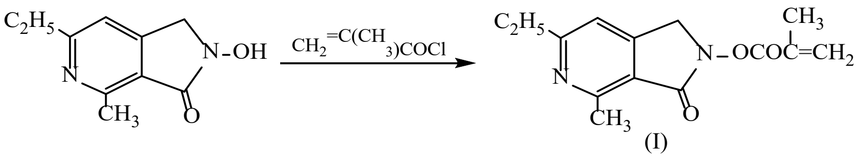
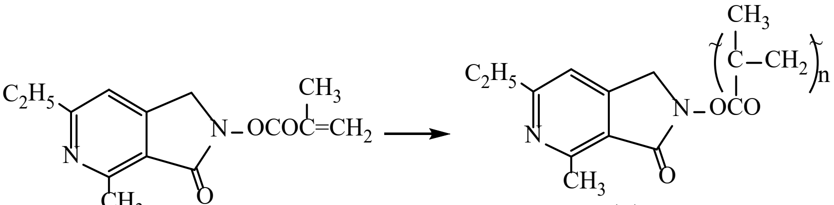
The heterocyclic compounds, whose cycle includes the nitrogen, oxygen and sulfur atoms, especially the first two, have been widely spread in nature as alkaloids, vitamins, antibiotics, etc. They perform vital physiological functions in the body. The heterocyclic compounds play a special role in medical chemistry – they form the basis of most drugs [1-4].

With the aim of preparation of the condensed heterocyclic monomers, the reaction of 2-methyl-4-(2-hydroxy)-3-oxo-7-ethyl-1,2-dihydropyrrolo[3,4-c]pyridine with chloroanhydride of methacrylic acid has been studied. It has been established that the interaction of these compounds in the presence of equimolar pyridine leads to the preparation of 2-methyl-7-ethyl-4-(2-methacryloyloxy)-3-oxo-1,2-dihydropyrrolo[3,4-c]pyridine (I).



(I)

The radical polymerization of 2-methyl-4-(2-methacryloyloxy)-3-oxo-7-ethyl-1,2-dihydropyrrolo[3,4-c]pyridine both in mass and in solution-dioxane (benzene) at temperature 70°C in the presence of AIBN has been studied. It has been established that the polymerization in mass leads to the formation of insoluble products. And in a case of polymerization in solution (30-50 wt%), the process proceeds smoothly with the formation of the soluble products (II). It has been established that the polymer yield increases with the increase of the experiment duration. However, at high conversions, the formation of cross-linked products is observed.



(II)

n = 5÷ 6

The structure of the synthesized compounds (I, II) has been confirmed by elemental analysis data, IR and NMR spectroscopy. The polymerization of pyrrolo-pyridine (I) containing monomer proceeds due to the opening of C = C double bond, as indicated by the disappearance of the absorption bands at 1625 cm^{-1} and 3110 cm^{-1}, characteristic for the methacryloyl group. In this case, the character of the unsaturated group in the pyrrole ring is not changed.

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Abstract

METAL-CONTAINING NANOCOMPOSITES ON THE BASIS OF POLYPROPYLENE AND BUTADIENE NITRILE RUBBER

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Now, thermoelastoplasts are one of the polymer materials with constantly growing fraction of world consumption. The most widespread were thermoelastoplasts produced on the basis of polypropylene (PP) with diene rubbers: butadiene nitrile (BNR), ethylene propylene diene, using various fillers or compatibilizers for improvement of their compatibility [1,2].

In this work, we have studied the influence of small additives of nanofillers (NF) containing nanoparticles (NPs) of oxides of various metals (NPCu_2O, NPNiO and NPCoO) stabilized by a polymer matrix of high-pressure polyethylene obtained by a mechano-chemical method in a polymer melt on the peculiarities of mixed TPE based on isotactic PP and BNR (18; 26 and 40% of acrylonitrile). The ratio of components of composition (mass %): PP/BNR (18; 26)/NF=50/50/ (0.5; 1.0; 2.0) and PP/BNR (40)/HH=70/30/ (0.5; 1.0; 2.0).

Nanocomposite polymer materials have been obtained by mixing of PP with BNR and metal–containing NF on laboratory rollers at temperature 165 - 170°C for 15 min. For carrying out of mechanical testing, the obtained mixtures were pressed as plates with thickness of 1 mm at 190°C and a pressure of 10 MPa.

The highest results of the physical-mechanical parameters of the composition are obtained in using 1.0 mass % of nanofillers PP/BNR(18)/NPCoO; PP/BNR(26)/NPCu_2O; PP/BNR(18;40)/NPNiO. It has been revealed the simultaneous improvement of the strength and deformation indices during the rupture of the composite, which, has been apparently connected with the synergetic effect of the interphase interaction of metal-containing nanoparticles in PE matrix with the components of PP/BNR polymer composition.

The introduction of metal-containing nanofillers into the composition of PP/BNR leads to an increase in the heat resistance index by 15-35°C.

The activation energy of thermal-oxidative destruction increases from 115.45 to 179.53 kJ/mol, which indicates higher thermal stability of the obtained nanocomposites.

The SEM-analysis of the obtained nanocomposites showed that the structure of the PP/BNR composite is shapeless, heterogeneous, since PP and BNR are polymers not combining with each other at the molecular level. In addition of metal oxide nanoparticles to PP/BNR, a relatively compatible consistency is formed in the interphase fields of the composite and a smooth surface with a fine-spherulite layered structure is formed.

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COPOLYMERIZATION OF N-VINYLPYRROLE WITH PROPARGYL ESTERS OF ACRYLIC AND METHACRYLIC ACID

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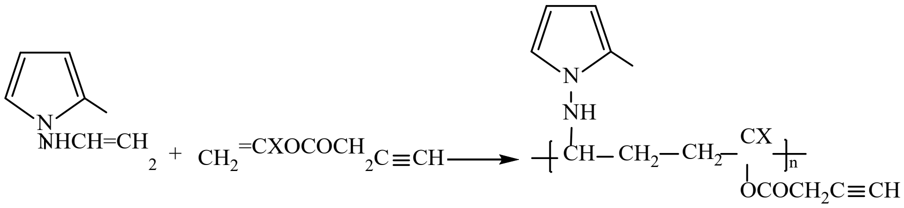
Interest to monomers – acetylene derivatives – is supported by their large synthetic potential, and also practically inexhaustible structural variety, which allows to obtain new unique polymer materials with given properties and prolonged-acting drugs on their basis. The increasing attention to these monomers has been stipulated by the orientation towards acetylene as a universal initial product for multipurpose application remaining in the world practice [1-3]. Such investigations have considerable scientific value, since the problems of the mechanism of chain growth and the structure of homo- and copolymers of bifunctional compounds with double and triple bonds in the molecule remain debatable.

Therefore, finding of the available methods of the synthesis of copolymers on the basis of N-vinylpyrrole with unsaturated esters of (meth)acrylic acids containing acetylene bonds are of not only theoretical but also practical interest.

In this connection, the object of our investigation was the study of the copolymerization of N-vinylpyrrole with propargyl esters of acrylic and methacrylic acids. The copolymerization was carried out at temperature 303 K in the presence of AIBN in a dioxane solution. The viscosity of the copolymer was measured in Ubbelode viscometer at 298K. For study of the influence of temperature on the copolymerization reaction, the process was carried out at temperatures 60°C, 65°C, 70°C, 75°C. The experimental data showed that with an increase of the reaction temperature, the copolymerization rate is increased, and the yield of copolymers, which are characteristic for radical polymerization is also increased.



The structure and composition of copolymers were determined by IR spectroscopy and on the results of elemental analysis. The comparison of the IR spectra of the monomer and the copolymers of PrA and PrMA with N-vinylpyrrole showed that the copolymerization took place via a double bond without the participation of an acetylene bond. There is no band corresponding to the double bond in the spectrum of polymer and the absorption band of the triple bond is kept. The intensive absorption band in the spectrum of copolymers at 2145 cm^{-1} is attributed to the valence vibrations of the acetylene bond.

With the aim of determination of the relative activities constants (r_1 and $r_2$0 for N-PB systems with PrA and N-PB with PrMA, the reactions were carried out at low degrees of conversions. The relative activities of monomers have been calculated using the Fineman-Ross method. The relative activity constants (r_1 and r_2) for N-PB with PrA are equal to 0.023 and for N-PB with PrMA – 0.025, which indicates a great tendency of the monomer links to alternation in the macromolecular chain of the copolymer.

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INVESTIGATION OF OLIGOPROPYLENE MACROMONOMER AND METHYLMETHACRYLATE RADICAL COPOLYMERIZATION REACTION

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The use of compounds based on olefins as a plasticizer comonomer for the production of high-impact copolymer based on styrene and methyl methacrylate (MMA) is considered an important area of research [1]. Taking into account these considerations, it seems interesting to use macromonomers of oligoethylene and oligopropylene (OPMM) as comonomers for the chemical modification of polymethyl methacrylate (PMMA) [1,2].

The reaction of radical copolymerization of oligopropylene macromonomer (M_1) with methyl methacrylate (M_2) has been carried out, the regularities of the reaction and the properties of the obtained products have been studied. The relative activity of monomers OPMM copolymerization (M_1) with MMA (M_2), in the radical reaction i.e. copolymerization constants (r_1=0.02 and r_2=12.20) were determined graphically using the Fineman-Ross equation. The results are shown in table 1. It was found that OPMM practically does not enter into the homopolymerization reaction and acts as a more passive monomer in the copolymerization reaction with MMA.

