MATERIALS RESEARCH SOCIETY OF SERBIA
INSTITUTE OF TECHNICAL SCIENCES OF SASA

Programme and the Book of Abstracts

EIGHTEENTH YOUNG RESEARCHERS' CONFERENCE
MATERIALS SCIENCE AND ENGINEERING

Belgrade, December 4–6, 2019

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&
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Aim of the Conference

Main aim of the conference is to enable young researchers (post-graduate, master or doctoral student, or a PhD holder younger than 35) working in the field of materials science and engineering, to meet their colleagues and exchange experiences about their research.

Topics

Biomaterials
Environmental science
Materials for high-technology applications
Materials for new generation solar cells
Nanostructured materials
New synthesis and processing methods
Theoretical modelling of materials

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Results of the Conference

Beside printed «Program and the Book of Abstracts», which is disseminated to all conference participants, selected and awarded peer-reviewed papers will be published in journal “Tehnika – Novi Materijali”. The best presented papers, suggested by Session Chairpersons and selected by Awards Committee, will be proclaimed at the Closing Ceremony. Part of the award is free-of-charge conference fee at YUCOMAT 2020.

Sponsors

ANALYSIS
LABORATORY EQUIPMENT

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Programme
Eighteenth Young Researchers Conference
Materials Science and Engineering

Wednesday, December 4, 2019

09.00 – 09.30 Opening Ceremony

09.30 – 11.15 1st Session – Biomaterials I
Chairpersons: Prof. Dr. Bojana Obradović and Željko Janićijević

09.30 – 09.45 Characterization of CeO_2-Fe_2O_3 nanoparticles as potential materials for biomedical applications
Šarolta Cako[1], Monika Jażdżewska[2,3], Svetlana Lukić-Petrović[1]
[1]University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Serbia, [2]Adam Mickiewicz University, Faculty of Physics, Poznan, Poland, [3]Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

09.45 – 10.00 Effect of chitosan on the behavior of biological membranes
Agata Ładniak, Małgorzata Jurak, Klaudia Woźniak, Agnieszka Ewa Wiącek
Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University, 20-031 Lublin, Poland

10.00 – 10.15 Synthesis, characterization and toxicity studies of gelatin modified zinc oxide nanoparticles
Željko Janićijević[1,2], Ana Stanković[2], Bojana Žegura[3], Đorđe Veljović[4], Metka Filipič[3], Magdalena Stevanović[2]
[1]University of Belgrade, School of Electrical Engineering, Bulevar kralja Aleksandra 73, 11120 Belgrade, Serbia, [2]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Knez Mihailova 35/IV, 11000 Belgrade, Serbia, [3]Department of Genetic Toxicology and Cancer Biology, National Institute of Biology, Večna pot 111, 1000 Ljubljana, Slovenia, [4]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11120 Belgrade, Serbia

10.15 – 10.30 Osteogenic differentiation of dental pulp stem cells influenced by synthesized calcium phosphate-based nanomaterial *in vitro*
Milica Tomić[1], Sanja Stojanović[1,2], Nenad Ignjatović[3], Stevo Najman[1,2]
[1]University of Niš, Faculty of Medicine, Scientific Research Center for Biomedicine, Department for Cell and Tissue Engineering, 18000 Niš, Serbia, [2]University of Niš, Faculty of Medicine, Department of Biology and Human Genetics, 18000 Niš, Serbia, [3]Institute of Technical Sciences of the Serbian Academy of Science and Arts, 11000 Belgrade, Serbia

10.30 – 10.45 Response of RAW 264.7 macrophages to the presence of bovine bone substitute particles *in vitro*

Sanja Stojanović and Stevo Najman
University of Niš, Faculty of Medicine, Department for Cell and Tissue Engineering and Department of Biology and Human Genetics, Niš, Serbia

10.45 – 11.00 Properties of the Langmuir monolayers of phospholipid-polypeptide on a liquid subphase

Klaudia Woźniak, Agata Ładniak, Kacper Przykaza, Małgorzata Jurak, Agnieszka Ewa Wiącek
Department of Interfacial Phenomena, Faculty of Chemistry, Maria Curie-Skłodowska University, M. Curie-Skłodowska Sq.3 20-031 Lublin, Poland

11.00 – 11.15 Single cell Raman scattering study of mesenchymal stem cells

Jasmina. J. Lazarević[1], Tamara Kukolj[2], Uroš Ralević[1], Diana Bugarski[2], Nenad Lazarević[1], Branko Bugarski[3], and Zoran V. Popović[1,4]
[1]Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade 11080, Serbia, [2]Laboratory for Experimental Hematology and Stem Cells, Institute for Medical Research, University of Belgrade, Belgrade, Serbia, [3]Department of Chemical Engineering, Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade 11060, Serbia, [4]Serbian Academy of Science and Arts, Knez Mihailova 35, Belgrade 11000, Serbia

11.15 – 11.30 Break

11.30 – 13.30 2nd Session – Biomaterials II
Chairpersons: Dr. Magdalena Stevanović and Dr. Nenad Filipović

11.30 – 11.45 Free-standing multilayer films as growth factor reservoirs for wound dressing applications

Adrian Hautmann[1], Devaki Kedilaya[1], Gurunath Apte[1], Sanja Stojanović[2,3], Stevo Najman[2,3], Thomas Groth[1,4]
[1]Department of Biomedical Materials, Institute of Pharmacy, Martin Luther University Halle Wittenberg, Germany, [2]Department of Biology and Human Genetics, Faculty of Medicine, University of Niš, Serbia, [3]Department for Cell and Tissue Engineering, Scientific Research Center for Biomedicine, Faculty of Medicine, University of Niš, Serbia, [4]Laboratory of Biomedical Nanotechnologies, Institute of Bionic Technologies and Engineering, I.M. Sechenov First Moscow State University, Moscow, Russian Federation

11.45 – 12.00 Effect of some biomolecules on the elimination of bubbles coused by decompression in biofluids

Katarina Jovičić Bubalo

Faculty of Mechanical Engineering, University of Belgrade, Serbia

12.00 – 12.15 Morphology, degradation, mechanical and biological properties of PHEMA/gelatin/alginate hydrogels
Jovana S. Vuković, Marija M. Babić, Simonida Lj. Tomić
Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

12.15 – 12.30 Structural, swelling, release and antimicrobial properties of hybrid PHEMA/gelatin/alginate/honey polymeric matrices
Ivana Vučinić, Jovana S. Vuković, Marija M. Babić, Simonida Lj. Tomić
Faculty of Technology and Metallurgy, University of Belgrade, Karnegijeva 4, Belgrade, Serbia

12.30 – 12.45 Chitosan microparticles: optimized synthesis and application
Ksenija Milošević[1], Antonije Mitrović[2], Marija Lučić Škorić[3], Melina Kalagasidis Krušić[2]
[1]ICTM-CCCI, Belgrade, Serbia, [2]TMF, Belgrade, Serbia, [3]ICTMF, Belgrade, Serbia

12.45 – 13.00 Design of the new particles for controlled release of bioactive peptides
Anđela Paunović, Zorica Knežević-Jugović, Jelena Jovanović, Neda Pavlović
Faculty of Technology and Metallurgy, University of Belgrade, Serbia

13.00 – 13.15 Optical and UV-VIS studies of genipin crosslinked chitosan hydrogels for drug delivery of methylene blue
Ana Stanojević[1], Luka Negrojević[1], Đurđa Vukajlović[2], Katarina Novaković[2]
[1]University of Belgrade - Faculty of Physical Chemistry, Belgrade, Serbia, [2]Newcastle University, School of Engineering, Newcastle Upon Tyne, United Kingdom

13.15 – 13.30 Investigation of antioxidant activity of 2-pyridone derivates
Vanja Verușevski, Jelena Lađarević, Dušan Mijin
University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

13.30 – 14.30 Lunch break

14.30 – 16.30 3rd Session – Biomaterials III
Chairpersons: Dr. Djordje Veljović and Sanja Stojanović

14.30 – 14.45 Study on the potential mechanism of anti-inflammatory activity of covalent versus layer by layer immobilized glycosaminoglycans
Hala AlKhoury[1], Adrian Hautmann[1], Frank Erdmann[2], Sanja Stojanović[3,4], Stevo Najman[3,4], Thomas Groth[1,5]

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14.45 – 15.00 Electrophoretic deposition of gentamicin-loaded hydroxyapatite/chitosan biocomposite coating on titanium
Tamara Kovačević, Milena Stevanović, Ivana Matić-Bujagić, Svetlana Grujić, Vesna Mišković-Stanković
University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia

15.00 – 15.15 Surface modification of Ti implants by electrophoretic deposition of hydroxyapatite/chitosan/graphene/gentamicin coating
Milena Stevanović[1], Ana Janković[1], Marija Đošić[2], Maja Vukašinović-Sekulić[1], Vesna Kojić[3], Vesna Mišković-Stanković[1]
[1]Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia, [2]Institute for technology of nuclear and other mineral raw materials, Bulevar Franš d'Eperea 86, Belgrade, Serbia, [3]Oncology Institute of Vojvodina, Faculty of Medicine, University of Novi Sad, Put Dr Goldmana 4, Sremska Kamenica, Serbia

15.15 – 15.30 Morphological changes of the biomedical titanium grade induced by laser treatment in air and nitrogen atmosphere
Slađana Laketić[1], Marko Rakin[2], Miloš Momčilović[1], Jovan Ciganović[1], Ivana Cvijović-Alagić[1]
[1]Institute of Nuclear Sciences „Vinča", University of Belgrade, Serbia, [2]Faculty of Technology and Metallurgy, University of Belgrade, Serbia

15.30 – 15.45 Polymer materials as substitutes in studies on human skin wettability
Joanna Krawczyk, Edyta Rekiel
Marie Curie-Skłodowska University in Lublin, Faculty of Chemistry, Department of Interfacial Phenomena, Maria Curie-Skłodowska Sq. 3, 20-031 Lublin, Poland

15.45 – 16.00 Mg^{2+}/Sr^{2+} co-doping of calcium hydroxyapatite: The effect on mechanical properties
Tamara Matić[1], Ivana Cvijović-Alagić[2], Rada Petrović[3], Đorđe Janaćković[3], Đorđe Veljović[3]
[1]University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia, [2]University of Belgrade, Institute of Nuclear Sciences „Vinča", Mike Petrovića Alasa 12–14, Belgrade, Serbia, [3]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia

16.00 – 16.15 Molecularly imprinted polymers: synthesis and application as therapeutic contact lenses

Filip Koldžić[1], Anamarija Nikoletić[2]
[1]Mathematical Grammar School, Belgrade, Serbia, [2]Faculty of Chemistry, University of Belgrade, Serbia

16.15 – 16.30 Electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol)/chitosan/graphene hydrogels and their applications as wound dressing materials

Katarina Nešović[1], Ana Janković[1], Maja Vukašinović-Sekulić[1], Ljiljana Živković[2], Tamara Radetić[1], Vesna Mišković-Stanković[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, Belgrade, Serbia, [2]University of Belgrade, Vinča Institute of Nuclear Sciences, Mike Petrovića Alasa 12–14, Belgrade, Serbia

16.30 – 16.45 Break

16.45 – 18.00 4th Session – Theoretical Modeling of Materials I
Chairpersons: Dr. Ana Dobrota and Dr. Marko Opačić

16.45 – 17.00 Citrate adsorption on Ag surfaces – establishing a DFT model

Dragana D. Vasić Anićijević
Vinca Institute of Nuclear Sciences, University of Belgrade, Mike Petrovića Alasa 12-14, Belgrade, Serbia

17.00 – 17.15 Tuning charge transfer states in the G-octet-metal ion complexes for the potential nanotechnological applications

Branislav Milovanović[1], Ivana M. Stanković[2], Milena Petković[1], Mihajlo Etinski[1]
[1]University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, [2]University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Belgrade, Serbia

17.15 – 17.30 Cytotoxic activity evaluation, molecular docking and molecular dynamics study of the newly synthesized 3-acetyl-4-hydroxycoumarin derivatives

Žiko Milanović[1], Edina Avdović[2], Dušan Dimić[3], Dejan Milenković[2], Zoran Marković[2]
[1]University of Kragujevac, Faculty of Science, Department of Chemistry, Radoja Domanovića 12, 34000 Kragujevac, Serbia, [2]Institute for Information Technologies, Department of Science, University of Kragujevac, 34000 Kragujevac, Serbia, [3]University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11000 Belgrade, Serbia

17.30 – 17.45 Apparent activation energy changes during structural units crystallization and melting in chalcogenide glass $Sb_{37}S_{45}I_{15}$

Radoš Raonić, Goran Štrbac, Nevena Ćelić, Svetlana Lukić-Petrović

University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000 Novi Sad, Serbia

17.45 – 18.00 DSC method application on analysis of the activation energy variation in crystallization processes of the As_2Se_3 glasses doped with copper
Stefan Jarić[1], Goran Štrbac[1], Dragana Štrbac[2], Svetlana Lukić-Petrović[1]
[1]*University of Novi Sad, Faculty of Sciences, Department of Physics, Trg Dositeja Obradovića 4, 21000 Novi Sad, Serbia,* [2]*University of Novi Sad, Faculty of Technical Sciences, Department of Environmental Engineering and Occupational Safety and Health, Trg Dositeja Obradovića 6, 21000 Novi Sad, Serbia*

18.00 – 18.15 Break

18.15 – 19.45 5th Session – Theoretical Modeling of Materials II
Chairpersons: Dr. Ana Dobrota and Dr. Marko Opačić

18.15 – 18.30 Curving graphene: a path towards enhanced reactivity?
Ana S. Dobrota[1], Igor A. Pašti[1], Natalia V. Skorodumova[2,3]
[1]*Faculty of Physical Chemistry, University of Belgrade,* [2]*Department of Materials Science and Engineering, School of Industrial Engineering and Management, KTH - Royal Institute of Technology,* [3]*Department of Physics and Astronomy, Uppsala University*

18.30 – 18.45 Theoretical investigation of structure and stability of small alkali halide clusters
Milan Milovanović, Marko Mitić, Stanka Jerosimić
University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia

18.45 – 19.00 Numerical confirmation of experimental tension test results during first fracture layer of carbon-epoxy material
Aleksandra Jelić[1], Slaviša Putić[2]
[1]*Innovation Centre, Faculty of Technology and Metallurgy, University of Belgrade,* [2]*Faculty of Technology and Metallurgy, University of Belgrade, Serbia*

19.00 – 19.15 Modeling of the optical gain in ZnO-based quantum cascade lasers
Aleksandar Atić, Jelena Radovanović, Vitomir Milanović
School of Electrical Engineering, University of Belgrade, Serbia

19.15 – 19.30 Numerical modeling of the deformation of steel X52 pipeline wall under pressurized gas flow effect: one way coupling approach of fluid-structure interaction
Zahreddine Hafsi

Laboratory of Applied Fluids Mechanics Process and Environment Engineering, National Engineering School of Sfax, University of Sfax, Sfax 3038, Tunisia

19.30 – 19.45 Leakage area variation through rounded-hole oppenings in visco-elastic piping systems
Oussama Choura, Sami Elaoud
Laboratory of Applied Fluids Mechanics Process and Environment Engineering,
National Engineering School of Sfax, University of Sfax, Sfax 3038, Tunisia

Thursday, December 5, 2019

09.00 – 10.45 6th Session – Nanostructured Materials I
Chairpersons: Dr. Vuk Radmilović and Željko Mravik

09.00 – 09.15 Effect of Gd^{3+} introduction on YF_3: Yb, Er structural, morphological and optical properties

Ivana Dinić[1], Marina Vuković[1], Predrag Vulić[2], Marko Nikolić[3], Olivera Milošević[4], Lidija Mančić[4]
[1]Innovation Center of the Faculty of Chemistry, University of Belgrade, Serbia, [2]Faculty of Mining and Geology, University of Belgrade, Serbia, [3]Photonic Center, Institute of Physics Belgrade, University of Belgrade, Serbia, [4]Institute of Technical Sciences of SASA, Belgrade, Serbia

09.15 – 09.30 Physicochemical properties of ion beam irradiated 12-tungstophosphoric acid

Željko Mravik[1,2], Danica Bajuk-Bogdanović[3], Ana Mraković[4], Ivan Trajić[1], Ljubiša Vukosavljević[1], Davor Peruško[5], Zoran Jovanović[1,2]
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09.30 – 09.45 Impact of the barium tytanyl oxalate precipitation condition on the aggregate formation characteristics

Olha Kovalenko[1], S. Škapin[2], M. Maček Kržmanc[2], S. Tkachenko[3], Ladislav Čelko[3], D. Vengust[2], N. Daneu[2], A. Kocjan[2], H. Hudelja[2], M. Spreitzer[2], S. Umerova[1], S. Ivanchenko[1], D. Baranovsky[1], A. Ragulya[1]
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09.45 – 10.00 Noble metals modified ZnO and TiO_2 for photocatalytic degradation of ceftriaxone using UV and solar radiation

Maria M. Uzelac[1], Nemanja D. Banić[1], Miljan D. Jelušić[1], Lokesh Kesavan[2], Carita Kvarnström[2], Biljana F. Abramović[1]
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Turku, Turku University Centre for Materials and Surfaces (MatSurf), Laboratory of Materials Chemistry and Chemical Analysis, Vatselankatu 2, FI-20014, Turku, Finland

10.00 – 10.15 Photodegradation of atenolol and salicylic acid using composites based on zeolites and TiO_2 nanoparticles
Srna Stojanović[1], Vladislav Rac[2], Mila Vranješ[3], Ljiljana Damjanović-Vasilić[1]
[1]University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, [2]University of Belgrade, Faculty of Agriculture, Belgrade, Serbia, [3]University of Belgrade,"Vinča" Institute of Nuclear Sciences, Belgrade, Serbia

10.15 – 10.30 Nickel doped titanate catalysts for photocatalytic hydrogen generation
Hristina Šalipur, Jasmina Dostanić, Davor Lončarević
University of Belgrade, Institute of Chemistry, Technology and Metallurgy-National institute, Department of Catalysis and Chemical Engineering, Njegoševa 12, 11000 Belgrade, Serbia

10.30 – 10.45 Synthesis of ZnO nanorods by spray pyrolysis for gas sensing application
Ganesh E. Patil and G. H. Jain
Department of Physics, SNJB's KKHA Arts, SMGL Commerce and SPHJ Science College, Chandwad, Dist- Nashik, 423101 India

10.45 – 11.00 Break

11.00 – 12.45 7th Session – Nanostructured Materials II
Chairpersons: Dr. Miloš Milović and Dr. Ivana Dinić

11.00 – 11.15 Development of nanoparticles-in-microparticles system for improved adsorption of arsenate (V) ions from water
Janko Živanić, Aleksandar Marinković, Antonije Onjia, Milan Milivojević
University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

11.15 – 11.30 Strong reversible rubber with self-healing properties, based on polydimethylsiloxane with liquid-crystalline pendant groups
Sabina Horodecka,[1,3] Adam Strachota,[1] Miroslav Šlouf,[1] Alexander Zhigounov,[1] Dana Kaňková,[1] Michaela Vyroubalová,[1] Miloš Netopilík,[1] Beata Mossety-Leszczak,[2]
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11.30 – 11.45 Study of electrical behavior of polymer-nanotubes composites
Dmytro Lykashevych[1], Illia Zhydenko[2], Dmytro Chalyy[2], Ivan Karbovnyk[3], Halyna Klym[1]

[1]Lviv Polytechnic National University, Lviv, Ukraine, [2]Lviv State University of Life Safety, Lviv, Ukraine, [3]Ivan Franko National University of Lviv, Lviv, Ukraine

11.45 – 12.00 Thermally induced microstructural changes in $Fe_{40}Ni_{40}B_{12}Si_8$ amorphous alloy
Milica M. Vasić[1], Tomáš Žák[2], Naděžda Pizúrová[2], Dragica M. Minić[1]
[1]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [2]Institute of Physics of Materials AS CR, Brno, Czech Republic

12.00 – 12.15 Probing subsequent charge density waves in 1T-TaS_2 by inelastic light scattering
S. Djurdjić-Mijin,[1] J. Bekaert,[2] A. Šolajić,[1] J. Pešić,[1] Y. Liu,[3] M. V. Milosevic,[2] C. Petrovic,[3] N. Lazarević,[1] and Z. V. Popović[1,4]
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12.15 – 12.30 Phonon thermal transport suppression in Si/SiO_2 crystalline/amorphous superlattices
Alexandr Cocemasov, Denis Nika
Moldova State University, Chisinau, Republic of Moldova

12.30 – 12.45 Nanostructural study of Ge-Ga-S glasses using multicomponent PAL analysis
Halyna Klym
Lviv Polytechnic National University, Lviv, Ukraine

12.45 – 13.45 Lunch break

13.45 – 15.15 8th Session – New Synthesis and Processing Methods I
Chairpersons: Dr. Nadica Abazović and Dr. Konrad Terpiłowski

13.45 – 14.00 Novel, eco-friendly approach for the oxidative polymerization of aniline using Fe_3O_4 nanoparticles/H_2O_2 catalytic system
Jana Mišurović, Gordana Ćirić-Marjanović
University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, 11158 Belgrade, Serbia

14.00 – 14.15 Electrochemical oxidation of maricite $NaFePO_4$ in mild aqueous solutions as a way to boost its charge storage capacity

Tamara Petrović[1], Miloš Milović[2], Danica Bajuk-Bogdanović[1], Milica Vujković[1]
[1]Faculty of Physical Chemistry, University of Belgrade, Belgrade, Serbia, [2]Institute of Technical Sciences of SASA, Belgrade, Serbia

14.15 – 14.30 The Briggs-Rauscher reaction as an unusual detector for a different type of bronzes

Tijana V. Maksimović[1], Jelena P. Maksimović[2], Tihana M. Mudrinić[3], Zoran P. Nedić[2], Ljubinka G. Joksović[1], Zorica D. Mojović[3], Maja C. Pagnacco[3]
[1]Faculty of Science, Department of Chemistry, University of Kragujevac, Radoja Domanovića 12, 34000 Kragujevac, Serbia, [2]Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, 11001 Belgrade, Serbia, [3]University of Belgrade, Institute of Chemistry, Technology and Metallurgy, Njegoševa 12, 11000 Belgrade, Serbia

14.30 – 14.45 UCST polymers based on dual pH- and thermo- sensitive copolymers obtained by free radical polymerization

Snežana Ilić-Stojanović[1], Zorica Eraković[2], Slobodan Petrović[1], Ljubiša Nikolić[1]
[1]University of Niš, Faculty of Technology, Leskovac, Serbia, [2]Scholar of the Ministry of Education, Science and Technological Development of the Republic of Serbia, University of Niš, Faculty of Technology, Leskovac, Serbia, [3]University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

14.45 – 15.00 Hot forged TiC/Al composite materials

Yulia Shishkina, Stepan Kyryliuk, Genadii Baglyuk, Maria Golovkova
IPMS NASU, Kyiv, Ukraine

15.00 – 15.15 Wettability of doped superhydrophobic silica coatings

Michał Chodkowski[1], Konrad Terpiłowski[1], Olena Goncharuk[2]
[1]Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin, Sq. M. Curie-Skłodowska 3, 20-031 Lublin, Poland, [2]Chuiko Institute of Surface Chemistry NASU, 17 General Naumov Str., Kyiv 03164, Ukraine

15.15 – 15.30 Break

15.30– 17.00 9th Session – New Synthesis and Processing Methods II
Chairpersons: Dr. Lidija Mančić and Dr. Tatiana Demina

15.30 – 15.45 Effect of water cooling system temperature on the cooling rate during solidification in the suction casting process

Krzysztof Pajor, Tomasz Kozieł
AGH University of Science and Technology, Facutly of Metals Engineering and Industrial Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland.

