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Dear Conference participants, Visitors and Colleagues,

We welcome you to the 3rd international biennial 'Nanomaterials and nanotechnology Meeting' in Ostrava, which is the centre of the Moravian-Silesian region and, at the same time, the third largest city in the Czech Republic. The symposium will be held at VŠB-Technical University of Ostrava, which has more than 160 years of existence. The University provides bachelor's, master's and doctoral studies at seven faculties and two university degree programs in full-time and combined forms.

The conference has been organized under cooperation of scientists from the Nanotechnology Centre (VŠB–TU of Ostrava), Institute of Geonics AS CR, Czech Chemical Society and Czech National Clay Group.

The meeting is a platform to facilitate open discussions between scientists, students and representatives from companies with a vested interest in furthering the development of nanomaterials and nanotechnology.

Conference will be organised in several sessions with plenary lectures focusing on important areas of Nanomaterials and Nanotechnologies.

1. Tools for preparation and characterization of nanomaterials
2. Nanomaterials and their properties
3. Nanotechnology for environment
4. Advances in nanomaterial technologies
5. Nanomaterials of clay minerals and zeolites
6. Education in nanotechnology

We wish you successful and fruitful conference – and enjoy Ostrava!

Organizing committee of NOM 2013

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Welcome from Nano Ostrava 2013 Organizing Committee Chair

On behalf of Nano Ostrava 2013 Organizing Committee, it is my honour and pleasure to welcome you to the Nano Ostrava 2013, 3rd Nanomaterials and Nanotechnology Meeting. The increasing demand for new, high-quality and effective products has resulted in rapid developments in area of nanostructured materials. The conference aims to bring together scientists, students and representatives from companies which deal with nanomaterials and nanotechnology.

Study and research at the VŠB- Technical University of Ostrava is closely related to the fact that Ostrava, the third largest city in the Czech Republic, is an important industrial centre of central Europe. VŠB-Technical University of Ostrava has more than 160 years of existence. It is the fourth largest university in the Czech Republic which provides bachelor, master, and doctoral studies at seven faculties and two University degree programs in full-time and combined forms.

Our Program Committee has prepared an interesting and informative technical program outlining current progress and activities in many research areas of nanotechnology. Over 90 papers from 10 countries have been accepted and scheduled for the 3-day conference.

I wish you to have beneficial conference and I hope that you will enjoy both scientific and cultural aspects of the conference programme as well as your stay in Ostrava.

Jaromír Pištora
Chairman, Nano Ostrava 2013

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The organizers would like to thank the following companies and Moravian-Silesian region for generously sponsoring this meeting:

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Near-IR spectroscopy in the organo-clays studies

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Clay minerals are an important class of materials utilized in a number of industrial and environmental applications. Their properties can be improved by chemical handling, e.g. by replacement of inorganic exchangeable cations by organic, most often alkylammonium cations, or by acid activation. A wide variety of instrumental techniques are used for characterization of organo-clays structure and properties. Present work introduces the potential of near infrared (NIR) spectroscopy to identify specific bonds "not visible" in the middle IR (MIR) region and to follow the effect of organic cation size on the stability organo-montmorillonite in HCl.

Na-saturated montmorillonite Jelšový Potok (Slovakia) and different surfactants containing octylammonium chain(s), hexadecylammonium chain(s) or a benzene ring with or without a reactive double bond were used for organo-montmorillonites preparation. Based on the fundamental vibrations observed in the MIR spectra the first overtone ($2\nu_{XH}$) and combination $(\nu+\delta)_{XH}$ bands of XH groups (X = O, C, N) were identified. While the presence of CH_3 and CH_2 groups was recognized in the 6000-5500 cm^{-1} ($2\nu_{CH}$) and 4450-4100 cm^{-1} $(\nu+\delta)_{CH}$ regions, the CH overtone and combination bands of benzene ring were clearly shifted to higher wavenumbers. The NIR spectra were found to be useful for identification of NH_2^+, NH^+ and vinyl groups, not-detectable in the traditionally used MIR region. The intensive bands of the first overtone and combination modes of NH_3^+ and NH_2^+ were found in the 6600-6050 cm^{-1} and 5000-4600 cm^{-1} regions, respectively. The presence of NH^+ confirmed $(\nu+\delta)_{NH+}$ band observed near 4750 cm^{-1}. The characteristic band assigned to $2\nu_{CH2}$ in $H_2C{=}C$ was detected at 6130 cm^{-1}.

Organo-montmorillonites prepared from Na-SAz montmorillonite (Cheto, Arizona) and tetraalkylammonium salts of alkyl-chains length increasing from methyl- to pentylammonium were dissolved in 6 M HCl for different time. Acid dissolution proceeded via replacement of the exchangeable cations with protons, which penetrated into the montmorillonite layers and attack the OH groups. Following dehydroxylation connected with the release of the central atoms from the octahedral sheets resulted in formation of amorphous, partly protonated silica phase. Gradual decrease of the intensities of the $2\nu_{CH}$ and $(\nu+\delta)_{CH}$ bands reflected the falling content of the alkylammonium cations, while the reduction of the structural OH overtone (~7060 cm^{-1}) and combination (~4520 cm^{-1}) bands intensities indicated gradual decomposition of montmorillonite structure. New band near 7315 cm^{-1} corresponding to SiOH overtone confirmed creation of protonated silica. NIR spectroscopy showed that the least stable were samples saturated with small cations while the most resistant to acid attack were organo-montmorillonites with large cations. They cover the inner and outer surfaces of montmorillonite, prevent the access of the protons to the layers and thus protect mineral from acid-degradation.

Characterization of polymeric drug carriers using molecular modeling

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Present work is devoted to the development of simple molecular modeling method for preliminary characterization of polymeric drug carriers. Six biodegradable polymers have been investigated as drug carriers using molecular simulations in Materials Studio modeling environment: L-polylactide, D-polylactide, chitosan, polyglycolic acid, polyethylene glycol and cellulose. Cyclosporine A (CsA) has been chosen as a model drug substance.

In order to characterize the suitability of a given polymer chain for non-bond anchoring of CsA molecule, four following parameters have been investigated: (1) non-bond interaction energy between polymer and CsA, (2) number of hydrogen bonds between CsA and polymer for optimized geometry of polymer/CsA model, (3) CsA-polymer miscibility using χ parameter from Flory-Huggins theory, and (4) flexibility of polymer chain characterized by means of gyration radius.

Molecular modeling using empirical force field revealed that the polymer-CsA interaction energy is a result of mutual cooperation of all the factors mentioned above, i.e. mutual miscibility, flexibility of polymer chain, mutual shape complementarity and chemical complementarity (number of functional groups on polymer and CsA molecule).

The main results can be summarized in three following points.

1. Miscibility dependens on length of polymer chain and this dependence is more noticeable for flexible chains.
2. The best miscibility is strongly correlated with the CsA-polymer interaction energy and with the number of hydrogen bonds between polymer and CsA molecule.
3. Two polymers (polychitosan and polycellulose) with the best miscibility and highest CsA-polymer adhesion exhibit surprisingly high rigidity. The reason is that these polymers are not so strongly coiled and remain much more open offering larger surface (and much more accessible functional groups) for interaction with CsA molecule.

Presented molecular modeling method is simple, cheap and relatively fast. Good agreement of obtained results with experimental data suggests that this method is a promising tool for the preliminary characterization of polymeric drug carriers

Keywords: molecular modeling, biodegradable polymer, structure, cyclosporine A

Magneto-optic activity of gold nanoparticles

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In this contribution the measurable magneto-optic (MO) activity of nanoparticles made out of noble metals is discussed. As some recently published works show, this phenomenon is observed when the localized plasmon waves are excited in the presence of external magnetic field. The origin of this MO effect consists in the resonance of permittivity that has been yet demonstrated. We confirmed these observations theoretically and by experimental way as well. The measurements presented here are related to Au nanostructure on SiO_2/Si substrate. They are compared to theoretical model based on effective medium approximation (EMA). Since the heterogeneous layer is formed as a field of randomly distributed spheroidal nanodots of various sizes having the same height and parallel symmetry axes, the Bragg-Pippard model of EMA is applied. Derived computational algorithm is implemented in Matlab code and successfully validated by comparison with the data published elsewhere. Realized simulations exhibit good agreement not only for own MO data, but also for obtained ellipsometrical outputs. Moreover, presented results illustrate plasmon excitation as an extinction peak in reflection response.

Keywords: Magneto-optics, Gold nanoparticles, Effective medium, Plasmonics

Physico-mechanical properties and electrical conductivity of the conductive plastic

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The paper deals with the research on a variety of non-standard samples of plastic material made by injection molding. The samples are made of a conductive plastic material (LNP Stat-kon Compound ZX05009. Brown Corundum F24 was used for blasting under different pressures. This conductive plastic material can be applied as a plastic electrode, therefore, there can be provided the measurements and examination of electrical conductivity. The experiment is used to in order to establish the extent to which the pressure used in blasting measurably affects the electrical conductivity of plastic electrode.

Keywords: physico-mechanical properties, blasting, plastic electrode, injection molding

Molecular modeling of PANI thin film on glass substrate

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Polyaniline (PANI) is nowadays the most studied conducting polymer exhibiting unique electrical and optical properties which make it an ideal candidate for wide range of practical applications. PANI can be prepared in powder form but the most frequently studied form of PANI is thin film deposited on various substrates: gold, quartz, zinc selenide and many others. Besides these supports, many research groups used glass slides which are transparent and chemically stable. The coating of glass surface with a thin PANI film can be achieved by using various precursors and preparation procedures. All the preparation methods, however, have the same base which is the polymerization in water solution of precursor and oxidizing agent in the presence of substrate on which the PANI film is formed. If the precursor can not served as cationic source, some acid has to be added. One of the key questions of this technology is the adhesion of PANI on the substrate and this feature can be studied using computer molecular modeling. The aim of present work is to give closer information about behaviour of PANI on glass substrate. For this purpose the molecular modeling with Universal force field as implemented in Materials Studio modeling environment was performed. Four glass surfaces with different values of total charge (0, -4, -8, -16 el.) were prepared, because of presence of surface charges in natural glass. Adhesion energies of PANI chains were computed from optimized models with respect to different glass substrates and the different number of PANI chains (from 1 to 4) present in the models. Octamers of PANI were used as a representatives of real PANI chains. PANI charges were compensated by glass substrate and appropriate number of Cl^- cations. Also the various positions of PANI chains before and after the optimization procedure were taken into account.

It was found that differences in adhesion energies of PANI chains are close related to the value of the total charge of the glass substrate. Models in which the charge of PANI chains is fully compensated by the charge of glass substrate exhibit the strongest adhesion. Resulting structural arrangement, leading to the lowest total potential energy, is always the same – PANI chains parallel to the glass surface. Molecular modeling showed that the glass charge may play a crucial role in the formation of PANI film.

Acknowledgement:

This work was supported by the European Regional Development Fund in the IT4Innovations Centre of Excellence project (CZ.1.05/1.1.00/02.0070).

Keywords: polyaniline, glass substrate, molecular modeling, adhesion

Identification of Stress - Deformation States in a Newly Created Material Produced by ECAP Technology

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This paper deals with the measurement of Young's modulus of elasticity on samples of alloy EN AW 6060, the material was pushed through the ECAP technology. Furthermore, focusing on the change of the material constants given the maximum possible deformation generated in these samples. With the increasing number of punching a measure of the energy embedded in the material decreases, while the value of E increases. You can use the evaluation of mechanical work (such as energy embedded in the material) and the prediction of the value of E (by regression function), then compare the measurement results and the theoretical prediction (depending on the number of punching) and determine to what extent could replace modeling real measurements.

Characterization of historical coins by X-ray powder diffraction analysis

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In the summer of 2012, an archaeological prospecting by a metal detector at locality Krnov-Cvilín (Czech Republic) was realized, in which a set of metallic archaeological artefacts was found. In the set, four modern historic coins were found. For determining the type of the historical coins, it was necessary to explore their relief by the means of optical microscopy and radiography. For illustration, a photograph of a relief of coins is shown in Fig. 1.

To determine the process of conservation and restoration, it was necessary to specify the composition of the original material the coins were made of. Also, the composition of corrosion products covering the coins needed to be determined. Based on the colour of the partially uncovered metallic core, the corrosion products and the fact that the coins are not magnetic, we assessed that they are made of copper or its alloys. The coins were investigated using X-ray powder diffraction analysis (XRPD). The main corrosion product, cuprite (Cu_2O) was identified on all four coins. XRPD patterns of the historical coins are presented in Fig. 2.



Fig. 1 Analyzed coins (a) SU 02/12-E100/60, (b) SU 02/12-C100/75, (c) SU 02/12-B100/78, (d) SU 02/12-K100/86.

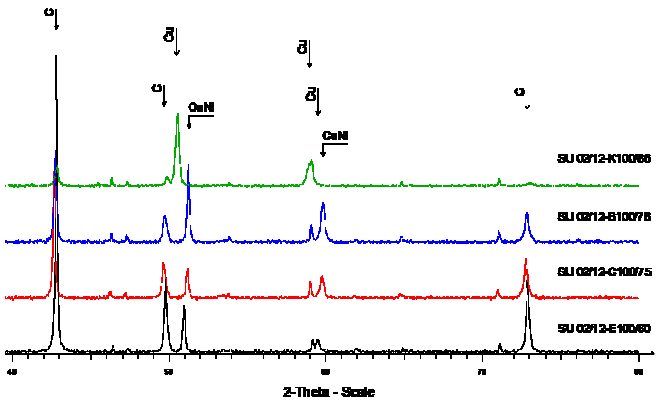


Fig. 2 XRPD patterns of the coins (Cu for copper, C for cuprite and CuNi for copper nickel).

Acknowledgement:
This paper has been elaborated in the framework of the Nanotechnology – the basis for international cooperation project, reg. no. CZ.1.07/2.3.00/20.0074 supported by Operational Programme 'Education for competitiveness' funded by Structural Funds of the European Union and state budget of the Czech Republic.