The value of $r_1 = 0.02$ in the studied monomer pair shows that the radical centers formed by OPMM are practically not bound to their monomer; they interact with MMA molecules in the process of copolymerization. This is due both to the electronic structure of OPMMs and to their large sizes, i.e. with spherical difficulties. The value of the copolymerization constant for a similar excess of MMA monomer in this reaction can be determined as r_2=12.2. Thus, MMA is a compound that polymerizes easily and binds MMA molecules at a faster rate when copolymerized with radical center of OPMM formed from this monomer. The resulting copolymer macromolecules with a statistical structure consist of oligopropylene units and blocks of methyl methacrylate. This is confirmed by the values of the parameters of the microstructure of the synthesized samples of the copolymer

The values of the copolymerization constants indicate that in the system OPMM + MMA OPMM is prone to copolymerization reaction, and formed copolymer macromolecules consisting of a random structure, OPMM units and blocks formed from MMA. The parameters of the microstructure of the copolymer macromolecules were calculated from the values of the copolymerization constants (fig. 1).

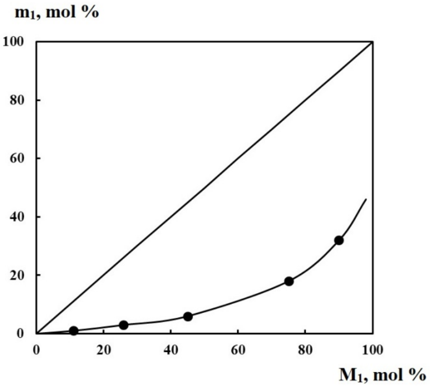

Figure 1. Dependence of the composition of copolymers on the composition of the mixture of monomers in the copolymerization reactions of OPMM and MMA

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COPOLYMERIZATION OF PARA-AMINOPYRIDINE METHACRYLATE WITH STYRENE

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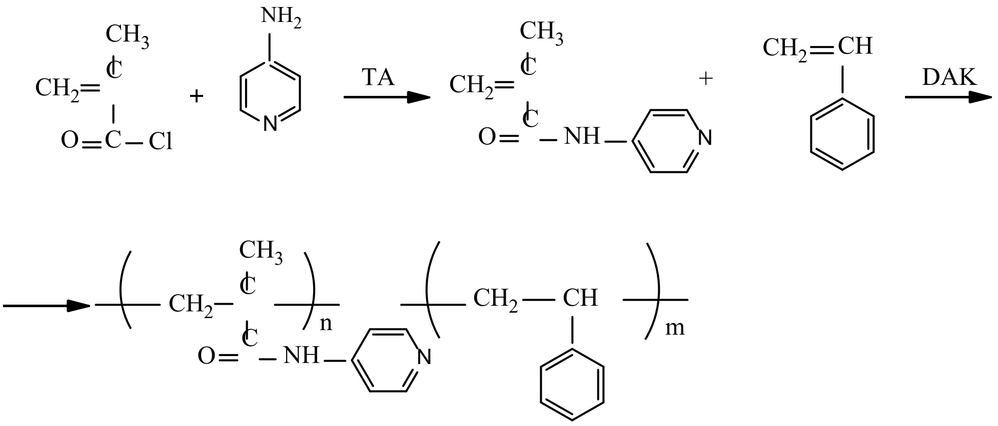
New antimicrobial copolymers containing biocidal fragments were synthesized by corresponding acrylic monomer and copolymerization with styrene different structures were investigated by different spectroscopic methods (IR, NMR).

This work is devoted to the synthesis of a new methacrylic monomer with styrene and the study of the regularities of its radical copolymerization with styrene and some antimicrobial properties of the resulting copolymer.

The synthesis of the new monomer and copolymer was carried out in the following reactions:



Copolymerization of the synthesized monomer with styrene was carried out in ampoules in a mass in a benzene solution in the presence of 0.3 % dinitrilazoisobutyric acid (DAA) of the total monomer mass at 70°C. The total concentration of the starting monomers was constant at 0.2 mol/l, and the ratio of the starting monomers varied over a wide range.

The resulting copolymer was purified by twofold redeposition from benzene solution to methanol and dried in vacuo (10-15 mm Hg) at 30 °C to a standing mass. The resulting copolymer in the form of white powder is well soluble in aromatic and chlorinated hydrocarbons. The characteristic viscosity (ɳ) was determined in benzene in an Ubbelode viscometer, which was 0.75 dl/g. Composition of the copolymer was determined by elemental analysis of nitrogen content.

The copolymerization constants (r_1, r_2) were determined by Feinman-Ross and the parameters were calculated by Alfrei-Price (*Q-e*).

It was shown that para-aminopyridine methacrylate constant r_1 is much more active in copolymerization than styrene r_1=0,85, r_2=0,52. This seems to be due to the influence of the aminopyridine fragment of methacrylate. The antimicrobial properties of the obtained polymer were studied and it was found that this polymer exhibits great antimicrobial properties. It was shown that the antimicrobial properties depend on the copolymer composition. When the macromolecule fragments of aminopyridine methacrylate increase, the antimicrobial properties increase. Thus, synthesized polymer has good antimicrobial properties which can be used in medicine.

PLASTICIZATION OF POLYVINYL CHLORIDE BY BIS-ADDUCTS OF ETHANEDITHIOL WITH ALKYL- AND CYCLOALKYL-SUBSTITUTED METHYLENE DIOXOLANES

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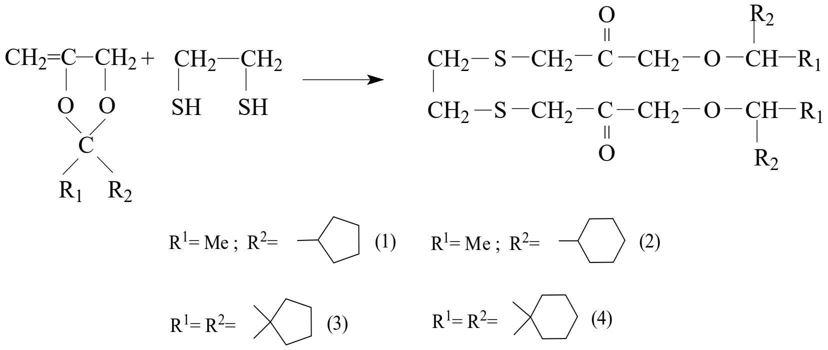
Polyvinyl chloride (PVC), due to a complex of useful technical properties, is used for preparation of a wide spectrum of materials for various purposes. The uniqueness of PVC is that this polymer gives a wide assortment of materials and products characterized by various physical-mechanical and exploitation properties: high resistance to aggressive medium and combustion, low water absorption, absence of unpleasant odor, etc.

Over a period of all term of exploitation, PVC materials and products are subjected to the action of aggressive media of various origins. Therefore, the creation of competitive PVC- plastics meeting the modern technological and operational requirements is of practical interest. In this connection, the problem of creation of the effective plasticizers is very relevant.

In this paper, it has been proposed to use bis-adducts on the basis of alkyl- and cycloalkyl-substituted methylene dioxolanes with ethanedithiol (EDT) as PVC plasticizers [1].

The bis-adducts of EDT with alkyl- and cycloalkyl-substituted methylene dioxolanes have been obtained by radical addition of EDT to alkyl- and cycloalkyl-substituted methylene dioxolanes at 70°C in the presence of azo-*bis*-isobutyronitrile. As a result of the addition reaction, the bis-adducts of linear structure containing ketoester fragments are mainly formed:



The obtained bis-adducts have been tested as PVC plasticizers.

It has been established that the sulfur-containing adducts of the compounds 1-4 are well combined with PVC and therefore their exudation from the composition during long-term storage is not observed.

It has been revealed that the introduction of bis-adducts into the composition of PVC compositions leads to an improvement of the physical-mechanical properties of the compositions. It has been established that the availability of sulfur atoms, carbonyl groups and ether bond in the composition of the obtained bis-adducts gives these compounds an improved plasticizing ability. The high physical-mechanical characteristics of the tested PVC plastics indicate that the compounds introduced into the compositions have plasticizing properties and, therefore, can be recommended for practical use.

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Abstract

ENANTIOSEPARATION STUDY OF OMEPRAZOLE WITH POLYSACCHARIDE-BASED CHIRAL SELECTORS IN HIGH PERFORMANCE LIQUID CHROMATOGRAPHY

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Chiral sulfoxides are mostly used as pesticides, drug compounds, etc. Omeprazole belongs to a class of drugs known as proton pump inhibitors (PPIs). The enantioselective biological activity of chiral sulfoxides is well known and became the reason for developing some of them as enantiomerically pure chiral drugs. Because of this, the separation of enantiomers is an actual matter, and chromatographic methods have been used for this purpose for many years [1, 2].

The goal of the present study was the screening of thirteen polysaccharide-based chiral columns for the separation of omeprazole enantiomers under the following mobile phases: methanol and methanol:water:formic acid 90:10:0.1 (v/v/v). During the research period, we also determined the enantiomer elution order.