15.45 – 16.00 Optimization of spray drying process for concentrated whey solutions
Luka Stević[1], Darko Jaćimovski[2], Milan Milivojević[1]
[1]*University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia,* [2]*University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Belgrade, Serbia*

16.00 – 16.15 The effect of biopolymer addition on the stability of the emulsion of essential oils
Michał Chodkowski[1], Jakub Matusiak[2], Konrad Terpiłowski[1], Salvador Pérez-Huertas[1], Elżbieta Grządka[2]
[1]*Deartment of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University in Lublin, Poland,* [2]*Department of Radiochemistry and Environmental Chemistry, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Sklodowska University in Lublin, Poland*

16.15 – 16.30 Optimization of parameters of polymeric microparticle fabrication through oil/water solvent evaporation technique
Tatiana S. Demina
[1]*Institute for Regenerative Medicine, Sechenov University, Moscow, Russia,* [2]*Enikolopov Institute of Synthetic Polymer Materials RAS, Moscow, Russia*

16.30 – 16.45 Reaction diffusion model for heterogenous N deacetylation of chitin into chitosan using catalytic alkaline solutions
Bojana Bradić, David Bajec, Andrej Pohar, Uroš Novak, Blaž Likozar
National Institute of Chemistry, Department of Catalysis and Chemical Reaction Engineering, Hajdrihova 19, 1000, Ljubljana, Slovenia

16.45 – 17.00 Development of a regression model for the eccentricity in tube drawing with tilted die process automation
Fariba Heidarian, Heinz Palkowski
IMET, Clausthal-Zellerfeld, Germany, Institute of Metallurgy

Friday, December 6, 2019

09.00 – 10.30 10th Session – Materials for High-technology Application I
Chairpersons: Dr. Dragana Jugović and Dr. Nikhil Dhawan

09.00 – 09.15 Synthesis temperature influence on the structure, morphology and electrochemical performance of Na_xMnO_2 as cathode materials for sodium-ion rechearchable batteries

Lazar Rakočević[1], Jelena Potočnik[2], Mirjana Novaković[2], Dragana Jugović[3], Ivana Stojković Simatović[1]
[1]University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia, [2] University of Belgrade, Vinča Institute of Nuclear Sciences, Serbia, [3]Institute of Technical Sciences of SASA, Belgrade, Serbia

09.15 – 09.30 Electrochemical properties of nanostructured composite $Li_{1.2}V_3O_8$/C in different aqueous electrolytes

Djurdjija Dzodan, Ivana Stojković Simatović
University of Belgrade, Faculty of Physical Chemistry, Belgrade, Serbia

09.30 – 09.45 Ion beam irradiated molybdenum disulfide for improved hydrogen evolution reaction

Jelena Rmuš[1], Ana Mraković[2], Željko Mravik[1], Anđela Mitrović[1], Igor Milanović[1], Ivana Stojković Simatović[3], Sandra Kurko[1]
[1]Laboratory of Physics, CONVINCE, Vinča Institute for Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia; [1]Laboratory of Theoretical Physics and Condensed Matter Physics, Vinča Institute for Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001 Belgrade, Serbia; [3]Faculty of Physical Chemistry, University of Belgrade, P.O. Box 47, 11158, Belgrade, Serbia

09.45 – 10.00 Processing of discarded lithium ion batteries for recovery of cobalt, manganese and lithium values

Nikhil Dhawan
Metallurgical and Materials Engineering, Indian Institute of Technology, IIT-Roorkee, Uttarakhand-247667, India

10.00 – 10.15 Investigation of the 4 MeV C and Si ion channeling implantation influence on the structure of 6H-SiC monocrystal

Marko Gloginjić[1], Srdjan Petrović[1], Marko Erich[1], Aikaterini Flessa[2], Eleni Ntemou[2], Michael Kokkoris[2], Efthymios Liarokapis[2], Stjepko Fazinić[3], Marko Karlušić[3], Kristina Tomić[3]
[1]Vinča INS, Belgrade, Serbia, [2]NTUA, Athens,Greece, [3]IRB, Zagreb, Croatia

10.15 – 10.30 Spin-phonon coupling in $CrSiTe_3$ and $CrSi_{0.8}Ge_{0.1}Te_3$

Ana Milosavljević[1], A. Šolajić[1], J. Pešić[1], B. Višić[1], M. Opačić[1], Yu Liu[2], C. Petrovic[2], N. Lazarević[1], Z. V. Popović[1,3]
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10.30 – 10.45 Break

10.45 – 12.00 11th Session – Materials for High-technology Application II
Chairpersons: Prof. Dr. Rastko Vasilić and Dragan Kukuruzović

10.45 – 11.00 Influence of coating defects on soldering resistance of CrAlN coated HPDC tools

Dragan Kukuruzović[1], Lazar Kovačević[1], Pal Terek[1], Vladimir Terek[1], Branko Škorić[1], Aleksandar Miletić[1], Peter Panjan[2], Miha Čekada[2]
[1]University of Novi Sad, Faculty of Technical Sciences, Novi Sad, Serbia, [2]Jozef Stefan Institute, Ljubljana, Slovenia

11.00 – 11.15 Effects of substrate material and rotation during deposition on topography of nanolayered TiAlSiN coating

Vladimir Terek[1], Lazar Kovačević[1], Aleksandar Miletić[1], Dragan Kukuruzović[1], Branko Škorić[1], Peter Panjan[2], Pal Terek[1]
[1]University of Novi Sad, Faculty of Technical Sciences, Trg Dositeja Obradovića 6, 21101, Novi Sad, Serbia, [2]Jožef Stefan Institute, Jamova 39, 1000, Ljubljana, Slovenia

11.15 – 11.30 Implementation of image analysis for cavitation erosion determination of refractory samples based on talc and domestic zeolite from Igros

Marko Simić[1], Sanja Martinović[2], Milica Vlahović[2], Tatjana Volkov Husović[1]
[1]University of Belgrade, Faculty of Technology and Metallurgy, Karnegijeva 4, 11000 Belgrade, Serbia, [2]University of Belgrade, Institute for Chemistry, Technology and Metallurgy, Njegoševa 12, 11000 Belgrade, Serbia

11.30 – 11.45 The mechanical aspects and the evaluation of the microstructure of the steel-aluminum explosive welded joins

Marcin Ptasiński
AGH University of Science and Technology, Faculty of Metals Engineering and Industrial Computer Science, al. Mickiewicza 30, 30-059 Krakow, Poland

11.45 – 12.00 The effect of additives of ultrafine titanium nitride nanopowder on the structure, phase composition and mechanical properties of chromium carbide steel

Yevhenia Karaimchuk, Vitaliy Maslyuk, Stepan Kyryliuk
Frantsevich Institute for Problems in Materials Science, NASU, Kyiv, Ukraine

12.00 – 12.15 Break

12.15 – 13.45 12th Session – Environmental Materials I
Chairpersons: Dr. Jasmina Dostanić and Dr. Tatjana Savić

12.15 – 12.30 Mechanochemically synthesized cobalt-ferrite and starch-coated cobalt-ferrite nanoparticles as efficient adsorbents for hexavalent chromium removal

Marija Šuljagić[1], Dejan Jeremić[2], Milica R. Milenković[3], Aleksandar S. Nikolić[3], Ljubica Andjelković[1]
[1]Department of Chemistry, IChTM, University of Belgrade, Studentski Trg 12-16, 11000, Belgrade, Serbia, [2]Innovation Center of the Faculty of Chemistry, University of Belgrade, Studentski Trg 12–16, 11000 Belgrade, Serbia, [3]Faculty of Chemistry, University of Belgrade, Studentski Trg 12-16, 11000 Belgrade, Serbia

12.30 – 12.45 Photocatalytic degradation of methylene blue and oxytetracycline via sol-gel synthesized pseudobrookite

Zorka Z. Vasiljević[1], Milena P. Dojčinović[2], Ivona Janković-Častvan[3], Jelena Vujančević[1], Nenad B. Tadić[4], Maria Vesna Nikolić[2]
[1]Institute of Technical Sciences of SASA, Belgrade, Serbia, [2]Institute for Multidisciplinary Research, University of Belgrade, Serbia, [3]Faculty of Technology and Metallurgy, University of Belgrade, Serbia, [4]Faculty of Physics, University of Belgrade, Serbia

12.45 – 13.00 Finding optimal conditions and investigating the structure & morphology of cobalt/magnesium ferrite based cubic spinels ($Co_xMg_{1-x}Fe_2O_4$) as photocatalysts

Milena P. Dojčinović[1], Zorka Z. Vasiljević[2], Nenad B. Tadić[3], Vera P. Pavlović[4], Dario Barišić[5], Damir Pajić[5], Maria Vesna Nikolić[1]
[1]Institute for Multidisciplinary Research, University of Belgrade, Serbia, [2]Institute of Technical Sciences of SASA, Serbia, [3]Faculty of Physics, University of Belgrade, Serbia, [4]Faculty of Mechanical Engineering, University of Belgrade, Serbia, [5]Department of Physics, Faculty of Science, University of Zagreb, Croatia

13.00 – 13.15 Development of nanoparticles-in-microparticles system for improved adsorption of chromium (VI) ions from water

Jelena Drčelić, Aleksandar Marinković, Milan Milivojević
University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

13.15 – 13.30 Mechanism of Rhodamine B photodegradation on hexagonal $ZnIn_2S_4$

Tatjana D. Savić

Laboratory for Radiation Chemistry and Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia

13.30 – 13.45 Biosorption of Cu^{2+} from aqueous solution by alkali modified waste jute woven fabrics

Aleksandra Ivanovska[1], Leposava Pavun[2], Koviljka Asanović[1], Mirjana Kostić[1]
[1]Faculty of Technology and Metallurgy, University of Belgrade, Serbia, [2]Faculty of Pharmacy, University of Belgrade, Serbia

13.45 – 14.45 Lunch break

14.45 – 16.30 13th Session – Environmental Materials II
Chairpersons: Prof. Dr. Ljiljana Damjanović Vasilić and Ana Kramar

14.45 – 15.00 Kinetic and equilibrium study on Cr(VI) removal from aqueous solutions using coconut shell activated carbon as adsorbent

Katarina Stanković, Marija Egerić, Radojka Vujasin, Ljiljana Matović, Daniela Dobrijević, Ksenija Kumrić
Vinča Institute of Nuclear Sciences, University of Belgrade, P. O. Box 522, 11001 Belgrade, Serbia

15.00 – 15.15 Hemp fibers and alginate biocomposite for the nickel ions adsorption

Jana Vujović, Borislav Savovski, Biljana Pejić, Marija Bačević, Milan Milivojević
University of Belgrade, Faculty of Technology and Metallurgy, Belgrade, Serbia

15.15 – 15.30 Glyphosate herbicide adsorption on the cross-linked environmental-responsive hydrogels

Snežana Ilić-Stojanović[1], Zorica Eraković[2], Aleksandar Lazarević[2], Jelena Zvezdanović[1], Ljubiša Nikolić[1]
[1]University of Niš, Faculty of Technology in Leskovac, Republic of Serbia, [2]Scholar of the Ministry of Education, Science and Technological Development of the Republic of Serbia, University of Niš, Faculty of Technology in Leskovac

15.30 – 15.45 Circular economy in textile industry - byproduct of textile bleaching as a novel material for textile wastewater treatment

Ana Kramar, Marina Knežević, Teodora Hajnrih, Mirjana Kostić
Faculty of Technology and Metallurgy, Department of Textile Engineering, University of Belgrade, Serbia

15.45 – 16.00 The application of the immobilized laccase from *Trametes versicolor* in the decolorization of textile dyes

Ana Vukoičić, Marija Ćorović, Dejan Bezbradica

Faculty of Technology and Metallurgy,University of Belgrade, Serbia

16.00 – 16.15 Natural clay pyrophyllite „Parsovići“ as electrochemical sensors for pesticides
Anđela Mitrović[1], Jelena Milićević[2], Sanja Milošević Govedarović[1], Sandra Kurko[1], Tijana Pantić[1], Jelena Rmuš[1], Željko Mravik[1], Jasmina Grbović Novaković[1]
[1]Centre of Excellence for Hydrogen and Renewable Energy, Laboratory of Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, POB 522, Serbia, [2]Laboratory for bioinformatics and computer chemistry, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, POB 522, Serbia

16.15 – 16.30 Synthesis, characterization and application of the zeolite/nano zero-valent iron composite for phosphates adsorption
Tara Veselinović, Ivona Janković-Častvan, Željko Radovanović, Slavica Lazarević, Vukašin Ugrinović, Rada Petrović
Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

16.30 – 16.45 Break

16.45 – 18.45 14th Session – Environmental Materials III
Chairpersons: Dr. Smilja Marković and Kristina Stevanović

16.45 – 17.00 Influence of raw seashells on pH and distribution of selected heavy metals in acidic soil near copper mining and smelting complex
Marija Egerić[1], Ivana Smičiklas[1], Mihajlo Jović[1], Marija Šljivić-Ivanović[1], Biljana Sikirić[2]
[1]University of Belgrade, Vinča Institute of Nuclear Sciences, P.O. Box 522, 11000 Belgrade, Serbia, [2]Institute of Soil Science, Teodora Drajzera 7, Belgrade, Serbia

17.00 – 17.15 Degradation of anthraquinone and sulphonthalein colors using laccase from Myceliophtora thermophila immobilized on primary amino carriers
Jana Vujadinović, Dejan Bezbradica, Marija Stojanović
Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

17.15 – 17.30 Recycling of waste industrial gypsum in different cement composites
Vesna Zalar Serjun, Mateja Štefančič, Ana Mladenovič
Slovenian National Building and Civil Engineering Institute, Ljubljana, Slovenia

17.30 – 17.45 Kaolin modified with cationic surfactant as a potential adsorbent for ketoprofen
Milena Obradović[1], Aleksandra Daković[1], George E. Rottinghaus[2], Milica Spasojević[1], Marija Marković[1]

[1]Institute for Technology of Nuclear and Other Mineral Raw Materials, Franše d' Epere 86, 11000 Belgrade, Serbia, [2]Veterinary Medical Diagnostic Laboratory, College of Veterinary Medicine, University of Missouri, Columbia, MO 65211, USA

17.45 – 18.00 Synthesis and characterization of Brushite-metakaolin-based geopolymer materials

Dunja Đukić[1], Snežana Nenadović[2], Ljiljana Kljajević[2], Vladimir Pavlović[3], Marija Ivanović[2], Miloš Nenadović[4], Miljana Mirković[2]

[1]Faculty of Biology, University of Belgrade, Studentski trg 16, 11158, Belgrade, Serbia, [2]Laboratory for Materials sciences, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001, Belgrade, Serbia, [3]Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Knez Mihailova 35/IV, University of Belgrade, 11000 Belgrade, Serbia, [4]Laboratory for Atomic Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, P.O. Box 522, 11001, Belgrade, Serbia

18.00 – 18.15 The influence of thermodynamic parameters of the alkaline activator on the mechanical properties of geopolymers

Marija Ivanović[1], Dunja Djukić[2], Nataša Mladenović[3], Ljiljana Kljajević[1], Vladimir Pavlović[4], Snežana Nenadović[1], Miljana Mirković[1]

[1]Laboratory for Materials Science, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [2]Faculty of Biology, University of Belgrade, Serbia [3]Laboratory for Nuclear and Plasma Physics, Vinča Institute of Nuclear Sciences, University of Belgrade, Belgrade, Serbia, [4]Institute of Technical Sciences of SASA, Knez Mihailova 35/IV, Belgrade, Serbia

18.15 – 18.30 Alizarin effects on two Iodate-based oscillators

Marko Pavlović[1], Kristina Stevanović[1], Jelena Senćanski[2], Jelena Maksimović[1], Maja Pagnacco[3]

[1]Faculty of Physical Chemistry, University of Belgrade, [2]Institute for General and Physical Chemistry, University of Belgrade, [3]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Serbia

18.30 – 18.45 Application of laccase in degradation of pesticide lindane and textile dyes

Milica Stojković, Dejan Bezbradica, Marija Stojanović

Faculty of Technology and Metallurgy, University of Belgrade, Belgrade, Serbia

18.45 Closing Ceremony

1-1

Characterization of CeO_2-Fe_2O_3 nanoparticles as potential materials for biomedical applications

Šarolta Cako[1], Monika Jażdżewska[2,3], Svetlana Lukić-Petrović[1]
[1]University of Novi Sad, Faculty of Sciences, Department of Physics, Novi Sad, Serbia, [2]Adam Mickiewicz University, Faculty of Physics, Poznan, Poland, [3]Frank Laboratory of Neutron Physics, Joint Institute for Nuclear Research, Dubna, Russia

The purpose of this study was to investigate the structure, morphology and magnetic properties, as well as the cytotoxicity of CeO_2-Fe_2O_3 nanoparticles. Structural characteristics were investigated by X-ray diffraction (XRD) and morphological information was obtained by transmission electron microscopy (TEM). Using Raman spectroscopy, the results obtained by X-ray diffraction were confirmed and complemented with the details provided by this technique. Analysis of magnetic properties was carried out by Mössbauer spectroscopy. Cytotoxicity was determined by MTT assay. X-ray diffraction data showed the presence of CeO_2 phase, while Raman spectrum revealed the presence of γ-Fe_2O_3. TEM images showed nearly spherical particles of about 5 nm, which is in good agreement with the XRD data. Mössbauer spectra indicated the superparamagnetic behaviour of the nanoparticles. Cytotoxicity analysis revealed that the toxicity on the metabolic activity of HeLa cells is minimal, which means that these nanoparticles can be considered as potential materials for biomedical application.

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1-2

Effect of chitosan on the behavior of biological membranes

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Department of Interfacial Phenomena, Institute of Chemical Sciences,
Faculty of Chemistry, Maria Curie-Skłodowska University, 20-031 Lublin, Poland

Recently, chitosan has been one of the most popular polymer used in the medical and cosmetics industry. Its biocompatibility, biodegradability in the human body and lack of cytotoxicity contributed to this. In addition, it exhibits antibacterial and antiviral properties by acting on a broad spectrum of these microorganisms. It is well known that the some polysaccharide characteristics may be enhancement as a result of combining it with other substances of both organic and inorganic nature. On the other hand, the addition of chitosan can improve the properties of materials, thus enabling them to be used in the above-mentioned areas of life.

The basis for product acceptance in the medical, pharmaceutical and cosmetics industries is also durability of the combination of ingredients. Therefore, it is necessary to carry out the research aimed at characterizing the interactions between individual components forming the cosmetic/medical/pharmaceutical product, as well as the behavior of the biological system in their presence.

Compounds called phospholipids quite often occur in living organisms (more precisely in its cytoplasmic membranes or blood). They have a specific - amphiphilic chemical structure and poor water solubility, thanks to that it is possible to study their properties at the different interfaces. Langmuir technique is a very useful analytic method that allows to easily predict the behavior of phospholipids as a result of contact with other substances. Using Langmuir monolayers, it is possible to obtain information on the interactions occur between the components of the aqueous solution/dispersion and the model biological membrane created from phospholipids, and as a result - a possible response from the biological environment.