Keywords: Historical coins, X-ray powder diffraction, Copper, Corrosion product

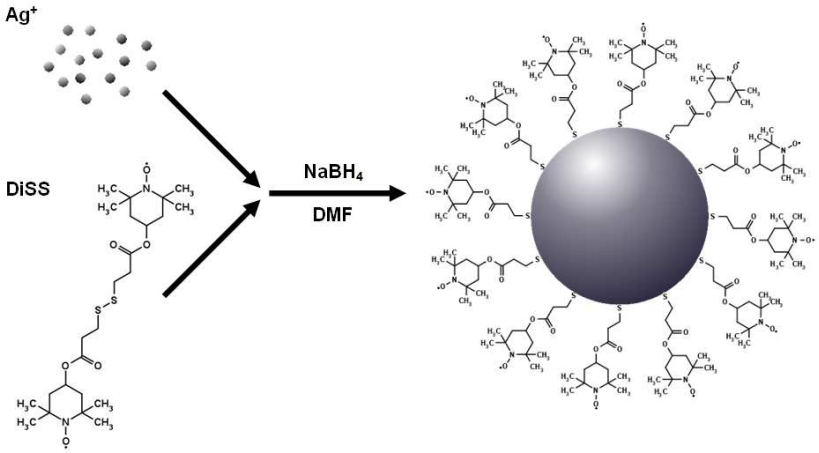
One-Phase Synthesis of TEMPO Coated Silver Nanoparticles

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Silver nanoparticles (AgNPs) have attracted a great interest in recent years due to extremely useful properties leading to a possibility of their utilization as antibacterial agents [1], catalysts in oxidation and oxidative coupling reactions, substrates for SERS spectroscopy, optical labels, enhancing agents in photocatalysis processes [2,3].
Nitroxides, in particular TEMPO (2,2,6,6-tetramethylpiperidine-1-oxyl), are well-known catalysts, excellent alkyl radicals scavengers, mediators in Nitroxide Mediated Polymerization and effective antioxidants [4]. Thus nitroxide coated decorated AgNPs, combining properties of silver nanoparticles with those of nitroxides, appear to be especially promising in design of new materials.
In this work, we report the one-phase synthesis of silver nanoparticles with spherical shape and relatively narrow size distribution (1.5 - 4 nm) covered with TEMPO radicals. The presented method of synthesis consists in direct grafting of nanoparticles with bisnitroxide disulfide, with dimethyl formamide (DMF) both as reaction medium and sodium borohydride solvent. The obtained material was characterized with UV-VIS spectroscopy, X-ray photoelectron spectroscopy (XPS), thermogravimetric and elemental analyses. FTIR and EPR spectra confirmed nitroxide functionalization of the synthesized nanoparticles. The synthesized AgNPs are soluble in most common organic polar solvents e.g. acetone, tetrahydrofuran, ethanol, methanol.



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Image statistical processing as a tool to nano-structured medium identification

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In this contribution the image analysis of nanostructure on SiO_2/Si substrate is described. The TEM image has been analyzed with the objective to describe basic geometrical characteristics of given heterogeneous layer. This medium is simulated as a field of randomly distributed spheroidal nanodots of various size having the same height and parallel symmetry axes. The size (height, diameter) of dots, their probability distribution, filling factor of nanodots and the other data being necessary to calculate the effective permittivity of heterogeneous medium were determined using the image processing. For this purpose two approaches EMA (effective medium approximations) were tested - Bragg-Pippard and Garnett-Maxwell model. The first one is preferred to describe material properties of nanoparticles made out of noble metals with regard to obtained results. Derived computational algorithm is completely implemented in Matlab code.

Keywords: Gold nanoparticles, Image analysis, Effective medium approximation

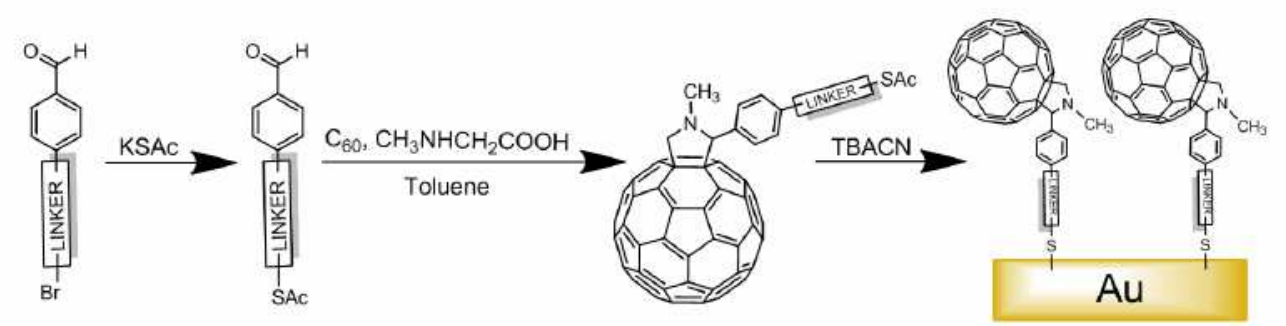
Synthesis of thioacetate-derivatized C60 fullerenes aimed to obtain fullerene-gold nanomaterial composites

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Starting from the discovery of fullerenes in 1985 [1], they have become an important focus of research in the rapidly developing field of nanotechnology. Simplification of their production technology has enabled the production of large-scale, lower prices and increased the chances of using fullerene based nanomaterials in practice. The largest research attention is focused on the chemical functionalization of C60 fullerene, which is the most abundant of fullerene family. Due to its solubility in organic solvents, various methods of surface modification and unique electron acceptor properties, including the ability of reversible 6-electron reduction [2], C60 fullerene and its derivatives are attractive candidates for the construction of advanced materials.



Functionalization of fullerenes by attaching aromatic rings leads to electroactive and photoactive fullerene derivatives. In the presented work we synthesized a series of new aromatic aldehydes terminated with S-acetyl group, which were subsequently used to produce thioacetate-derivatized fullerenes using Prato method [3]. Identification and detailed characterization of the newly obtained compounds was made using spectral methods: mass spectrometry (ESI-MS), Magnetic Resonance Spectroscopy 1H NMR, IR spectroscopy (FT-IR), UV-Vis spectroscopy. In addition, experimental results were supported by quantum mechanical calculations made by semiempirical PM3 method. According to literature data [4], including our recent results [5], thioacetate derivatives synthesized in this work can be efficiently deprotected *in-situ* using tetrabutylammonium cyanide (TBACN) and form well ordered and stable self-assembled monolayers on gold surface. This gives a chance to produce nanocomposites by their chemisorption on Au (111) surface (gold electrode, Au nanoparticles) [6,7].

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Keywords: fullerene, functionalization, nanomaterials

Metal-nanocarbon interactions in nanocomposites

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The interaction of two inorganic materials in composite is facing most of the time obstacles and difficulties to get homogenous material with least possible faults. Interaction of metals and nanocarbons is one of them. Nanocarbons in many of their variation brought interesting opportunities for metals to improve many properties such as mechanical strength, friction parameters or electrical characteristics. Junctions between ferromagnetic metals and carbon nanomaterials are of particular interest in spinronics. Due to self-lubrication and topological structure of C-nanotubes, the friction coefficient of the composite decreases and shows a steadily lower value than that of the reference probe. Increasing of hardness of metal matrix nanocomposites is studied for metals with more ductile properties.

In our study experiments on compatibility were conducted and simulation of possible interaction among carbon nanotube- modifying substance and metals (Au, Ag and Cu) was studied. The structural changes were evaluated using X-ray diffraction methods and Raman spectroscopy. Modeling was performed in Material Studio software environment. The properties concerning mechanical parameters were highlighted in modeling results.

Keywords: nanocarbons, metals, modeling, modification

Identification of relation between the topography of surfaces of classical materials and nanomaterials generated by multiple plastic deformation to the technological process

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In the present paper, there is described the method of identifying the relationship between the surface topography of traditional materials and nanomaterials generated by multiple plastic deformation in relation to the technological process. There are also analyzed the relationships between changes in surface roughness on walls of extruded samples especially in relation to structural changes in grain size and strength of material.

Keywords: multiple plastic deformation, surface topography, technological process, materials

Analysis of Surfaces of Cold Rolled Sheets using Digital Camera

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A new area scan camera system for surface analysis is introduced in this paper. The system is composed of Basler area scan digital camera and Schneider Kreucnach lens mounted on a frame with a controllable LED illuminator. Several measurements of surfaces of cold rolled sheets were done using this camera system. The results of this measurement along with spectral analysis of acquired data are presented in this paper.

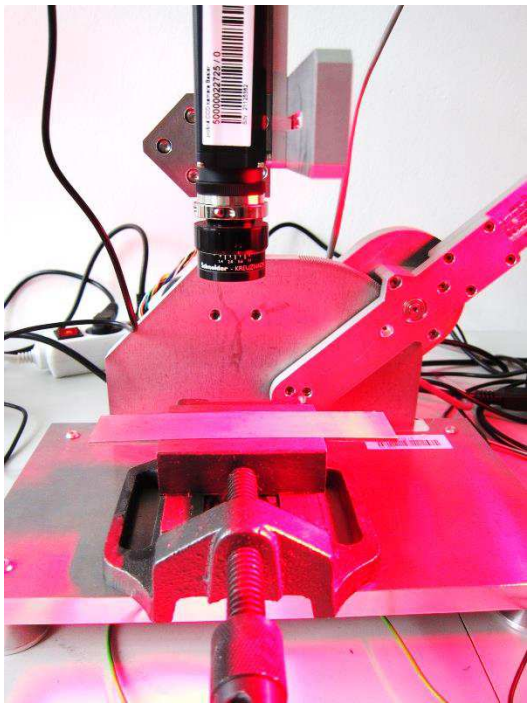


Fig. 1 Area scan camera system for surface analysis.

Keywords: spectral analysis, surface topography, camera system, cold rolled sheets

Advanced Nanocomposite Anode Materials For Li Batteries: Preparation and Characterization

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Lithium batteries are most commonly employed as power sources for portable electronic devices. Limited capacity, high cost, and safety problems associated with the commercially used graphite anode materials are hampering the use of lithium batteries in larger-scale applications such as the electric vehicle. Nanocomposites have shown promise as new anode materials because of their better safety due to higher operating potential, increased energy density, low cost, and straightforward synthesis as compared to graphite.

New materials hold the key to fundamental advances in energy conversion and storage, both of which are vital in order to meet the challenge of global warming and the finite nature of fossil fuels. Nanocomposite materials in particular offer unique properties or combinations of properties as electrodes in a range of energy devices. Nanocomposites consisting of active grains which can alloy with lithium and “inactive” grains which cannot have been made by mechanical alloying of elemental powders. The inactive grains act as a matrix to hold the active grains as they repeatedly alloy with lithium during the operation of a lithium battery. A microscopic mixture of (active) and (inactive) shows a volumetric capacity for which is more than twice that of the graphite materials, which are now the anode of choice for the battery. Unlike pure and alloys, the nanocomposites retain this capacity for many charge-discharge cycles suggesting that materials like this will be the anodes of choice for the next generation of compact, high energy, batteries. This review paper describes some recent developments in the discovery of nanocomposite anode materials and their advanced characterization techniques for lithium batteries. The advantages and disadvantages of the nano-scale in composite anode materials preparation and the new characterization methods are highlighted.

Keywords: Li batteries, nanocomposite anode, preparation, characterization

Single-Photon Nanophotonics

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Most of the past and present research results may be referred to as conventional photonics. Even when various functions such as switching or sensing are implemented with modern nanoscale technologies, the actual use of photons is still far from the ultimate level of exploitation, i.e. at the quantum limit level whereby the underlying principle is to generate, detect and manipulate single photons. However, challenging issues of theoretical and experimental studies of optical effects at the single-photon level have become a focus of recent research worldwide. Some proof-of-concept demonstrations have been highly promising, including photonic quantum circuits on a silicon chip, high-efficiency photon-number-resolving detectors based on superconducting nanowires, semiconductor-cavity-quantum-dot single-photon sources, photonic crystal quantum-dot-based single-photon nonlinearities, or photon-induced tunneling and blockade in a solid-state system.

The goal of our research is to utilize unique properties of various optical effects at the single-photon level for establishing photonic functionalities based on optical gain and optical nonlinear interactions of single photons. Nanoscale waveguide, plasmonic, periodic and nonlinear optical structures are investigated for control, manipulation, amplification, and storage of photons. Semiconductor materials such as silicon and gallium arsenide are the media of choice for given single-photon propagation and interaction studies. For optical gain studies, our research concentrates on understanding and possible exploitation of ways, via material nonlinear and plasmonic interactions, for obtaining single-photon energy gain other than known spontaneous and stimulated emission effects. For nonlinear interactions, the research activities center around understanding the behavior of single photons in electron's environments in semiconductors and how a photon interacts individually and how it can be brought into- and utilize in a nonlinear interaction with another individual photon via their mutual interactions within and via the material.

Complementarily to semiconductor materials, the material structuring (e.g. quantum dots, photonic crystals, nanostructures, nanoresonators, nanofilters) is being studied in detail with a goal of designing and implementing configurations that accommodate best the desired interaction and functionality.The strategy is to design and implement a single-photon ultra-fast switching element with built-in optoelectronic amplification. Ourlong-term goal is to establish theoretical, experimental, and technological platforms for single-photon functionalities and functional elements and devices with built-in optoelectronic gain and storage capabilities in order to be able to control and manipulate photons for applications in engineering, biomedicine, and other fields.

Recent results are reported in designing nanophotonic structures for applications in light collection and manipulation for solar cells, and optical nanofilters for high-resolution microscopy. Structures utilize metals as well as semiconductors (e.g. silicon) and exploit extraordinary transmission (EOT) effects existing due to wave-plasmon interactions.

Keywords: Nanophotonics, Optical plasmons, Light-matter interactions, Semicodnuctors

Analysis of parabolic gold nanooptical antenna for high directivity applications

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Optical antennas are metal nanostructures designed to convert localized energy into optical radiation and vice versa. The behavior of metals at optical frequencies is different from that at microwave and RF frequencies. Metals cease to behave as perfect conductors at terahertz frequencies and show dielectric properties. The optical properties of metals are strongly affected by the existence of Surface Plasmon Polariton(SPP) resonances as shown in Fig.1. These modes are highly confined and can be controlled at the nanoscale by shape, size, structure and type of materials. The electromagnetic field is not restricted to the surface of the metal but depending on the permittivity of the material, the field penetrates the surface to an extent given by the skin depth.

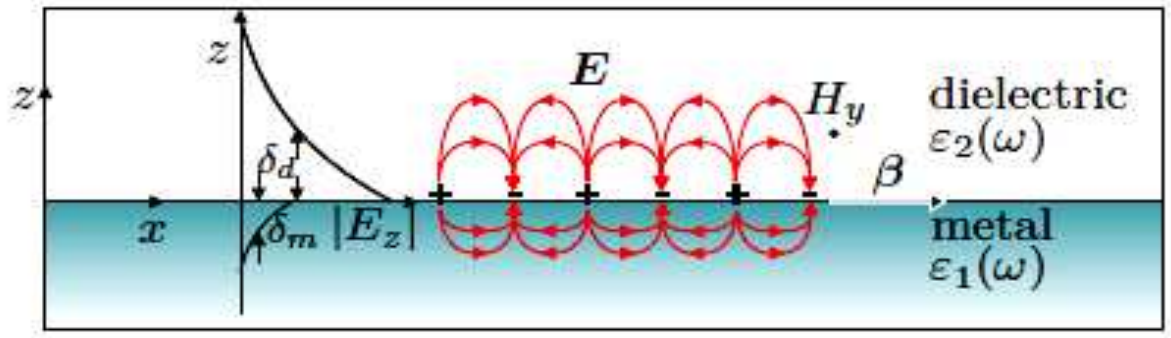


Fig. 1 SPPs at metal dielectric interface.