The enantiomerically pure analogue of omeprazole is widely used in clinical practice, and it is important to determine whether the content of a minor enantiomer corresponds to the norms. In the present study, a method was derived for the determination of a minor enantiomeric impurity of R-omeprazole in commercially available S-omeprazole formulations (esomeprazole). The most optimal method for the separation of enantiomers was under mobile phase methanol and with column Lux 5u-Cellulose-4.

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EXTRACTING OPTICAL PARAMETERS OF BIOTISSUES BY OPTICAL SPECTROSCOPY OF SKIN *IN VIVO*

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Institute of Cybernetics and the Joe Ann University Clinic is currently conducting a study on the optical characteristics of the skin related to cardiovascular pathologies. This study likely involves using diffuse reflectance spectroscopy (DRS) to analyze tissue composition and determine the optical properties of the skin.

In the context of the study, we are likely using DRS to investigate how cardiovascular pathologies affect the optical characteristics of the skin. They may be comparing the optical properties of healthy skin, as represented by the time-averaged reflectance spectrum shown in Figure 1, with the optical properties of skin affected by cardiovascular conditions.

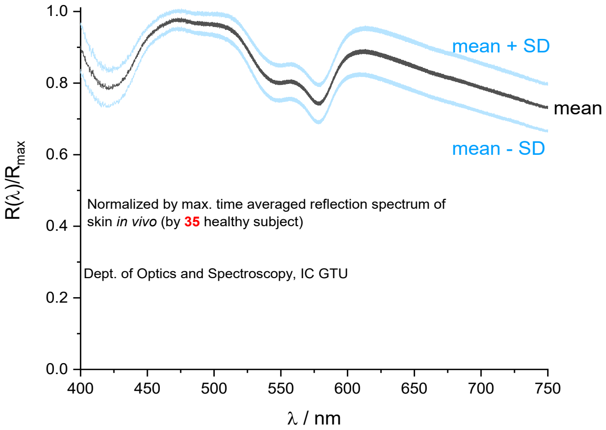

Figure 1. Time-averaged reflectance spectrum of a healthy human

To determine the optical properties of the skin, a mathematical model is used, considering diffuse reflection and taking into account the distance between the light source and the detector. This model is fitted to the experimental data, as shown in Figure 2, to extract various parameters such as the absorption coefficient, blood concentration, average diameter of blood capillaries, oxy- and deoxyhemoglobin concentrations, melanin concentration, and exponent of wavelength dependence of Mie scattering.

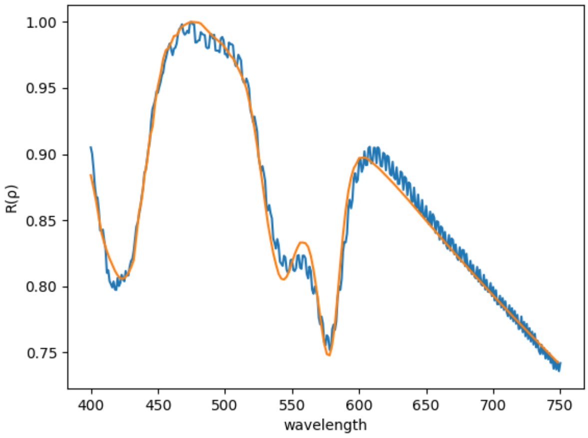

Figure 2. Experimental (zigzag) and fitted (smooth) curves

By studying the optical characteristics of the skin affected by cardiovascular pathologies, we aim to gain insights into how these conditions influence the optical properties of the skin. This research may have implications for the development of non-invasive diagnostic tools or monitoring techniques for cardiovascular health.

ON MACHINE LEARNING ALGORITHMS TO PREDICT THE PROPERTIES OF POLYMER MATERIALS

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Machine learning (ML) has been proved to be useful in various applications thought multiple fields [1-7]. More and more ML algorithms that use statistical models have been applied to predict the properties of polymer materials. They can be used to identify patterns and relationships between the chemical structure of polymers and their properties [8]. Several machine learning algorithms like Random Forests, Support Vector Machines, Artificial Neural Networks, Gaussian Process Regression and Principal Component Analysis were used for polymer property prediction.

In the work we consider each of the above-mentioned algorithms along their application possibilities for polymers-based prediction, define their main characteristics, strengths and weaknesses, in order to simplify the choice based on needs of the user [9].

In addition, in the work there are two different machine learning algorithms Random Forest and Deep Learning compared and contrast for the task of prediction of the glass transition temperature of polymers based on their molecular structure [10].

Finally, it must be noticed that the choice of algorithm depends on the specific task being addressed, the desired level of accuracy and speed as well as the size and quality or dataset used for data processing.

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WOOD POLYMER COMPOSITES ON THE BASIS OF SILYLATED POLYSTYRENE

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Polymer composites are widely used in various applications due to their unique properties such as high strength, durability, and lightweight. However, the widespread use of polymer composites has led to environmental concerns due to their non-biodegradable nature and harmful effects on the environment. To address these concerns, eco-friendly polymer composites are being developed that are biodegradable and sustainable. [1]

In our work, we obtained a new eco-friendly polymer composite based on vinyltrimethoxysililatedpolystyrene (15%, 20%, 25%, 30%, 35%) and bamboo in the presence of various organ /inorganic additives, fire retardants, antioxidants, made at different temperatures and pressures via hot press method at 15 MPa under 200 and 220 Celsius temperatures. The aim of this study is to investigate the mechanical, thermal, and morphological properties of the composite.

The results showed that the addition of bamboo into the polymer matrix improved the mechanical properties of the composite. The tensile strength of the composite increased from 50 MPa to 60 MPa with the addition of 10 wt% bamboo. Moreover, the thermal stability of the composite was also improved due to the presence of bamboo. The composite exhibited good thermal stability up to 300 Celsius. The morphological analysis of the composite using scanning electron microscopy (SEM) showed good interfacial adhesion between the polymer matrix and bamboo particles. [2]

Overall, our study demonstrates that the use of bamboo as a reinforcement in polymer composites based on vinyltrimethoxysililatedpolystyrene can lead to the development of eco-friendly and sustainable materials with improved mechanical and thermal properties. The developed composite has the potential to be used in various applications such as automotive, construction, and packaging industries.

Acknowledgment: The financial support of the Georgian National Science Foundation (Grant #FR-21-4630) is gratefully acknowledged.

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MANGANESE DIOXIDE NANOFILMS FOR SUPERCAPACITORS

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Electrochemical capacitors are becoming promising energy storage systems, especially for high power devices. Supercapacitors are energy storage devices with a higher energy density than conventional capacitors and with a higher power density than batteries. The performance of supercapacitors depends on their electrode material. Among other transition metal oxide, manganese dioxide (MD) is one of most promising, affordable, cheap and environmentally friendly electrode material with high electrochemical activity, high theoretical specific capacitance and wide potential range.

The effect of the presence of Fe (II) or Fe (III) ions in solutions for obtaining thin films of manganese dioxide on their capacitive properties has been studied by the cyclic voltammetry. We have shown in our work that during electrochemical deposition of manganese dioxide on a platinum substrate, Fe^{2+} ions transfer from the electrolyte solution into its structure and dramatically change the electrochemical properties of MD. It was found that the Fe ion-modified MD films have capacitive properties. Based on the experiments, the optimal conditions for film formation were developed. The specific capacity of the obtained films was 500 F/g. As the film thickness changed from 50 nm to 200 nm, the capacity increased in direct proportion, indicating progress of the process across the entire mass, not on the surface. Such behavior is explained by the influence of iron on the structure and properties of the MD.

To study the effect of Fe^{3+} ions on the electrochemical properties of the manganese dioxide, we used a cell with separated anode and cathode spaces. Deposition of the film was carried out on the platinum rotating disk electrode. The highest capacity shown the film obtained at a speed of 400 rpm. The capacity of the films obtained under such conditions was increased to 650 F/g, while the shape of the cyclic voltammetric curve was improved. Experiments have shown that Fe^{2+} ions are electrochemically oxidized, while Fe^{3+} ions are adsorbed on the surface of the manganese dioxide and are introduced into its crystalline structure.

Examination of the samples by X-ray fluorescence and infrared spectroscopy showed that the introduction of iron into the hydroxide groups in the structure of the manganese dioxide increases the length and polarization of the O-H bond. This facilitates the proton jump over the neighboring atom and facilitates the proton migration and diffusion into the solid phase, which improves the electrode properties of the film.

The series of cycles for electrochemically deposited MD film on platinum substrate were recorded for 9 hours and the number of cycles reached 1000. Capacity loss was 10%. After 400 cycles the shape and capacity of the voltammograms practically did not change, thus, the degree of cycling was far from exhausted.

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STUDY OF PELETTES OBTAINED FROM BIOMASS

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The most important problem of world's energy is development of technologies for saving natural energy resources. One of the urgent tasks in this direction is to find alternative sources of energy. Among them, the most time–tested is production of fuel pellets based on the utilization of renewable secondary raw materials and agricultural wastes (biomass).

The main task for us was obtaining of combustible pellets with different compositions using available in Georgia wastes of energy-bearing raw materials such as Caucasian pine cones and their unused seeds, as well as of corn root residues, assessment of physical-chemical, mechanical and technical characteristics, commodity properties of secondary raw materials and of the obtained pellets.