The aim of the study was to determine the effect of a mixture containing, among others, chitosan on a model biological membrane, based on the changes in surface pressure as a function of area per molecule (compression isotherms) and analysis of compresion modules. The obtained data allow to estimate the type and strength of interactions occurring between individual system components, which can be useful for determining toxicity and biocompatibility. Such analysis will be helpfull to further applications of antibacterial products or skin substitutes.

1-3

Synthesis, characterization and toxicity studies of gelatin modified zinc oxide nanoparticles

Željko Janićijević[1,2], Ana Stanković[2], Bojana Žegura[3],
Đorđe Veljović[4], Metka Filipič[3], Magdalena Stevanović[2]
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Nanostructured zinc oxides are promising materials for numerous biomedical applications where they can serve as therapeutic agents or tools for sensing and imaging. Despite their favorable properties, wider use of zinc oxide nanoparticles in biomedicine is limited by toxicity issues. Therefore, new synthesis approaches should be devised to obtain zinc oxide nanoparticles which are safe-by-design. We present an innovative low-cost wet precipitation synthesis of gelatin modified zinc oxide nanoparticles at the gel/liquid interface. The diffusion of ammonia through the gelatin hydrogels of different porosities induces precipitation of the product in contact with the surface of the aqueous solution of zinc ions. After thermal treatment of the precipitate, adsorbed organic residues of decomposed gelatin act as modifiers of zinc oxide nanoparticles. We characterized the physicochemical properties of obtained gelatin modified zinc oxide nanoparticles by XRD, FTIR, DTA/TG, and SEM. The synthesized nanoparticles show hexagonal wurtzite structure and form flake-like aggregates. FTIR and DTA/TG analyses indicate that the thermal decomposition of adsorbed gelatin depends on the gelatin content of the hydrogel used in the synthesis. We also examined the viability of HepG2 cells, generation of intracellular reactive oxygen species, and genotoxicity using the MTS, DCFH-DA, and alkaline comet assay, respectively. Fabricated gelatin modified zinc oxide nanoparticles show very low toxicity potential at doses relevant for human exposure.

1-4

Osteogenic differentiation of dental pulp stem cells influenced by synthesized calcium phosphate-based nanomaterial *in vitro*

Milica Tomić[1], Sanja Stojanović[1,2], Nenad Ignjatović[3], Stevo Najman[1,2]
[1]University of Niš, Faculty of Medicine, Scientific Research Center for Biomedicine, Department for Cell and Tissue Engineering, 18000 Niš, Serbia, [2]University of Niš, Faculty of Medicine, Department of Biology and Human Genetics, 18000 Niš, Serbia, [3]Institute of Technical Sciences of the Serbian Academy of Science and Arts, 11000 Belgrade, Serbia

Dental pulp stem cells (DPSCs) are mesenchymal stem cells that may have a versatile and abundant application in regenerative medicine and dentistry due to their availability, possibility of isolation from different types of teeth and potential to differentiate into several cell types. In recent years, there is an emerging trend of the use of nanomaterials in medicine and dentistry that, by virtue of their unique properties, have become very attractive as a tool for the treatment of bone tissue defects. The aim of our study was to examine the potential of synthesized nanomaterial, intended for bone tissue engineering and regenerative applications, biphasic calcium phosphate coated with poly-D,L-lactide-co-glycolide (CP/PLGA), to influence the osteogenic differentiation of DPSCs. Cells were obtained from the mature healthy teeth by outgrowth of the cells from undigested pulp pieces during culturing, in standard cell culture conditions. Cells were subjected to osteogenic differentiation for seven and 14 days by culturing the cells with two concentrations of CP/PLGA nanoparticles in the presence or absence of osteogenic supplements in the media. Osteogenic differentiation was assessed by phase contrast microscopy as well as by Von Kossa and Alizarin Red S staining of formed inorganic deposits. The results showed that CP/PLGA influenced osteogenesis in concentration-dependent manner and differently in osteogenic and standard cell culture media. The use of calcium phosphate-based nanomaterials in combination with DPSCs, under certain conditions, could be a promising approach in regenerative medicine and dentistry.

Acknowledgment: This study was supported by the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. III 41017).

1-5

Response of RAW 264.7 macrophages to the presence of bovine bone substitute particles *in vitro*

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Macrophages (MΦs) play a key role in tissue response to implanted biomaterial and determine the biomaterial faith and further course of tissue reaction. MΦs may respond in different ways that depends on the properties of biomaterials and cell/tissue microenvironment. The aim of our study was to examine *in vitro* response of MΦs to Bio-Oss®, a commonly used bovine bone substitute material. Murine RAW 264.7 macrophages were incubated with Bio-Oss® particles in different concentrations for 24 hours (short-term exposure) in standard cell culture conditions. Phagocytic activity and functional activation of MΦs was assessed by phase contrast microscopy, NBT test, MTT test and Neutral red uptake (NRU) assay. Secretion of inflammatory products by MΦs was determined by L929 bioassay. Phagocytosis of Bio-Oss® particles by unstimulated MΦs was not microscopically observed in examined model after short-term exposure that supports the general consideration that Bio-Oss® is a non-resorbable bone substitute material and also is in accordance with some of our *in vivo* results obtained in different animal models. Formation of multinucleated giant cells was observed especially in the case of higher examined concentrations of biomaterial. Reduction of MTT, as a measure of cell metabolic activity, was slightly increased with decreased concentration of biomaterial's particles compared to untreated cells. The same pattern was observed in NRU assay (indicator of pinocytic activity) while the reduction of NBT, as a measure of intracellular superoxide anion production, was increased only in the case of the highest examined concentration of biomaterial's particles. Crystal violet test did not show the reduction in cell number. L929 bioassay showed an absence of secretory inflammatory molecules by MΦs short-term incubated with Bio-Oss® particles. These results indicate that Bio-Oss® was not phagocytable by unstimulated MΦs in examined concentrations and applied model while led to the concentration-dependent functional activation of MΦs that might resulted in the foreign body-like reaction of cells.

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1-6

Properties of the Langmuir monolayers of phospholipid-polypeptide on a liquid subphase

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Using the Langmuir technique coupled with BAM (a Brewster Angle Microscope) properties of the Langmuir monolayers of phospholipid-polypeptide on a liquid subphase were studied. The Langmuir technique enables thin films of amphiphilic substances at the liquid-air interface. Langmuir monolayers are produced and characterized by a Langmuir trough. The classic experiment consists of placing onto the subphase a substance dissolved in an organic solvent and immiscible with water. After the solvent evaporation, during symmetrical compression a monolayer is formed and the π-A isotherm, the dependence between surface pressure and the surface per one molecule in the monolayer, is recorded. The π-A isotherm provides information about the monolayer stability on the surface of the subphase, molecule reorientation, phase transitions and conformation changes. Moreover, BAM facilitates a broad description of films by providing information on emerging domains, their size, shape or density.

The properties and morphology of mixed monolayers of phospholipid 1,2-dipalmitoyl-*sn*-glycero-3-phosphocholine (DPPC) with the polypeptide cyclosporine A (CsA) were studied. DPPC was chosen because is the main building component of biological membranes, while CsA is an immunosuppressive drug used in medicine mainly to the prevention of transplant rejections. From the tissue engineering point of view, it is important to study the interactions between membrane components and the drug.

We hope that these preliminary studies will be helpful in the aspect of designing modern systems of controlled release of the active substance, the development of biocompatible tissue or bone substitute material.

1-7

Single cell Raman scattering study of mesenchymal stem cells

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Mesenchymal stem cells (MSCs) are multipotent adult stem cells present in tissues throughout organism. The International Society for Cell Therapy defines MSCs by three characteristics: adhesion to plastic, expression of specific set of membrane molecules with lack of hematopoietic markers and human leukocyte antigen-DR, and ability to differentiate towards three lineages: osteogenic, chondrogenic, and adipogenic. Having in mind that the isolation process of these cells is not related to ethical issues of any kind, they are potent cell source for tissues engineering and regenerative medicine, meaning that in the near future currently incurable illnesses could be eradicated. Due to various culture conditions, different tissues of origin, donor age, etc. MSCs present heterogenic group of cells. Moreover, before any manipulation, they have to be adequately characterized and purified. Numerous methods and techniques are used for these purposes, but most of them are time-consuming and demanding in terms of sample preparation. Most importantly, many of these techniques are invasive and destructive. Owing to its features, Raman spectroscopy is ideal candidate to become the method of choice for characterization and monitoring of changes occurring in cells, on a single cell level. It overcomes all above mentioned issues. We utilized Raman spectroscopy for tracing changes in MSCs during the fixation process performed with fixatives witch have different chemical mechanism of action, formaldehyde and methanol. Furthermore, this optical technique was employed for probing differentiation status of MSCs after the differentiation was induced towards osteogenic, adipogenic, and chondrogenic lineages.

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2-1

Free-standing multilayer films as growth factor reservoirs for wound dressing applications

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Introduction: Chronic skin wounds place a high burden on patients and health systems. The use of mitogenic growth factors could facilitate the healing process. Unfortunately, they are easily inactivated by the wound environment. We propose layer-by-layer (LbL) based growth factor releasing multilayer films as the basis for a novel wound dressing design.

Experimental methods: Free standing multilayer films were constructed by employing Chitosan and Alginate as opposing polyelectrolytes. 100 bilayers were applied and subsequently crosslinked to create a thick detachable film. Two crosslinking strategies were compared to the non-crosslinked films, using EDC combined with NHS and Genipin. Wetting, swelling, visco-elastic properties and crosslinking density were characterized. After crosslinking, fibroblast growth factor 2 (FGF2) was loaded into the films and its release was evaluated by ELISA. The films were added on top of normal human dermal fibroblasts (NHDFs). For these cells the metabolic cell activity, growth, migration and morphology was studied with the help of MTT and Qblue assays as well as immunohistochemical staining.

Results and discussions: EDC/NHS and Genipin cross-linked films showed improved mechanical strength, while retaining most of their swelling abilities necessary to take up wound exudates. Additionally, they showed sustained release of FGF2, which is beneficial in an oxidative wound environment. All films showed no cytotoxicity. Cell Proliferation and Migration was greatly improved by the cross-linked and FGF-2 loaded films. Genipin cross-linked film demonstrated a slight advantage over the EDC/NHS films. Interestingly the direct contact of films with the cells had a beneficial effect on cell growth compared to equal amounts of soluble FGF2.

Conclusions: The results show that the proposed free standing multilayer films are able to act as a reservoir for the sustained local release of FGF2, which alleviates chronic wounds by stimulating granulation tissue formation. At the same time, they show properties that make them suitable as wound dressings by forming a physical barrier, showing mechanical resistance and swelling capabilities. This makes them a promising starting point for the design of active wound dressing.

2-2

Effect of some biomolecules on the elimination of bubbles coused by decompression in biofluids

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One of the biggest problems with diving is the barotraumatic effect of air bubbles in the bloodstream and tissues. Bubbles can cause mechanical problems such as reduced circulation through the blood vessel, blockage of blood vessels, displacement of tissues, or inducing inflammatory reactions if it stays in the body for too long.

The first part of the research explains the reason for the formation and composition of the bubbles in the body. Key characteristics that influence to bubble formation are given, such as biofluid gas saturation, biofluid surface tension, and viscosity. Then, it was analyzed the physiological impact of the bubbles that can form in the biofluids during and after diving.

In addition, it was explained the potential effect of surfactants on the elimination of bubbles in the bloodstream. It was defined and explained the concept of surface tension and its influence on bubbles. Also, it was given the dependence of surface tension on some fluid characteristics.

It was described Young-Laplace's law that concerning the pressure difference along the boundary of the bubble-biofluid phase. Also, it was analyzed the equations for stress tensor of static and dynamic interface. Finally, it was explained the Maragoni effect, which shows the existence of mass transfer at the interface between fluids due to the surface tension gradient.

2-3

Morphology, degradation, mechanical and biological properties of PHEMA/gelatin/alginate hydrogels

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Focus of tissue engineering is repair, replacement or regeneration of damaged tissue, which occurs as a consequence of various defects, injuries and trauma. The discovery of novel efficient treatment demands multidisciplinary approach, connecting life sciences and engineering for the same purpose. The application of biomaterial scaffolds should offer the support and control of cell growth, as well as the transport of nutrients and methabolic waste, due to porous three-dimensional structure with controlable degradation and suitable mechanical properties. Hydrogels are attractive scaffolding materials owing to their unique compositional and structural similarities to the natural extracellular matrix.

In present study, we synthesized novel hydrogels based on 2-hydroxyethyl methacrylate, gelatine, and alginate, by porogenation and cryogelation method. Morphology and mechanical properties of the hydrogels were investigated by scanning electron microsscopy (SEM) and universal testing machine (Galdabini Quasar). *In vitro* degradation study was conducted during 16 weeks, within the weight loss of the hydrogels was monitored. Antibacterial potential of the hydrogels against Gram-negative bacteria *Escherichia coli* was studied. The MTT test was conducted on L929, HCT 116, and K562 cell lines. Based on the obtained results, the hydrogels have a great potential as biomaterials for tissue regeneration.

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2-4

Structural, swelling, release and antimicrobial properties of hybrid PHEMA/gelatin/alginate/honey polymeric matrices

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Combinations of synthetic and biopolymers have been widely used in medical application due to its biocompatibility, biodegradability and properties that are similar to the human tissues. Gelatin and alginate are biopolymers that are commonly used in wound healing, drug delivery, soft tissue engineering, cell delivery, and in pharmaceutics. HEMA component contributes to preserving the structural integrity of biomaterials. Honey was added as a component contributing to bioactivity.

In this scenario, the present work reveals synthesis and behavior of hybrid PHEMA/gelatin/alginate/honey polymeric matrices. Polymeric matrices based on 2-hydroxyethyl methacrylate and natural polymers of gelatin, alginate and honey were synthesized by the cryogelation. Active agent curcumin was loaded into matrices by the diffusion method. Structural characterization of samples was performed using Fourier transform infrared spectroscopy. Effect of different fraction of honey, as honey and curcumin on the degree of swelling and controlled release of curcumin from matrices were tested. The antimicrobial activity of all samples within and without curcumin for microbial culture *Escherichia coli, Candida albicans* i *Staphylococcus aureus* was examined. The obtained results showed a great potential of the prepared polymeric matrices for tissue regeneration.

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2-5

Chitosan microparticles: optimized synthesis and application

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Chitosan crosslinked particles are very interesting as carriers for controlled release of active substances. Crosslinking of chitosan and producing spherical particles of different dimensions can be accomplished in a number of ways. Desirable crosslinking for pharmaceutical application is established by ionic interactions. In like manner, the most commonly used crosslinker is sodium tripolyphosphate. The degree of particles' crosslinking, and thus the ability to release the active substance, is affected by crosslinking time and the pH of the sodium tripolyphosphate. Also, the particle size, which has the significant influence on the particle release capacity, can be adjusted in several ways, for example choosing the appropriate synthesis method.

In this paper, properties of chitosan particles obtained by emulsion technique and drop-by-drop method were examined. During the particle synthesis by the emulsion technique, concentration of the crosslinker, mixing time, type and content of the emulsifier were varied. Likewise, in the drop-by-drop method, the influence of needle diameter and concentration of the crosslinker was investigated. Optical microscopy and FTIR spectroscopy were used for the characterization of the obtained particles, and their swelling capacity in solutions simulating intestinal and gastrointestinal fluids was examined. The potential use of synthetized particles was studied: 1) as a carrier for controlled release of the active substance with paracetamol as a model drug; 2) as a part of chitosan/polyvinyl alcohol based hydrogels, crosslinked by tripolyphosphate and boric acid, for controlled release of insulin; and 3) as a part of the chitosan/silver nanocomposite system for glucose detection. Encapsulation of paracetamol and insulin was carried out by two different methods: a) dip-coating method and b) *in situ* encapsulation during hydrogel synthesis. In order to determine glucose and insulin concentrations in the solutions, the DNS and Bradford method were used. Presence of glucose and insulin was monitored using an UV/Vis spectrophotometer. The best results were achieved by the particles obtained by drop-by-drop method with the lowest concentration of the sodium tripolyphosphate.

2-6

Design of the new particles for controlled release of bioactive peptides

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Bioactive peptides carry antioxidative activity and have the potential to be used as additives in food formulation. When incorporated, major instability of peptides is imposed within heterogeneous products, as well as the loss of biological activity in the gastrointestinal system before absorption into the bloodstream and manifestation of biological activity at the target site in the body. A good solution as a controlled release system is liposomes – particles made out of phospholipids, natural molecules and a building block of the cell membrane. Therefore, the aim of this study was to prepare new systems for the encapsulation and controlled release of soybean antioxidant peptides.

Liposome preparation was performed by forming a uniform thin film of phospholipon 90-G and hydrating it with an aqueous solution of soy protein concentrate hydrolyzate prepared by a two-step enzymatic process. The last step of liposome preparation was ultrasonic treatment. The size distribution, surface charge, degree of encapsulation and stability of multilamellar liposomes were characterized. A thin film method provided a satisfying percentage of encapsulation of soybean antioxidant peptides (19%). The ultrasonic homogenizer proved to be three times better than the ultrasonic bath while reducing the size of the particles. The antioxidant activity was tested by neultralization of the ABTS • + radical cation method and by Fe2+ ion chelation method. The test have shown that encapsulation of the peptide activity was partially retained. In the simulated gastrointestinal system, diffusion experiments have shown that liposomes slow down the release of antioxidant peptides.

The presented results represent important information for the specific application of liposomes with encapsulated soybean peptides in functional food products.

2-7

Optical and UV-VIS studies of genipin crosslinked chitosan hydrogels for drug delivery of methylene blue

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Series of crosslinked chitosan-genipin hydrogels were prepared with addition of methylene blue. The methylene blue was loaded into the hydrogel solutions prior to polymerisation. The hydrogels were evaluated for swelling and drug release.

The swelling studies were performed in an optical reactor using simulated body fluid at 37˚C for a 24 hour period. The degree of swelling was measured by images taken from 2 cameras which were then analysed using ImageJ software. Results showed that those hydrogels are not swelling, but shrinking. Also, addition of methylene blue changed the rate of shrinking and the shrinking equilibrium value compared to hydrogels without it.

Drug release was investigated by UV-VIS studies. The release of methylene blue from chitosan hydrogels was studied for a 24 hour period in simulated body fluid. The mechanism of release was determined to be diffusion with heavy influence from surface diffusion in the first 30 minutes.

2-8

Investigation of antioxidant activity of 2-pyridone derivates

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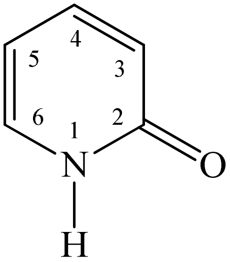
Significant interests in the study of the antioxidant activity of the compounds are the result of the harmful effect of free radicals on humans and animals. Any substance that can delay or completely inhibit oxidation processes, participate as a protection from the various negative effects caused by free radical attacks and has a role in the defense mechanism of the organism is known as an antioxidant. Pyridones are essential heterocyclic compounds present in diverse compounds of natural origin and are believed to be a cause of strong biological activity of these natural substances. In this study, the antioxidative activity of 24 diverse 2-pyridones has been determined, in order to consider the influence of various groups in different positions of the pyridone ring on the activity of the compounds. This activity investigation was accomplished using two tests: ABTS and DPPH. ABTS method involves measuring the ability of the compound to neutralize stabile bis radical cations 2,2'-azino-bis-3-ethylbenzothiazoline-6-sulfonic acid ($ABTS^{\bullet +}$) and DPPH test the ability of the compound to reduce 2,2-diphenyl-1-pykrilhydrazyl (DPPH). Antioxidative activity of 2-pyridones has been analysed considering the various effects of substituents in the positions 1, 3, 4, 5 and 6. According to the results of this study, the derivatives of pyridone with hydroxyl-group in the position 6 are shown to be outstanding candidates for antioxidants. Moreover, it has been established that the compounds with methyl- and phenyl-groups in position 6 have low antioxidative activity.



Structure of 2-pyridone

3-1

Study on the potential mechanism of anti-inflammatory activity of covalent versus layer by layer immobilized glycosaminoglycans

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Biomaterial implants are targeted to improve the patient's quality of life. However, the implantation process can initiate an inflammatory cascade ending with foreign body response (FBR) and fibrous encapsulation. Thus, surface modification may prevent opsonization of biomaterials and suppress this undesirable effect. Macrophages represent key players in orchestrating inflammation. Glycosaminoglycans (GAG) like heparin (HEP) and high molecular weight hyaluronic acid (HA) possess a valuable anti-inflammatory potential related to the inhibition of NF-κB signalling and transcription. Hence, we used here HEP and HA as biomaterials coating which were either covalently immobilized on amino-terminated glass surfaces or physically adsorbed as multilayer system in combination with chitosan (Chi) using the layer-by-layer (LBL) technique. The samples were characerized toward topography and wettability while cell studies examined the anti-inflammatory potentials. Western blotting (WB), internalisation of Fluorescein isothiocyanate (FITC)-labelled-GAG and NF-κB content in macrophages were performed. Immunofluorescence (IF) staining as well as the flow cytometry indicated that FITC-labelled GAGs were internalized by macrophages. Studies with WB together with IF staining of p65 showed also effects on the NF-κB that are related to inhibition of macrophage activation by GAGs. The aforementioned results proved one mechanism of action of GAG by suppressing the NF-κB transcription factor together with their wettability due to the sulphate and carboxylic groups. Overall, both immobilization techniques show promising results for future applications on biomaterial implants to avoid fibrosis.