Based on the theory of conventional parabolic dish as an efficient structure for transmission and reception of energy, the focus of this research is to analyze the scattering cross section of parabolic gold nano-disc which relates to the ability of the antenna to absorb, scatter and reradiate the incident radiation. Analyzing the near-field and far-field profiles of the nano-disc provides insight into the behavior of the antenna with respect to directivity, polarization and field-enhancement. The near and far field radiation patterns, electric field distribution on the antenna surface, effect of cylindrical and circular wave front polarizations and field gains have been obtained for various antenna dimensions and dielectric materials through this analysis. The COMSOL Multiphysics software has been used for simulations.

Keywords: Nanoantenna, Surface Plasmon Polariton (SPP), Finite Element Method (FEM), Polarizability

Probing the quantum levels of individual semiconductor impurities

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A transformation is occurring in electronic technologies – with the goal of developing semiconductor devices based on manipulating the charge and spin of individual dopant atoms. As the size of conventional components is reduced to nanometer scales, driven by the desire to maintain Moore's Law, the exponential improvement in the performance is determined by ever fewer numbers of dopants. The ultimate limit is that of a single impurity atom. Elucidating the physics of these minute systems is a difficult technical challenge. We have developed a capacitance-based scanned-probe method that can detect individual electrons entering impurities. Single-electron peaks have been observed in the capacitance-versus-voltage curves for both donors and acceptors in silicon and gallium-arsenide materials. We find that the quantum states in these systems can be understood in terms of dopant molecules, effectively formed by nearest-neighbor dopant pairs.

Keywords: scanning probe microscopy, capacitance, single-electron tunneling, dopant molecules, subsurface dopants

Silicon/Nickel core-shell negative electrodesusing electroless process for li-ion batteries

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In this work, core-shell Si/Ni composite powders were produced using an electroless deposition process. The nickel content on the surface of silicon powders was varied by using different concentrations of $NiCl_2$ in the plating bath. The surface morphology of the produced Si/Ni composite powders were characterized using scanning electron microscopy (SEM) attached with an energy dispersive spectroscopy (EDS) which was used to determine the elemental surface composition of the composites. X-ray diffraction (XRD) analysis was performed to investigate the structure of the Si/Ni composite powders.

Keywords: Si/Ni, Composite Powders, Electroless, Characterization

Effective silica coating strategy on hydrophobic quantum dots toward sensitive biological imaging and labeling detection

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Compared with florescent protein and organic dyes, quantum dots (QDs) possesses several advantages in bioimaging such as high Quantum Yield (QY), tunable color emission from UV to NIR, low photobleaching and multicolor emission under single excitation wavelength [1]. However, there are still several challenging problems in the biological application field of QDs. First, how to achieve highly bright and stable water soluble QDs just as their organically synthesized counterparts with high quantum yield and hydrophobic surface. Second, how to enhance the florescent brightness in terms of the single QD that usually used. Third, how to prepare efficient QDs assemblies with nano-carriers for signal amplification and ultra sensitive labeling detection.

In current work, we demonstrated an effective and versatile silica coating strategy on hydrophobic QDs based on organosilane micellization and silicate deposition. This method skipped the conventional water solubilization step for oil-soluble QDs and greatly favored the fluorescence preservation by confining the QDs in a lipophilic interior of a silica bead. The facile ultrasonic fragmentation of organosilane precursor enabled an easy scaling over silica bead size and their loading amount of hydrophobic contents. By this manner, we created a serious of CdSe/ZnS@SiO_2 nano-spheres ranging from 16 nm to 38 nm with multi-core structure (enhance the brightness and reduce the blinking) and a tunable silica shell thickness [2]. These nano-spheres exhibited a quantum yield of 45% (90% relative to the oil sample), robust photochemical and colloidal stability in biological medium. We applied the transferrin labeled fluorescent beads for targeted HeLa cell imaging (Fig. 1).

The coating strategy not only works for II-VI semiconductor QDs but also fulfill the water solubilization of different surface capped QDs including the most promising and challenging I-III-VI QDs [3]. In this case we incorporated single or multiple hydrophobic $CuInS_2$/ZnS directly into silica beads with a relative small of 17-25 nm. The silica coating maintained the emission properties of $CuInS_2$/ZnS regarding the photolumilescent spectrum, quantum yield above 60% in aqueous solution and the PL lifetime. The obtained $CuInS_2$/ZnS@SiO_2 nanoparticles exhibited advanced PL stability in aqueous phase along with the low cytotoxicity (MTT test) which favoured their biomedical fluorescent imaging. More interestingly, the strategy is applicable for hydrophobic assemblies such as silica@QDs nano-spheres with high packing density. This allows the fluorescent nano-spheres water soluble with high quantum yield. One can use the assembly-silication-assembly circle to prepare fluorescent encoded nano-spheres, noble metal and magnetic particles encapsulated QDs@SiO_2 multifunctional nanocomposites.

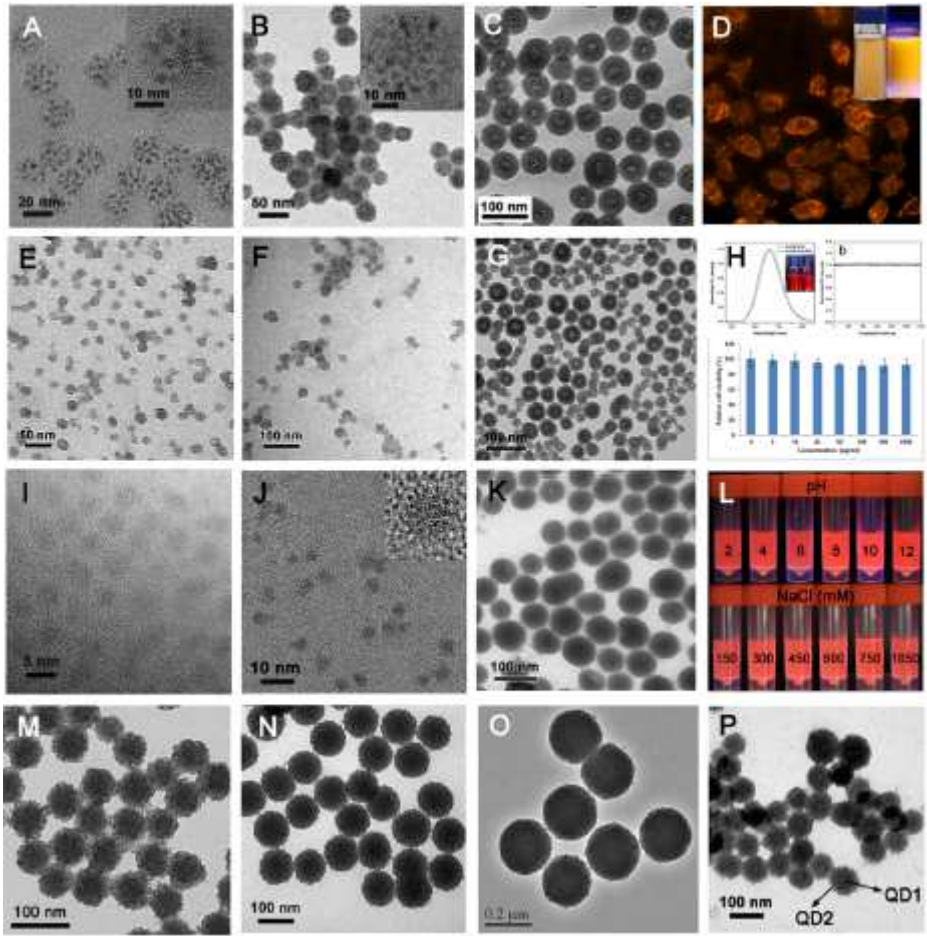


Fig. 1 Strategy I (A-D): Direct organosilica coating on CdSe/ZnS QDs to form multi-core silica beads for cell imaging. **Strategy II (E-H):** Silica coating on $CuInS_2$/ZnS QDs toward non-toxic and NIR emitting labels. **Strategy III (I-L):** Single QD per-micelle as ultra small, stable and brilliant fluorescent probe. **Strategy IV (M-P):** Silica coating on metal affinity induced QDs nano assemblies towards ultra bright, stable and color encoded fluorescent spheres.

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Keywords: Organosilane micellization, $CuInS_2$/ZnS@SiO_2, silica nanospheres, fluorescent sensing

Muller matrix ellipsometry of 1D periodic nanostructures with non-reciprocal optical response

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In recent work in magneto-optical transverse Kerr effect (TMOKE) domain it was presented how the TMOKE can be strongly enhanced in a periodic structure supporting both plasmonic and magneto-optic effect [1,2]. Up till now this magnetoplasmonic enhancement was mainly attributed to a nonreciprocal shift of the dispersion of the surface plasmon polariton resonances at the interface with the magnetized substrate. It was theoretically demonstrated that the amplitude of the transverse Kerr effect can be further enhanced by tuning of geometry of the grating, namely its thickness [3].

In this paper we present precise characterization of structure of the gold grating on MO garnet (Bi-substited yttrium iron garnet $Bi_xY_{3-x}Fe5O_{12}$ or pure BIG, $Bi_3Fe_5O_{12}$) in transversal magneto-optical configuration. In first step we present dielectric function of used materials and precise geometrical parameters of the structure. The main part of paper is focused to study of nonreciprocal transverse MO effect for different geometry of the grating by spectroscopic ellipsometry. We show how amplitude of the TMOKE can be significantly affected by the geometry of the structure, namely by its air fill-factor. Two-rotating compensator ellipsometer Woolam RC2-DI with spectral range from 193 nm to 1.7 μm (0.72 – 6.4 eV) is used for optical characterization.

Acknowledgements:
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Keywords: transverse Kerr effect, plasmonics, surface plasmon polaritons, magnetooptics

Well dispersion of MWCNTs within Al based matrix by controlling ball movement

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Recently, metal matrix composites reinforced by carbon nanotubes have been developed because of their applied mechanical and thermal properties. Low quality dispersion of carbon nanotubes within matrix is an important parameter to achieve good properties that are still challenging.
In this research work, a new procedure including acidic treatment of CNTs, mixing with Al powder by ultrasonic and ball milling by an improved method was used to achieve high quality dispersion. Moreover, the effect of some parameters such as CNT aspect ratio and weight percent on dispersion of CNTs in matrix were investigated. The results showed functionalization of CNTs using Nitric/Sulfuric acid has a marked effect on homogenous dispersion of CNTs with Al powder in Ethanol. Also, by controlling the ball movement using an external magnet in a horizontal ball mill, The dispersion of CNT within matrix can be improved greatly. Furthermore, time and energy consumptions were decreased so that carbon nanotubes dispersed in the matrix with appropriate bond at initial times. The results revealed the agglomeration and grinding of 2 wt. % CNTs with high aspect ratio fabricated by conventional horizontal ball milling. In this matter, the dispersion improved slightly by decreasing the weight percent to 1wt%,. On the other hand, CNTs with low aspect ratio showed more clustering and minor damage in both 1 and 2 wt.%. In modified milling process, both types of carbon nanotubes dispersed well in the matrix at initial times. Also, the particle size of grain structure of composite containing carbon nanotubes determined to find the influence of aspect ratio on grain growth.

Keywords: Metal matrix composite, characterization, multiwall carbon nanotube, mechanical alloying, dispersion

Structural and electrochemical studies on $Li_4Ti_5O_{12}$ spinel decorated by Ag nanoparticles

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Secondary lithium-ion batteries (LIBs) have attracted great attention for their widespread applications in various electronic device and electric vehicles. LIBs were found to be the most promising systems to conquer that challenges, owing to its high power capacity, good cyclability, flat charge/discharge profiles and high operating voltage. Nevertheless, high costs of the electrode materials, low current densities acquired from the cells and safety concerns make Li-ion systems as still demanding improvement.

One of the objectives is to replace a costly and unsafe graphite anode with a new type of anodic material - $Li_4Ti_5O_{12}$ (LTO) of spinel structure. LTO is cheaper and more safe compared to graphite, due to high potential of 1,55 V vs Li/Li^+ which prevent metallic lithium plating on negative electrode during overcharge. Due to no structural change during lithiation/delithiation processes („zero-strain" electrode) the material shows excellent cyclability. However, $Li_4Ti_5O_{12}$ suffer from lower theoretical specific capacity compared to graphite, which is 175 mAh/g and its insulating character, which prevents using it in high current applications. The conductivity of lithium-titanium oxide can be greatly improved by various surface modifications, cation doping or preparing this material in the nanocrystalline form.

In this work we present the surface modification of LTO using Ag nanoparticles. Also our studies demonstrate, that highly dispersed Ag nanoparticles on the surface of $Li_4Ti_5O_{12}$ grains, greatly improve their high-rate capability and cyclability.

The three-step solid state synthesis including ball-milling process of nanocrystalline lithium titanium oxide ($Li_4Ti_5O_{12}$) of spinel structure and surface modification (decoration by Ag nanoparticles) of LTO grains by a new low temperature wet chemical method will be presented.

All the prepared powders have been characterized by a numbers of methods: X-ray powder diffraction (XRD), Raman spectroscopy, X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM). Also the electrochemical tests were performed.

Acknowledgments:

This work was supported by The National Science Centre through the research grant DEC-2011/03/N/ST5/04389. Monika Michalska would like to thank for the scholarship awarded by the Mazovia Voivod ship Office.

Nanogratings with sinusoidal modulation of optical properties

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Anisotropic gratings with sinusoidal modulation of permittivity tensor take place in many applications as volume holograms, liquid crystals, magneto-optic films with magnonic waves, photorefractive, and nonlinear optical media. Despite the modelling of grating optical properties using numerical methods based on Rigorous Coupled Wave Algorithm (RCWA) give precise results in a real computation time, it is often usefull and needed to describe the system response using an approximative effective medium model. Such approximation can give (i) symbolic relations especially usefull to describe and understand the complex response of anisotropic gratings and analytical dependence on particular anisotropy parameters and (ii) for cases of subwavelength or quasistatic limit $\Lambda << \lambda$, where Λ and λ denote the grating period and light wavelength, the effective medium approximation (EMA) gives reasonable and precise results.

Figure 1 shows schematically the anisotropic grating with sinusoidal profiles of the permittivity tensor components described using the effective permittivity. Based on boundary conditions of field components perpendicular to the grating gradient [1] the effective permittivity tensor is obtained in general form and in special configurations. We discuss the biaxial crystal in special non-mode-conversion geometry and mode conversion magneto-optical configuration. The grating modulation causes enhanced quadratic magneto-optical effect observed in pump-probe magneto-optic measurement of magnonic waves. Validity and limits of the effective medium approximation is demonstrated by comparison with rigorous Coupled Wave Algorithm (RCWA) models.