Combustible pellets from Caucasian pine cones, as well as from their compositions with 15% and 35% sawdust were developed and manufactured for heating of various purpose buildings (small boilers, production, energy, household stoves and fireplaces).

The Caucasian pine cones were used by us for production of pellets for the first time. A study of chemical composition of the cones was carried out also for the first time. It is estimated that Caucasian pine cones contain 37.50% polysaccharides, 40.20% lignin and 7.3% polyphenolic compounds, 13.1% of lipids, 11.9% of protein compounds and 0.54% of essential oils. In addition, cones and their seeds contain micro and macroelements, which determines their physical properties. It is also advisable to make biologically active extracts using crushed cones and seeds, and corn root residues (biomass).

Characteristics of the obtained pellets were studied. These were: calorific value 15-17.2 MJ/kg, humidity 10-12%, ash content varies within 3-4.4%, stability (60–95 kg/cm^2). Stability seems to be given by the glue contained in the composition. Their burning duration is 4.5 times higher than burning duration of the original material. These pellets are characterized by a small amount of smoke released during burning and thus they have no negative impact of the environment. Their mechanical and technical characteristics are in compliance with the requirements of the standard. Moreover, the ash obtained as a result of burning of pellets is the best potassium containing fertilizer.

As a result of the performed investigational analysis it can be concluded that on the basis of utilization of renewable secondary and agricultural wastes available in Georgia it is possible to develop and obtain high-calorific alternative briquette fuel. The obtained samples are in line with the standard requirements in terms of economy and ecology. They can be used to obtain additional thermal energy, which provides development of energy efficient technology and reduction environmental burden.

MORPHOLOGICAL AND OPTICAL PROPERTIES OF MANGANESE-DOPED ZINC OXIDE/NANOSILICA DESIGNED FOR THE VISIBLE LIGHT PHOTOCATALYSIS

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The present study`s scope rests on determination of manganese dopant`s role upon optical and, consequently, photocatalytic properties of non-porous crystalline zinc oxide deposited over the nanosilica (SiO_2, $S_{BET} = 380$ m^2 g^{-1}, Evonik). The latter serves as a matrix of the textural porosity (meso- and macropores) controlling formation and growth of the photo-active phase (Mn-doped ZnO) over the amorphous surface. A series of three samples (Mn-ZnO/SiO_2) was synthesized at 3, 6, and 9 mmol of ZnO per gram of SiO_2 using commercially available acetate precursors of manganese or zinc. The samples are designed for the visible light-induced photocatalytic applications in gas and liquid environment.

In order to understand the impact of the Mn dopant upon the optical parameters of the synthesized materials, digital colorimetric analysis and photoluminescence measurements were undertaken. The analysis of morphology and porosity, which are important for the gas-phase photocatalysis in terms of adsorption accompanying the photodegradation, was conducted by means of scanning electron microscopy (SEM) and low-temperature nitrogen adsorption/desorption. The textural properties were calculated via standard BET method (S_{BET}), the maximal adsorption point (V_p) and using the modified Nguyen-Do method (pore size distribution by volume, PSD_V).

With the help of digital colorimetry, the blue component was discovered to be the most aligned with the concentration of ZnO ($R^2_{red} = 0.873$; $R^2_{green} = 0.963$; $R^2_{blue} = 0.999$) (Fig.1a). This can be utilized for in-depth chemometric studies to predict the composition of the subject nanomaterials. All three samples are luminescent ($\lambda_{exc} = 473$ nm) representing the absorbance maxima within $\lambda = 550 - 570$ nm (Fig.1b). The ZnO nanocrystals (< 100 nm) were proven to be well distributed over the nanosilica surface, and their concentrations determined via EDS, were proportional to the fore-mentioned nominal molar concentrations of ZnO. The PSD_V-s revealed that the textural mesoporosity reduced together with S_{BET} (from 160 to 110 m^2 g^{-1}) proportionally to the growing concentration of ZnO. Also, it has been shown, that S_{BET} depends not only on the crystallites` formation and their aggregation, but also on the reduction of the voids among the composite nanoparticles.

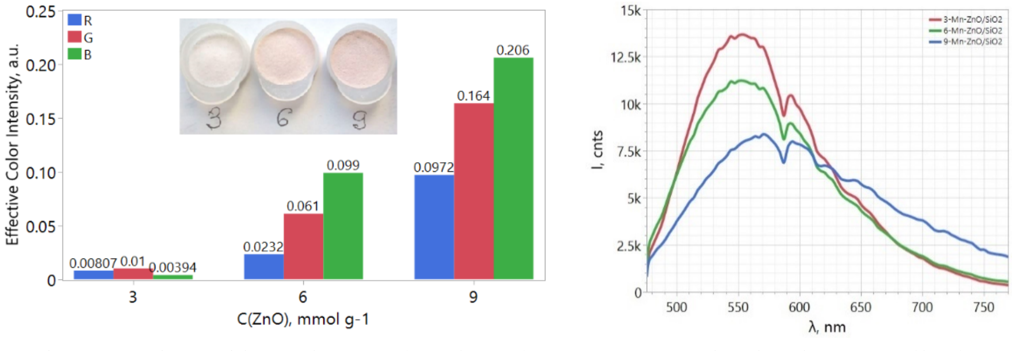

Figure 1. The RGB channel intensity as a function of ZnO concentration in SiO_2: contribution of the color components *(a)*; photoluminescence emission spectra *(b)*

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INTERCALATION OF HEXAGONAL BORON NITRIDE AND GRAPHENE OXIDE BY MAGNETIC CLUSTERS

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Iron(0) pentacarbonyl $Fe(CO)_5$ is widely used to obtain magnetic materials containing ultra-disperse iron of different functional applications. By its impregnation and subsequent transformation, it becomes possible to get nano-zero valent iron and oxides of iron supported in various (organic and inorganic) matrixes. Previously, we carried out chemical transformation of $Fe(CO)_5$ impregnated in porous sorbents and biopolymers. The aim of this work is to intercalate magnetic clusters (Fe and Fe_3O_4) in 2D compounds such as hexagonal boron nitride h-BN and graphene oxide (GO) or reduced graphene oxide (rGO). The structural similarity of these compounds determines the similarity of their chemical properties. h-BN:Fe, h-BN:Fe_3O_4, rGO:Fe and rGO:Fe_3O_4 composites obtained by thermal treatment of h-BN–$Fe(CO)_5$, h-BN–$Fe(CO)_5$–H_2O, GO–$Fe(CO)_5$, GO–$Fe(CO)_5$–H_2O systems in autoclave at 200°C. h-BN doped with ferromagnetic iron (Fe) or its ferrimagnetic oxide – magnetite Fe_3O_4 can serve for delivery agents of boron ^{10}B isotope atoms to cancer cells. Nanopowders of pure h-BN and h-BN:Fe and h-BN:Fe_3O_4 composites were obtained; and their chemical and phase compositions, crystal structure and morphology were investigated (Fig. 1a). In the case of thermal treatment of the GO–$Fe(CO)_5$–H_2O system in an autoclave, rGO is obtained from GO, on which magnetite (Fe_3O_4) is deposited, the particle size of which is 20-60 nm. In this case, exfoliation of GO and formation of bulky rGO:Fe_3O_4 composite powder does not occur, as it happens with vacuum-thermal treatment of GO–$Fe(NO_3)_3$ complex at 130°C. XRD pattern of rGO:Fe_3O_4 composite obtained in autoclave is given in Fig. 1b.

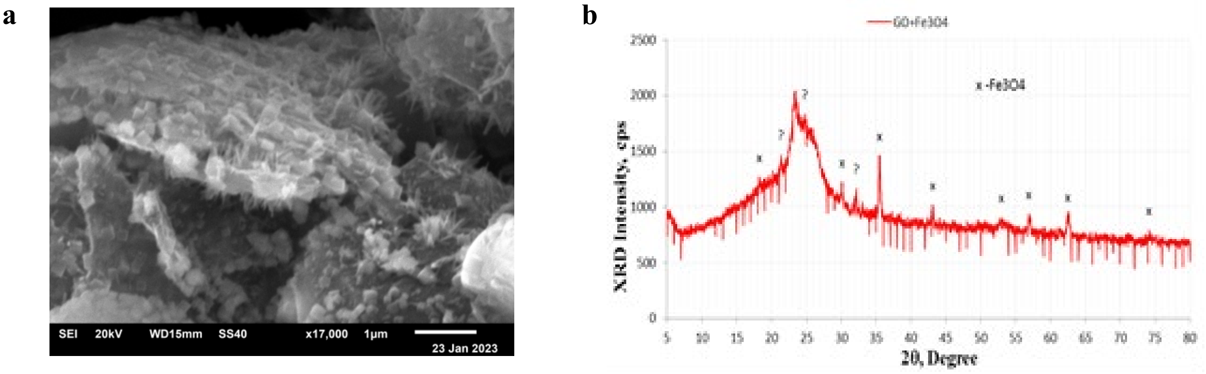

Figure 1. (a) SEM images h-BN:Fe_3O_4 and **(b)** XRD pattern of rGO:Fe_3O_4 composites obtained by thermal treatment of h-BN–$Fe(CO)_5$–H_2O and GO-$Fe(CO)_5$–H_2O systems in autoclave at 200°C.