3-2

Electrophoretic deposition of gentamicin-loaded hydroxyapatite/chitosan biocomposite coating on titanium

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In an effort to reduce dosage of systemic drug administration during major orthopedic procedures due to the rising problems of antibiotic resistance, a novel approach of producing gentamicin loaded coating on titanium implant *via* electrophoretic deposition and subsequent drug-release monitoring of such local administration was investigated.

The research was conducted analyzing requirements of biocompatibility, bioactivity, non-cytotoxicity, good adhesion and antibacterial properties. Titanium plate was used as a substrate due to its high corrosion resistance and good mechanical characteristics. In order to improve Ti bioactivity, a composite coating of hydroxyapatite (HAP), natural polymer chitosan (CS) and antibiotic gentamicin (Gent) was assessed. Composite coatings were successfully formed using cathodic electrophoretic deposition (EPD) from aqueous HAP/CS/Gent and HAP/CS suspensions. EPD was performed under previously determined optimal conditions of 5V and 12 min. Bioactivity of obtained composite coatings was monitored over several time periods of exposure to simulated body fluid (SBF) at 37°C. The biomimetic growth of new apatite layer was evaluated by electrochemical impedance spectroscopy (EIS) and potentiodynamic sweep (PDS) measurements. A qualitative assessment of the coating adhesion properties was done according to ISO 2409 standard for HAP/CS/Gent HAP/CS coatings. Gentamicin release was monitored over a predetermined periods of time. The amount of released gentamicin was quantified by high-performance liquid chromatography–mass spectrometry (HPLC-MS). Formation of a new apatite layer and initial burst release of gentamicin in the case of HAP/CS/Gent biocomposite coating on titanium indicated the high potential for application in medicine.

3-3

Surface modification of Ti implants by electrophoretic deposition of hydroxyapatite/chitosan/graphene/gentamicin coating

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Bone diseases and especially prevalent surgical procedures of total joint replacements in aging population, cause the need for swift development of new biomaterials for bone tissue implants. Nowadays, Ti implants are by far most commonly used in orthopedics, due to their excellent mechanical properties and biocompatibility. Having in mind that biomaterials should stimulate bone tissue regeneration while providing strong support, the Ti implant surface requires modifications to facilitate improved osteointegration. In this work, modification of the titanium surface was carried out by depositing novel composite hydroxyapatite/chitosan/graphene (HAP/CS/Gr) and hydroxyapatite/chitosan/graphene/gentamicin (HAP/CS/Gr/Gent) coatings. Deposition was performed by single-step electrophoretic deposition (EPD) technique from aqueous suspension at constant voltage on pure titanium plates. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR) and field-emission scanning electron microscopy (FE-SEM) were used to characterize obtained composites and to explore the graphene influence on the composites properties. The results of all performed analyses confirmed the formation of new composite HAP/CS/Gr and HAP/CS/Gr /Gent coatings on Ti. Antibacterial activity kinetics against *Staphylococcus aureus* and *Escherichia coli* was performed in order to evaluate the antibacterial properties of obtained composites. HAP/CS/Gr/Gent coating exhibited excellent antibacterial properties, justifying the gentamicin addition to composites. Encouraging results for potential applications were obtained for cytotoxicity testing towards MRC-5 and L929 cell lines. Good biocompatibility of composites was proven towards both cell lines, with slightly more pronounced effect for human MRC-5 cell line. Summarizing the obtained results it could be safe to state that HAP/CS/Gr/Gent composite represents a prospective material for bone implant coating.

3-4

Morphological changes of the biomedical titanium grade induced by laser treatment in air and nitrogen atmosphere

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Cell/tissue interaction with biomaterials can cause damage or rejection of hard-tissue implants; therefore, the proper material surface characteristics are a major requirement for their functionality and extended lifespan in the human body. The commercially pure titanium (CP-Ti) is one of the most biocompatible metallic implant materials used for medical applications. In order to provide specific surface characteristics, which can ensure improved biointegration, the CP-Ti grade 2 was subjected to laser surface modification in air and nitrogen atmosphere. During the material surface irradiation using a picosecond Nd:YAG laser, operated at a 1064 nm wavelength with a typical repetition rate of 10 Hz and as a function of laser pulse energy (5 and 15 mJ) and accumulated laser pulses (50, 150 and 300 pulses), energy was partially absorbed resulting in the appearance of various surface morphological features. These features were examined by light optical microscopy (LOM) and optical profilometry. It was found that the process of laser interaction with the CP-Ti was accompanied by surface melting and plasma formation. Analysis of the morphological changes that emerged as a result of the interaction of laser irradiation with the material, revealed that at a small number of accumulated pulses and low pulse energy the surface damage in the form of shallow craters was induced. An increase in the number of accumulated pulses and the laser pulse energy led to the appearance of more pronounced surface craters, as well as an increase of the damaged area dimensions. The presence of microcracks and hydrodynamic effects was detected. Moreover, the increase in the number of accumulated pulses led to an increase of the damage degree along the depth of the material, as well as the increase of the surface roughness. The higher damage degree was achieved in the nitrogen atmosphere, while the higher surface roughness was observed after the irradiation in air. Based on the obtained results, it can be concluded that the laser irradiation in the nitrogen atmosphere resulted in the appearance of the more pronounced surface morphological features which can show a higher impact on the material biointegration abilities.

3-5

Polymer materials as substitutes in studies on human skin wettability

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Skin is the largest organ in the body. It plays many different and important roles, especially in human sensing of the surrounding world. Skin is the most efficient barrier in protecting against harmful environment and UV radiation. Nerve endings located in skin inform about heat, pain and cold. Skin is responsible for many autoimmune responses, helps in maintaining proper balance of fluids and electrolytes as well as allows to control temperature of the organism [1-2]. Human skin surface properties contribute to adsorption of cosmetics, such as creams, salves or ointments containing drugs. Adsorption as well as wetting process of the skin are the key for proper skin permeability (especially for microorganisms), protecting natural skin ecosystem and stability of the lipid barrier [3].

Most of the cosmetic formulations are based on water. Water has a naturally high surface tension (72.8 mN/m) which causes lack of spontaneous wettability. To obtain better conditions of this process, many surfactants are used. They have close contact with human skin, sometimes causing allergies and immune responses. Wettability of the skin surface is quite poorly investigated because of high individuality of skin composition. For many investigations and researches, human skin is substituted by polymers such as PTFE or PMMA [4].

Measurements of contact angle of aqueous solutions of some anionic, cationic and non-ionic surfactants as well as formamide, diiodomethane and water as model liquids were performed. Obtained results were compared with the values obtained for polymeric materials: PMMA and PTFE.

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3-6

Mg^{2+}/ Sr^{2+} co-doping of calcium hydroxyapatite: The effect on mechanical properties

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Calcium hydroxyapatite (HAP) is the main mineral component of human bones and teeth. HAP is never found pure in nature due to its flexible lattice that allows a wide variety of ion substitutions. Magnesium ions are found to promote cell proliferation and mechanical properties of HAP, while strontium ions decrease bone resorption and enhance bone formation. Upon heating above 800 °C pure HAP undergoes phase transformation to β–TCP and, if heated further above 1150 °C it transforms to α–TCP phase. Substitution of Ca with smaller ions such as Mg, or larger ions, such as Sr, raises strain in the HAP lattice which favours phase transitions. The presence of Mg ions stabilizes β–TCP phase during heating, unlike Sr ions that stabilize α–TCP phase, which result in impaired mechanical properties. The aim of this study was to investigate mechanical properties of Mg/Sr co-doped HAP with different Sr^{2+} and Mg^{2+} content and its potential use as a bone and dentin substitute. Nanostructured Sr/Mg-HAP powders were obtained hydrothermally, pressed into cylindrical compacts and sintered at 1200 °C for 2 h. Hardness by Vickers and fracture toughness values of sintered compacts were found to be the greatest when Ca^{2+} ions were simultaneously substituted with 3 mol. % Sr^{2+} and 3 mol. Mg^{2+} or 5 mol. % Sr^{2+} and 3 mol. % Mg^{2+}.

3-7

Molecularly imprinted polymers: synthesis and application as therapeutic contact lenses

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Eye drops are the most used type of medication for eye diseases, but only a small part of the drug reaches the infected area due to the intense draining effect of blinking and lachrymal fluid removal. Hence, patients need to take large amounts of medication. This problem could be overcome by extending the duration of a drug's spent time on the eye surface. The most common eye disease is conjunctivitis, which is usually caused by infection, as a consequence of poor hygiene. One of the most efficient drugs for conjunctivitis treatment is chloramphenicol. Because of their unique properties, hydrogels are used for contact lens production. The aim of this research was the synthesis of new hydrogels molecularly imprinted for chloramphenicol and the investigation of their potential application as therapeutic contact lenses. The influence of different comonomers on hydrogel's loading and releasing properties was investigated. Six various poly(2-hydroxyethyl methacrylate) (HEMA) based hydrogels imprinted for chloramphenicol were successfully synthesized. Five of them meet the norms for soft contact lens material. The swelling and releasing kinetics were studied at conditions that represent the human eye. It was proven that HEMA copolymer with methacrylic acid was the most efficient for releasing of chloramphenicol, almost linearly during a 24-hour period. This suggests that synthesized hydrogels present a promising solution to the problem of sustained chloramphenicol delivery.

3-8

Electrochemical synthesis of silver nanoparticles in poly(vinyl alcohol)/chitosan/graphene hydrogels and their applications as wound dressing materials

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The need for constant improvements of wound dressing materials and advancement of their properties is an ever-present element of (bio)materials science research. The biomaterials field is always evolving towards finding new wound dressing formulations which can provide active protection of the wound from bacterial infections, rather than just being a passive barrier for infiltration of bacteria. Hydrogel-based materials are especially interesting for such a purpose, considering their favorable biocompatibility, sorption and mechanical properties, as well as the potential for immobilization and incorporation of antibacterial agents, such as silver nanoparticles (AgNPs). In this work, we attempt to synthesize new wound dressing materials based on poly(vinyl alcohol)/chitosan (PVA/CHI) hydrogels with electrochemically synthesized silver nanoparticles. The electrochemical synthesis parameters (time, voltage, resistance) were varied in order to ensure optimal conditions, whereas the different amounts of chitosan in the hydrogel were pursued to elucidate the effect of CHI on the AgNPs synthesis. Thus obtained nanocomposite hydrogels were characterized using UV-visible spectroscopy, transmission electron microscopy and dynamic light scattering in order to confirm the successful incorporation of AgNPs. Further, the kinetics of swelling and silver release were monitored in the simulated physiological conditions (phosphate buffer, 37 °C) and subsequently fitted with several models that helped resolve the governing mechanisms of swelling and release. Finally, the potent antibacterial properties of the obtained silver/poly(vinyl alcohol)/chitosan (Ag/PVA/CHI) hydrogels were confirmed using quantitative test in suspension against two most common wound infection culprits – *Staphylococcus aureus* and *Escherichia coli*. The obtained results indicated that the prepared materials could be used as active wound dressing materials with improved properties.

4-1

Citrate adsorption on Ag surfaces – establishing a DFT model

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Ag nanoparticles stabilized by citrate capping have various biomedical applications as imaging agents, drug delivery agents, in biolabelling and immunosensing. Citrate adsorption on metallic Ag surface, playing an important role in any of these applications, can be studied by DFT as an attratctive, cheap, computational method. On the other hand, large size and negative charge of the system are somewhat discouraging. In this contribution, a DFT-GGA method using plane wave basis set is applied to study adsorption of citrate on different Ag surface models, including: 1-Ag-atom model, Ag - cluster and periodic Ag111 surface. Adsorption energetics and charge distribution were analyzed, depending on the surface model and the initial charge (i.e. ionic state) of the citrate anion. Results are discussed in view of the available literature data in order to evaluate their reliability, and make a step towards establishing a general model to study the adsorption of more complex, biologically important molecules on nanoparticle surfaces, using computational chemistry methods.

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4-2

Tuning charge transfer states in the G-octet-metal ion complexes for the potential nanotechnological applications

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At the telomeric, guanine (G) rich region of the DNA, non-canonical biologically relevant nanostructures can be formed including G-quadruplexes. To further improve their stability, binding of the monovalent/bivalent cations is also possible within the G-quadruplex cavity. Due to their unique topological pluralism and self-assembly tendency, they can be used to prepare functional supramolecular assemblies. These structures can be easily integrated in nanodevices. Exploring their excited state properties is of interest for the application in the molecular electronics and optoelectronics. Here we study G-octet-metal ion complexes ($M-G_8$) which act as models for the G-quadruplex supramolecular arrangement within DNA. We used DFT based molecular dynamics (BLYP-D3/DZVP+PW+GTH) for the configuration sampling purposes and calculated electronic excitations to initially populated (Franck-Condon) states. We use descriptors based on one-electron transition density matrix to seize charge transfer content of the selected excited states. We use TDDFT formalism (CAM-B3LYP/6-31G(d)) to calculate one-electron transition density matrices and absorption spectrum. Results indicate that the $M-G_8$ ($M=Li^+$, Na^+, K^+, Mg^{2+}, Ca^{2+}) systems absorption spectrum is slightly modulated by introducing alkali metal ions compared to the empty scaffold. On the other hand, earth-alkali metal ions have somewhat larger impact on the broadness and the red tail of the spectrum. Beside this, charge transfer content is highly modulated and shifted towards lower energies for the $Mg^{2+}-G_8$ and $Ca^{2+}-G_8$ systems making them accessible more easily. This feature is not in the correlation with structural arrangement but probably with charge of the templating cation. These results indicate that earth-alkali $M-G_8$ complexes are more suitable for potential technological applications.

4-3

Cytotoxic activity evaluation, molecular docking and molecular dynamics study of the newly synthesized 3-acetyl-4-hydroxycoumarin derivatives

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In this contribution, we have prepared new coumarin derivatives, namely 3-(1-((3-chlorophenyl) amino) ethylidene)-chroman-2,4-dione (L1) and 3-(1-((4-chlorophenyl) amino) ethylidene)-chroman-2,4-dione (L2), in reaction between 3-acetyl-4-hydroxycoumarin and *-meta* and *-para* chloraniline. The obtained compounds were characterized using spectroscopic techniques (^{1}H NMR, ^{13}C NMR, IR) in combination with theoretical methods (DFT). *In vitro* anticancer potential of investigated compounds was determined by the MTT assay on human colorectal carcinoma, HCT-116. The results have shown that L2 is more potent substance towards this cell line. Vascular endothelial growth factor A (VEGFA) receptor was chosen for molecular docking and molecular dynamics studies. Several studies have previously shown that VEGFA represents potential therapeutic target for the treatment of variety of tumors such as colorectal. Based on the thermodynamic parameters, obtained after molecular docking and during molecular dynamics simulation time, it is was observed that VEGFA-L2 complex had lower binding free energy and higher value of the inhibition constant than VEGFA-L1. This means that L2 compound shows better inhibitory activity towards VEGFA receptor than L1. Investigated compounds form several types of interactions in the active site of protein, such as conventional hydrogen bonds, hydrophobic and electrostatic interactions. These interactions are established between polar functional groups and aromatic rings of investigated compounds and amino acids of VEGFR receptor: B:ILE22, B:CYS53, C:THR24, C:LEU25, C:ASP27, and C:CYS44. Based on the results, obtained *in vitro* and in theoretical studies, it can be concluded that the obtained compounds are promising anticancer agents.

4-4

Apparent activation energy changes during structural units crystallization and melting in chalcogenide glass $Sb_{37}S_{45}I_{15}$

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In this paper analysis of thermally stimulated processes of crystallization and melting in $Sb_{37}S_{45}I_{15}$ chalcogenide glass were carried out. The investigated glass composion was analyzed by a non-isothermal differential scanning calorimetry, whereby different heating rates have been applied. Apparent activation energies were determined using the Vyazovkin and Kissinger isoconversional methods, and the changes in activation energy as a function of extent of conversion and temperature were examined. Crystallization of $Sb_{37}S_{45}I_{15}$ has shown complex character and it has consisted of crystallization of at least two structural units, SbSI and Sb_2S_3, at close temperatures. Obtained results indicate that the crystallization of SbSI increases with extent of conversion from about 100 kJ mol^{-1} to 160 kJ mol^{-1} while analysis of crystallization of Sb_2S_3 structural unit has shown that the activation energy first increases and then remains approximately constant during the process with value of about 165 kJ mol^{-1}. Crystalizations of two structural units affect each other. Analysis of the melting process of the SbSI structural unit has shown that it is not a single step process and that the energy decreases with the increase in the extent of conversion. The values of activation energies obtained by using the equations given by Vyazovkin and Kissinger were in accordance.

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4-5

DSC method application on analysis of the activation energy variation in crystallization processes of the As_2Se_3 glasses doped with copper

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In this paper the isoconversional analysis of thermally stimulated process of crystallization in As_2Se_3 chalcogenide glass doped with 1, 5, 10 and 15 at. % of copper has been realized. Experimental results were obtained by differential scanning calorimetry under non-isothermal conditions at different heating rates. The analysis has been performed according to three different methods in order to determine variability of the apparent activation energy with the extent of transformation: advanced isoconversional method proposed by Vyazovkin, and isoconversional forms of relations of Kissinger and Moynihan. The crystallization processes of three structural units from two glass compounds have been analysed: As_2Se_3 unit (in $Cu_1(As_2Se_3)_{99}$ composition), $CuAsSe_2$ and Cu_2Se (in $Cu_{10}(As_2Se_3)_{90}$ composition). All three isoconversional methods gave similar results with respect to the detected measurement uncertainties. Effective activation energy shows decreasing trend with increase of the extent of transormation for As_2Se_3 and $CuAsSe_2$ units. For Cu_2Se structural unit effective activation energy showed increase at first, then slight decrease with increase of the extent of transformation. Obviously, this tendency has been dictated by the incomplete crystallization of the $CuAsSe_2$ structural unit.

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5-1

Curving graphene: a path towards enhanced reactivity?

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The world is facing serious energy-related issues and the pursuit for novel materials which will help solve them is in place. Pristine graphene is chemically inert, *i.e.* it interacts rather weakly with species of interest in the world of novel energy conversion and storage systems. These species include metal ions (for metal-ion batteries applications) and hydrogen (for hydrogen production and storage). As graphene is quite unique in terms of many of its properties, different strategies are being developed with the goal of making it more reactive towards the aforementioned species. It is known in Materials Science that deviations from perfection can lead to new achievements. Therefore, defects in the form of dopant atoms and/or functional groups are often introduced to graphene in the attempt of targeted tuning of its electronic structure and reactivity. However, another plausible strategy is curvature of the graphene layer. In this contribution, using Density Functional Calculations we demonstrate the effects of introducing strain (up to ±5%) into the graphene layer, and how it combines with the presence of N and P dopants. We probe the reactivity of non-doped, N-doped and P-doped strained graphene with H and Na, as the representatives of covalent and ionic interactions with graphene, which are of great electrochemical interest in energy conversion and storage applications.

5-2

Theoretical investigation of structure and stability of small alkali halide clusters

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Clusters are small stable or metastable groups of atoms, which exhibit collective properties different from those of constituting atoms, and by general properties clusters are between molecules and bulk materials. Investigation of clusters is significant because of connection with nanoscale science where they could serve as building blocks for new materials, with tailored properties.

In present work, heterogeneous clusters of lithium and potassium with iodide, chloride and bromide, up to seven atoms, were examined. The structures of low-lying isomers of clusters were obtained by using a random-kick procedure and DFT calculations. As consequences of flat potential energy surfaces for the ground states of these clusters, there are many local minima with similar energies. In order to calculate the stability parameters (binding, ionization, and dissociation energies) more accurate coupled clusters calculations were carried out. The alterantion of stability for closed-shell and open-shell clusters were noticed. The electronic structure and chemical bonding phenomena were analyzed using natural bond orbital analysis (NBO). Higher stability of closed-shell over the open-shell clusters were explained by the delocalization of electrons over the alkali cage, which is more energetically favored than the localization of electron between two alkali atoms.

5-3

Numerical confirmation of experimental tension test results during first fracture layer of carbon-epoxy material

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The different structure of laminate composite materials allows the composite material to carry the load up to final fracture. The subject of the test is a carbon-epoxy composite material loaded on tensile mechanical testing to obtain tensile strength and modulus of elasticity, data required for numerical analysis based on the mechanics of laminated composite materials. The obtained results give an insight into the assessment of the possibilities of the examined structures of composite materials. The main objective of this paper is to obtain data on the prediction life of the composite material until the final fracture.

5-4

Modeling of the optical gain in ZnO-based quantum cascade lasers

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ZnO has been proposed recently as a good base material for high-power terahertz quantum cascade lasers (QCLs) operating at room temperature. We have developed a theoretical model for calculation of the optical gain, based on solving the system of rate equations and taking into account relevant scattering mechanisms. This model has been implemented to perform numerical simulations using ZnO/ZnMgO material combination, starting from the conventional design with three well within the active region of the structure. The influence of the layer widths and composition on the output properties has been considered, together with the variation of the number of quantum wells per QCL period.