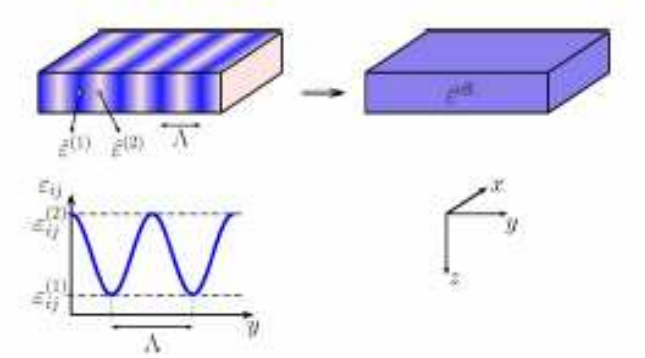


Fig. 1 Grating with sinusoidal variation of permittivity tensor is described by the effective medium approximation.

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Keywords: Effective medium approximation, sinusoidal grating, pump-probe experiments

Synthesis, and purification of Nano (Na)[$^{57}Fe(CN)_5NO$]

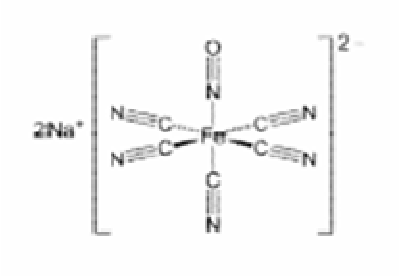
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Pentacyanonitrosylferrate (II) complex with $Na_2[Fe(CN)_5NO]\cdot 2H_2O$ general formula and below structure is synthesized.



Its sodium salt (SNP) under the pharmacological and commercial name nipride is an effective vasodilator in lowering blood pressure. In summary nipride is an effective drug for the treatment of two conditions, high blood pressure and heart attack, which are common and wide-spread.

The main purpose of this work has been to find and evaluate a production, synthesis and purification method for nanoparticles pentacyanonitrosylferrate (II).
Finally drug synthesis and purification of nano dimensions, and is analysed by (FT/IR) spectroscopy method and (UV/VIS) spectroscopy method. The results of micro structure analysis with scanning electron microscopy (SEM) and X-ray diffraction (XRD). The FT-IR of pentacyanonitrosylferrate(II) was observed to exhibit two absorption bands at 2202 cm^{-1} and 1960 cm^{-1}, attributed to stretching of νs (C≡N) and νs (NO), respectively.
The best size for nanoparticles obtained 14 nm respectively that show these nanoparticles are suitable for drug delivery systems.

Keywords: Synthesis, purification, (Na)[$^{57}Fe(CN)_5NO$], (FT/IR)spectroscopy, (UV/VIS) spectroscopy, scanning electron microscopy (SEM), X-ray diffraction (XRD)

Antibacterial effect of Ag, Cu–vermiculite filler in polyethylene

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Vermiculite (Ver) enriched with Ag and/or Cu was tested for antibacterial effect and used as nanofiller to the polyethylene (PE) matrix. The samples Ver-Ag, Ver-Cu and Ver-AgCu were prepared by shaking of Ver with the aqueous solutions of silver and copper nitrate (0.1 mol.dm^{-3}) at room temperature. The mixtures of the Ver nanofillers (7 wt.% and 3.5 wt.%) and PE was homogenized by the melt compounding at 160°C. The thin foils of PE/Ver-nanocomposites were pressed from stiff mixtures.

The exfoliation of the powder Ver nanofillers in PE matrix was characterized by the X-ray diffraction analysis of the nanocomposite foils. Distribution of Ver nanofiller in PE matrix was observed by Light microscopy (Fig. 1). The creep data of nanocomposites were measured and the changes of the PE properties were studied.

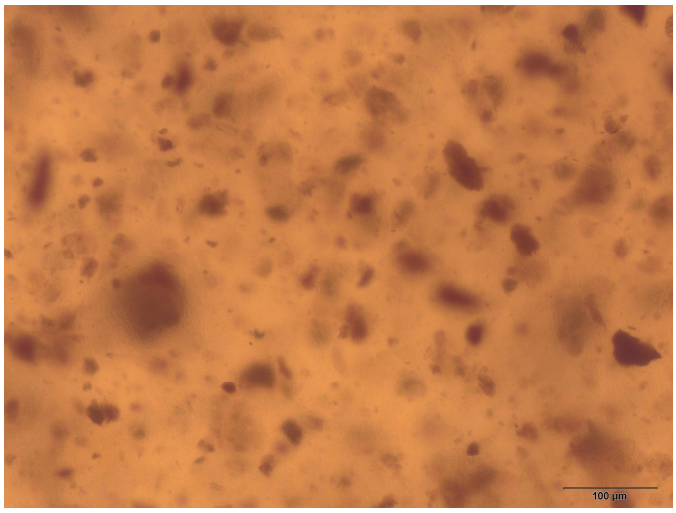


Fig. 1 Vermiculite filler Ver-AgCu distributed in polyethylene matrix (sample PE/Ver-AgCu/3.5).

Antibacterial behaviour of nanocomposites' surface were studied against the Grampositive bacteria *Enterococcus faecalis* by the fingerprints method and counting the CFU (colony forming unit) number of the viable bacteria after 24 h, 48 h, 72 h and 96 h of contact time. All tested nanocomposites showed good antibacterial behaviour after 24 h in comparison with pure PE. The number of colonies decreased from the countless number to several hundred colonies (decrease about four orders).

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This work was supported by projects: IT4Innovations Centre of Excellence project reg. no.cz.1.05/1.1.00/02.0070; Czech Grant Agency P210/11/2215 and Ministry of Education, Youth and Sport of Czech Republic SP2013/78.

Keywords: vermiculite, polyethylene, nanocomposite, x-ray diffraction, antibacterial activity

Features the introduction of additives nanopowder Al_2O_3 in the production of ceramic materials based YSZ

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In recent years, some new ways of improving properties of structural materials were developed based on purposeful formation of micro-and nano-crystalline structures. Considerable interest to voluminal nanomaterials is caused by the fact that their structural and functional properties differ significantly from the properties of coarse analogues. Ceramic structural nanomaterials can be prepared by various techniques with powder metallurgy occupying amongst them not the last place. The method of nanomodification of ceramic materials is currently the most promising way of improving characteristics of these materials. This technique is optimal from the both economic and technological points of view. Furthermore, the ceramic materials modified in such may exhibit unique properties.

In the present study the effect of adding modifying additives of Al_2O_3 nanopowder (up to 15%) on the properties of ceramics based on zirconium oxide partially stabilized by yttrium oxide was examined. Application of partially stabilized zirconia causes primordially high tensile properties of the ceramic matrix.

Density of the hot-pressed ceramics was measured by hydrostatic weighing employing Mettler Toledo XP205 instrument. Density of the prepared ceramic samples is close to the theoretical values (with the maximum of 99.23% of the theoretical density) thus indicating the correct choice of pressing conditions. Also, judging by the low spread of the apparent density values of different samples, it can be concluded that high-quality and uniform mixing of the starting powders was achieved using ultrasound in acetone as the working medium.

Mechanical properties of ceramics were determined by three-point bending method. Tensile strength of the samples containing 10% of alumina nanopowder was nearly 40% higher than that of the samples made of pure partially stabilized zirconia ($\sigma_{bend.}$ *ca*. 520 MPa).

Keywords: Nanopowder, hot-pressed ceramics, YSZ

Back-to-back Schottky barriers model applied to Zn_3P_2 nanowires

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Zn_3P_2 nanowires were grown by vapour-liquid-solid (VLS) mechanism on Si substrates covered with gold nanoparticles. The obtained nanowires were morphologically and structurally characterized by X-ray diffraction (XRD), field emission scanning electronic microscopy (FEM-SEM) and transmission electronic microscopy (TEM) with an energy dispersive X-ray spectroscopy module. This analysis showed high crystalline Zn_3P_2 nanowires with diameters between 50 and 200 nm and lengths ranging from tenths to hundreds of micrometers. In order to study the electric contacts made to Zn_3P_2 nanowires, a single nanowire device was fabricated using conventional litography techniques and lift-off processes, defining Ti electrodes. The current-voltage measurements exhibited Schottky behavior with different barrier heights for each contact to the nanowire, which can be explained by the expected non-uniform surface of nanowires grown by self-organized mechanisms, since the surface plays a very important role on nanostructures due to the high surface-volume ratio. Thus, the most suitable way to treat these data is to use a model considering two Schottky barriers, which can also have different heights. A back-to-back Schottky barriers model was used as fitting to the experimental data and provided both, barrier heights and ideality factors for each contact.

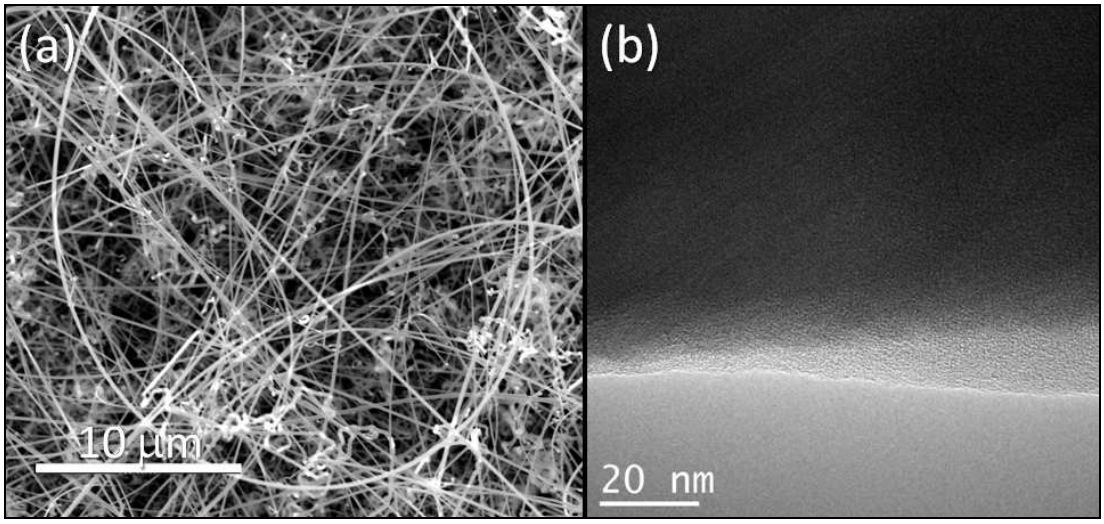


Fig. 1 (a) FEG-SEM image of as-grown Zn_3P_2 nanowires. (b) HRTEM image showing the non-uniformity of the oxide layer on the surface along the nanowire.

Keywords: crystal growth, nanowires, electrical characterization, Schottky barriers

Multilayer nanostructured thick-film structures for integrated sensors application

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The problem of simultaneous temperature and relative humidity T/RH control consists in principally different sensitivities of monitored solid-state system to thermally- and moisture-activated environmentally-induced processes. The basis functioning principle of T-measuring systems are grounded, as a rule, on some changes in their physical properties, such as electrical conductivity, resistance, capacity etc. stimulated by ambient temperature variations. Despite time delaying in system response on these variations caused by relative durability of T-influenced effects, the controlled parameter can be determined finally with a high accuracy. In contrast, the RH measurements are based on changes in physical properties of solid bulk or surface produced by absorbed water. The greater amount of absorbed water molecules, the better exploitation sensitivity of RH-measuring solid systems can be achieved.

Spinel ceramics based on mixed transition-metal manganites and/or magnesium aluminates are known to be widely used for temperature measurement, in-rush current limiting, gas sensing, flow rate monitoring etc. But their sensing functionality is sufficiently restricted because of bulk performance allowing, as a rule, no more than one kind of application.

Thick-film performance of mixed spinel-type manganites restricted by $NiMn_2O_4$-$CuMn_2O_4$-$MnCo_2O_4$ concentration triangle has a number of essential advantages, non-available for other ceramic composites. Within the above system, the fine-grained semiconductor materials possessing p^+-type $Cu_{0.1}Ni_{0.1}Mn_{1.2}Co_{1.6}O_4$ and p-type $Cu_{0.1}Ni_{0.8}Mn_{1.9}Co_{0.2}O_4$ conductivity can be easily prepared. The multilayer thick-film structures involving semiconductor $NiMn_2O_4$-$CuMn_2O_4$-$MnCo_2O_4$ and dielectric (d-type) $MgAl_2O_4$ spinels can be used as simultaneous thermistors and integrated RH/T sensors with extremely rich range of exploitation properties. The aim of this work is development of T/RH-sensitive thick-film structures for ecological environment control and monitoring.

The T-sensitive thick film p^+-p structures based on spinel-type $NiMn_2O_4$-$CuMn_2O_4$-$MnCo_2O_4$ ceramics possess good linear electrophysical characteristics in the region from 298 to 358 K. The values of B constants were 3615 K. The RH-sensitive d-type $MgAl_2O_4$ thick films possess linear dependence of electrical resistance from relative humidity without hysteresis in the range of RH ~ 40-99 %.

By using spinel-type ceramics of mixed Mn-Co-Ni system with RuO_2 additives, the temperature-sensitive elements prepared in thick-film performance attain additionally a better RH sensitivity. Despite improved long-term stability and good temperature-sensitive properties with character material B constant value, such thick-film elements possess only small RH sensitivity. This disadvantage occurred, because of relatively poor intrinsic pore topology proper to semiconducting

mixed transition-metal manganited in contrast to dielectric aluminates with the same spinel-type structure.

So, novel separate T- and RH-sensitive thick-film elements based on spinel-type $NiMn_2O_4$-$CuMn_2O_4$-$MnCo_2O_4$ manganites, p^+-p structures and dielectric magnesium aluminate $MgAl_2O_4$ can be used to produce T/RH-sensitive thick-film structures for ecological environment monitoring and control.

Keywords: nanostructures, spinel, thick film, ceramics

Titanium dioxide nanoparticles prepared using $TiOSO_4$ precursor

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Nanostructured titanium dioxide is an outstanding photocatalyst finding a variety of applications ranging from the water treatment to the preparation of the self-cleaning surfaces. There are several techniques and precursors employed for preparation of nanosized TiO_2. One of the most widespread techniques is sol-gel method which utilizes different organotitanates as precursors. This technique enables preparation of highly photoactive TiO_2 but its drawback is relatively high price. Other techniques utilize the combustion of titanium tetra chloride or thermal hydrolysis of titanyl sulphate or its reaction with alkali hydroxides. Titanium tetra chloride and titanyl sulphate are intermediate products originated during industrial manufacturing of TiO_2 white pigment using chlorine or sulphate process, thus these precursors are available in large quantities and their price is lower in comparison to organotitanates.

The aqueous solution of titanyl sulphate has acidic character and addition of sodium hydroxide directly leads to formation of white slurry of hydrous TiO_2. After the drying the resulting TiO_2 has amorphous structure and its subsequent heat treatment results in formation of anatase (at lower temperatures) and rutile (at higher temperatures). The properties of resulting TiO_2 particles are significantly influenced by reaction condition e.g. heating of reaction mixture, time for reaction with NaOH, even sequence and speediness of the addition of NaOH or presence of nucleation centers.