Magnetization curves at room temperature have also been measured for composites containing a magnetic phase and there are established the numerical values of their main parameters (saturation and remanent magnetizations and coercive force). It is concluded that the nanocomposite powder of hexagonal boron nitride doped with magnetite nanoclusters h-BN:Fe_3O_4 will be an effective nanoagent for delivering boron ^{10}B isotope atoms to tumor cells in BNCT (Boron Neutron Capture Therapy).

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CHARACTERISTICS OF GAS-FILLED PITCH-THERMOPLASTICS

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Gas-filled pitch-thermoplastics are the solid foams in which a pitch-thermoplastic is used as a matrix. Pitch-thermoplastic is a thermoplastic material based on coal tar pitch, which is characterized by polymeric properties [1].

Pitch-thermoplastic is a product of the interaction of coal pitch with active polymers PVC, PMMA in various ratios at a temperature of up to 170 °C. The properties of pitch-thermoplastic depend on the time of heat treatment, consumption and ratio of polymer additives [2,3].

The developed method for pitch-thermoplastic producing allows, by changing the conditions for modifying coal tar pitch, as well as the component composition of active polymer additives, to control its viscosity and thus provide the required characteristics for the foaming process [4].

Gas-filled pitch-thermoplastics were obtained by foaming and subsequent curing of a plastic-viscous composition. The exothermic chemical blowing agent azodicarbonamide (ADCA) was used to foam the pitch-thermoplastic (PTP). Exothermic chemical blowing agents mainly release nitrogen, which is a more efficient blowing gas than CO_2 due to its slower diffusion rate through polymers.

The influence of the pressure, amount of a complex blowing agent (a mixture of azodicarbonamide with zinc stearate) and technological additive $ZnSt_2/CaSt_2$, as well as the viscosity of the pitch-thermoplastic on the maximum foaming ratio of solid foam samples and their properties were determined.

The study of the kinetics of pitch-thermoplastic foaming under a pressure showed that the maximum foaming ratio of the studied PTP samples at a CBA amount of 1-3 phr reached 1.5-2.5. The higher viscosity of the PTP sample led to the lower foaming ratio. The increase of the pressure from 0.145 MPa to 0.265 MPa during the PTP foaming reduced the foaming ratio.

Technological additive surfactant (ZnSt2/CaSt2) reduced the viscosity of the melt (an increase in MFI by 2–3 times), and regardless of the pitch-thermoplastic composition.

The porous structure of solid foams, depending on viscosity and pressure, was characterized by ellipsoidal cells ranging in size from 20 μm to 250 μm, elongated in the direction of material movement from the extrusion chamber opening. With an increase in viscosity and pressure, the cells acquired an irregular (torn) shape.

The authors proved the possibility of using pitch-thermoplastic as a precursor for obtaining solid foams using the chemical blowing agent at relatively low foaming temperature (150°C). Solid foam obtained by pitch-thermoplastic foaming (MFI=4.76 g/10 min) under a pressure of 0.265 MPa was characterized by porosity of 36-42%, apparent density of 760-850 kg/m^3, thermal conductivity coefficient of 0.068-0.073 W/(m·K) and compressive strength in the range of 3.4–3.6 kgf/cm^2.

The received solid foams based on pitch-thermoplastic belong to non-carbonized materials, have heat-insulating properties and are resistant to the action of aggressive environments.

The prospect of pitch-thermoplastic use for the production of a new material - pitch-thermoplastic foams is due to its low cost and excellent ability to be modified with various polymers and additives.

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Abstract

PRODUCTION OF ETHANOL FROM BIOMASS – RESEARCH AND PERSPECTIVES

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Change of climate in the present-day world, being one of the most serious environmental problems, is associated with the "greenhouse effect", caused by a drastic increase in the concentration of carbon dioxide (CO_2) in the atmosphere, the main part of which comes from transport vehicles. This is contrary to the regulations of the Kyoto Protocol and the Rio de Janeiro Climate Convention, which declare significant reductions in greenhouse gas emissions in the 21st century.

Identifying alternatives to fossil fuels is considered an urgent priority for all the developed nations. During the last few decades, the demand for energy increased due to industrialization, increase in population and geopolitical factors. It leads to scarcity of carbon based energy sources which in turn lead to discover a suitable alternative energy source. With agriculture occupying more than 10% of land use, biomass presents a potential resource for the synthesis of ethanol through different methods. This alternative source of bio-energy is found to be renewable, cost-effective, ecologically friendly and can overcome all worldwide problems related to the use of fossil fuels.

Biofuels like biogas, biodiesel, and bioethanol are produced from organic materials, known as biomass. Bioethanol, identified as a sustainable solution to fossil fuel problem, has gained significant attention with an annual global production of 29 billion tonnes.

Conversion of biomass into ethanol presents combined advantages of waste to value conversion and alternative fuel generation. The research interest of bioethanol has not only focused on the issues of energy crises but also provides to the diversification of the economy all the way.

Ethanol is a colorless volatile liquid with a pleasant smell. It is used as solvent and fuel in a wide variety of industries and in healthcare as desinfectant.

Combustible ethanol was obtained by us from agricultural waste. Test samples of ethanol/benzene mixture – E0 (petroleum gazoline) and E5 (5% of ethanol + 95% petroleum gasoline), E10 (10% ethanol + 90% petroleum gasoline) and E20 (20% ethanol + 80% petroleum gazoline) – were prepared and their physical, chemical and technical characteristics were studied. The group composition of the samples was studied on PerkinElmer Spectrum version 10.4.2 and individual composition – on gas chromatograph Crystallux-4000M with NetChrom, v2 software. The effect of bioethanol on the ecological compatibility of the automobile engine has been studied. The objects of research were Regular, Premium and Super brands of petroleum gazoline samples, as well as a of 10%, 20% and 30% bioethanol/gazoline mixtures. The study of the ecological properties of the test additive was carried out at the stand of automobile engines SAK-670 (Germany), on which the engine of a BMW-316 car with coupling sleeve and a transmission assembly was installed. The stand was equipped with brakes and torque sensors, as well as with crankshaft speed and fuel consumption measuring instruments. The test mixtures during an idle running of engine cause a decrease in the CO content in the exhaust gases by 10-16%, and this taking into account their low cost, indicate the prospect of expanding the use of fuel ethanol. The obtained samples were found to meet requirements of EN228 and EN15376 standards.

Thus, it is established that addition of 5-10% of bioethanol fuel to petroleum benzene ensures normal operation of BMV car engine without its modifying. In addition, since the obtained blends contain oxygen, complete combustion of the fuel takes place. And thus, adding of bioethanol the ecological properties of fuel are improved.

Abstract

PATTERNS OF HUMIC SUBSTANCE IN SURFACE WATERS OF UKRAINE

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Humic substances (HS) are the main component of organic matter in surface waters. They are complex ensembles of macromolecules with variable composition and irregular structure and consist of 2 main fractions: humic (HA) and fulvic acids (FA).

The spatial differentiation of the HS content in the surface waters of Ukraine largely corresponds to the law of latitudinal zonation and is closely related to the zonal genetic features of humus formation. Quantitative parameters of HS leaching into water depend on the stock of humus in the soil as well as its fractional composition, which, in turn, is determined by physical and geographical conditions. The analysis of the humus patterns in the main types of soils in Ukraine and the spatial differentiation of HS in surface waters has shown their different direction. The highest humus content is observed in the forest zone, in areas of peat bog soils, whose absorption complex is dominated by H^+ ions. This causes the existence of HS in free form, which can be easily washed away by surface water. The high ratio of C_{HA}:C_{FA} indicates a predominantly fulvate composition of humus.

The average humus content in soils of certain physiographical zones increases from the mixed forest zone to the forest-steppe zone, while in the steppe zone its relative decrease is noted. On the contrary, the content of HS in surface waters decreases as much as twice in the direction from the mixed to the broadleaf forest zone. This is explained by a decrease in free mobile forms of HS due to saturation of the soil absorption complex with bases (primarily Ca^{2+})· which causes humus inertia. While in the coniferous forest zone, 100% of HS is in mobile form, in the broadleaf forest zone it is 20-30%, and in the direction of the forest-steppe and steppe this amount decreases to 15-20% and 10-15%, respectively. Seasonal variations in the content of HS are determined by changes in river water flow.

The Dnipro reservoir cascade is an azonal system. The upper part of the Dnipro basin contains tributaries with the highest water runoff and maximum concentrations of HS. The large mass of humus that enters the first Kyiv reservoir, mainly with the waters of the Pripyat River, is gradually redistributed from the upper to the lower part of the cascade. Intra-water processes that contribute to the formation of planktonic humus play a role in the formation of the HS to.

We have calculated the coefficient of water migration (K_{vm}) for HS. It reflects the ratio of HS content in water to its amount in the surface soil layer. This coefficient was determined by GIS as a weighted average value for each studied basin. Depending on the value of K_{vm}, 3 main zones were identified in which similar conditions are observed regarding the ability of the HS to migrate in water. The selected zones are based on the physical and geographical zoning of Ukraine as the most comprehensive characteristic for determining the factors of chemical substances migration.