5-5

Numerical modeling of the deformation of steel X52 pipeline wall under pressurized gas flow effect: one way coupling approach of fluid-structure interaction

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API X52 steel grade is a widely used material for pipelines dedicated to gas transport in large scale networks. Assessment of the capability of the pipeline material to maintain its integrity under the internal load of pressurized gas mainly during transient pressure fluctuations is a major concern for engineers and designers. The present work is devoted to numerically model the behavior of X52 steel pipeline wall carrying natural gas under pressure. The numerical model is built through a one way coupling approach of the interaction between the gas flow and the material behavior. Partial differential equations describing steady and transient gas flow are numerically solved. Then, obtained pressure variations are taken as a boundary load on the internal X52 pipe wall and thus displacement equation describing pipe structure deformation is numerically solved. To describe the material behavior, two techniques were used to obtain the transient pipe displacement field. For the first technique, the displacement equation is solved for the transient case considering the time dependent boundary load resulted from the transient gas pressure. The second way to obtain the displacement field is to solve the displacement equation considering a stationary case with a formal time dependencies. Indeed, a sweep method over a parameter "*t*" that stands for time is used to solve a set of stationary forms of the displacement equation. The effectiveness of both techniques was discussed. The reliability of the numerical model is proved through comparison of obtained steady state pipe wall deformation with the analytical solution of the internally pressurized cylinder problem.

5-6

Leakage area variation through rounded-hole oppenings in visco-elastic piping systems

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In water distribution systems, leaks of different shapes and sizes are likely to occur, leading to major losses in energy and decreasing the water quality. Previous research works have related the change of the leak discharge area to the internal pressure in the water pipe. This variation depends also on the shape and the size of the leak itself. The relationship between the applied pressure and the leak discharge area variation for visco-elastic material pipes is linear when long-time approach is followed. However, no accurate model for the deformation of rounded holes in different axis has been yet established. The presented work is devoted to modeling the deformation of a rounded hole-shaped leak under a bi-axial load approach during transients. The pipe has been considered as a finite width plate with a round hole where the distribution of stress around the circular fault has been studied. Linear superposition is used to obtain analytical solutions for the stress field and the deformation under the loading conditions. The longitudinal and circumferential stresses, due to the pressure applied on the visco-elastic pipe wall, affect the background small leak size. Indeed, the discharge has been analyzed to verify the linear pressure-discharge relationship. Deformation as a function of the applied pressure relationships were implanted in a method of characteristics based solver to simulate the behavior of the surges in a visco-elastic pipe material with a leak of circular shape. The proposed model permits to follow up the effect of leak area variation on transient pressure waves. The reliability of the developed model of area variations, and therefore the leak discharge, has been proved through comparison of obtained fast transient simulations to long-term approaches and previous experimental results.

6-1

Effect of Gd^{3+} introduction on YF_3: Yb, Er structural, morphological and optical properties

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Monosized up-converting nanoparticles (UCNPs) with a spherical shape and biocompatible surface have a wide application in biomedicine as new cell markers or light-triggered drug delivery agents. The synthesis of the hexagonal β-$NaYF_4$:Yb/Er phase is of a great interest, because of its most efficient up-conversion luminescence. Beside it, synthesis of the UCNPs based on YF_3:Yb/Er phase is also attractive due to its orthorhombic phase arrangement and fact that higher concentration of dopants could be introduced in such crystal lattice. In this work the synthesis of pure and Gd-doped YF_3:Yb/Er phases were performed through hydro/solvo thermal method using a biocompatible chitosan as a surfactant. The XRD analysis showed that independently of the gadolinium content formation of the orthorhombic phase is achieved, but intensity of the green emission due to the $({}^2H_{11/2}, {}^4S_{3/2}) \rightarrow {}^4I_{15/2}$ electronic transitions was highest for un-doped YF_3:Yb/Er sample.

6-2

Physicochemical properties of ion beam irradiated 12-tungstophosphoric acid

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Ion beam irradiation is a useful tool for modification of physicochemical properties of materials. In this work 10 keV C^+ ions at fluences between 5×10^{14} and 2.5×10^{15} ions/cm^2 were used for irradiation of 12-tungstophoshoric acid (WPA). For that purpose, 120 nm thick films of WPA on platinized silicon substrate were prepared via spin-coating method from the ethanol solution. The pristine and irradiated samples were characterized by attenuated total reflectance-Fourier transform infrared spectroscopy (ATR-FTIR), Raman spectroscopy, UV–Vis diffuse reflectance spectroscopy (UV-VIS DRS), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and atomic force microscopy (AFM). Infrared and Raman spectra of irradiated samples showed shifts and widening of WPA vibrational bands as well as the appearance of new vibrational bands that indicate structural transformation of WPA to phosphate tungsten bronzes. This modification also led to morphology changes which included agglomeration of WPA grains with an increase of fluence. Transformation of WPA to bronze-like structure was confirmed by band gap energy values obtained from UV-VIS DRS spectra and partial decrease of oxidation state as manifested by peak shifts in W 1f spectra.

6-3

Impact of the barium tytanyl oxalate precipitation condition on the aggregate formation characteristics

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Barium titanate ($BaTiO_3$) is well known material for its unique ferroelectric and dielectric properties, which widely used in electronics production. For the effective use of the $BaTiO_3$ it is important to synthesize nanosized powders and precisely control the properties of the obtained nanopowder. In term of obtaining stoichiometric BaTiO3 nanopowder with controlled particle size and size distribution the most appropriate method is Pechini method. This technic based on the precipitation of the metal-based complex with subsequent decomposition of this complex under high temperature to the BaTiO3. Setting of the barium tytanyl oxalate precipitation parameters permit regulate homogeneity, stoichiometry, crystallinity, aggregation and morphology of the precipitated complex, which, in turn, allow regulate more finely particle size and size distribution of the heat treated particles on the calcination step. Thus it is important to understand the precipitation process features and barium tytanyl oxalate formation to finely control the parameters on the subsequent step. In the present work barium tytanyl oxalate precipitation under pH range of 1-6 and reagent concentration in the range of 0,1-1,5 M was performed. Aggregation of the barium tytanyl oxalate in rod-like blocks was observed. The synthesis parameters impact on the rod-like blocks aggregate formation was investigated. According to the zeta-potential measurement, isoelectric point for barium tytanyl oxalate is around pH 10,5. According to the SEM analysis, barium tytanyl oxalate aggregation morphology retain after heat treatment and consist of the units with size of 7-90 nm. The condition for the stoichiometric barium tytanyl oxalate deposition was determined.

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6-4

Noble metals modified ZnO and TiO_2 for photocatalytic degradation of ceftriaxone using UV and solar radiation

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Pharmaceuticals are manmade persistent substances which are intended for human and veterinary medical purposes. Compared to other pharmaceutical substances, the β-lactam antibiotics, such as cephalosporins are the largest and most frequently used group of antibiotics. Ceftriaxone as one of the most widely used antibiotics in treating urinary, respiratory tract infections, and sexually transmitted disease like gonorrhea, brought potential risk to the environment especially aquatic ecosystems, upon its waste disposal. The ceftriaxone contaminated water causes side effects in human and aquatic well-being. Therefore, it is necessary to find a green and safe method to effectively remove the ceftriaxone residues from the water bodies. Application of solar photocatalysis using semiconductor materials for water treatment has been intensively studied in recent times. The synthesis of various nanometal-semiconductor composites has been achieved by numerous physical and chemical methods. Recently, the development of oxides supported bimetallic nanoparticles has resulted in considerable performance in photocatalytic activity and selectivity due to the exceptional electronic, optical, and photocatalytic properties of their nanosized metallic constituents. In this work, the photocatalytic efficiency of supported noble metal nanoparticles synthesized using the chemical wetness impregnation method (Pd/ZnO, Pt/ZnO, Ag/ZnO, and Au/ZnO) and sol-immobilization method (Au/ZnO, Pd/ZnO, Au–Pd/ZnO, Au/TiO_2, Pd/TiO_2, and Au–Pd/ZnO) were compared for degradation of ceftriaxone as the model contaminant. All photocatalysts were tested under UV and solar radiation. The effect of noble metal content on the efficiency of ceftriaxone degradation and mineralization was very dependent upon the nature of noble metal used.

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6-5

Photodegradation of atenolol and salicylic acid using composites based on zeolites and TiO_2 nanoparticles

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Pharmaceutically active compounds are frequently detected in small concentrations in both waste water effluents and surface waters because conventional wastewater treatments cannot ensure their complete removal.

In this work the photodegradation of atenolol (β blocker) and salicylic acid (transformation product of aspirin) was studied using composite materials based on different zeolites and TiO_2 nanoparticles under simulated solar irradiation. The aim was to develop efficient and economically justified photocatalysts for waste water treatment. The catalysts preparation consisted of mechanical mixing of TiO_2 (10 and 20 wt% loading) and starting zeolites (ZSM-5, 13X and natural zeolite-clinoptilolite), their sonication with ethanol for 4 h on 80 ^{o}C, and calcination in air for 5 h at 500 ^{o}C. The crystal structure and optical properties of the obtained catalysts were studied using X-ray powder diffraction, FT-IR and UV VIS diffuse reflectance spectroscopy. This study has shown that composite materials based on ZSM-5 zeolite displayed the best photocatalytic activity and the highest removal rate for both atenolol and salicylic acid compared to all other investigated photocatalysts including the pure TiO_2. The composite made of ZSM-5 zeolite and 20 wt% of TiO_2 nanoparticles, successfully eliminated 80 % of atenolol and 70 % of salicylic acid after 70 min of irradiation. The enhanced photodegradation of these composites is achieved because of simultaneous adsorption of pollutants on ZSM-5 surface and TiO_2 photocatalysis.

6-6

Nickel doped titanate catalysts for photocatalytic hydrogen generation

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Decrease of fossil fuels reserves coupled with their harmful environmental impact have moved the interest toward new, environment friendly energy sources. During the past decades the interest in hydrogen as a green and sustainable fuel has increased. Photocatalytic water splitting has been considered as a promising method for storing and converting solar energy into clean, renewable hydrogen fuel. Among various used photocatalysts, one-dimensional titanate nanomaterials attracted considerable attention, due to their favorable physicochemical properties (excellent ion-exchange activity, high specific surface area, high surface charge density, etc.).

This study will focus on investigation of photocatalytic hydrogen production activity over low cost Ni modified titanates, as alternatives for highly cost and low-abundance noble metal based catalysts. The catalysts with different nickel loading were synthesized by deposition of predetermined amount of nickel on hydrothermally prepared titanate support, followed by hydrogen temperature programmed reduction (TPR). The final catalysts were characterized using various methods, such as N_2 physisorption, XRD, TPR. The study showed that adequate selection of synthesis parameters results in catalyst with improved textural, morphological and structural properties. The investigation on the effect of the nickel content on the photocatalytic hydrogen production allowed us to define the optimal metal content in the synthesized catalysts.

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6-7

Synthesis of ZnO nanorods by spray pyrolysis for gas sensing application

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Hexagonal pillar shaped ZnO nanorods with different sizes have been successfully synthesized by Spray Pyrolysis Technique (SPT). The equal amount of methanol and water is used as a solvent to dissolve the AR grade Zinc acetate for precursor solution. This solution is sprayed on to the glass substrate heated at 350 ^{o}C. The films were characterized by Ultra-Violet spectroscopy (UV), X-ray diffraction (XRD), Field emission scanning electron microscopy (FESEM) and transmission electron microscopy (TEM). The deposition of thin films results in a layer comprising well-shaped hexagonal ZnO nanorods with diameter of 90-120 nm and length of up to 200 nm. The gas sensing properties of these films have been investigated for various interfering gases such as CO_2, CO, Ethanol, NH_3 and H_2S etc at operating temperature from 30^{o} (room temperature) to 450 ^{o}C. The results indicate that the ZnO nanorods thin films showed much better sensitivity and stability than the conventional materials to H_2S gas (100 ppm) at 50 ^{o}C. The Hexagonal pillar shaped ZnO nanorods can improve the sensitivity and selectivity of the sensors.

7-1

Development of nanoparticles-in-microparticles system for improved adsorption of arsenate (V) ions from water

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Arsenic ions in drinking water are very often unwanted pollutants especially when they are present above the permitted concentrations, so the development of methods for their removal is very up-to-date. One of the most efficient and inexpensive methods for their removal is adsorption on metal powders because they have very advantageous properties as adsorbents. However, the use of adsorbents in powder form is complicated mainly due to the separating of very small particles from solution after adsorption. In order to overcome this problem, in this work, immobilized iron oxides in the alginate gel particles were used as adsorbent, in order to facilitate the separation of the adsorbent after adsorption, with minimum adverse effects on the adsorption kinetics.

The goal of this research was removal of arsenic (V) ions from aqueous solutions. Adsorption was done with iron oxide nanoparticles immobilized in Ca-, Al-, and Cu-ions gelled alginate particles as adsorbents. Analyzing the adsorption of arsenic (V) ions, we determined the kinetic parameters for pseudo-first and pseudo-second order model, adsorption capacity and adsorption efficiency. The atomic adsorption spectrophotometry (AAS) was used for measuring the concentrations of arsenic ions after the adsorption. Acquired kinetic parameters for pseudo-second order model showed that adsorbents have encouraging potential for rapid reduction of arsenic (V) ion concentration to an acceptable level, therefore they could be used in waters affected by this type of pollution.

7-2

Strong reversible rubber with self-healing properties, based on polydimethylsiloxane with liquid-crystalline pendant groups

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The aim of this study was to develop rubbery copolymers, which could be melt-processed, solvent-processed (reversible rubbers) and would be able of self-healing. For this purpose, several structures were synthesized, starting from alpha-omega-hydrido-bifunctional poly(dimethylsiloxane)s of various length or from polydimethylsiloxane containing Si-H repeat units in pendant positions, and from several vinyl-functional mesogens as the second component. Three groups of liquid-crystalline copolymers were obtained in this way: linear infinite PDMS-LC copolymers, linear α,ω-LC-terminated short PDMS polymers, as well as LC-grafted PDMS polymers, which will be discussed in detail. The latter materials were synthesized via hydrosilylation reactions between the pendant-Si-H-functional polydimethylsiloxanes "HMS 301" or "HMS 064" and the mono-vinyl-functional azobenzene-based mesogen "BAFKU". The product "$(\text{BAFKU})_{45}$-HMS 064" appears to be a good reversible elastomer (extent of rubbery plateau: 100 °C, modulus slightly above 1MPa in this region), crosslinked by the reversible aggregation of the "BAFKU" mesogens. It is fusible (gradual melting between 50 and 80°C) and soluble in some organic solvents like chloroform, toluene or tetrahydrofuran. BAFKU units' aggregation generated extended anisotropic domains visible via polarized light microscopy, which completely disappear above 80°C (isotropic melt state). The product "$(\text{BAFKU})_{45}$-HMS 064" combines properties of covalently crosslinked polymers with the processibility (injection-moulding, recycling) of the linear ones, and is hence attractive also in view of possible applications in 3D-printing or as elastic self-healing material in protective coatings, seals, or in viscoelastic couplings (melting behavior).

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7-3

Study of electrical behavior of polymer-nanotubes composites

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Nanocomposites into polymer matrix are known to have extraordinary mechanical, thermal and electrical properties. Among such nanocomposites of significant interest are PEDOT:PSS polymer matrices with carbon nanotubes. In this of work we analyze electrical behavior of PEDOT:PSS layers with high-purity single-walled (SWCNTs) or multi-walled carbon nanotubes (MWCNTs).

Electrical studies were performed using E7-20 RLC measuring instrument. This instrument is designed to measure the parameters of samples represented by a parallel or serial two-element equivalent circuit. Harmonic voltage (1 V) in the frequency range from 1000 Hz up to 1 MHz was used as an excitation signal. The instrument ensures the 3% accuracy of impedance absolute value measurements. To see the difference in the electrical performance of obtained samples, impedance tests were carried out. Based on the readings from E7-20 instrument, which initially measures absolute value of the impedance of the sample and phase angle between applied voltage and current through the sample, we have recalculated real and imaginary parts of the impedance.

It is established that all investigated samples show lowest impedance (highest conductivity) at room temperature and electrical conductivity decrease upon cooling. General trend is that Re(Z) slightly increases with frequency from 1 kHz to up to some threshold frequency and then drops rapidly. This threshold frequency for pure PEDOT:PSS and PEDOT:PSS/SWCNTs samples is about 100 kHz and is somewhat lower for composite layers with MWCNTs.

Most notable temperature effect on the real part of the impedance of fabricated polymer/CNTs composite layers is that Re (Z) increases drastically starting from certain temperature, which is different for samples with different composition. For pure polymer this occurs already at 80…90 K and below 60 K Re (Z) is almost out of the measurable range. For layers reinforced with SWCNTs, increase of impedance is more gradual and even more so for MWCNTs-reinforced composites. In the latter case, reliable measurements can be performed even at temperatures as low as 40K.

7-4

Thermally induced microstructural changes in $Fe_{40}Ni_{40}B_{12}Si_8$ amorphous alloy

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Fe-Ni-M amorphous alloys (M is a metalloid element) have been attracting considerable scientific attention because of their interesting magnetic properties, high strength and good corrosion resistance.

Amorphous $Fe_{40}Ni_{40}B_{12}Si_8$ alloy was obtained by rapid quenching technique. Thermally induced microstructural transformations, from purely amorphous to purely crystalline structure, were followed using different analytical techniques. The formation of γ-(Fe,Ni), $(Fe,Ni)_3(B,Si)$, $Ni_{31}Si_{12}$ and $(Fe,Ni)_2B$ crystalline phases was observed by XRD and Mössbauer spectroscopy. Thermal treatment at increasing temperatures provoked the changes in average crystallite size and minimum dislocation density of the formed crystalline phases. Deconvolution of the complex DTA peaks was carried out to study the kinetics of individual crystallization steps. For kinetic description of crystallization of individual phases, the autocatalytic kinetic model was suggested as the most suitable one. The observed thermally induced microstructural transformations were shown to influence significantly functional properties of the alloy.

7-5

Probing subsequent charge density waves in 1T-TaS_2 by inelastic light scattering

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Two-dimensional layered transition-metal dichalcogenides (TMDs) have attracted attention for over 30 years mostly due to multiple charge-density wave (CDW) states that had been observed. Prime candidate is 1T-TaS_2 because of its unique and opulent electronic phase diagram. It experiences various phase transitions at high temperature, starting from the normal metallic to the incommensurate charge-density wave (IC-CDW) phase transition, at T= 554 K. At T=355 K 1T-TaS_2 CDW state changes to nearly-commensurate CDW (NC-CDW) phase, eventually leading to commensurate CDW (C-CDW) phase at approximately T= 180 K. Recent discoveries indicate the possibility of yet another phase transition in 1T-TaS_2 at T= 80 K. The new state is identified as hidden CDW (H-CDW) state, and can be induced using ultra-fast laser pulse. We present a detailed Raman spectroscopy study on CDW transitions. Our data indicate the coexistence of different CDW states, as well as strong electron-phonon interaction in the IC-CDW state. The experimental results presented in this work are supported by density functional theory (DFT) calculations.

7-6

Phonon thermal transport suppression in Si/SiO$_2$ crystalline/amorphous superlattices

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Clear understanding of phonon properties in nanostructures is instrumental in design of novel thermoelectric materials [1-3]. Crystalline/amorphous superlattices (CASLs) consisting of alternated crystalline and amorphous layers are promising in tailoring the thermoelectric properties because they can be made of materials with distinctly different physical and chemical properties. Here we report on theoretical study of phonon thermal transport in c-Si/a-SiO$_2$ CASLs, which remain less explored in the literature [4]. Comparing equations for lattice thermal conductivity within linearized Boltzmann transport equation [5-6] and Allen-Feldman theory of diffusive thermal transport [7-8] we have obtained an expression for the rate of diffusion of lattice vibrations in a-SiO$_2$ layers. The obtained expression is parameter-free and can be used for a wide range of amorphous materials. The performed theoretical study have showed, that heat transport in c-Si/a-SiO$_2$ CASLs is strongly suppressed as compared to purely crystalline c-Si/c-SiO$_2$ superlattices. Owing to the reduced lattice thermal conductivity, we conclude that c-Si/a-SiO$_2$ CASLs show promise for thermoelectric applications.

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7-7

Nanostructural study of Ge-Ga-S glasses using multicomponent PAL analysis

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The GeS_2–Ga_2S_3 chalcogenide glasses (ChG) have shown many advantages for potential applications of optical modulator, efficient laser host materials, fiber-optical amplifier in the IR region. Atomic arrangement in such ChG can be studied with numerous techniques, while number of probes available to study atomic-deficient distribution is rather limited, especially at a sub-nanometer scale. One of the best techniques capable to probe such fine free volumes is the positron annihilation lifetime (PAL) spectroscopy. In the present paper, we imply the PAL method to study of free-volume structure of GeS_2-Ga_2S_3 ChG.

The PAL spectra were recorded with conventional fast-fast coincidence system ORTEC. The measured PAL spectra of ChG were processed with standard LT 9.0 computer program, the obtained curve being fitted by two components with tau$_1$, tau$_2$ lifetimes and I_1, I_2 intensities. The positron trapping modes in the studied ChG were calculated using a formalism of two-states trapping model. Since (τ_1, I_1) component has no strong physical meaning within accepted two-state positron trapping model, we focused our further analysis on second component, where tau$_2$ lifetime is directly related to a size of free-volume entity and the intensity I_2 is proportional to the number of such “defects”. At values of PAL fitting parameters for $80GeS_2$-$20Ga_2S_3$ system, bulk positron lifetime is near 0.28 ns and average lifetime is 0.32 ns. It is shown that the size of free-volume trapping centers in the $80GeS_2$-$20Ga_2S_3$ system is higher than in the $80GeSe_2$-$20Ga_2Se_3$ glasses, weak increases of I_2 intensities testify growing behaviour in the number of corresponding free-volume entities. Other positron trapping parameters for Ge-Ga-S system are similar to Ge-Ga-Se glasses.