Two procedures has been tested for preparation of nanosized TiO_2 using the reaction of titanyl sulphate with sodium hydroxide. The first is based on direct reaction of both substances at the temperature 100 °C, the second method can be divided into two steps, whereas during the first step the nucleation centers in the form of in-situ prepared colloid TiO_2 particles are prepared and within the second step the growing of TiO_2 particles occur on nucleation centers prepared during the first step. The obtained TiO_2 particles were isolated by the means of filtration, washed several times with distilled water, then dried at 105°C and calcined at the selected temperatures 200, 400, 600 and 800 °C. The samples were characterized using TG-analysis, X-ray diffraction analysis, the photodegradation activity of the prepared samples was evaluated by the means of photodegradation of azo dye acid orange 7.

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Keywords: Titanium Dioxide, Preparation, Characterization, Photodegradation Activity

Comparative study on the nanotubes decorated with metal nanoparticles via different synthesis methods

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In this work we present a comparison study of different preparation methods of nanotubes decorated with metal nanoparticles. For the decoration of nanotubes with nanoparticles acetates of iron, nickel and cobalt have been used. Metal nanoparticles synthesis was performed by two methods. The first method was the reflux of functionalized nanotubes in salt aqua solution. The second method was the impregnation of the raw carbon nanotubes followed by the vacuum calcination. In both methods hybrids of nanotubes with metal nanoparticles were obtained. Metal nanoparticle sizes depend on the process conditions. The effectiveness of both methods and the morphology of the obtained samples were analyzed by the transmission electron microscope (TEM) and a scanning electron microscope (SEM). EDX analysis confirmed distribution of metal on the surface of the nanotubes. The composition of the metallic phase was determined by X-ray diffraction. In addition, Raman spectroscopy allowed to determine the quality of the material in terms of the number of defects in the structure of the nanotubes. The obtained products can be used as selective absorbents, new catalysts for chemical synthesis and as fillers for plastics.

Keywords: nanotubes, metal nanoparticles, nanotubes decoration

Improvement of the capacity retention of $LiMn_2O_4$ by ceramic coatings

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Lithium-ion batteries have been commonly used in many portable electronic devices, such as: cell phones, notebooks, tablets, ipods, media players, as well as in hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), owing to its high energy density and working voltage, long lifecycle, small dimensions and weight.

Lithium manganese oxide ($LiMn_2O_4$) of spinel (cubic) structure is one of the most promising material as a positive electrode (cathode) due to its low cost and easy preparation, environmentally friendly, high discharge potential (4V vs. lithium metal) and good safety compared with the lithium cobalt $LiCoO_2$ or lithium nickel $LiNiO_2$ oxides. In spite of these advantages, $LiMn_2O_4$ electrodes at the 4V potential (vs. Li/Li^+) region suffers from capacity fading during charge-discharge cycles, especially at elevated temperature (50-60°C), which limits the application in commercial lithium-ion batteries. The capacity loss has been ascribed to three main factors: (**1**) dissolution of Mn^{2+} ions; (**2**) Jahn-Teller (J-T) distortion effect; (**3**) decomposition of organic solvents in electrolyte. In order to resolve this complicated problem many approaches including metal doping at Mn-sites (Fe, Ni, Cr) and surface coating with metal or ceramic oxides to minimize the surface area of $LiMn_2O_4$ contacting with the electrolyte have been proposed. Finally, it should to improve the capacity retention.

In this work, we investigated and compared the electrochemical performance of $LiMn_2O_4$ coated by various ceramic oxides. The wet chemical method was used to modify the surface grains of LMO.

Firstly, pure stoichiometric nanopowder of $LiMn_2O_4$ was prepared by modified sol-gel method using lithium and manganese salts. Secondly, we used wet chemical method for the surface modification by ceramic oxides (like i.e. La_2O_3, Al_2O_3, CeO_2, SiO_2) of LMO spinel.

The crystal structures of all samples were characterized by X-ray powder diffraction (XRD) and Raman spectroscopy. The particle size and morphology were observed by: SEM, HRSEM, TEM. Also the electrochemical tests were performed.

Acknowledgments:

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Shape, sizes, anisometricity and volumes of nanoparticle supramolecular aggregates in lyotropic liquid crystalline nematic mesophases

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Lyotropic liquid crystals are the binary, ternary or multi-component systems. In definite concentration, temperature and pressure conditions in these systems the single axis and biaxial anisotropic nematic mesophases are formed. Structure units in these mesophases are the nanoparticle supramolecular aggregates with the rod-like and disc-like shape.

The physical and physicochemical properties of lyotropic nematic mesophases are generally determined by the structural peculiarities, shapes and sizes of the supramolecular aggregates and also by character of packing of amphiphile molecules in these supramolecular aggregates. Therefore determination of the shapes, sizes, anisometricity and form factors of the aggregates, the investigation of transformation dynamics of these parameters under different external influences is an important topic both from fundamental and application points of view.

In this work we are interested in sizes, anisometricity, form factors and volumes of the nanoparticle supramolecular aggregates in nematic-calamitic (N_C) and nematic-discotic (N_D) mesophases of lyotropic liquid crystalline system based on sodium dodecyl sulphate as the amphiphile. The method of compulsory orientation of the supramolecular aggregates in the shear flow has been used. The effective length of the rod-like supramolecular aggregates in N_C mesophases and the effective diameter of the disk-like supramolecular aggregates in N_D mesophases have been estimated by consideration of the rod-like and disc-like aggregates as lengthened and flattened ellipsoids, respectively.

The anisometric and space parameters of the rod-like and disc-like nanoparticle supramolecular aggregates of N_C and N_D mesophases and the dependences of the electrical conductivity anisotropy vs. velocity gradient for the X-, Y- and Z-direction to the shift flow will be presented.

Keywords: Nanoparticle supramolecular aggregates, Liquid crystals, Nematic-calamitic, Nematic-discotic

Conductivity of PANI and PANI/MMT pellets in dependence on the high pressure

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Pure polyaniline (PANI) r and composite polyaniline/montmorillonite (PANI/MMT) powders have been prepared. Powder sample of pure PANI have been prepared from anilinium sulfate using ammonium peroxodisulfate as an oxidizing agent. PANI/MMT composite has been prepared using one step process of anilinium sulfate polymerization induced by ammonium peroxodisulfate in the presence of montmorillonite matrix in the reaction mixture at room temperature. For both samples the polymerization of aniline was completed within 40 minutes; in the case of composite PANI/MMT subsequent stirring of the suspension for 6 hours was proceed with the aim to capture PANI at the surface of MMT matrix. The green solid portion was separated from supernatant liquor using filtration, and was washed several times with distilled water and dried at 40°C.

Pressed pellets from powder samples have been prepared using high pressure in the range from 50 to 400 MPa. Mechanical press ZWICK 1494 for the controlled compression of pellets (controlled speed and time of "compaction", progressive excavation and controlled pressure) was used. All pellets were pressed without any binder and matrix was not lubricated with oil.

DC conductivity was measured in two perpendicular directions: in the pellet plane and in the orthogonal direction to the pellet plane. Conductivity of pressed pellets of composites PANI/MMT has been compared with the conductivity of pressed pellets of pure PANI.

Acknowledgement:
This study was supported by project the Grant Agency of Czech Republic (project P108/11/1057).

Keywords: Polyaniline, Composite, Pressed pellets, Conductivity

Photoluminescence of ZnO nanopowders after laser shockwave treatment

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Investigation of structure and photoluminescence of ZnO that we made helped us to detect changes in defect structure after laser shockwave treatment [1]. In laser treatment we used energies E_{av}=5-12 J/pulse, with an average power density P=5.8*10^8 W/sm^2 and following diameter of the treated surface D=4mm^2. In this work we used ZnO nanopowder obtained by pulsed laser reactive technology [2]. Treated ZnO sample was purchased between copper plate (d=100μm) and steel plate (d=4.51 mm). ZnO nanopowders was treated in three stages that differs by energy applied and quantity of laser pulses for each sample (sample 1: 7 pulses, E_{av}=8 J/pulse; sample 2: 14 pulses, E_{av}=8.5 J/pulse; sample 3: 21 pulses, E_{av}=9.3 J/pulse). Photoluminescence experiments was held in vacuum (P=10 Pa). After laser treatment we have noticed significant changes in photoluminescence properties of the treated ZnO samples. Other interesting feature we have been observing intensity growth of photoluminescence peak (λ=430nm) and weak decreasing of intensity of the main peak (λ=510 nm). Further treatment energy growth revealed photoluminescence intensity decreasing for both peaks in comparison with ZnO samples without laser shockwave treatment.

Intensity growth of the photoluminescence peak (λ=430nm) can be connected with releasing of large amount of defects created by laser shockwave treatment. In our opinion intensity growth of photoluminescence peak (λ=430nm) can be induced by laser annealing on the sample of ZnO nanopowder in nanosecond pulsed mode. We assumed that such defects which induced by laser shockwave treatment are acceptor oxygen vacancies V_O. Laser shockwave treatment of ZnO nanopowder can be used as simple and convenient method of obtaining structures with controllable features.

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Keywords: laser shockwave treatment, ZnO nanopowder, photoluminescence

Modified organovermiculite for cordierite ceramic nanocomposites

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Ceramics based on the cordierite ($Mg_2Al_4Si_5O_{18}$) have a wide range of applications as electrical insulators, low-expansion refractory's and semiconductor packing materials, an excellent thermal shock resistant material for industrial furnaces, heat exchangers, gas turbine engines and honeycomb catalyst carriers in automobile exhaust systems.

The basic powder mixture of the clay minerals kaolinite (Kaol), talc (Tlc) and vermiculite (Ver) was prepared for sintering in the oxide ratio $2MgO•2Al_2O_3•5SiO_2$ of cordierite. Other derived mixtures contained oganovermiculite (ODA-VER) obtained using intercalation of Ver with octadecylamine (ODA).

Solving the problem includes finding answer to the question how differ ceramic cordierite nanocomposites when sintered with various content of organovermiculite in powder mixture of clay minerals.

The X-ray powder diffraction mineral phase analysis and analysis of pores and pore size distribution allowed characterization of a new cordierite ceramic nanocomposite.

Acknowledgements:
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Keywords: Organovermiculite, Sintering, Cordierite, Nanocomposite, X-ray powder diffraction, Structural characterization

Preparation and properties study of ceramic materials under hot pressure YSZ-WC

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In the present work the process of preparing powder composite materials based on zirconium oxide partially stabilized by yttrium oxide and containing various amounts of tungsten carbide additive, as well as physical and mechanical properties of these materials were investigated. Hot-pressing method was employed for preparing the samples for this study. Similar to Al_2O_3, WC additives increase the strength of the materials prepared by hot pressing. Addition of WC to the YSZ matrix results in increasing the density and strength of the composites due to the differences in indices of linear thermal expansion and elasticity modulus.

Physical and mechanical properties of the hot-pressed materials were measured. Analysis of the experimental results showed that increasing content of finely dispersed tungsten carbide results in increasing strength of the samples. Maximum strength value was obtained with WC content of 30 wt. %. The strength equaled to 943 MPa, which is significantly higher than the value for pure partially stabilized zirconia (710 MPa). The increasing of strength amounted to about 33%. The surface topography of the samples was determined using an atomic force microscope.

Surface geometry and strength properties of the samples produced from the stabilized zirconium oxide containing tungsten carbide additives allows using these compositions for manufacturing special-purpose items, where there is constant friction contact with the material which is being processed.

Keywords: Composite materials, hot-pressed ceramics, YSZ, WC

Study of the conditions of synthesis forsterite ceramic from the original and modified talc

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Forsterite represents crystalline magnesium silicate which belongs to the olivine group, with chemical formula Mg_2SiO_4. Forsterite exhibits extremely low electrical conductivity, good refractoriness due to its relatively high melting point of 1890 °C, good chemical stability even at high temperatures, low thermal expansion and good biocompatibility.

Various methods have been used for preparation of forsterite ceramic including the solid state reaction of SiO_2 and MgO and/or bauxite and $MgCO_3$ and sol-gel techniques. The main constituents of talc are SiO_2 and MgO and therefore, talc is the very good material for synthesis of forsterite ceramics.

For synthesizing forsterite ceramic is important to avoid the formation of secondary phases such as enstatite ($MgSiO_3$) and periclase (MgO). These secondary phases may reduce the good properties of forsterite and they should be removed from the final product. Pure forsterite is very difficult to prepare. The purpose of this work was to prepare monophasic forsterite ceramic from mixtures of talc (original and/or acidified), magnesium oxide (MgO) and magnesium carbonate ($MgCO_3$) mixtures. The mixtures before sintering at 1200 °C for 1h were mechanically homogenized by milling for 1h or 2h.

Forsterite ceramic material was investigated using the X-ray powder diffraction (XRD) analysis and also by scanning electron microscopy (SEM).

Acknowledgements:
The financial support of the Ministry of Education, Youth and Sport of the Czech Republic (project SP2013/78) and the IT4Innovations Centre of Excellence (project reg. No. cz.1.05/1.1.00/02.0070) are gratefully acknowledged.

Keywords: talc, $MgCO_3$, MgO, acidification, forsterite, sintering, XRD, mineral phase analysis

Transmission electron microscope analysis of different silica, carbon, iron oxide nanomaterials whit potential application in fields of microbiology and environmental science

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High resolution electron microscopy analysis is one of more important methods for detailed characterization of nanoparticles and nanocomposites. The electron microscopy can be dividing in to two main visualization techniques: scanning (SEM) and transmission microscopy (TEM). Main differences between the scanning and transmission microscopy is the obtained date on the morphology of studied materials and resolution of the image. Transmission electron microscopy is more powerful device, capable in detailed morphology visualization at the molecular level. Due to the high tension of the transmission microscopy obtained images clearly shows the inner structure of the nanomaterials like: core-shell structure, hollow space, guest molecules in the composites or porous structure of the nanomaterials. Additional source of the image in the electron microscope enables for more special analysis of the chemical and physical structure of the studied material. TEM in the combination with Energy-dispersive X-ray spectroscopy (EDS) allows to identification of the elements that studied material is composed, calculation quantitative composition of the elements, distribution of the elements on the obtained image. Other highly important application of the electron microscope is characterization of the crystallographic structure of the studied material. The electron high-resolution visualization method at molecular level finds application in many fields of science, from characterization of crystallographic structure of mono and polycrystalline, visualization micro and nanomaterials, identification and distribution of the elements, analysis interaction and influence of the materials on the morphology of the micro-organism.