The solubility limits of HSs in the soil complex have been identified. FAs are highly soluble substances, thereby ensuring the transport function of HS in the environment. The mass fraction of soluble HA under the most typical conditions for Ukrainian surface waters does not exceed 2.2% what was found experimentally.

The hydrophilic fractions of soil HA with the lowest molecular mass have the greatest ability to dissolve. Because of precipitation, they diffuse into solution and then transported into river systems with water runoff. The most finely dispersed fractions of soil are predominant in the composition of HA and FA of rivers. High-molecular weight, low-dispersed HA particles tend to be retained in the soil formation zone.

DSORPTION OF METHYLENE BLUE BY THE ETHYL CELLULOSE/HALLOYSITE COMPOSITE MATERIALS

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At present, much attention of researchers is paid to composite materials based on biocompatible natural polymers containing inorganic micro- and nanoparticles as fillers. Such composites can be used in various industries due to their unique physical and chemical properties: mechanical, gas barrier, adsorption, resistance to UV radiation.

Among nanosized fillers for polymers, halloysite, which consists of multilayer aluminosilicate nanotubes, is of great interest. The introduction of halloysite nanoparticles into the polymer matrix will make it possible to obtain composite materials for various purposes with improved physico-mechanical and adsorption properties.

The purpose of the current work is to prepare the ethyl cellulose (EC)/halloysite film composites, to study their structure, morphology, and adsorption properties with respect to the thiazine dye methylene blue (MB).

EC/halloysite composites were obtained by mechanical dispersion of layered silicate particles in an ethyl cellulose matrix. The content of the inorganic filler in the composite varied from 0 to 6 wt %.
Studies carried out by scanning electron microscopy have shown that the initial EC films are characterized by a uniform structure. At the same time, aggregates of filler particles of various shapes and sizes are visible on the SEM images of the composite surface.

The adsorption-kinetic characteristics of film composites with different halloysite contents were determined by studying the influence of the contact time between the phases of the adsorbent and the methylene blue solution on the amount of dye in the adsorbent phase. It has been found that the kinetics of MB adsorption on EC films and composites is described by a pseudosecond order reaction equation. The rate constants of the sorption process were determined. It was found that the equilibrium of the process of MB adsorption on the EC film and the EC/(6 wt % of halloysite) composite is described by the Langmuir isotherm. A tenfold increase in the limiting adsorption capacity and the specific surface area of the composite compared to unmodified EC was found.

Studies of the physico-mechanical properties of the obtained polymer-silicate film materials showed that the introduction of halloysite into the ethyl cellulose matrix led to an increase in tensile strength and relative elongation.

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THERMAL PROPERTIES OF NANOCOMPOSITES BASED ON POLYCYANURATE/POLYBENZOXAZINE HYBRID THERMOSETS AND EPOXY-POSS

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Polymer nanocomposites containing polyhedral oligomeric silsesquioxanes (POSS) are of considerable scientific and practical interest because they are characterized by a valuable and improved complex of properties even with a low (<1 wt.%) content of POSS compared to the corresponding microcomposites or individual polymers. In the present study, the structure and properties of novel high-performance thermostable nanocomposites based on polycyanurate/polybenzoxazine (PCN/PBA) hybrid thermosets and epoxycyclohexyl POSS (ECH-POSS) were synthesized and investigated, and the influence of nanofiller content on their final thermal properties was studied.

The nanocomposites were synthesized as follows. At first, the nanofiller ECH-POSS (in the amount of 0.025, 0.05 or 0.5 wt.%) was dispersed in liquid dicyanate ester of bisphenol E (DCBE) (Primaset® LECy, Lonza, Switzerland) with a magnetic stirrer at 165 ºC for 2 h. Then the temperature was decreased to 120 ºC and bisphenol A based benzoxazine (BA) (Araldite® MT 35600, Huntsman Advanced Materials, Switzerland) was added and vigorously stirred for 15 min. The filled compositions were cured from 20 to 300 ºC at a heating rate of 0.5 ºC /min. For comparison, a sample of unfilled PCN/PBA hybrid thermoset was synthesized using the same curing schedule. The ratio between DCBE and BA was equal to 75:25 wt.% for all the compositions synthesized. The thermal properties of the nanocomposites were estimated by DSC and TGA. It was found that the T_g values of the PCN/PBA/ECH-POSS nanocomposites shifted to higher temperatures by 14-21 ºC compared to that of the neat PCN/PBA matrix. TGA measurements have shown that for all the PCN/PBA/ECH-POSS nanocomposites studied an improvement of their thermal stability is observed, and the higher the nanoparticles content, the higher the positive effect is reached.

Acknowledgement: CNRS and NAS of Ukraine are gratefully acknowledged for financial support through French-Ukrainian POLYTHERMAT International Research Project

SYNTHESIS AND CHARACTERAZATION OF PSEUDOPROTEINS MODIFIED BY POLYAMIDES - POLY (ESTER AMIDE-CO-AMIDE)S

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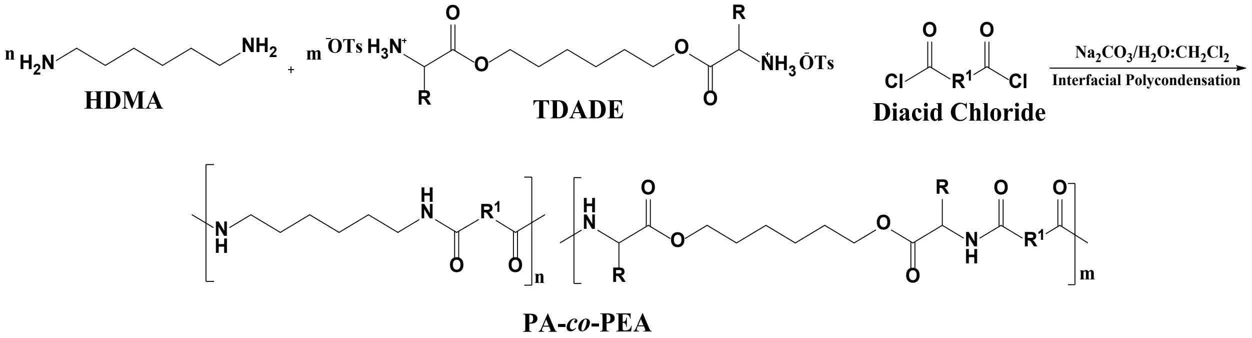
The development of synthetic chemistry in the 20th century was followed by the creation of synthetic polymers, that possessed desirable technical properties and were inexpensive. However, their uncontrolled accumulation and inability to degrade caused environmental problems. This situation increased the demand for materials that could degrade and disappear after fulfilling their intended purpose, without harming the environment. Biodegradable polymers (**BP**) are a category of materials that fit this description. They can break down into natural components, thus minimizing the environmental impact of plastic waste. Among the various types of biodegradable polymers, polyamides (PA), commonly known as Nylons, are noteworthy due to their exceptional mechanical properties resulting from strong intermolecular interactions between the bonds of polymer chains. However, the presence of amide bonds makes PA resistant to degradation [1]. One approach to enhance the biodegradability of polymers is to incorporate better hydrolysable groups into their structure. Pseudoproteins (**PP**) are particularly significant among biodegradable polymers. They belong to a relatively new family of polymers based on natural α-amino acids [2]. PP possess several advantageous qualities, including the non-toxicity of their decomposition products, ease of synthesis, and environmental friendliness. These characteristics contribute to their high technological value and cost-effectiveness.

Poly(ester amide-*co*-amide)s were synthesized by the method of interfacial polycondensations at room temperature between difference ration of monomers: Hexamethyldiamine (HDMA) and Tosyl diamine diesters (TDADE) with various diacid chlorides as depicted in Scheme 1.



Scheme 1. Synthesis of Poly (ester amide-co-amide)s

HMDA is cost-effective, leading to reduced material expenses. The addition of pseudoprotein moiety substantially increases biodegradability. The solubility of the obtained products was examined, and their structures were verified through FTIR and NMR spectroscopy techniques. Furthermore, the mechanical properties were assessed using a Tensile Testing Machine.

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NOVEL CERAMIC-POLYMER BONE CEMENT BASED ON MAGNESIUM PHOSPHATE MODIFIED WITH pHEMA HYDROGEL

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Bone tissue has an innate regenerative potential and the ability to self-healing after various defects. However, using biomaterials dedicated to support regeneration is sometimes advisable and necessary. Due to self-hardening and injectability, bone cements are extremely interesting functional biomaterials that may be applied in minimally invasive procedures. These materials usually consist of a liquid component and a powder component, which, after mixing, form a paste intended for application directly to the treatment site [1]. More recently, research on novel and/or composite kinds has been underway due to various disadvantages of the used cements. Magnesium phosphate cements (MPC) are characterized by a fast setting time, high initial mechanical strength, favorable resorbability and osteogenic potential. However, there are still some problems to solve, such as high brittleness, leachability of the paste and its difficult injectability [2,3]. Therefore, the novel cement formula based on MPC enriched with 2-hydroxyethyl methacrylate (HEMA) was proposed in this work.