8-1

Novel, eco-friendly approach for the oxidative polymerization of aniline using Fe_3O_4 nanoparticles/H_2O_2 catalytic system

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Leading research in the field of conductive polymers continues to focus largely on polyaniline (PANI) as one of the most important of this group. Following the latest tendencies to sustainable and green processes, more and more investigations are aimed at developing eco-friendly polymerization routes. For now enzymatic polymerizations are one of the most promising in this manner due to the usage of hydrogen peroxide (H_2O_2), an oxidant which does not produce harmful byproducts as in the case of the most used ammonium peroxydisulphate (APS). However, there are still many disadvantages involving the high price of enzymes, their sensitivity to different reaction conditions and time-consuming extraction and purification processes. Thus, an idea of finding other appropriate materials, which behave as catalysts with H_2O_2 emerged.

In this work Fe_3O_4 (magnetite) nanoparticles (NPs) have been used as a catalyst for aniline oxidation with H_2O_2 as an oxidant and a very small amount of APS has been added as an initiator to speed up the reaction. The prepared Fe_3O_4 NPs were characterized by X-ray powder diffraction (XRPD) and scanning electron microscopy (SEM) which revealed uniform, roughly spherical nanoparticles (10–50 nm). The polymerization reaction was monitored by UV-Vis-NIR spectroscopy that clearly showed the development of the bands characteristic of conductive PANI emeraldine salt (ES) with reaction time. The influence of reaction time on the structure and physicochemical properties of isolated, powdered products was investigated by means of FTIR, Raman and EPR spectroscopies. All spectra contained characteristic bands confirming that the obtained products are in the PANI-ES form and indicated their relatively high electrical conductivity ($\sim 10^{-2}$ S·cm^{-1}). Both EPR and XRPD measurements stated the presence of the Fe_3O_4 NPs in the final products, which is an important evidence of their catalyst role. Their irreplaceable effect in this system was confirmed by setting the reaction without Fe_3O_4 NPs, under the same other conditions, which did not yield PANI products. SEM micrographs of the reaction products revealed that their morphology was, in major extent, controlled by magnetic nanoparticles, but that there is also a certain amount of ideal spherical structures of a diameter from 1 to 5 μm. Furthermore, charge storage ability of the obtained materials was preliminary examined and discussed.

8-2

Electrochemical oxidation of maricite $NaFePO_4$ in mild aqueous solutions as a way to boost its charge storage capacity

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Lithium has a low abundance in the Earth's crust, which in a few years will lead to difficult lithium production, and therefore difficult production of lithium-ion batteries. Sodium-ion batteries, on the other hand, have been proven to be a good replacement. The material obtained from iron combined with the phosphate and pyrophosphate compounds of sodium has attracted attention as a possible cathode material for sodium-ion batteries. $NaFePO_4$ exists in two polymorphic structures (triphylite and maricite). Maricite $NaFePO_4$ is a more thermodynamically stable structure than triphylite NaFePO4 but doesn't have channels for Na^+ movement and electrochemical performance of this structure is low. In comparison to maricite $NaFePO_4$, triphylite $NaFePO_4$ (structural analogue to $LiFePO_4$) has one-dimensional channels for Na^+-ions movement and better electrochemical activity but it is not stable and is difficult to synthesize. Herein, the maricite $NaFePO_4$ can be obtained by sintering a polyanionic compound, $Na_4Fe_3(PO_4)_2P_2O_7$, at temperatures above 600 °C, as shown by XRD. $Na_4Fe_3(PO_4)_2P_2O_7$ is synthesized by the glycine-nitrate process after which it was sintered at temperatures above 500 °C. The glycine-nitrate process was found to catalyze the decomposition of the sintered $Na_4Fe_3(PO_4)_2P_2O_7$ to the $NaFePO_4$ maricite. The electrochemical characterization of the sintered material, evaluated in aqueous $NaNO_3$ and $LiNO_3$ electrolyte by cyclic voltammetry, showed poor electrochemical activity of maricite $NaFePO_4$. By exposing the sintered material to high anodic potentials, the electrochemical activity and specific capacity of the material were increased by 50% in case of $NaNO_3$ and 80% in case of $LiNO_3$ relative to the pristine with low activity. After electrochemical measurements, residual powder was characterized by FTIR and Raman spectroscopy. It was shown that high anodic polarization of the material tested in $LiNO_3$ causes the formation of triphylite $LiFePO_4$. Similarly, it is assumed that the electrochemical activity obtained by deep anodic polarization of the material in $NaNO_3$ electrolyte originates from the formed triphylite $NaFePO_4$. The obtained results open novel directions regarding the use of $NaFePO_4$ in metal-ion rechargeable batteries.

8-3

The Briggs-Rauscher reaction as an unusual detector for a different type of bronzes

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The Briggs-Rauscher (BR) reaction is an oscillating reaction in which the oxidation of malonic acid ($CH_2(COOH)_2$) in the presence of hydrogen peroxide (H_2O_2) and potassium iodate (KIO_3) is catalyzed with a metal ion (usually manganese ion (Mn^{2+})) in an acid solution ($HClO_4$). It is well known that the BR reaction represents a chemical system that is extremely sensitive to the addition of different types of analytes. Every change in oscillatory dynamics, caused by analyte addition, can be used for the assessment of analyte concentration, as well as its potential antiradical activities.

The basic idea of this work is to use the oscillatory reaction, as an unusual and novel system for distinguishing different types of insoluble materials such as bronzes, specifically phosphate tungsten bronze (PWB) and phosphate molybdenum bronze (PMoB). Regarding the results obtained, the increasing mass of PWB leads to a significant decrease of BR oscillatory time, while the addition of PMoB has not affected the BR reaction dynamics. The obtained different behavior of PWB and PMoB introduced the BR reaction as a system-detector for these two types of bronzes. In order to investigate the mechanism of bronzes action in BR oscillatory reaction, the pH and electric conductivity measurements, as well as inductively coupled plasma and the cyclic voltammetry measurements were done. This work extends the practical aspect of the BR reaction for the examination of solid materials. Furthermore, the obtained results open a new section of oscillatory reaction usage in material science and catalysis in general.

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8-4

UCST polymers based on dual pH- and thermo- sensitive copolymers obtained by free radical polymerization

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Positively thermosensitive polymers have an upper critical solution temperature (UCST), defined as the critical temperature, above which the polymer swells in the solution, and under which polymer contracts. UCST type polymers are poorly researched. The main goal of this investigation was synthesis and characterization series of copolymer based of methacrylic and acrylic acid with different cross-linker content. These cross-linked copolymer hydrogels were obtained by free radical polymerization process. FTIR spectra of poly(methacrylic acid-*co*-acrylic acid) hydrogels confirm that polymerization was performed by breaking the double bonds. Also, the amount of unreacted monomers, monitored by high-pressure liquid chromatography (HPLC) method, confirms successful copolymer synthesis. Thermal characterization of obtained hydrogels was analyzed using differential scanning calorimetry (DSC) method. The swelling study showed that synthesized copolymer hydrogels swell intensively in basic medium at higher temperature (40 °C), compared to swelling capacity in acidic medium at room temperature (40 °C). Poly(methacrylic acid-*co*-acrylic acid) hydrogels showed characteristic swelling properties as UCST polymers.

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8-5

Hot forged TiC/Al composite materials

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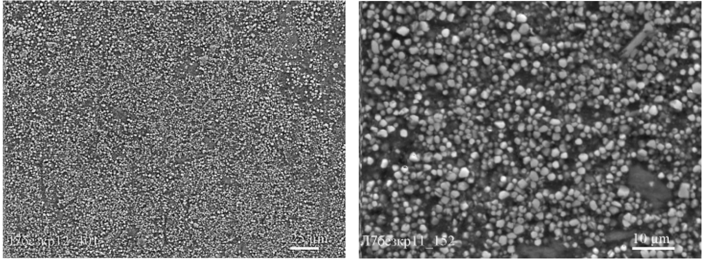
TiC-based cermets are extensively used as advanced structural materials due to their unique mechanical properties. In particular, TiC/Al composites combines metallic and ceramic characteristics - toughness and ductility with high strengths and modulus of elasticity, which helps to overcome one of the most undesired properties of cermet materials - the lack of impact strength. Traditionally, cermets have been produced by various casting methods and by spray depositions or infiltration of porous ceramic frames. Hot forging of porous preforms is alternative method for manufacturing fully-dense composite materials with high carbide content, that also ensure possibility for production of material with fine stricture, advanced and service characteristics. Therefore, the aim of this work was the investigation for effect of hot plastic deformation of hot forging on structure and properties of TiC/Al composite materials.

The TiC was synthesized in-situ from the blend of 45Al (wt.%), 44Ti (wt.%) and 11 C (wt.%) powders by thermal synthesized at 900 ^{o}C through exothermic reaction. The porous preforms obtained after thermal synthesis were milled to produce a composite powder, which, according to the X-ray phase analysis, consist of Al, TiC and some amount $AlTi_3$, Al_2Ti. This composite powder was compacted in steel shell in a cylindrical die (40 mm in diameter) at 500 MPa, then heated to a 600 °C for 20 min and hot forged.

The microstructure of the composites materials after hot forging consists fine TiC particles with a size of 1-1.5 microns or les, uniformly distributed in aluminum matrix (fig. 1).



a *b*

Fig. 1 Microstructures of 55TiC-45Al (wt.%) composite materials
with different resolution (×400 and ×1500 accordingly)

The Vickers hardness value is 300-314 HV and the density value close to theoretical one.

8-6

Wettability of doped superhydrophobic silica coatings

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A hydrophobic surface is defined as the surface on which the water contact angle is greater than 150° [1]. These types of surfaces have very interesting functional features, such as ability to repel water and self-clean.

The aim of the experiment was to obtain hydrophobic layers based on tetraethoxysilane (TEOS) and modified silicas. The layers were deposited on glass supports by dip coating in the sol-gel solution. Furthermore, the effect of support cold plasma activation on the properties of obtained surfaces was also examined.

Measurements of the water contact angle using the tilting plate method were made in order to determine the surface properties of the obtained layers. The XPS and FT-IR/PAS spectra as well as optical profilometers and SEM images of the surfaces were also made to characterize their structures.

The wettability measurements revealed that the obtained surfaces are hydrophobic – their water contact angle was in the range of 140-150 degrees.

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9-1

Effect of water cooling system temperature on the cooling rate during solidification in the suction casting process

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Bulk metallic glasses (BMGs) are characterized by interesting both physical and mechanical properties due to their amorphous structure. For this reason, BMGs are subject of continuous studies, which focus mainly on increasing the critical diameter (D_c – the largest diameter of alloy with an amorphous structure) and the plasticity of these materials [1]. Among many glass forming systems, the Zr-Cu-Al alloys deserve a special attention due to their relatively low cost and high glass forming ability (GFA) [1-3].

In order to produce a metallic glass, the alloy should be cooled at a sufficient cooling rate (R_c – critical cooling rate) during solidification to prevent crystallization [4]. The R_c can differ from 10^6 K/s for marginal glasses to less than 1 K/s for the best glass formers. However, in the case of metallic glass in a bulk form (min. 1 mm of thickness) the critical cooling rate should be lower than 1000 K/s. The cooling rate during solidification can be controlled by changing the diameter of the mold and/or its temperature. Knowledge of this correlation allows predicting the critical diameter as well as synthesis of in-situ formed amorphous-crystalline composites with a controlled volume fraction of the crystalline phase.

The R_c parameter seems to be better reflect the GFA compared to D_c because it is more effective and excludes other conditions influencing the casting process. However, it is very difficult to be measured accurately. Alternatively, indirect methods based on the microstructural features of the as-cast alloys can be used to estimate cooling rates during solidification.

In this work, the cooling rates were estimated based on measurements of the dendrite arm spacing in the Fe-25wt%Ni alloy. This alloy was produced by arc melting of constituent elements followed by suction casting into copper moulds of different inner cavities and/or water cooling system temperatures.

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9-2

Optimization of spray drying process for concentrated whey solutions

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The spray drying process is common way for treatment of whey solutions with mass concentrations between 40-60%. Usual temperatures of inlet hot air for this process are between 150 and 200 °C. The aim of this work was the reduction of operating costs and the optimization of separation efficiency of the dryed particles with desired moisture content (< 10%).

Modeling will be primary used to determine the optimal temperature of the inlet hot air which will cause the reduction of the electrical energy used for the calorifier heating. The two main variables in the model are pressure in the two-fluid nozzle and the flow of the concentrated whey solutions. The optimal concentration of the concentrated whey solutions was also determined by analyzing the diameter of dry particles and their moisture content. Calculation of water mass transfer rate during drying was compared with retention time of the solution in the columnin order to determine the right size of the spray drying column. The impact of the agglomeration of dry particles upon the process of separation in the cyclone separator due to lactose crystallization was also investigated.

9-3

The effect of biopolymer addition on the stability of the emulsion of essential oils

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Biopolymers are obtained from natural sources, often referred to as renewable sources, in contrast to synthetic polymers produced from a non-renewable source, which is crude oil. Polymers of natural origin are biodegradable and therefore not harmful to the environment. For this reason, production branches are of great importance [1].

The purpose of the work is to create a stable emulsion containing essential oils. The emulsion should be stabilized with biopolymers. As biopolymers, fucoidan, carrageenan, carboxymethylcellulose [2], chitosan [3] and guar gum were used. The resulting emulsions were additionally thickened by the addition of xanthan gum. The resulting product was to be stable for 40 days at 40°C. Stability was tested using Turbiscan Lab^{Expert}, this device works in the technique of multiple light scattering. After formulation and stability testing, chitosan and fucoidan may not be suitable for stabilizing this type of emulsion. The best results were obtained when the stabilizer was guar gum. The stability of the emulsion system is obtained by macromolecular and steric stabilization. Turbiscan Stability Index (TSI) coefficient proposed by the turbiscan manufacturer is well suited for analyzing the stability of systems of this type.

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9-4

Optimization of parameters of polymeric microparticle fabrication through oil/water solvent evaporation technique

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Oil/water solvent evaporation technique is one of the most widely used methods for fabrication of polymeric microparticles, which could be used as multifunction cell microcarriers or building blocks for fabrication of 3D structures. A number of emulsification parameters, such as temperature, agitation mode and speed, etc. as well as compositions of oil and water phase could be varied, that provides a possibility to adjust characteristics of fabricated microparticles. This work was aimed to evaluate an effect of various emulsification parameters on characteristics (total yield, mean size, size distribution and morphology) of polyester-based microparticles fabricated though oil/water emulsion technique using different emulsifiers in aqueous phase. Increase of agitation speed allows to decrease a mean size of the microparticles, while an agitation mode plays an important role in total yield of the microparticles. An increase of molecular weight or concentration of polymer dissolved in oil phase as well as decrease of temperature of emulsification led to an increase of mean size of the microparticles. Different approached to optimization of characteristics of polymeric microparticle based on various polyesters and its mixtures will be highlighted within this presentation as well. Modification of composition of aqueous phase led to a more complex effect on parameters of fabricated microparticles. As a first point, macromolecular features of polymers used as emulsifier in aqueous phase should provide them an ability to stabilize oil/water interface. A variety of water-soluble polymers including polysaccharides, their derivatives/copolymers and proteins were tested in terms of their ability to stabilize the microparticles in a course of their preparation. From another point of view, variation of molecular weight of the polymer dissolved in aqueous phase could also affect not only mean size and size distribution of the microparticles, but their other characteristics as well. An application of nanoparticles for stabilization of oil/water interface will be also discussed in a frame of this presentation.

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9-5

Reaction diffusion model for heterogenous N deacetylation of chitin into chitosan using catalytic alkaline solutions

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For industrial chitosan production, chemical deacetylation in heterogeneous media involving strong alkaline solutions remains the most studied one.[1] So far, the complete deacetylation of chitin was not attained in a single-stage treatment with concentrated alkali.[2] This conversion study provides a new mechanistic insight into the modelling of the heterogeneous N-deacetylation step of α-chitin, obtained from waste crustacean shells, using a catalytic alkaline solution at different operating temperatures (25–80 °C) and concentrations (50–80 wt%). Transient particle-size distributions for two separate experiments with smaller powder or larger flake morphologies were obtained by applying an inline tracking probe. The degree of deacetylation (DDA), polymer molecular mass and viscosity of the deacetylated raw sources were continuously monitored with time until the maximum DDA was reached. The mechanism of the conversion of an average biopolymer chain was described with a reaction–diffusion kinetic model, solved for all fraction intervals, and optimised. Additionally, several analytical tools such as scanning electron microscopy (SEM) was employed as well as specific porosity measurements to get a deeper phenomenological understanding of the material's morphological transformation. The selected mathematical relationship granted a relatively good agreement for the cumulative experimental data by regarding the kinetics in the initial consumption phase, as well as the subsequent transport resistance for OH^-.

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9-6

Development of a regression model for the eccentricity in tube drawing with tilted die process automation

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The purpose of this study is finding the relationship between the effective parameters of tube drawing with a tilted die and the tube's eccentricity leading to design an in-line thickness measurement and adjustable die for tube drawing processes. During drawing the wall thickness of tubes will be measured: These data and the regression model will be applied to predict the optimum angle and position of die's tilting. The importance of this research lies in the uniqueness and effectiveness of the regression model for process automation. The eccentricity after tube drawing is considered as a dependent variable while the independent variables include the tilting angle of the die, material properties and the geometry of the tubes. To this end, the results of tube drawing with tilted die for different materials and tilting angles are conducted and applied for developing the regression model. Minitab software as statistic tool was used to determine and to select the effective independent variables predictively and to develop the regression models.

This paper includes different regression models: the initial goal was to develop a specific regression model for each material separately. Finally a general regression model predicting the eccentricity of the tubes after drawing regardless of material category was developed.

A multiple regression model - for more than one independent variable - is applied to predict the new eccentricity. Tensile and hardness tests will be conducted to determine the change of mechanical properties before and after processing considering tube drawing with a tilted die. Two factors - squares residual and p-value - are considered to evaluate the models. The developed model is applied to improve the performance of the tube drawing process by applying an online measuring self-regulation tilted die machine in order to change the eccentricity. The results indicate that through applying such an adjustable dynamic system, the eccentricity after tube drawing can be improved by 50% in one process step.

10-1

Synthesis temperature influence on the structure, morphology and electrochemical performance of Na_xMnO_2 as cathode materials for sodium-ion rechearchable batteries

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The lithium-ion batteries are the most commonly used for energy storage in portable devices. Since lithium is relatively rare on earth but rapidly consumed, it is necessary to find an adequate replacement. Owing to the similar chemical properties of sodium and lithium, but much higher availability, sodium ion batteries are one of the best candidates to replace lithium-ion batteries. A variety of materials such as manganese oxide, vanadium oxide or phosphate can be used as an electrode material (anode and cathode) in sodium ion batteries due to the high ability of intercalation of sodium.

In this work, Na_xMnO_2 powder was synthesized by glycine nitrate method. The precursor powder was annealed for four hours at different temperatures: 800, 850, 900 and 950 °C. The characterization of the obtained materials was carried out using following methods: X-ray diffraction (XRD), scanning electron spectroscopy with energy dispersive X-ray spectroscopy (SEM/EDS) and transmission electron spectroscopy with energy dispersive X-ray spectroscopy (TEM/EDS). Electrochemical properties were studied using cyclic voltammetry and chronopotentiometry in an aqueous solution of $NaNO_3$.

The layer structured $Na_{0.7}MnO_{2.05}$ with sheet-like morphology and $Na_{0.4}MnO_2$ with 3-D tunnel structure and rod-like morphology was obtained at 800 ^oC and 900 ^oC respectively. $Na_{0.44}MnO_2$ with rod-like morphology was annealed at 900 and 950 ^oC. 3D-tunnel structure $Na_{0.44}MnO_2$ obtained at 900 ^oC showed the best electrochemical behaviour in aqueous $NaNO_3$ solution.

10-2

Electrochemical properties of nanostructured composite $Li_{1.2}V_3O_8$/C in different aqueous electrolytes

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Today, rechargeable Li^+-ion batteries experienced widespread use as power sources in mobile electronic devices and electric cars. However, there is a strong demand, especially in the field of large scale systems, for cheaper and safer batteries that would be comparable to the Li^+-ion batteries in both energy and power. Some of the scientists' attempts are orientated towards developing different rechargeable batteries that use aqueous instead of flammable organic solvents and some other non-toxic and more abundant metals instead of lithium. Thus far, different forms of vanadium oxides were investigated as electrode materials in different aqueous electrolyte solutions. Among them, a lithiated form $Li_{1+x}V_3O_8$ was used very frequently. In the scope of this research, $Li_{1.2}V_3O_8$/graphite composite was synthesized and subjected to electrochemical characterization by using cyclic voltammetry and chronopotentiometry in aqueous $LiNO_3$, $NaNO_3$ and KNO_3 solutions in order to investigate possibility of potential use of nanostructured composite $Li_{1.2}V_3O_8$/graphite as an electrode material in Li^+, Na^+ and K^+- ion aqueous rechargeable batteries. The discharge capacity, cyclic stability and Li, Na, K - ion insertion behavior of $Li_{1.2}V_3O_8$/graphite in the above mentioned aqueous solutions was studied. The cyclic stability and discharge capacity of $Li_{1.2}V_3O_8$/graphite were found to be the best in $LiNO_3$ solution.