Keywords: Transmission electron microscope, microscopic analysis, nanomaterials characterization

Bioelectronics and bionanotechnology: From novel concepts towards practical applications

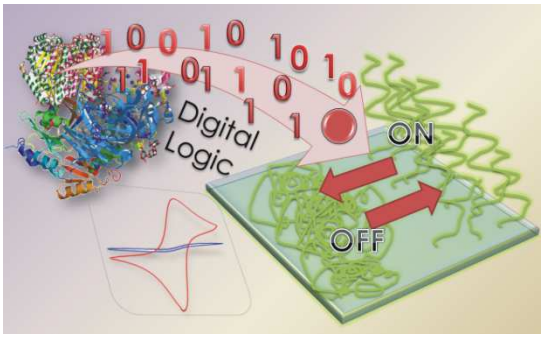
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The talk will outline the conceptual foundations of the novel approach to biosensing and bioactuating based on multi-step processing of biochemical signals through biocatalytic/biorecognition processes, adapting ideas recently developed in the field of bioelectronics and biocomputing (biomolecular logic). Extensive ongoing research in biocomputing, mimicking Boolean logic gates has been motivated by potential applications in bionanotechnology and medicine.



Furthermore, novel "Sense/Release" concepts have been contemplated with multiple inputs processed biochemically before the final output is coupled to transducing "smart-material" electrodes and other architectures. We review and exemplify these developments, as well as offer an outlook for possible future research foci.

Recent advances in biomedical applications of enzyme-based logic systems, particularly for the analysis of pathophysiological conditions associated with various injuries will be briefly reviewed.

Other developments in the general area of bioelectronics and bionanotechnology include novel biofuel cells operating *in vivo*. The first fully implanted biofuel cell continuously operating in aanimal and producing electrical power over long period of time using physiologically produced glucose as a fuel will be discussed.The "electrified" animals demonstrated the possibility of activating electrical/electronic devices using energy produced *in vivo*. Implanted biofuel cell will be able to operate in a natural environment producing sustainable electrical micro-power for activating various implantable bioelectronic devices.

The presented studiesare the first steps in the long way to the design of bioelectronic self-powered "cyborgs" which can autonomously operate using power from biological sources.

Overall, integration of bioelectronics, biocomputing, materials science, and bionanotechnology resulted in the novel "smart" bioelectronic systems for medical, environmental and homeland security applications.

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Keywords: bionanotechnology, bioelectronics, "smart" electrodes, biofuel cells, bioactuators

Adsorption of Aromatics from Waste Water by Multi Walled Carbon Nanotubes

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There are many developed methods for wastewater treatment; their application depends on source and type of contamination, on level of contamination and on origin of present contaminants. Some of procedures are available only for inorganic or organic contaminants; some of them are versatile without any modification or with various alterations. Adsorption of organic and inorganic compounds is one of the best available technologies (BAT) which is used for decontamination of highly polluted waste water. It is also used for surface and ground water treatment in case of accident consequence elimination or in case of remediation. There are many adsorbent materials, such as activated carbon, clay minerals in natural or modified forms, polymeric adsorbents, and alternative sorbents on the basis of waste materials.

One of the very promising materials in future can be carbon nanotubes. Sorption efficiency of single and multi-wall carbon nanotubes was studied for many organic or inorganic compounds, as well as for pathogenic microorganisms in many research studies. Higher efficiency as compared with commonly used active carbon was confirmed in most published observations. Only higher economic costs and lack of knowledge about their behaviour in the Environment hinder their larger application in that sphere. However, further studies are required for observations of their interactions with chemicals and the Environment to identify their possible interactions with living organisms and their surroundings.

The contribution is aimed to describing interactions of multi-walled carbon nanotubes with aromatic organic compounds occurring in real waste water samples.

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The study was supported by the projects Ministry of education, youth and sports CZ.1.07/2.3.00/20.0074 and CZ.1.05/2.1.00/03.0069 from the state budget of the Czech Republic.

Keywords: carbon nanotubes, aromatic organic compounds, adsorption, waste water

Magnetically responsive biocomposites for xenobiotics removal

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Magnetic materials exhibiting different types of response to external magnetic field have already found many important applications in various areas of biosciences, medicine, biotechnology, environmental technology etc. In most cases they can be described as composite materials, where the magnetic properties are caused by the presence of iron oxides nano- or microparticles. In the presentation the main attention will be paid to magnetically modified biopolymers, plant-derived materials and microbial cells and their applications for the removal of xenobiotics such as organic dyes, heavy metal ions and radionuclides.

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Keywords: magnetic materials, magnetic separations, biological materials, xenobiotics

Nanotechnologies in field of pharmacy

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Precipitation belongs among bottom-up techniques of nanoparticle preparation. It is a simple and fast method, which main principle is preparation of two solutions (the first with a stabilizer (polymer or surfactant) and the second with an active pharmaceutical ingredient, API) and subsequent mixing of both with continuous stirring. A solvent in which the API is very soluble is used, and the stabilizer is solved in water. The organic solvent is evaporated after mixing. The result is stabilized nano-precipitated APIs in aqueous medium.

The mechanism of nanoparticle preparation by this method depends on the used solvent. When the API is dissolved in a polar solvent and then mixed with water containing the stabilizer, one-phase solution is generated, and nanoparticles are formed spontaneously and immediately upon mixing. This technique is called antisolvent precipitation/solvent evaporation. When a nonpolar solvent is used and then mixed with water containing stabilizers, a two-phase system (emulsion – o/w type) is formed. The API is clustered by the excipient, which results in the encapsulation of the API into nano-vesicula. For generation of nanoparticles under this conditions additional energy, e.g., ultrasound, is needed to be supplied. This combination of emulsification and solvent evaporation can be called emulsion/solvent evaporation

APIs are chosen based on the Biopharmaceutical Classification System. This system classifies drugs into four groups based on their solubility and permeability. In this study, for example, sodium cholate from BCS II (high permeable, low soluble) and cimetidine from BCS III (low permeable, high soluble) are used. As stabilizers the following excipients are chosen from Pharmacopoeia: sodium dodecyl sulfate and Tween 80 as surfactants and macrogol 6000, carboxymethyl cellulose sodium of mass weight 250 and 700 and carboxymethyl dextran sodium as polymers. The most convenient excipient/combination of excipients and their concentrations for nanoparticles preparation are discussed.

Hardly soluble and/or permeable APIs were chosen for the above discussed technique of nanoparticles preparation. The aim was to prepare nanoparticles, characterize them (particle size distribution) and to evaluate solubility and permeability of prepared nanoparticles. The PAMPA (parallel artificial membrane permeability assay) system was used for test of permeability.

Acknowledgement:
This study was supported by the Czech Science Foundation – GACR P304/11/2246.

Keywords: drug nanoparticles, precipitation, permeability, solubility

Ecotoxicological evaluation of leachates of sewage sludge contaminated with ZnO nanoparticles

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Substantial proliferation of nanotechnologies and the uses in consumer products, raise environmental concern about adverse ecological effects of nanoparticles. Sewage treatment plants are considered to be intermediate stations that control the flows of nanoparticles between anthropogenic and environmental compartments. During wastewater treatment processes, nanoparticles may be incorporated into the sewage sludge matrix and may be concentrated over time. When sewage sludge materials re-enter the environment through agricultural land application, contaminated sludge can have consequences not only on terrestrial communities, but also on aquatic species. Because of the present lack of experimental data, the disposal of nanomaterials is not regulated. There is a strong need to clarify possible entrances of nanoparticles into the aquatic environment.

The present work investigates the toxicological effects of leachates of sludge amendments on agricultural lands contaminated with zinc oxide nanoparticles (ZnO-NPs). The sewage sludge application represented a dose of 5% dry weight. ZnO-NPs treatments were 0.12, 0.25, 0.5 and 1g NPs (Zn based)/Kg amended soil. For the generation of leachates, a standard DIN 38414-S4 method was applied to the samples. The zinc concentrations in all of the extracts obtained were determined using flame/graphite furnace atomic absorption spectrometry. Ecotoxicity was assessed by using freshwater species representing three trophic levels. Extracts were tested *in vivo* using *Chlorella vulgaris* (acute growth inhibition test) and *Daphnia magna* (acute immobilisation test) following the OECD methods (201 and 202 respectively), and *in vitro* with the rainbow trout gonad cell line RTG-2, using a battery of well known biomarkers, that evaluate Ah receptor-mediated toxic effect (EROD activity assay), lisosomal function (NRR assay), cell growth (KBP assay), reductase enzyme activity (AB assay), membrane function (CFDA-AM assay) and reactive oxygen species cell production (ROS assay).

The sensitivity and the complementarity of these aquatic species would be in favour of their incorporation in a “battery” of tests used for toxicological screening studies to predict potential aquatic ecosystem risk of ZnO-NPs from contaminated sludge.

Acknowledgements:
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Keywords: ZnO-NPs, , ecotoxicity, leachate

Influence of microemulsion on the release of terbinafine hydrochloride from xanthan gum gel

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In nowadays, the issue of poorly soluble drugs is extensively expanded in pharmaceutical research. Their formulation into conventional dosage forms and thereby ensure the bioavailability is difficult. Microemulsion, as dispersion of water, oil and surfactants, could be one of the solution. Due to their composition, they are able to solubilize hydrophilic an lipophilic substances, too. Also the microemulsions are capable improving and increasing the release of drugs from dosage forms.

The aim of this work was to evaluated microemulsions and their influence on the release of poorly soluble drug.
In this study, terbinafine hydrochloride was used as active substance. Terbinafine is synthetic, allylamine antifungal drug against superficial cutaneous fungal infections. It is a poorly soluble drug therefore it´s formulation into the topical dosage form is limitated by the solvent and vehicles, which can affect drug permeation through the skin.

Three microemulsions o/w were determinated in formulation with Xanthan gum as gelling agent. The amount of released terbinafine was assessed in vitro throught dialysis membrane.
Microemulsion 1 and 3 reduced the released amount of terbinafine. Microemulsion containing oleic acid as oil phase and Tween 80 as surfactant, showed significantly increase in drug release compared to other formulations. The amount of terbinafine after 6h was 1,5 fold higher than formulation without microemulsion. The presence of propylene glycol had positive effect on the release.

Keywords: Microemulsions, Xanthan gum, Terbinafine hydrochloride, Drug release

Characterization methods of metal-based particles in human amniotic fluids

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Bodyfluids (e.g. blood, plasma, amniotic fluid) make internal environment of tissues and organs, therefore changes in their composition may potentially affect organ and tissue functions. Suspended solid particles due to their size below 100 nm are able to penetrate into bodyfluids through biomembranes and subsequently into target organs and tissues. Solid particles, which penetrate through the placenta, can seriously affect fetus evolution. Amniotic fluids of healthy fetuses and also amniotic fluids of fetuses with diagosed congenital anomalies were analysed. The samples were analyzed using the selected techniques: Raman microspectroscopy, (scanning electron microscopy with energy-dispersed spectrometer (SEM-EDS), Fourier transformed infrared spectroscopy (FTIR) and X-ray diffraction (XRD) analysis. Major natural compounds in human amniotic fluid are sodium chloride and organic compounds, mainly proteins, that were analyzed by XRD, SEM-EDS, FTIR and Raman microspectroscopy. XRD and FTIR weren´t able to detect metal and its compounds presence. SEM-EDS (see Fig.1) analysis seems to be most suitable, because it is quite fast and precise data obtaining. Compared to Raman microspectroscopy, which is more time-consuming method. However, Raman microspectroscopy is a valuable tool for point-phase-analysis.

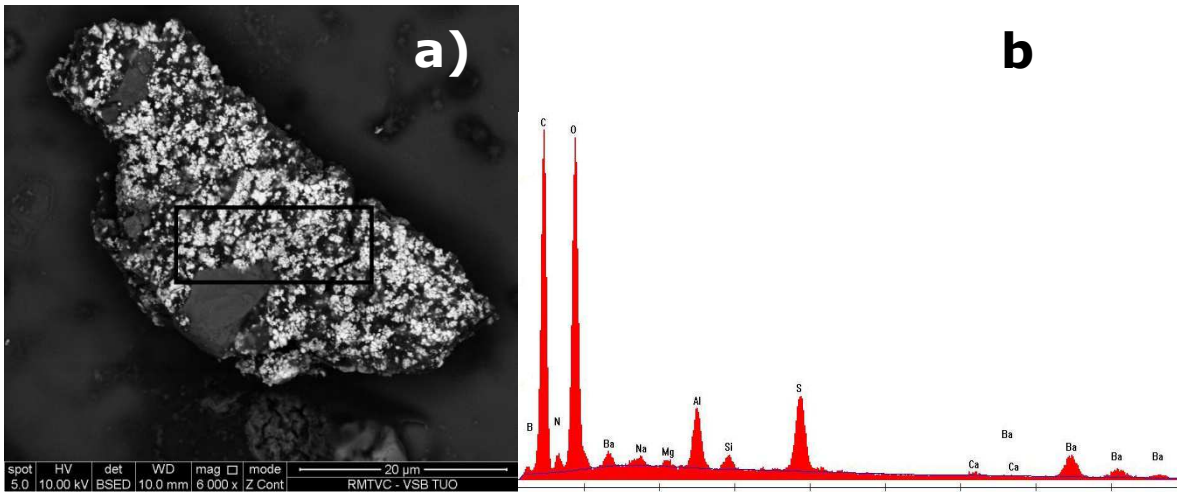


Fig. 1 SEM image of detected Ba particles in one of the samples (a) with corresponding EDS spectra (b).

Acknowledgement:
The study was supported by the project reg. No. MPO FR-TI3/818.

Keywords: Human amniotic fluid, Raman spectroscopy, Scanning electron microscopy, Metal-based particles

Adsorption of substituted aromatics from aqueous solutions by multi walled carbon nanotubes

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Carbon nanotubes can be one of promising materials for waste water treatment in future. Sorption efficiency of single and multi-wall carbon nanotubes was studied for many organic or inorganic compounds, as well as for pathogenic microorganisms in many research studies and it was determined to be higher than sorption efficiency of commonly used active carbon. Higher costs and incompletely explored effects on living organisms and entire ecosystems hinder their rapid expansion to those applications. Observation of compound sorption processes in systems of aqueous solution-sorbent is very interesting also with respect to interactions of organic compounds with carbon nanotubes.

The contribution is aimed to describing interactions of multi-walled carbon nanotubes with monosubstituted aromatic compounds with pristine carbon nanotubes and after their modification. Affinity of selected compounds to adsorbent surface was evaluated.

Acknowledgements:
The study was supported by the projects Ministry of education, youth and sports CZ.1.07/2.3.00/20.0074, CZ.1.05/2.1.00/03.0069 and MPO FR-TI3/818 from the state budget of the Czech Republic.

Keywords: carbon nanotubes, aromatic organic compounds, adsorption, sorption isotherm

Removing toxic ions by TiO_2 composite nanomaterial

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The environmental pollution by industrial activities significantly affects the health of the population. It is therefore in the constant interest of search for new procedures how pollution can be prevented or how to remove presence pollutants from the environment. The nanoparticles of metal oxides, such as TiO_2, are a very effective sorbent according to literature data. Due to the potential toxicity of nanoparticles, it is preferable to use them in the form of a composite in which the nanoparticles are anchored to the inert material. Study of adsorption of toxic substances onto specially modified composite nanomaterials is a first necessary step before their industrial use. The present article is a preliminary study and it is focused on the possibility of using TiO_2/kaolinite composition for removal of toxic ions from aqueous solutions. The selected toxic ions were thallium, cadmium, chromium or copper ion. The effect of various parameters was investigated, such as the concentration of toxic ions in solution and the contact time of adsorbate with sorbent to the adsorption process. The concentration of absorbate was determined by AAS-FA and ICP-AES. The adsorption capacities were calculated from the measured results, eventually were constructed adsorption isotherms.