The powder component was tri-magnesium phosphate mixed with 0.5 M di-ammonium hydrogen phosphate in a 4:1 mass ratio, and the liquid components were HEMA solutions (15, 20, 25%). The pHEMA polymerization was received by ammonium persulfate (APS, 2.5 µg/mL) and N,N,N′,N′-tetramethylethylenediamine (TEMED, 2.5 µl/mL). The hydrogel reaction started with different premix times (2 or 4 min) before cement components were mixed. The specimens were prepared by manually mixing components (2.5 g/mL powder-liquid ratio) until obtained a homogenous paste, which was then transferred into molds and stored for 24 h (37°C, > 90% humidity). The following properties were tested: setting time, microstructure (SEM microscopy), phase and chemical composition (XRD diffractometry, FTIR spectroscopy), compressive strength, porosity changes and degradation behavior (PBS incubation). Moreover, cytocompatibility was evaluated on human osteoblast cells (hFOB 1.19, ATCC; MTT test).

A novel dual-setting composite cement based on MPC and HEMA was developed in this work. The addition of the hydrogel component significantly influenced the main properties of the cement. It was found that both HEMA content and premix time significantly influenced the formation of hydrogel agglomerates in the cement matrix. Both reactions, polymerization and cement crystallization, were confirmed as effective.The mechanical strength improvement was found for a longer premix time and 15-20% HEMA content.

The cements obtained with a shorter premix time contribute to faster and more effective degradation of the matrix. The observed cytotoxic effect of cultured osteoblasts of MPC-HEMA cements was related to the polymer itself and was probably due to using TEMED as a polymerization agent. Despite obtaining favorable functional and mechanical properties of the developed cement, future research should focus on selecting a different hydrogel additive or HEMA polymerization process.

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STUDY OF BELOUSOV-ZHABOTINSKY REACTION IN WATER DROPLETS OF SODIUM BIS(2-ETHYLHEXYL)SULFOSUCCINATE REVERSED MICROEMULSIONS

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Study of Belousov-Zhabotinsky (BZ) reaction in reversed microemulsions is important from the point of view that the oscillation reaction is studied via nano-sized droplets interacting with each other. In this way, it is possible to observe the nonlinear properties of oscillation reactions not only in individual water droplets, but also in the process of interaction between droplets [1-2]. New features of the BZ-reaction in reversed microemulsions are determined by the concentration of surfactants and the degree of their aggregation, the size of the droplets, the distance between them, etc.

The aim of the work was to study the BZ oscillation chemical reaction in the reversed microemulsions of the anionic surfactant sodium bis(2-ethylhexyl) sulfosuccinate (AOT), in particular, to study the dependence of the induction period of the reaction and concentration fluctuations in the water droplets on the following factors: a) amount of sulfuric acid; b) ratio of sulfuric and chloric acids in their mixture; c) amount of potassium bromate, d) presence of kosmotropic and chaotropic non-ionic additives, e) temperature f) concentration of AOT, etc.

It was found that the induction period of BZ-reaction increases with decreasing concentration of sulfuric acid and potassium bromate, also with increasing of content of perchloric acid in the sulfuric acid-perchloric acid mixture. In addition, influence of some factors, viz. concentration of AOT, also concentration of kosmotropic and chaotropic non-ionic additives causes nonlinear changes in the basic oscillation characteristics of the BZ-reaction in AOT reversed microemulsions.

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Abstract

DETERMINATION OF TECHNOLOGICAL PARAMETERS FOR THE PRODUCTION OF ALUMINUM ALLOYS BY THE METHOD OF "WITHOUT INGOT ROLLING"

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For several years Georgian Institute of Metallurgy and Materials Science has been actively working now to develop the technology of "without ingot rolling". where casting and rolling plant was designed and pilot version constructed. The method is a combination of two independent processes (continuous casting, hot rolling). This work discusses in detail the mechanism for the formation of the primary billet in a combined mold. The article discusses the methodology for determining the basic technological parameters of the process "without ingot rolling " of their relationship with structural, powerful energy parameters and mechanical properties of the work pieces. The values of all parameters and their interdependence are provided in the paper as nomogram. The experiments show that the difference between theoretical computations and experimental data is no more than 5-7%. The specified method has mastered the technology of producing aluminum leaves with a thickness of 8,10,16,22 mm by the method "without ingot rolling."

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QUANTUM-CHEMICAL MODELING OF THE HYDRIDE ADDITION REACTION OF α,ω-BIS(TRIMETHYLSILOXY) METHYLHYDRIDSILOXANE WITH METHYLACRYLATE

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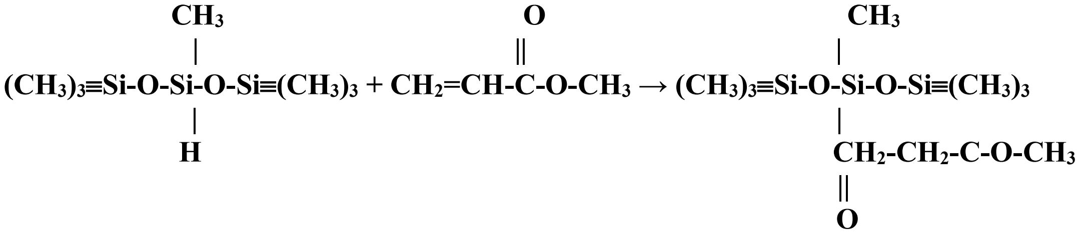
Two possible variants of the bimolecular reaction were considered: according to Farmer's and Markovnikov's rules.

Quantum-chemical calculations were performed using the non-empirical density functional theory (DFT) method. The program "Priroda-04" [1] was used.

For the first time, we discussed a variant of the Farmer's rule.



$$\mathrm{(CH_3)_3{\equiv}Si\text{-}O\text{-}\underset{H}{\underset{|}{\overset{CH_3}{\overset{|}{Si}}}}\text{-}O\text{-}Si{\equiv}(CH_3)_3 + CH_2{=}CH\text{-}\overset{O}{\overset{\|}{C}}\text{-}O\text{-}CH_3 \rightarrow (CH_3)_3{\equiv}Si\text{-}O\text{-}\underset{CH_2\text{-}CH_2\text{-}\underset{O}{\underset{\|}{C}}\text{-}O\text{-}CH_3}{\underset{|}{\overset{CH_3}{\overset{|}{Si}}}}\text{-}O\text{-}Si{\equiv}(CH_3)_3}$$

The dependence of the system energy change (ΔE) on the distance between atoms is shown in **Figure 1.**

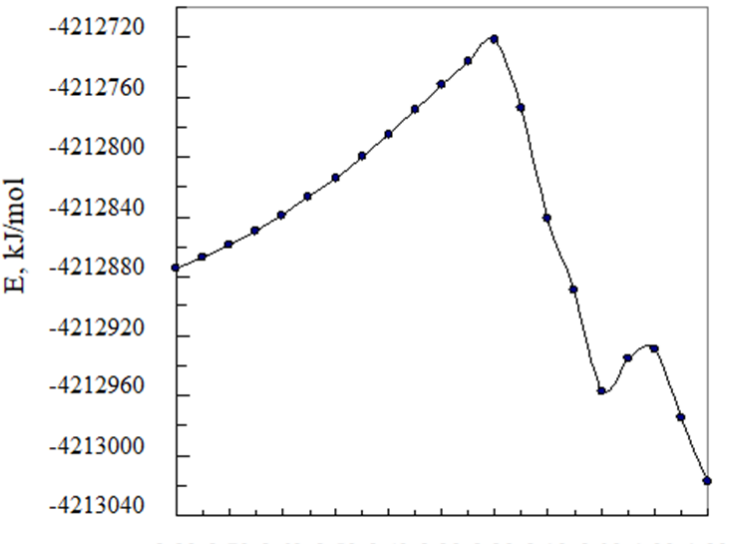
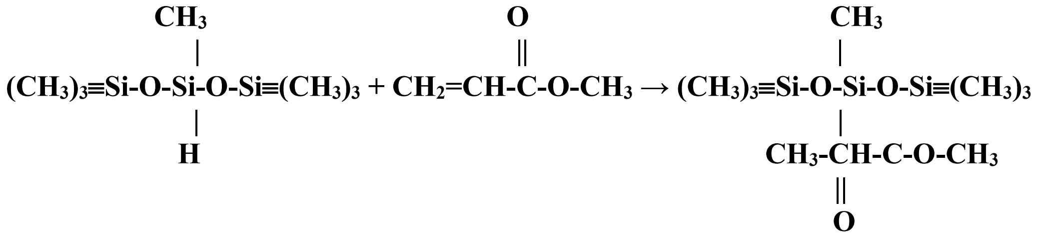


Figure 1. Dependence of system energy change (ΔE) on distance between silicon and carbon atoms ($R_{Si3\text{-}C35}$).