10-3

Ion beam irradiated molybdenum disulfide for improved hydrogen evolution reaction

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Various catalysts based on low-cost, earth-abundant transition metals oxides and dichalcogenides have been studied for hydrogen evolution reaction (HER). Among them molybdenum disulfide (MoS_2) has emerged as potential candidate. In order to enhance catalytic activity and increase number of active sites, low energy ion beam irradiation is used. MoS_2 was synthesized via facile hydrothermal method. Obtained powder was irradiated with carbon and hydrogen ions of different energy and fluences. Both modified and pristine samples are characterized via various physicochemical techniques and ion beam induced changes in sample are observed. Scanning electron microscopy images show spherical, flower-like structures which are composed of nano-sheets. The X-ray diffraction patterns indicate hexagonal type of structure denoted as 2H. Raman spectroscopy reveals vibrations corresponding to Mo-S in-plane and out-of-plane vibrational modes. Hydrogen evolution is examined with impedance spectroscopy, linear sweep and cyclic voltammetry in an acidic electrolyte solution (0.1M H_2SO_4) at room temperature. The results indicate enhanced hydrogen evolution for irradiated samples with shifting of required potential to achieve a current density of 10 mA/cm^2 for 100mV compared to as-prepared sample.

10-4

Processing of discarded lithium ion batteries for recovery of cobalt, manganese and lithium values

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Lithium-ion batteries have a limited lifespan; ever-growing demand and adequate presence of critical metals such as lithium and cobalt make their recycling inevitable. In this study, discarded mixed mobile batteries were discharged, dismantled, and separated into cathode and anode sheets, followed by crushing in an attritor. The cathode material comprises $LiCoO_2$ and $LiMn_2O_4$, while graphite is present in the anode material. The cathode material was indigenously reduced with purified graphite at different times and dosages. A statistical design is employed for optimization of reduction parameters and obtained magnetic fraction contains cobalt and manganese oxide whereas graphite and lithium carbonate were found in nonmagnetic fraction and dried solution. The composition, saturation magnetization and product phases obtained at optimum conditions (900 °C, 7.5 % graphite, 45 min and 800 °C, 7.5 % graphite, 45 min) are Co: ~80-84 %, Mn: 6~10 %, saturation magnetization:105-114 emu/g with Co, CoO and MnO phases, respectively.

10-5

Investigation of the 4 MeV C and Si ion channeling implantation influence on the structure of 6H-SiC monocrystal

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Due to its exceptional physicochemical properties, SiC stands out as a material for wide range of applications, from the production of high-power, high-frequency and high-temperature electronic devices to the uses in the extreme environmental conditions like those that exist in nuclear reactors. In modern semiconductor industry, doping method through ion implantation is very popular due to its ability to successfully control depth and thickness of the implanted layer. This process can induce defects in the crystal. Therefore, study of defects impact on crystal properties is of great importance.

In order to achieve greater penatration depths of ions, as well as to cause less damage to the crystal lattice, we performed ion implantation in the crystal channeling orientation. To study radiation damage, C^{3+} and Si^{3+} ions of 4 MeV energy were implanted along [0001] 6H-SiC crystal axis, with the fluenses ranging from $4.17 \cdot 10^{14}$ to $2.02 \cdot 10^{16}$ cm^{-2}. Elastic backscattering spectrometry in channeling mode (EBS/C) and micro-Raman spectroscopy (µR) conducted by surface side mapping of transversally cleaved irradiated crystal, were used for determining of induced lattice damage. EBS/C analysis showed that damage of the crystal lattice is more pronounced in the case of Si ions and at the same time having shallower implantation depths as a consequence of their greater mass. A minor modification of the crystal surface was observed. However, significantly more pronounced crystal modification was observed in the ion's end of the range region. µR spectroscopy showed a very good reproduction of the conclusions obtained regarding the depths of modified zones, the influence of the ion types and fluences compare with the EBS/C and SEM techniques. It confirmed greater implantation depths and less damaged crystal lattice in the case of channeling compered to random ion implantation. µR obtained depth profile evolution of the FWHM of F_2-FTO(2/6) peak at 790 cm^{-1} very well describes the physical profile of the modified zone coinciding with the SEM image. The results also indicate the existence of a critical fluence above which crystal lattice is fully modified (amorphized). Tracking the characteristic evolution of µR spectra, we concluded that ions gradually interrupted the long-range crystalline order, which only remained crystalline within small domains embeded in the amorphus phase.

10-6

Spin-phonon coupling in $CrSiTe_3$ and $CrSi_{0.8}Ge_{0.1}Te_3$

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Trichalcogenides $CrXTe_3$ (X = Si, Ge) are semiconducting representatives of the van der Waals materials, with ferromagnetic order and band gap of 0.4 eV for Si and 0.7 eV for Ge compound, and Curie temperatures of 32 K and 61 K, respectively. Their layered structure provided exfoliation to mono and few-layer nanosheets, due to the weak van der Waals inter-layer bonding. This possibility togeather with their semiconducting and magnetic properties makes them ideal candidates for applications in optoelectronics and nano-spintronics.

Here we present temperature dependent Raman scattering study on $CrSiTe_3$ and $CrSi_{0.8}Ge_{0.1}Te_3$. Four and eight out of ten Raman active modes were assigned and observed for pure and slightly doped compound, respectively. The self-energies of A_g^3 and E_g^3 symmetry modes of $CrSiTe_3$ compound exhibit unconventional temperature evolution around 180 K. In addition, doubly degenerate E_g^3 mode shows a clear change of asymmetry in the same temperature region. The observed behavior is consistent with the previously reported presence of short-range magnetic order and strong spin-phonon coupling. Changing the concentrations of elements in parent compounds and doping plays a significant role in semiconducting physics and can lead to surprising physical properties, like considerable change in magnetic transition temperature or structural modifications. SEM measurements performed on our CrSi0.8Ge0.1Te3 single crystals revealed the 10% concentration of Ge atoms and the same amount of vacancies. Inelastic scattering results on CrSi0.8Ge0.1Te3 in addition to symmetry predicted modes, shows the presence of one mode attributed to the inhomogeneous distribution of Ge atoms, and two overtones, all obeying pure A_g selection rules. All analyzed modes display unconventional behavior, but in a difference from the pure compound on a higher temperature of 210 K.

11-1

Influence of coating defects on soldering resistance of CrAlN coated HPDC tools

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High-Pressure Die Casting (HPDC) is a high-volume manufacturing process for components of different sizes and shapes. In this process, a molten metal, commonly an aluminum alloy, is injected into the die cavity under high pressure and high velocity. This has a high impact on tool degradation and wear, which as a result leads to significant financial losses. Modifying surface layers by applying hard ceramic coatings, tool durability can be significantly increased. In this study, a nanolayered CrAlN coating with three different chemical compositions was evaluated. The performance of the coating was examined in terms of its soldering tendency to Al-Si-Cu alloy, by using a detachment test. Analyzing the contact surfaces, it was found that sticking tendencies and soldering mechanisms of cast alloy toward the investigated surfaces occurred. The contact surfaces were analyzed using a 3D profilometer and different microscopy techniques. The molten metal was kept in contact with the analyzed coatings for defined time periods. A detachment of the solidified metal and the samples were conducted using a tensile test. Scanning electron microscopy (SEM) analyses of contact surfaces reveled remains of solder and partial coating delamination. By comparing the amount of soldered material to the sample surfaces and the amount of coating delamination, it was found that those amounts varied for different time periods of contact. However, the amount of coatings delaminated area is different and closely correlates with sample detachment force. Higher detachment force is addressed to larger coating delamination area. It was found that the chemical composition of investigated coatings has a modest influence on the soldering phenomena, but the number of coating defects displayed the highest influence on soldering resistance of coatings.

11-2

Effects of substrate material and rotation during deposition on topography of nanolayered TiAlSiN coating

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Nanolayered TiAlSiN coating deposited by magnetron sputtering is one of the most advanced contemporary wear resistant coatings. It is suitable for various tribological applications which sometimes require complex elements rotation during the coating deposition. It is known that substrate material and the degree of rotation in coating deposition process affect the coating growth and its topography. The coating grain morphology governs the coating mechanical properties while surface topography affects its tribological behavior and performance in corrosive environment. However, in literature, systematic investigations on these topics are scarce and therefore this was a motivation for conducting the following investigation. This investigation evaluated the properties of nanolayered TiAlSiN coating produced by industrial magnetron sputtering unit on: cold-working tool steel (X153CrMoV12), hot-working tool steel (X38CrMoV5), plasma nitrided hot-working tool steel, implant stainless steel (X2CrNiMo18-15-3) and cemented carbide (WCCo). The effect of substrate rotation during deposition (1-fold, 2-fold, 3-fold) was evaluated on cold-working tool steel samples. 3D stylus profilometry and atomic force microscopy (AFM) were employed for evaluation of micro and nano topography of produced coatings coupled with use of software for image analysis. Surface of coated implant steel has the highest roughness (Sa) which corresponds to the highest concentration of growth defects, determined for this steel. However, for implant steel the overall volume of defects is considerably smaller than for other substrates. The observed difference is linked to differences in the concentration of specific carbides, contained in steel, and differences in their sputtering rate which directly affect defect density. AFM analysis revealed that coating on implant steel exhibited the smallest diameter of coating columnar grains (columns) and their highest uniformity. Diameters of columns on other substrates are twice that size, while nitrided hot-working tool steel has the largest columns. Such finding suggests that differences in mechanical properties should be expected too. Coatings produced with higher degree of rotation (2-fold, 3-fold) are characterized by lesser defects, they are smoother and have finer columns of more uniform size.

11-3

Implementation of image analysis for cavitation erosion determination of refractory samples based on talc and domestic zeolite from Igros

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Domestic zeolite from Igroš as raw material for ceramic samples for application in condition of cavitation erosion was used. Samples based on talc with 15% of zeolite, from Igroš sintered at 1200ºC were used in this investigation. The ultrasonic vibratory cavitation set up with stacionary specimen was used. Mass loss was measured as well as the degradation level of the samples using image analysis. Image analysis was used for level of damage determinatios, as well for number and area of the formed pits. Analysis of the pits formation and growing will be used for description of mechanism of degradation during cavitation erosion testing. Obtained resultes showed good resistance of the sample to the cavitation erosion, which gives the possibility for future application of ceramic samples based on talc and zeolite in conditions where cavitation erosion is expected.

11-4

The mechanical aspects and the evaluation of the microstructure of the steel-aluminum explosive welded joins

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Explosion-welded sheets are used in various industries, including shipbuilding, where steel sheets clad with aluminium and its alloys are used. Connecting steel with aluminum and its alloys is important for building structures with a low center of gravity, such as ships. The steel from which the hull of the ship is made is responsible for transferring loads under fatigue and dynamic loads. The lightweight aluminum superstructure reduces the center of gravity, which reduces the risk of the ship tipping over in waves.

Such construction of ships, forces the use of well-weldable materials such as non-alloy steel and aluminum and aluminum alloys of the 5xxx series, due to the lack of mutual solubility and the creation of hard and brittle phases, it is not possible to make steel-aluminum alloy welded joints. In this case, it is necessary to used welding connectors made by explosive welding method. In the structure of welding connectors, a flyer plate sheet, it can be aluminum and its alloys or other materials providing the desired properties. Aluminum is used due to its relatively good corrosion resistance and action of concentrated nitric acid as well as organic acids and hydrogen sulfide. Satisfactory corrosion resistance of aluminum is the result of self-passivation, i.e. aluminum oxide spontaneously arising in the presence of oxygen.

The research focused on the analysis of the structure and hardness of the welding joint made by the method of explosive welding using S235 non-alloy steel, pure aluminum used as a buffer layer (1xxx) and aluminum-magnesium alloy (5xxx). In the analyzed case, non-alloy steel and aluminum alloy have good weldability.

11-5

The effect of additives of ultrafine titanium nitride nanopowder on the structure, phase composition and mechanical properties of chromium carbidesteel

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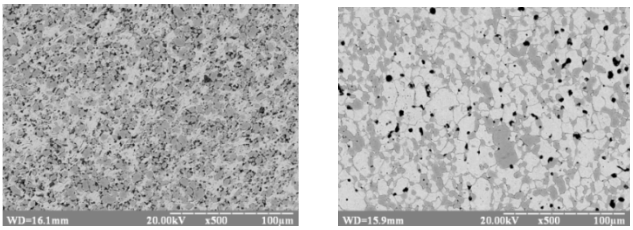
Nowadays, the use of alloying and modifying additives in the ultrafine state (nanopowders TiCN, TiN, SiC, WC, Al_2O_3 and in.) is considered particularly promising in increasing the dispersion of the metal matrixstructureand leading to the destruction of the carbide network and spheroidization of the carbide grains.

In this work, we studied the structure, phase composition, and mechanical properties of steel in the Fe-Cr-C system alloyed with 0.0002% (mass.) TiN. The size of the initial TiN powder is<0.05 µm. The composite material was obtained by powder metallurgy route. Sintering is carried out in vacuum at temperatures of 1150 -1250°C. After the introduction of TiN nanopowder (Fig. 1), the structure of the material changes from two-phase structure to the three-phase structure, and is also significantly ground. The grain size of the matrix phase decreased from 17-18 to 8-10 µm., and for the carbide grains from 10-13 to 4-7 µm.



a b

Fig. 1 – Microstructure of steel a (with 0.0002% TiN), b (withoutadditives)

Additives of TiN nanopowder lead to the formation of a black phase with a size of 2–3 µm, which consists of 68.05% Cr-31.39% Fe-0.1% TiN. The mechanical properties of steels were also investigated. After the introduction of the additive, the bending strength significantly increased (1117 to 1840 MPa), however, the hardness of the material remained unchanged at 74 HRA.

12-1

Mechanochemically synthesized cobalt-ferrite and starch-coated cobalt-ferrite nanoparticles as efficient adsorbents for hexavalent chromium removal

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Cobalt-ferrite ($CoFe_2O_4$) and starch-coated $CoFe_2O_4$ nanoparticles were prepared by the mechanochemical method and carefully chosen as adsorbents for Cr(VI) removal from wastewater. The kinetic study, adsorption isotherms and influence of pH, contact time and interfering ions were investigated to have deeper insight into adsorbent quality. UV/Vis spectroscopy confirmed that the dominant adsorption mechanism is the electrostatic attraction at lower pH values. The study showed there was no significant change in adsorption efficiency for starch-coated nanoparticles. However, starch as a natural and biocompatible compound can enhance nanoparticles water dispersibility. The advantage of such materials is that saturation time does not exceed 20 minutes. Therefore, the as-prepared and starch-coated $CoFe_2O_4$ presents very efficient material for application in the field of water remediation.

12-2

Photocatalytic degradation of methylene blue and oxytetracycline via sol-gel synthesized pseudobrookite

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Fe_2TiO_5 nanoparticles were synthesized by modified sol-gel method using $Fe(NO_3)_3{\cdot}9H_2O$ and $Ti(OC_3H_7)_4$ as starting reagents, oxalic acid as chilate agent and cetyltrimethylammonium bromide as surfactant. The aim of this study was to asses the photocatalytic degradaton of water pollutants, methylene blue and the antibiotic Oxytetracycline (OTC) using natural sunlight irradiation. As prepared nanoparticles were characterized by XRD, BET, FESEM and UV-vis DRS. The optimal operating conditions of photocatalytic degradation of water pollutants were achived by changing the pH of the solution and changing the concentration of photocatalyst.

12-3

Finding optimal conditions and investigating the structure & morphology of cobalt/magnesium ferrite based cubic spinels ($Co_xMg_{1-x}Fe_2O_4$) as photocatalysts

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Cobalt/magnesium ferrites with various mole percentage ratio of the metals (obtained structures are $Co_xMg_{1-x}Fe_2O_4$ with x being 0, 0.1, 0.3, 0.5, 0.7, 0.9, 1.0) were synthesized by sol-gel combustion synthesis using glycine as fuel, following the rules of propellant chemistry. The powders were then sintered at 700 °C for 3 hours. Obtained powders were characterized by X-Ray diffraction (XRD), scanning electron microscopy (SEM), Raman spectroscopy, UV/*vis* diffuse reflectance spectroscopy (DRS). Investigation of the magnetic properties was also conducted by vibrating sample magnetometry (VSM). The obtained powders were proved to be phase-pure cubic spinels which formed agglomerated micrograins. Series of photocatalytic experiments of methylene blue degradation were done. The influence of different experimental conditions was investigated including variations of: pH values, concentrations of the pollutant, masses of the photocatalyst, different light sources and therefore different light irradiation. Interesting results, including enhancement of the degradation rate with the introduction of cobalt into $MgFe_2O_4$ and decrease of the degradation rate with further increase of cobalt content and formation of hard agglomerates, open new possibilities for further investigation of the utilisation of Co/Mg ferrites as photocatalysts.

12-4

Development of nanoparticles-in-microparticles system for improved adsorption of chromium (VI) ions from water

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Chromium ions are often present in the drinking water above allowed limits and their removal is a very actual topic. One of the most efficient and cheap process for their removal is adsorption on metal powders because they have fast kinetics and high adsorption capacities. However, those powders are usually hard to remove from solution after the adsorption. In order to overcome this problem in this work metal powder of ferric oxides was immobilized within the alginate beads geled by calcium (II), aluminum (II) and copper (II) ions. Thus separation process of the adsorbent from the mixture is facilitated but with minimal loss of adsorption speed and adsorption capacity.

The aim of this paper is to investigate the kinetic of so formed adsorbents for adsorption of chromium (VI) ions from water solutions. The results obtained were processed applying kinetic models pseudo-first and pseudo-second order. Based on the results, adsorption capacity and adsorption efficiency of chromium (VI) ions were defined. The results confirmed that metal oxides immobilized in alginate particles can be very successfully used as adsorbents for the removal of chromium ions from aqueous solutions.

12-5

Mechanism of Rhodamine B photodegradation on hexagonal $ZnIn_2S_4$

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Textile industry is the greatest consumer of synthetic organic dyes and consequently, the greatest producer of water polluting effluents [REF.] Because of emerging global problem with drinkable water it is necessary to find easy applicable methods for water purification, at least for possible industry re-use. Photocatalytic degradation of pollutants can be that method of choice, but in order to lower the price of its application, selected photocatalyst must be active under Solar light illumination.

$ZnIn_2S_4$ (ZIS) fulfils this request; additionally, its hexagonal form is resistible to photocorrosion, and can be easily synthesized in 2D morphology (as sheets), which provide larger available surface area for dyes adsorption.

However, in process of dyes photodegradation, organic intermediates that are even more harmful for the environment than original compound can be produced. Thus, deep understanding of photocatalyst/dye interaction is necessary.

Here, mechanism of ZIS/Rhodamine B (RhB) interaction under simulated Solar light irradiation will be discussed. RhB is xanthene, cationic dye which readily adsorbs on sulphur-rich, negative surface of ZIS. Under solar light illumination, both, RhB and ZIS are excited and due to convenient potential positions of LUMO of RhB and conduction band of ZIS, electron-transfer process occurs, leading to step-by-step de-ethylation of RhB structure. As a result of this process, pale yellow conjugated structure of RhB stays in the system. In that case we cannot talk about photodegradation, but only about decolourization of the dye.

However, due to convenient potential values of valence band of ZIS and HOMO of RhB, direct oxidation of RhB by photogenerated hole in ZIS is possible, and this process leads to destruction of conjugated part of the dye. This route is dominant, and consequently in illuminated RhB/ZIS system, dye is majorly degraded.

12-6

Biosorption of Cu^{2+} from aqueous solution by alkali modified waste jute woven fabrics

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Waste jute fabrics (raw and alkali modified), acquired as waste from different industries were used as an efficient biosorbent for removal of Cu^{2+} ions from aqueous solution. All woven jute fabrics (raw as well as alkali modified) were characterized by determination of their chemical composition and amount of carboxyl groups. The effect of solution pH, contact time and initial metal ion concentration on the biosorption were studied. The alkali modifications lead to hemicelluloses removal and an increased amount of carboxyl groups. The maximum biosorption capacity for Cu^{2+} was observed at pH 5.5. Concerning the contact time, more than 80% of total Cu^{2+} uptake by the raw jute fabric was removed within 1 h. On the other hand, in the case of alkali modified jute fabrics, between 70-75% of the total Cu^{2+} uptake was removed within 3 h. Increased initial ion concentration from 10 to 20 mg/l caused an increase in the total uptake capacity of alkali modified jute fabrics for 42-55%. It was found that the biosorption properties of waste jute fabrics are predominantly influenced by the amount of carboxyl groups, while fabric chemical composition (i.e. hemicelluloses content) has a secondary role in the biosorption of Cu^{2+} ions. The best biosorption performance possesses alkali modified jute fabric with 58% higher amount of carboxyl groups; its total uptake capacity towards Cu^{2+} ions (at 20 mg/l) is about 2 times higher compared to the raw jute fabric.

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13-1

Kinetic and equilibrium study on Cr(VI) removal from aqueous solutions using coconut shell activated carbon as adsorbent

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Chromium is toxic metal and its poisonous hexavalent form, Cr(VI), in water can cause serious harm to ecological environments. In this study, the adsorption of Cr(VI) from aqueous solutions by coconut shell activated carbon (CSAC) was investigated. The influence of various parameters, such as pH, contact time, adsorbent and initial Cr(VI) concentration, was examined. Results revealed that removal efficiency of Cr(VI) was the highest in the pH interval from 2.0 to 3.5, while the equilibrium was restored after 60 minutes. Further, the adsorption kinetics of Cr(VI) can be described using a pseudo second-order kinetic model. Two equilibrium adsorption models, the Langmuir and Freundlich, were used to fit the obtained data. The adsorption equilibrium data fit the Langmir isotherm and the maximum adsorption capacity was found to be 31.2 mg/g. The results on the removal of Cr(VI) from aqueous solutions by CSAC indicated the possibility of using this low-cost material in the treatment of wastewaters containing toxic chromium.