Keywords: composite TiO_2/kaolinite, sorption, remove inorganic pollutants

Fabrication of Chitosan scaffolds as multifunctional household water filtering media by lyophilization method

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Multi-functional chitosan scaffolds as household water filtering medium were prepared by tuning preparation parameters and subsequent freeze-drying conditions.
The morphology and pore size of the chitosan scaffolds were studied by scanning electron microscope. It was found that pores in the scaffolds were interconnected with pore diameter around 5μm.The surface charge polarities of scaffolds (positive, negative and neutral) were tuned by addition of functional additives. It is advantageous as scaffolds bearing different charges can be used to filter off specific charged species and/or polar chemicals and also micro-organisms (e.g. bacteria) which are charge sensitive. The mechanical strength of scaffolds was improved by cross-linking chitosan with environmentally benign additives. The prepared samples are more versatile than conventional filtering media which based on size-exclusion only. The chitosan scaffolds demonstrated bacteria retention property with 95% retention rate for *Escherichia coli*.
Self-regeneration capability was shown as removal of more than 90% of organic contaminants in water after 10 generation cycles. Heavy metals (Pb^{2+}, Cd^{2+} and Hg^{2+}) absorption ability were found to be more than 8mg/g respectively by inductively coupled plasma optical emission spectrometer. Filtration efficiencies were correlated to the pore size of the scaffolds and the intrinsic properties of chitosan.

Keywords: Chitosan, Freeze-drying, Self-regeneration

Sol-gel derived Au-enriched TiO_2 and TiO_2-ZrO_2 photocatalysts and their examination in photocatalytic reduction of carbon dioxide

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Since Fujishima and Honda in 1972 reported in Nature on the electrochemical photolysis of water at a semiconductor electrode [1], namely the split water into hydrogen and oxygen in the presence of TiO_2 electrode under VUV light irradiation, the scientific interest in the heterogeneous photocatalysis over semiconductors has dramatically raised. From the group of semiconductors TiO_2 has been stood in the forefront of scientific research. Researches have started keenly investigate the positive effect of various forms (i.e. nanoparticulate powders and thin films) of TiO_2 for various applications, e.g. degradation of organic pollutants in air and water, sensing films of gas sensors, coatings for self-cleaning surfaces, an electrode material or a support of noble metal catalysts. The development of highly efficient TiO_2-based photocatalysts, which would be reactive even under solar light irradiation, has become a challenge and a subject of current intense research.

Considering the aspects of preparation of gold-based photocatalysts and gold photocatalysis, it is worth a mention that it is more complicated issue than in the case of other noble metals due to the gold crystallinity. In this contribution some critical aspects of the gold photocatalysis will be discussed. Au-supported TiO_2 and TiO_2-ZrO_2 photocatalysts and their pristine counterparts were prepared by using the sol-gel process controlled within reverse micelles environment and by impregnation under vacuum. All photocatalysts were characterized by organic elementary analysis (OEA), inductively coupled plasma mass spectrometry (ICP MS), N_2 physisorption, powder X-ray diffraction (XRD), transmission electron microscopy combined with electron diffraction (TEM/SEAD) and UV-Vis spectroscopy. The performance of laboratory-prepared photocatalysts was examined in CO_2 photocatalytic reduction and was compared with the catalytic performance of commercial TiO_2 Evonic P25. Logically, the determined physicochemical and optical properties of photocatalysts were correlated with their catalytic performance and some interesting aspects of gold photocatalysis were revealed.

Acknowledgements:
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Keywords: TiO_2, TiO_2-ZrO_2, gold, photocatalysis, carbon dioxide

Metal finishing waste water treatment by zero valent iron nanoparticles

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Wastewater from metal finishing industry contains high concentrations of contaminants, e.g. cyanides and heavy metals. This kind of pollution is slowly degradable by conventional treatment processes and hazardous to the environment. There is a growing need for more efficient and cost effective methods to remove heavy metals as the regulation of the water quality become more stringent We focused to the application of zero valent iron nanoparticles (NZVI) for heavy metal removal with processing wastewater from metal finishing industry.

The application of iron nanoparticles is promising for both municipal and industrial waste water treatment. Zero valent iron nanoparticles are strong reducing agents with high reactivity and surface area. This environmentally friendly technology has great potential to combine redox processes with sorption and coagulation effect in one technological step. Reaction mechanisms vary for different types of pollutants. Reaction products are non-toxic iron compounds.

Tests were carried out in lab-scale. NZVI was commercially available sample from Nanoiron, s.r.o. Iron nanoparticles were applied in the form of aqueous suspension with 17 wt.% Fe(0). Tests were performed with processing rinsing water from cyanide copper plating (pH = 10, high concentration of copper-30 mg/L and nickel- 70 mg/L). Both metals were bound in complex compounds and difficult to remove from wastewater by conventional treatment. Reaction time was set to 4 hours. Unreacted NZVI was separated by coagulation and flocculation.

Results showed more than 99% Ni and Cu removal efficiency at the NZVI dose 3 g/L. This dose was required to reach the limits for water discharge into the sewer (Cu = 0.5 mg/L and Ni = 0.8 mg/L). Reaction mechanism has not been determined yet. ZVI as a strong reducing agent could break the complex bounds and transform Cu and Ni to easily separable form.

Metal finishing operators face the problem with residual heavy metal concentration in outlet. NZVI showed possibility to solve the problem via environmentally friendly way. Therefore, we are going to focus on tertiary treatment of metal finishing wastewater as required dosage is proportionally lower.

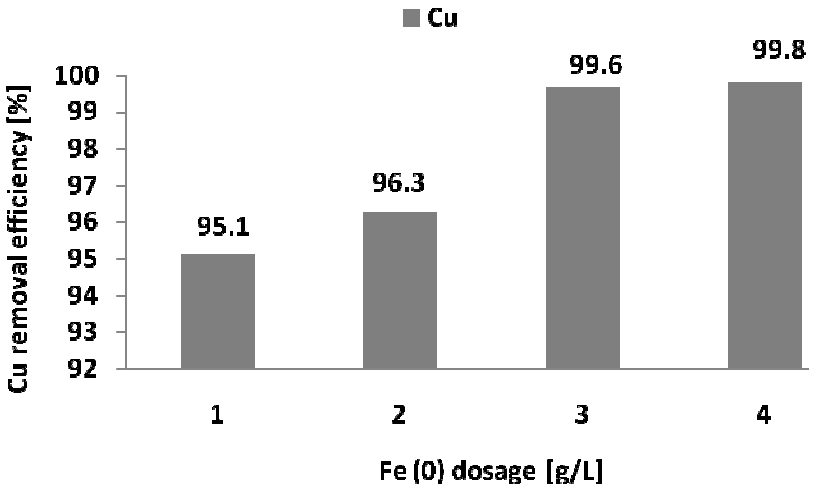


Fig. 1 Effect of different NZVI doses on Cu removal.

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Keywords: zero valent iron nanoparticles, heavy metals removal, metal finishing wastewater

Nanoparticle Determination in real Soil, Road Dust and Sludge in the Environment

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Occurrence of nanoparticles in the Environment is perceived as potential threat for living organisms in future as consequence of huge increase in their manufacture and use. Increasing human and environmental exposition to nanoparticles will occur as consequence of that rapid development, when production of engineered nanoparticles is estimated to be approximately tens of thousands tons in 2011-2020.Nanoparticles are divided from their origin to two main groups:1) natural and 2) anthropogenic. The anthropogenic nanoparticles can be produced intentionally, they are called engineered or manufactured or unintentional as by-product during various industrial processes.

The town Ostrava is known to be one of the most polluted areas in the Europe. Due to the industry that is localised in the town and its environment, occurrence of unintentional nanoparticles especially of many metals and their oxides can be expected. Thus, several samples of soils and road dusts from proximity of possible nanoparticle emission source were taken and observed with SEM. Also samples of sludge from waste water treatment facility of this source were investigated. The samples were compared to samples of soil, road dust and sludge from area out of possible nanoparticle emission source in Ostrava. Interesting results were confirmed.

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The study was supported by the projects Ministry of education, youth and sports SP2013/71, CZ.1.07/2.3.00/20.0074and CZ.1.05/2.1.00/03.0069 from the state budget of the Czech Republic.

Keywords: nanoparticles, soil, road dust, sludge, SEM

Magnetically modified tea for lead sorption

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Lead is one of the elements dangerous for the environment it occurs in soil and also in water. Therefore, the content of Pb ions should be controlled and their concentration in wastewater must be reduced. There are several methods used for removing lead ions from wastewater, for example ion exchange resins, chemical precipitation, electroflotation and reverse osmosis. But all these methods are generally expensive. Sorption is less expensive method of elimination. Magnetically modified material seems to be potentional new material for sorption lead ions from aqueous solutions.

Article deals with sorption properties of the magnetically modified biological material which was developed from a used tea leaves. Magnetically modified tea was suspended in methanol and then was added ferrofluid (magnetic iron oxide nanoparticles). Prepared material was characterized by using scanning electron microscopy, RTG diffraction and X-ray fluorescence spectrometry. Studies were focused on the sorption and desorption properties. The changes of Fe content in magnetically modified material after treatment were observed as well. A flame atomic absorption spectrometer was used for determination the Pb (II) and Fe concentration in solution after treatment. Scanning electron microscopy was used to study surface of material after sorption. Adsorption and desorption processes have been modelled by Langmuir and Freundlich isotherms.

Keywords: lead sorption, magnetically modified biological material

Formulation and evaluation of microemulsion-based gel with indomethacin

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The purpose of this study was to develop and evaluate microemulsion-based gel formulation of indomethacin for topical delivery with an objective to increase the solubility of the drug. Microemulsions are spontaneously formed, single-phase colloidal dispersions of either oil in water (o/w) or water in oil (w/o), stabilized by an interfacial film of surfactants and cosurfactants.

The pseudo-ternary phase diagrams for microemulsion regions were constructed using water, isopropyl myristate, surfactant and cosurfactant. The most suitable microemulsion with surfactant:cosurfactant ratio 1:1 and with appropriate viscosity was chosen. Carrageenan (1%, 2%) as a gel matrix was used to create the microemulsion-based gel for improving the viscosity of microemulsion for topical administration. The optimized microemulsion-based gel was evaluated for viscosity. Indomethacin was dissolved either in carrageenan gels or microemulsion-based gels or in microemulsion and subsequently dispersed in gels (1:5). The solubility of the drug was observed. The abilities of various microemulsion systems to deliver indomethacin through SpectraPor® membrane were evaluated in vitro using Franz diffusion cells.

The mechanism of drug release from the microemulsion-based gels was followed zero order kinetics. The studied optimized microemulsion-based gels showed a good stability over the period of 1 month but permeability of drug from microemulsion-based gel within 6 h was found approximately six-times less than from gel with content of the microemulsion (5:1) and ten-times less than from carrageenan gels without microemulsion.

The results indicate that the studied microemulsion-based gels improve the solubility of indomethacin but they are not suitable for dosage forms with rapid onset of action required.

Keywords: Microemulsion-based gel, Indomethacin, Carrageenan, SpectraPor®

Liberation of terbinafine from chitosan gels containing microemulsion

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Chitosan is a natural based-polymer of N-acetylglucosamine and glucosamine obtained by alkaline deacetylation of chitin. Chitosan is of major importance in pharmaceutical preparations because it possesses excellent properties such as biocompatibility, biodegradability, non toxicity and absorption properties. These properties make chitosan a good candidate for the development of conventional and novel drug delivery systems. Chitosan is used as a coating material in drug delivery applications as it has a good film forming properties and also due to its good mucoadhesive property. Chitosan exerts immuno-stimulating effects, and it is not seen as a foreign body by human cells. The antimicrobial activity of chitosans has been elucidated for numerous bacteria and some fungi.

Microemulsions are promising delivery systems which allow sustained or controlled drug release for topical administration of medicaments. They offer the advantage of spontaneous formation, ease of manufacturing and scale-up, thermodynamic stability, improved drug solubilization of hydrophobic drugs and bioavailability. In topical drug delivery systems, during terbinafine administration a major problem that exists with lipophilic drugs is related to the compromised absorption due to its low aqueous solubility.

The aim of this work was to study microemulsion type O/W. As drug was estimated drug - terbinafine hydrochloride which was used in 1%, 2% and 3% chitosane glycerogels. Physical and chemical properties of formulation dosage form were adjusted for the convenient topical application and dispersion stability. Prepared dispersions of drug in gels mixed with microemulsion type O/W were convenient from the standpoint of solubilization and rheological properties. The influence of aqueous microemulsion on the liberation of 1% terbinafine from different concentrations of chitosan glycerogels and their mixtures with the microemulsion was evaluated in vitro. Liberation of terbinafine is much higher when the chitosan gel is added to microemulsion type O/W.
It can be concluded that the highest percentage of terbinafine, 10.2% of total drug concentration, was released after 6h from a mixture of microemulsion and 3% glycerogel of chitosan. Depending of in vitro liberation of drugs, it was concluded that the O/W microemulsion is convenient for formulation of terbinafine into the gels of chitosan like topical dosage form. Enhancement of the efficacy and toxicity reduction can be achieved by encapsulation of the drug in aqueous microemulsion.

Keywords: Microemulsion, Topical delivery, Terbinafine, Chitosan gels

Sorption of strontium from aqueous solution

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Isotopes of strontium are one the major radioactive contaminants in surface water and shallow groundwater. Groundwater contamination by radionuclides were caused of many sources such as dismantlement of medical instruments containing radioisotopes, radioactive waste produced from nuclear power plants and nuclear fission products routinely or accidentally released. The sorption of strontium on different natural materials has been the subject of many studies. Batch experiments have been performed to study the sorption of strontium from aqueous solution on different clay minerals already established to be predominantly montmorillonite, bentonite and activated carbon. The authors described effect of various factors such as pH, initial concentration of strontium, particle size and temperature on strontium sorption. The results show that 92-100 % of the Sr was rapidly adsorbed onto montmorillonite while bentonite was adsorbed about 90 % Sr from solution. This paper describes the sorption of dissolved strontium in solution prepared from $Sr(NO_3)_2$ on montmorillonite and its magnetically modified form. Sorption of on montmorillonite was studied as a function to several factors. The study focused on effect of solution pH and present of magnetic particle in montmorillonite structure. The experiments were carried out in bats reactor at 25 °C. Concentration of strontium and others dissolved ions in filtrate were determined by AES-ICP. The changes of sorbents composition were described also. Selected experiments were examined by sorption isotherm.