Activation energy ΔE* = 152.90 kJ/mol, and reaction heat effect ΔE = - 142.40 kJ/mol. As we can see, the reaction is exothermic. The second time we discussed the variant of Markovnikov's rule.



$$(CH_3)_3{\equiv}Si\text{-}O\text{-}\underset{\displaystyle H}{\overset{\displaystyle CH_3}{Si}}\text{-}O\text{-}Si{\equiv}(CH_3)_3 + CH_2{=}CH\text{-}\overset{\displaystyle O}{\overset{\|}{C}}\text{-}O\text{-}CH_3 \rightarrow (CH_3)_3{\equiv}Si\text{-}O\text{-}\underset{\displaystyle CH_3\text{-}CH\text{-}\underset{\displaystyle O}{\underset{\|}{C}}\text{-}O\text{-}CH_3}{\overset{\displaystyle CH_3}{Si}}\text{-}O\text{-}Si{\equiv}(CH_3)_3$$

The dependence of the system energy change (ΔE) on the distance between atoms is shown in **Figure 2.**

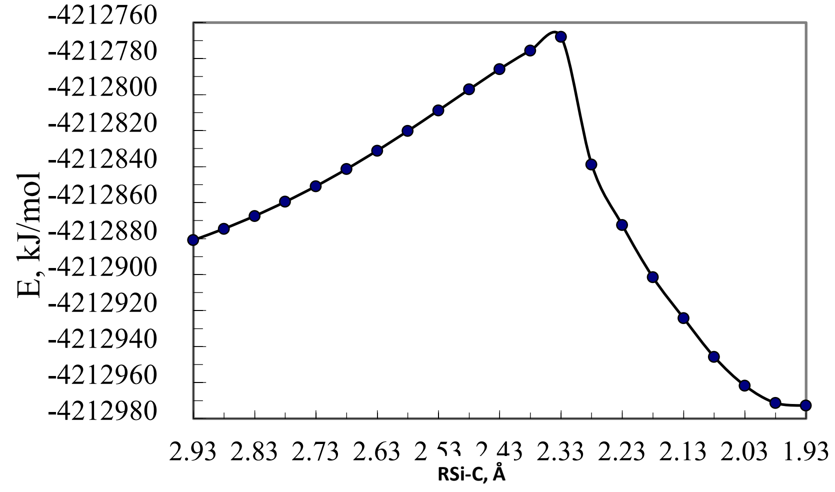


Figure 2. Dependence of system energy change (ΔE) on distance between silicon and carbon atoms ($R_{Si3\text{-}C35}$).

Activation energy ΔE* = 113.00 kJ/mol, and reaction heat effect ΔE = - 91.89 kJ/mol. As we can see, the reaction is exothermic.

Based on the comparison of the activation energies and heat effects of the reaction, the experiment between α,ω-bis(trimethylsiloxy)methylhydridsiloxane and methylacrylate is energetically more favorable with the second scheme[2,3]. The structure of the synthesized oligomer was confirmed by with functional and elemental analysis IR, ^{1}H and ^{13}C NMR spectral data. The order of hydrosilylation reaction, rate constants and activation energy are determined. Synthesized oligomer were studied by DSC, HPLC and wide-angle X-ray methods. The obtained oligomer are transparent products that are well soluble in common organic solvents $\eta_{sp} \approx 0{,}05$. To establish the truth, it is necessary to conduct a simple experiment and use more complete non-empirical methods of quantum-chemical calculations.

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Abstract

STUDY OF MIXED REVERSE MICROEMULSIONS ON THE BASIS OF SODIUM BIS (2-ETHYLHEXYL) SULFOSUCCINATE: APPLICATION IN DRUG RELEASE PROCESS

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Microemulsions prepared on the basis of two different surfactants or mixed microemulsions possess an average degree of hydrophilicity. They also are characterized with properties significantly different from those of the original surfactants separately. Water solubilization capacity, elastic rigidity of the interface, microviscosity of the confined water, percolation of electrical conductance, the dynamics of entrapped water, etc. are considerably changed after mixing [1-3].

The purposes of the proposed work were: i) to study the structure of polyoxyethylene (4) lauryl ether (Brij-30) and sodium bis (2-ethylhexyl) sulfosuccinate (AOT) mixed reverse micelles via with infrared, UV-visible spectroscopy, light scattering and conductivity measurements; ii) use of mentioned mixed microemulsions in the drug release process.

The O-H stretching vibrational absorption spectra in the region of 3000-3800 cm^{-1} were fitted into three subpeaks with the help of a Gaussian curve fitting program. The microenvironment of (AOT+Brij-30) mixed reverse micelles was investigated by UV-visible spectroscopy via o-nitroaniline as optical probe. Electrical conductivity of the reversed mixed micellar solutions was measured with conductometer Orion Star A215.

The microenvironment of mixed reversed microemulsions was investigated with an ultraviolet-visible spectroscopy by using of ortho-nitroaniline and methyl orange as molecular probes. The values of binding constants and association degrees of ortho-nitroaniline and methyl orange with AOT reverse micelles were determined.

Water-induced electrical percolation in reverse microemulsions prepared on the basis of sodium bis (2-ethylhexyl) sulfosuccinate occurs at relatively low values of water/surfactant molar ratio (W) in the presence of additives of nonionic surfactant. Electrical percolation in mixed (ionic and non-ionic surfactant mixtures) microemulsions with a fixed value of water-to-surfactant molar ratio takes place at relatively lower temperature than for reversed microemulsion based on sodium bis (2-ethylhexyl) sulfosuccinate alone. The activation energy of temperature induced electrical percolation was calculated for each investigated microemulsion.

Release profile of promethazine hydrochloride from mixed microemulsion systems was studied. Release of promethazine hydrochloride from aqueous system obeys Fick's diffusion law, but release of promethazine hydrochloride from mixed microemulsions is based on non-Fickian or anomalous diffusion.

Results may be will useful to clarify the complex structure and properties of mixed reverse microemulsions as they widely are applied in mimicking of biomembranes, enzymatic catalysis, drug delivery, extraction processes, etc.

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SYNTHESIS OF LITHIUM TETRATHIOANTIMONATE(V) AND LITHIUM METAANTIMONATE(V)

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The subject of our research was the study of LiOH - Sb_2S_3 - S - H2O interaction products of starting substances.

We took the reactants in molar ratio:

$$\mathbf{LiOH : Sb_2S_3 : S = 9 : 2 : 4}$$

After 5 hour of constant stirring (magnetic stirrer) and heating, the contents of the flask separated into solid (light gray powdery substance) and liquid (golden solid solution) phases.

When maintaining optimal conditions of the process, the yield of lithium metaantimonate(V) exceeds 90%, the non-quantitative precipitation of the latter from the reaction area is explained by its low solubility in the mother solution. It is possible to free the filtrate from lithium metaantimonate(V) by precipitating it with ethyl alcohol and filtering the mother solution. After that, it is not a problem to isolate lithium tetrathioantimonate(V) in its individual state by carefully evaporating the filtrate on a water bath.

This is how the current reaction should be presented as the following:

$$\mathbf{18\ LiOH + 4\ Sb_2S_3 + 8\ S + 46\ H_2O \rightarrow 5\ Li_3SbS_4 \cdot 9{,}5\ H_2O + 3\ LiSbO_3 \cdot 2{,}5H_2O}$$

As a result of the research, it was determined that the transformation products of the LiOH - Sb2S3 - S - H2O system are crystalline hydrate salts containing tetrathioantimonate and metaantimonate anions, molecular formulas of which can be expressed as follows: $Li_3SbS_4 \cdot 9{,}5H_2O$ და $LiSbO_3 \cdot 2{,}5H_2O$

Thus, a new method for the simultaneous synthesis of lithium tetrathioantimonate(V) and lithium metaantimonate(V) crystal hydrates has been developed. Crystal hydrates of lithium tetrathioantimonate(V) and trioxoantimonate(V) represent the products of surmium(III) sulfide oxidation with elemental sulfur in a molar ratio of 5:3.

PREPARATION AND PROPERTIES OF HEMOSTATIC SPONGES BASED ON CHITOSAN WITH MICROPARTICLES AND WATER-SOLUBLE POLYSACCHARIDES

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Current requirements for wound dressings include gas exchange capacity, maintaining of a moist microenvironment, protection of the wound from external microorganisms, absorption of excess fluid and wound exudate. In particular, this material should be comfortable for the patient and easily replaceable with a new dressing [1,2]. Modern wound dressings are designed according to the theory of wound healing, which can maintain wound moisture by absorbing excess fluid from the wound or retaining water. Biomedical sponges are a type of soft and flexible scaffold with interconnected porous structures. Their high swelling capacity and rapid hemostatic capacity make them suitable for preventing exudate accumulation [2,3].

Chitosan (CS) gives significant antibacterial activity against a broad spectrum of pathogenic bacteria and fungi [4]. It can also accelerate wound healing when using as powders, different types of particles, sponges, or with other materials as composite materials [4].

We fabricated, characterized and evaluated a series of cross-linked sponges with different ratios of chitosan to cross-linker (sodium tripolyphosphate, TPP) for potential wound dressings. For CS/TPP ratios of 2:1; 5:1 and 10:1, the structure of the sponges obtained was a combination of lamellae and microparticles. This may be an advantage when using such materials for the fabrication of hemostatic sponges. The presence of microparticles may promote prolonged release of hemostatic drugs. The presence of lamellae may contribute to the strengthening of the hemostatic material.

The use of soluble polysaccharides for wound dressings, such as konjac glucomannan (KG), can provide a moist environment for wound healing, absorb excess exudates, have air permeability, and which make them be readily accepted [5].

Addition of KG substantially increased the swelling ratio of the crosslinked sponges made them suitable for promoting wound healing.

These studies revealed that the CS/KG sponges with microparticles might be used as potential wound dressing materials.

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