13-2

Hemp fibers and alginate biocomposite for the nickel ions adsorption

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Due to the more excessive industrial activity, the pollution of the environment has been worsening through the years. Sustainable solutions for the pollution problems are the ones that not only provide a method for removal of the pollutants, but guarantee that the method is ecologically and economically efficient. The number of existing pollutants is enormous, but the ones which may be considered as the most dangerous are heavy metals. Due to the fact that heavy metals are non-degradable and that they bioaccumulate, they are considered as very hazardous pollutants. Nickel is one of the toxic heavy metals, which is mainly present in waste waters coming from electrochemical industries, or in waste waters which are polluted by substances from used batteries. Numerous methods for removal of heavy metals have been developed, but we chose biosorption as an adequate one for nickel removal. Biosorption is a process where biological materials bind and accumulate heavy metals. Most frequently used biosorbents are biopolymers, like lignocellulosis biomass, alginates, chitosan etc.

In this work short, intricate hemp fibers, obtained as a waste from textile industry, were used as cost-efficient biosorbents. Alginates, which also have noticeable sorption capacity towards heavy metal ions, were used as coating of hemp fibers. Therefore, the idea of this research was to combine the biosorption abilities of hemp fibers and alginates by creating a biocomposite, which could have better adsorption properties – adsorption capacity and kinetic parameters than individual biosorbents. In order to produce the adequate biocomposite for nickel adsorption, the adsorption parameters were investigated by measuring nickel concentrations during the adsorption, and then performing the analysis. Acquired results showed that this biocomposite has very good potential for nickel removal, in terms of both adsorption capacity and kinetic parameters.

13-3

Glyphosate herbicide adsorption on the cross-linked environmental-responsive hydrogels

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Extensive use of pesticides to increase crop yields has been significantly increased, as has the number of agrochemicals present in the environment. The main idea of environmental-responsive hydrogels application is to minimize the nonselective use of conventional pesticides for improving their safe environmental utilization. Glyphosate, *N*-(phosphonomethyl) glycine, is a widely used herbicide throughout the world. The adsorption of glyphosate in soils is of great interest for the minimization of its impact on the soil and water environment. The aim of this study was to examine the environmentally sensitive hydrogels for absorption of glyphosate residues in aqueous environment. In this reason, by free radical polymerization of monomers *N*-isopropylacrylamide and 2-hydroxypropyl methacrylate synthesized was a series of copolymer samples with different content of ethylene glycol dimethacrylate as crosslinker with benzoyl peroxideas initiator and dioxane as solvent. The swelling capacity of synthesized poly(*N*-isopropylacrylamide-*co*-2-hydroxypropyl methacrylate), p(NIPAM-HPMet), hydrogels enable their potential use as adsorbers to remove glyphosate from the aqueous mixture. The residual concentration of glyphosate during adsorption was monitored by the high-pressure liquid chromatography (HPLC) method. The adsorption efficiency of glyphosate from aqueous solutions (pH 6.0) by p(NIPAM-HPMet) hydrogels has been monitored based on the residual concentration of glyphosate in the aqueous solution. Adsorption of glyphosate was found to be decreased with increasing cross-linking degree of hydrogels. The maximum adsorption capacity of glyphosate herbicide was achieved by the hydrogel with the lowest cross-linker content. The results obtained indicated that the synthesized cross-linked hydrogels exhibited adsorption properties and making them potential candidates for use as next-generation adsorption materials.

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13-4

Circular economy in textile industry - byproduct of textile bleaching as a novel material for textile wastewater treatment

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Textile industry has long been recognized as one of the major waste generating industry. Large waste is generated in every segment of textile processing, from the solid (fiber and fabrics) waste, to the large volumes of chemically contaminated wastewater. Particularly, output of textile dyeing operations is reflecting in extremely high amounts of wastewater containing chemicals and dyes, dangerous to the environment, requiring very expensive and time consuming methods for handling and disposal. Therefore, there is an urgent need for implementation of solutions which will provide easy, inexpensive, practical and efficient textile wastewater treatments.

Textile bleaching is a process where raw fibers are subjected to chemical treatment in order to remove impurities and to obtain proper whiteness before dyeing operation. Bleaching with potassium permanganate is a traditional process which implies procedure of fibers treatment with $KMnO_4$ solution, followed by washing with $Na_2S_2O_5$ in order to remove deposited MnO_2 on fibers as unwanted byproduct of bleaching. However, MnO_2 has a potential for decolorization of various dye solutions. Knowing this, we analyzed the byproduct of $KMnO_4$ bleaching, cotton with deposited MnO_2, for decolorization of methylene blue and basic fuchsine dye solutions and concluded that it can be successfully used for removal of selected dyes from solutions. The decolorization efficiency of semi-bleached cotton is over 98% in 10 minutes of solution treatment, using solid to liquid ratio of 1:500. We propose an organizational model, where textile waste fibers are subjected to the first step of existing bleaching procedure, in order to obtain novel product for wastewater treatment in textile industry. Remodeling and reusability of textile waste in existing textile industrial operations is in accordance with circular economy, a targeted model of modern industrial organizations.

13-5

The application of the immobilized laccase from *Trametes versicolor* in the decolorization of textile dyes

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Laccases (EC 1.10.3.2, benzenediol: oxidoreductases) are enzymes which catalyze the oxidation of various aromatic compounds with the reduction of molecular oxygen to water. Because of their high affinity towards a wide spectrum of aromatic compounds which includes dyes used in different industrial branches, the use of laccases in the process of purification of industrial effluents is becoming very appealing for researchers. An important limitation in the development of these processes is high price of the enzymes therefore it is of great importance to make efficient immobilized laccase preparations.

In this work, a commercial carrier Lifetech^{TM} ECR8285, poly(metacrylate) functionalized with butyl and epoxy groups was used for the immobilization of laccase from *Trametes versicolor*. During the optimization of the key factors of the immobilization (the protein concentration, pH, immobilization buffer molarity) the concentration of proteins was monitored by spectrophotometric Bradford method and the activity of the laccase, also spectopfotometricaly, with syringaldazine as a substrate. Immobilization was performed at the conditions suitable for covalent bond forming between the functional groups of the carrier and amino groups on the surface of the enzyme- buffer molarity 1 mol/dm^3 pH 7, during 24h at 25 °C. After varying the protein concentration in the immobilization solution, an optimal concentration of 24mg/g of the carrier was established for the laccasse from *T.versicolor*.

Immobilized preparation with the highest enzyme activity was applied in the decolorization of dyes bromophenol blue, bromocresol green, bromothymol blue, Lanaset violet B and Lanaset blue 2R which was determined by spectrophotometric method. Immobilized preparation of the laccasse from *T.versicolor* was successfully applied in the decolorisation of dyes bromocresol green, bromothymol blue, Lanaset violet B and Lanaset blue 2R and was very stable during the seven reaction cycles, while it did not show any activity in the reaction with dye bromophenol blue.

13-6

Natural clay pyrophyllite „Parsovići“ as electrochemical sensors for pesticides

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Pyrophyllite $Al_2Si_4O_{10}(OH)_2$) is phyllosilicate mineral composed of aluminium silicate hydroxide containing an Al octahedral sheet condensed between two tetrahedral Si sheets (2:1 structure). Pyrophyllite shows excellent physicochemical characteristics, such as low thermal and electrical conductivity, low expansion coefficient, low reversible thermal expansion and excellent reheating stability. The aim of this study is to examine pyrophyllite for its potential application like electrochemical sensors for pesticides. Mechanochemical modification using SPEX Mixer/Mill 5100 was used to generate desired products with fine structures. This treatment offers an advantage because it does not use harmful chemicals and has no negative impact on the environment. The structural changes of pyrophyllite before and after the milling process have been investigated by means of PSD (particle size distribution, XRD (X-ray diffraction), FTIR (Fourier-transform infrared spectroscopy, DTA-TG (Differential thermal analysis-thermogravimetric analysis) and Raman spectroscopy. Pyrophyllite carbon paste electrode based on tricresyl phosphate as a binding liquid has been applied as working electrode for the voltammetric characterization and determination of the carbendazim fungicide. It is demonstrated that carbon paste electrode modificate with pyrophyllite can be use like electrochemical sensors for pesticides.

13-7

Synthesis, characterization and application of the zeolite/nano zero-valent iron composite for phosphates adsorption

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Nano zero-valent iron particles (nZVI) and composite nano zero-valent iron particles and zeolite were synthesized and analysed as phosphate adsorbents. Agglomeration of iron nanoparticles restricts its application in remediation. Natural zeolite was used for nZVI immobilisation in order to enhance the efficiency of nZVI. Adsorption properties of nZVI and composite material, containing ~30 mass % were analysed and compared. Samples characterization was performed using scanning electron microscopy (SEM), energy-dispersive spectroscopy (EDS), determining textural properties using BET method. Scanning electron microscopy confirmed that zeolite provided better dispersibility of nZVI. Presence of iron was confirmed by energy-dispersive spectroscopy. Determination of adsorption isotherms demonstrated that maximum adsorption capacities of pure nZVI and composite have the same value of ~12.8 mgP/g, meaning capacity of ~40 mgP/g nZVI in the composite sample, while zeolite doesn’t have any adsorption capacity for phosphates. Therefore, zeolite used as a support provided better nZVI dispersibility and efficiency.

14-1

Influence of raw seashells on pH and distribution of selected heavy metals in acidic soil near copper mining and smelting complex

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Acidification of soil near mining and smelting complexes and the contamination with heavy metals are the issues that can be solved by liming. Such a process aims at pH regulation and simultaneous reduction of toxic metals solubility, leaching, and phytotoxicity, and improving overall agrochemical properties of the soil. To preserve the natural sources of a common liming agent (limestone), alternative materials rich in calcium carbonate, such as waste seashells, are considered. This study intended to determine the influence of raw waste seashells on soil pH and the distribution of trace metals. The soil was sampled in the vicinity of the mining and smelting complex near Bor, Serbia and characterized as acidic (pH 4.93) and Cu contaminated (219.2 mg/kg) with a very low level of P supply (3.61 mg P_2O_5/100 g). The soil was amended with 0.15%, 0.3%, 2%, and 5% of grounded raw seashells and incubated in the pots for two months, with periodic addition of distilled water. The total content of Cu and selected trace elements, Zn, Pb, Ni, Cd, and Mn, in control soil and amended soil samples was determined following the microwave-assisted acid digestion method US EPA 3051A, while modified Tessier extraction protocol was applied as a tool for assessment of the metal distribution. The addition of raw seashells caused the increase in soil pH in all soil samples. Furthermore, the reduction of the ion-exchangeable content of the selected metals in the soil was observed and associated with the treatments. The favorable soil pH level for most crops (pH 6.35) and reduced mobility of Cu were gained with a seashell dose of 0.3% (10 t/ha), indicating that the seashell waste can be used as an effective liming additive. The small effect of various doses of the seashell material onto the available content of P implies that the application of phosphate fertilizer is necessary in order to balance the essential agrochemical properties of the soil.

14-2

Degradation of anthraquinone and sulphonthalein colors using laccase from Myceliophtora thermophila immobilized on primary amino carriers

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Laccase belong to the group of poly-phenols (p-diphenol oxidase, EC 1.10.3.2) who their catalytic capabilities exhibit through electron transfer and oxidation of different phenol and non-phenolic substances where the main by-product is water.

In this paper, the immobilization of laccase of Myceliophthora thermophila was done on multiple macroporous carriers. The immobilization on carrier Purolite® A109 (polystyrene crosslinked with divinyl-benzene, primary amino groups), a distinctly hydrophobic carrier LifeTechTM ECR8806M (polystyrene with octadecyl groups) and SiO2 mesoporous nanoparticles with propylamino groups receive preparations of significantly less activity relative to the methacrylate carrier LifeTechTM ECR8409F (amino group receipts), with which further optimization of immobilization conditions was carried. Immobilization was performed at low ionic strength (50 mM buffer) and pH value of 5. Analyzing the effect of initial protein concentration on activity of immobilized laccase and monitoring the immobilization flow, it was found that the most active preparation, 203 IU / g carriers, was obtained after 4 hours of immobilization in an initial protein concentration of 160 mg/g of carrier. The obtained immobilized enzyme preparation was used in the decolorization of three sulphonthalein and two anthraquinone colors. In addition to the decolorization effect by adsorption onto the carrier particles observed, a significant effect of degradation by the catalytic action of immobilized laccase was detected in the case of anthraquinone colors. In case of sulphonthalein colors the adsorption effect was dominant (except for bromtimol blue). After seven successive reaction cycles, the degree of color de-colouration of the Lanaset violet B has been achieved, from 84 to 50%, while further use has resulted in a significant loss of activity. From the color solution Lanaset blue 2R, 91 to 55% of the initial amount was removed during the ten reaction cycles.

14-3

Recycling of waste industrial gypsum in different cement composites

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Waste industrial gypsum is a waste or a by-product generated during various chemical processes. Numerous different types of industrial residues have been routinely recycled in the construction sector, however in the case of waste industrial gypsum this practice has not yet been widely implemented.

Gypsum is as a setting regulator which is used as an essential ingredient in the production of cement. The increased amount of gypsum used in the preparation of cement composites can, on the other hand, be reflected in the lowered mechanical properties. However, it has been established that the quantities of susceptible components in the cement composite incorporating increased amount of gypsum could be minimized through the use of recycling materials in a form of supplementary cementitious material.

The primary focus of this research project is synthesis and optimization of multi-component cement composites in which increased amount of waste gypsum is used, in order to obtain green cement composites that would, on the one hand, have appropriate properties for use, as well as sufficient durability and functionality over their life span, on the other hand.

Detailed characterization of several different recycling materials (eight ashes and two slags) has been performed in order to gain generic knowledge about their behaviour as supplementary cementitious materials. For the preparation of cement composites, two different cements (Portland cement (PC), calcium aluminate cement (CAC)) and two different waste gypsums (white and red gypsum form TiO_2 production) were used. Waste gypsum was blended in two different ratios (10 and 20 wt. %). The results showed, that in the cement composites with white gypsum, the concentrations of the sulphate in the leachates were generally higher than in leachates from the composites with red gypsum on account to its higher purity. The gypsum composite with PC showed lower early age strengths values than the gypsum composite with CAC, due to the differences in their composition. The results of the time dependent phase characterization of investigated composites enabled the identification of the development of hydration products. On the basis of the results obtained, the optimization of cement composites with larger amount of waste gypsum is in progress together with the identification of their long term characteristics.

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14-4

Kaolin modified with cationic surfactant as a potential adsorbent for ketoprofen

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The contamination of the natural aquatic environment by pharmaceuticals is a serious environmental problem due to their extensive use in human health and animal husbandry. One of the most efficient technique for removal of pharmaceuticals from water is their adsorption on activated carbons, clays and zeolites. In this study adsorption of ketoprofen (KETO), widely used non-steroidal anti-inflammatory drug, on modified kaolin was invesitgated. The natural kaolin (from Rgotina, Serbia) was modified with cationic surfactant hexadecyltrimethyl ammonium bromide in amounts equivalent to 50% and 90% of kaolin cationic exchange capacity. FTIR and DTA/TGA were used for characterisation of materials. The obtained data showed that adsorption of KETO by modified kaolin increased with increasing the amount of surfactant, as well as with increasing the amount of solid phase in the suspension (0.5 – 5.0 mg/ml). According to obtained results modified kaolin may be used as adsobent for removal of KETO from contaminated water.

14-5

Synthesis and characterization of Brushite-metakaolin-based geopolymer materials

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In a field of green chemistry, environmental protection and ecological conservation of the environment there are ways to come up with new and more advanced materials using on the one hand natural, recyceled or waste materials and on the other hand syntethic materials obtained by using green chemistry synthesis procedures. The aim of this paper was to synthesize and characterize Brushite-metakaolin-based geopolymer materials and to examine the possibility of using these materials in the fields of construction, cement industry, as well as in environmental protection as potential adsorbents. Initial materials which were used for geopolymer synthesis was Brushite ($CaHPO_4·2H_2O$) which was obtained by solution-precipitation reaction form acetate solutions and Kaolinite clay from Rudovci deposit (Serbia). The obtained mixture powders were dissolved in a strong alcaline solution with addiction of water glass. Produced geopolymers was cast into mods and preserved for 28 days. The starting materials and the synthesized Brushite-metakaolin-based geopolymer material were examined using XRPD, FTIR SEM-EDS methods. The contact angle measurements were made to test hydrophilic and wettable properties of synthesized material.

14-6

The influence of thermodynamic parameters of the alkaline activator on the mechanical properties of geopolymers

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In order to optimize process of geopolymerization, the investigation of thermodynamic parameters of alkali activators are important. The aim of this research was to investigate the influence of thermodynamic parameters (density, viscosity, refractive index and sound velocity) of alkaline activators on mechanical properties (compressive strength and hardness) of synthesized geopolymer samples. Geopolymers were synthetized by alkaline activation of metakaolin, having the density 2.524 g/cm^3, using the activators at elevated temperature of 60 ^{o}C for two days. Based on the obtained results thermodynamic properties has been selected to predict the properties of materials.

Four series of alkaline activators have been used. Activators remarked as AA1, AA2, AA3 and AA4 present the mixtures of Na_2SiO_3 and solutions of NaOH, of different molarities 2M, 4M, 6M and 8M respectively. The volume ratio of Na_2SiO_3 and aqueous solution of NaOH was the same for all samples. Densities, viscosities and refractive indices of alkaline activators were determined over the temperature range 15-60 ^{o}C of process of geopolymerizations. The values of density, viscosity and refractive index decrease with temperature increase over the investigated temperature range. Increasing molarity of alkali activator solutions, the sound velocity of activators is changed. For sample AA2 the values of sound velocity rises from room temperature to 45 °C and then begins to decrease while for the sample AA3 sound velocity grows until 30 °C and then starts to decrease with further increasing of temperature. Four series of geopolymer samples GP1 to GP4 were synthesiyed using the constant ratio of solid and liquid phase. FTIR, XRD, SEM-EDS methods were used for physicochemical further characterization of geopolymer samples.

14-7

Alizarin effects on two Iodate-based oscillators

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The alizarin (1,2-Dihydroxyanthracene-9,10-dione) effects in two different iodate-based oscillators: Bray-Liebhafsky (BL) and Briggs-Rauscher (BR) were investigated. The Bray-Liebhafsky (BL) reaction is the oldest known chemical oscillator. It consists only of three reactants potassium iodate (KIO_3), sulfuric acid (H_2SO_4) and hydrogen-peroxide (H_2O_2), while the Briggs-Rauscher reaction besides inorganic part (hydrogen-peroxide and iodate in acidic solution), has an organic upgrade in the form of malonic acid. Therefore, in the BR reaction the oxidation of malonic acid ($CH_2(COOH)_2$) by a mixture of hydrogen peroxide (H_2O_2) and iodate (KIO_3) is catalyzed by metal ion (usually Mn^{2+}) in acidic aqueous solution. In general, two chemical mechanisms, non–radical and radical are related to BL and BR oscillators, respectively. In this work, the alizarin effects on BL and BR reaction dynamics is investigated. The alizarin (also known as a Turkey red) has been usually used as a prominent red dye, principally for dyeing textile fabrics, and it was derived from the roots of plants. The different alizarin concentrations have been added in oscillatory mode in both systems. Surprisingly, only BL system is satisfactory sensitive to alizarin addition. Due to the BL reaction is the one subsystem of BR reaction, the different alizarin behavior in these two iodate-based oscillators should be addressed to different experimental temperatures (usually 60 ^{o}C for BL and 25 ^{o}C for BR) at which these oscillatory reactions take place.

14-8

Application of laccase in degradation of pesticide lindane and textile dyes

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Laccases are enzymes which belong to the group of oxidoreductases. They catalyze direct oxidation of many aromatic compounds. Because of their properties they are used in bioremediation of soil and purification of effluents from multiple industries. Aim of this paper was to investigate potential use of microbial laccases produced by *Miceliophthora thermophila* (Novozym 51003) and *Trametes versicolor* in degradation of several selected pollutants.

Preparation Novozym 51003 was used in degradation of lindane which belongs to the group of organochlorine pesticides and its chemical structure is γ -hexachlorocyclohexane (HCH). At optimal conditions (pH 6.5, 25 °C), the enzyme was applied in its free and its immobilized form on SiO_2 nanoparticles. Through application of gas chromatography coupled with mass spectrometry (GC-MS) qualitative and quantitative analysis was performed. Final degree of degradation was 50% after 6 days in both cases.

Two anthraquinone – Lanaset violet B and Lanaset blue 2R and three sulphonphtalein colors – bromophenol blue, bromothymol blue and bromocresol green were examined. Two free laccase from *T. versicolor* and *M. thermophila* were used and degree of decolorisation was monitored using spectrophotometry. Novozym 51003 demonstrated highest activity in degradation of anthraquinone colors – 70% after 28h. Laccase from *T. versicolor* showed significant efficiency and after 5 hours degree decolorisation of 90% was accomplished. Both enzymes showed lower efficiency when used in decolorisation of sulphonphtalein dyes.