Keywords: Sorption, strontium, montmorillonite

Using Montmorillonite and Bentonite for Phosphate Removal

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Industrial fertilization, the use of detergents with polyphosphates and other chemicals cause excessive amounts of phosphates (concentration more than 0.03 mg/l) in waste and natural waters. Phosphates increase the amount of nutrients and growth of algae and cyanobacteria. This process causes eutrophication of water and complicates the treatment of water for drinking water. There are number methods of remove of phosphorus from waste water. Some of those are used in industrial scale, others only in laboratory conditions and exist only as theoretical studies. Most phosphates are removed as an insoluble salts. The processes using adsorbents, ion exchange, electrocoagulation, etc. are not exception. The literature pays attention to the use of natural clay minerals (especially bentonites and montmorillonites), which for the removal of phosphates were modified. For example, the inorganic-organic bentonite (IOBs) which are used for simultaneous removal of phosphates and organic pollutants can be mentioned. Modification is performed by using cetyltrimethylammonium bromide (CTMAB) and oktadecyltrimethylammonium chloride (OTMAC) and inorganic hydroxide, aluminium and iron (III) ions respectively. Changes of Fe(III) content in bentonite has been achieved higher adsorption capacity of phosphate. The adsorption capacity of phosphate depends on pH of solution also. Another possibility of clay modification is simulations intercalation of OH^-, Al(III) and Fe(III) ions into bentonite. There are always described sorption orthophosphate in literature. Behaviour of other forms of phosphorus anions in contact with the sorbent is not sufficiently described. This work presents results of comparison of the sorption properties of montmorillonite and bentonite for removing of metaphosphate (PO^{3-}) and phosphite (PO^{2-}) ions at laboratory temperature. The obtained dependencies are processed by sorption isotherm.

Keywords: Sorption, Bentonite, Montmorillonite, Metaphosphate, Orthophosphate

The influence of microemulsion on liberation of indomethacin from hydrogel vehicles

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Microemulsions represent modern colloidal carriers for dermal and transdermal drug delivery. They belong among colloidal application systems that have common characteristic, their size lower than 300 nm, as their droplet size range from 10 to 100 nm. They are formed spontaneously combining appropriate amount of a lipophilic, hydrophilic substance, surfactant and co-surfactant. Among all the colloidal drug delivery carriers, the unique features of microemulsions offer several advantages over other dosage forms, such as easy preparation, long term stability, high solubilization capacity for drugs sparingly soluble in water and improved dermal drug delivery. The ingredients of microemulsions could facilitate the permeation rate of the drug by reducing the diffusion barrier of the stratum corneum. Their size enables them to bring a drug to specific organ or tissue (drug targeting). On the other hand, microemulsions have low viscosity and less retention capacity in the skin which limits their application. Therefore new approaches have been studied to overcome this disadvantage. Gelling agents of different origin have been added into the microemulsion to form microemulsion based gel in order to increase its viscosity to be suitable for topical application.

Indomethacin belongs to Non-steroidal anti-inflammatory drugs (NSAIDs), which are used in treatment of various rheumatic or similar diseases. However, their unfavourable effect on gastric mucosa manifested from dyspepsia to peptic ulcer force scientists to look for other options for their administration. Percutaneous and transdermal application offer alternative possibility.

Conventional dermal dosage forms, such as gels, creams, ointments allow reaching only upper layers of the skin. As the NSAID drug concentration should reach therapeutic level in the synovial tissue, synovial fluid and intra-articular tissues during dermal application, novel drug delivery systems have been extensively investigated.

The aim of the present investigation was to evaluate an influence of microemulsion on liberation of indomethacin from various types of vehicles. Hydrogels as Metolose® 4000, Tylose SL®, Carbopol® 940 were used, all in concentration of 0.5 %. Indomethacin was incorporated in two different concetrations, namely 0.5 % and 1%. Microemulsion was processed with each hydrogel in two proportions: 1:9 and 1:4 for microemulsion to hydrogel, respectively. Liberation was performed through semipermeable artificial membrane in *in vitro* conditions. The liberation medium was a buffer with pH 7,4. The microemulsion of W/O type was used.

The microemulsion influenced the liberation of indomethacin in all studied samples in positive way. The highest amount of liberated indomethacin in 0.5% and 1% concentration from pure hydrogel was observed in samples with Tylose SL®. From the mixture of microemulsion and hydrogel, processed in ratio 1:9, respectively, higher amount of indomethacin was released from vehicle with Metolose® 4000 containing 0,5% indomethacin, in comparison with samples containing higher concentration of indomethacin (1%). It turned out that microemulsion added to hydrogels in proportion 1:4, respectively, reached higher values of liberated indomethacin than in proportion 1:9, respectively. From the mixture of microemulsion and Carbopol® 940 (ratio 1:4) the highest amount of indomethacin was released from all liberated samples.

Keywords: Microemulsion, Indomethacin, Liberation, Vehicles

Magnetic Silica Nanotubes - Synthesis, Drug Release, and Feasibility for Magnetic Hyperthermia

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A new kind of silica nanotube with incorporated γ-Fe_2O_3 nanoparticles has been successfully prepared through sol−gel processes. Hematite particles supported on carbon nanotubes served as templates for the fabrication of the magnetic silica nanotubes. The obtained nanostructures consisting of magnetic Fe_2O_3 nanoparticles protected by a silica shell were fully characterized by transmission electron microscopy (TEM), X-ray diffraction (XRD), N_2 sorption and desorption, and magnetization studies. The hollow inner space and the magnetic functionalization render the material promising for applications in biology and medicine. This is underlined by studies in alternating magnetic fields which show a significant heating effect, i.e., the feasibility for applications in hyperthermia therapies. In addition, the material exhibits enhanced drug-loading capacity which is demonstrated by loading with rhodamine B molecules as drugs and corresponding release experiments. The results show that magnetic silica nanotubes can be straightforwardly synthesized and have a great potential as a multifunctional drug carrier system.

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Nano-oxide modified graphite felt for all vanadium flow redox battery

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All vanadium flow redox battery (VFB) is a new type of energy storage batteries. It has the advantages of high-power, large current charge and discharge, and without geographical restrictions.

The graphite felt becomes one of the most extensive use of the VFB electrode materials due to it's the large specific surface area, acid and alkali resistance and good mechanical properties. In order to improve the efficiency of the VFB, graphite felt must be subjected to surface treatment to increase the surface functional groups and wet ability for further improving the electrochemical activity of the electrode.

In this study, bismuth oxide and indium oxide nano-particles were used to modify graphite felt. The characteristics of the modified graphite felt were analyzed by SEM and EDS. Cyclic voltammetry, AC impedance and potentiodynamic scan found that graphite oxide nanoparticles modified superior to that of untreated graphite felt. A large number of nano-oxide adsorbed on the graphite surface of the felt fiber, nano-bismuth oxide aggregate particle size and number are significantly smaller than the indium oxide nanoparticles. This may be due to the heat treatment of nano-bismuth oxide played a catalytic graphite felt fibers lead to oxidation.

Keywords: vanadium redox flow battery, graphite felt, nano-oxide modified

Synthesis and potential application of phosphazene derivatives

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Most synthetic polymers are totally organic macromolecules. One of the exceptions is the class of polymers with an inorganic backbone – polyphosphazenes. These polymers contain a backbone or rings of alternating phosphorus and nitrogen atoms, with two organic or inorganic groups linked to each phosphorous atom. Organic and inorganic phosphazene derivatives could find practical application in various industries. They can be used as an admixture e.g. to lubricants and flame retardants.

Our research focuses on synthesizing cyclic phosphazene derivatives with mostly flame retardant properties which are suitable for creating nanofibres made from their mixture with common polymers.
Two types of synthesis have been investigated in our work, synthesis fully substituted phosphazene derivatives from monomer phosphazene and from trimer derivatives. $P_3N_3(PhO)_4(NH_2)_2$, $P_3N_3(PhO)_6$ were synthesized by substitution reactions from the most common cyclic phosphazene structure $P_3N_3Cl_6$, the other derivative, $P_3N_3(Ph)_3(C{\equiv}CPh)_3$, was synthesized by condensation method from $(Me_3Si)_2NH$ and $PPhCl_2$.
Our prepared derivatives can positively affect final nanofibre properties with regard to their potential application as flame retardants.

Keywords: phosphazene, synthesis, nanofibres

Impact of plastically deformed steel surface on magnetic measurements

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Durability and usability of the steel products strongly depends on the state of surface, which can be expressed in the terms of final microstructure and residual stresses. Therefore a non-destructive testing methods (NDT) are needed which can detect unacceptable discrepancies. Magnetic methods have gained significant importance in modern industrial processes due to its robustness and relatively simple implementation.

A very thin surface layer of material has a transformed microstructure after hard turning operation due to the significant plastic deformation and due to a temperature exposure exceeding the Currie temperature in the cutting zone. The state of this thin layer significantly affects the surface magnetic properties of the material which can be measured by magnetic NDT methods.

This paper deals with a pronounced magnetic anisotropy found in a hard turned surface and a grinded surface of bearing steel. The microstructural changes of surface layer after machining are correlated with surface magnetic anisotropy measured by different methods. The magnetic properties of the studied surfaces are analyzed by Barkhausen noise emission as well as magneto-optical methods.

Keywords: magnetic anisotropy, surface, bearing steel, Barkhausen noise, magneto-optical Kerr effect

Influence of the microstructural parts interaction on the electrochemical properties of Mg-Al-Zn alloys

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The corrosion resistance of materials is dependent also on their microstructure. Microstructural parts can have different electrochemical properties as the base material. This is the cause of the inductive current formation in the structure which has a negative effect on the corrosion resistance of materials.

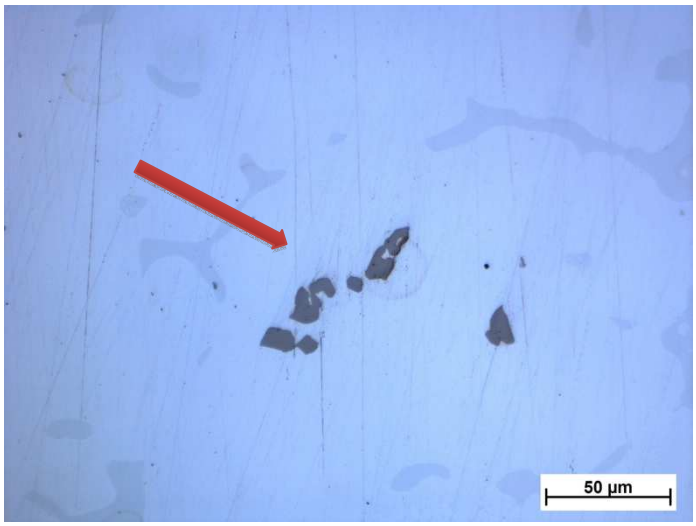


Fig. 1 Phase Mg_{17} Al_{12} with different surface potential as the base material.

The paper deals with the influence of microstructural parts on the corrosion resistance of magnesium alloy AZ 91. Corrosion characteristics were measured using electrochemical impedance spectroscopy (EIS) method in a standard 0.1 M NaCl solution at 22 °C. The results of EIS measurements are supplemented by measurements of surface potential of structural parts at the AFM microscope.

Keywords: EIS, corrosion resistance, magnesium alloy AZ 91, AFM, surface potential

Electrodeposition of the calcium phosphate coatings on the Mg-Al-Zn alloys surfaces

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Magnesium alloys are very reactive in corrosion media containing aggressive chloride ions. They are very interesting and perspective material for biodegradable implants but it is problem with very high corrosion rate in simulated body fluids. Besides the corrosion rate there is the problem with evolution of very high amount of hydrogen as product of cathodic reaction. Several possibilities exist to tailor the corrosion rate of magnesium by using alloying elements and protective coatings, processes that of course must lead to a non-toxic, biologically compatible material.

Calcium phosphates have been researched extensively for biomedical applications due to their high biocompatibility and bioactivity. Unfortunately, these ceramic biomaterials do not have the mechanical strength to enable them to succeed in load bearing applications. However, implant materials such as stainless steels and titanium alloys are coated with calcium phosphates. Compared to conventional preparation methods, such as hot spraying or laser cladding, the structure of Ca–P coatings formed in solution is closer to that of the bone minerals.

This paper deals with evaluation of dicalcium phosphate dihydrate (DCPD) thin layer formation on the surface of magnesium alloy AZ31 by electrodeposition and evaluation of biodegradation process of Mg-3Al-1Zn alloy surfaces after grinding and grinding followed by electrodeposition of (DCPD). The electrodeposition cathodic treatment process was performed in water solution of $Ca(NO_3)_2.4H_2O$, $NH_4H_2PO_4$ and H_2O_2.The corrosion processes of untreated and treated specimens were evaluated by electrochemical impedance spectroscopy method.

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Keywords: magnesium alloy, dicalcium phosphate layer, electrodeposition, electrochemical impedance spectroscopy

Micromagnetic evaluation of surfaces after grinding

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Despite properly suggested grinding operations grinding burn can randomly occurs due to many variable parameters affecting grinding. Thermal softening due to elevated temperatures in the grinding wheel – work piece contact is the most usual case of surface damage in grinding. Chemical activation is very often used as a nondestructive testing of ground surfaces. However, when grinding large parts chemical indications should be replaced by micromagnetic technique since this technique is very fast, portable and well suited for automated cycles.

This paper deals with detection of surface burn after grinding operations on larger bearing rings made of case - hardened steels. The paper reports about calibration of Barkhausen noise technique for non destructive monitoring of grinding operations for rings of diameter in the range of 600 up to 4000 mm. Properly suggested monitoring concept enables to detect thermal damage due to grinding wheel wear as well as insufficient coolant supply. Results of the study indicate that higher values of Barkhausen noise correlated with more pronounced thickness of heat affected zone found in the ground surfaces. Correlation between micromagnetic parameters and heat affected zone (its thickness) enable to set up the critical limit for surface burn detection as well as needed allowances for additional regrinding of the surface.

Further, grinding burn associated with lack of coolant can be clearly distinguished from damage corresponding grinding wheel wear. While thermal affected zone is clearly separated from the untouched structure in the case of wet grinding, subsurface layers after dry grinding can be defined as a mixed zone where thermal softening and raw structure occurs. The paper also discusses increasing magnetoelastic responses obtained after grinding rings of higher diameters as a result of increasing grinding wheel wear. The paper also reports about higher risk of grinding burn when grinding rings of higher diameter. Results of hardness measurement as well as corresponding X - ray diffraction are also reported in the paper to verify information about surface integrity obtained through micromagnetic technique.

Keywords: grinding, Barkhausen noise, monitoring, thermal softening

Influence of nanostructured surface layer obtained by severe shot peening on the ultra-high cycle fatigue life of 50CrMo4 steel

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This contribution deals with the use of severe shot peening to obtain nanostructured surface layer and deep compression residual stress field which can significantly improve fatigue properties of materials. Quenched and tempered steel 50CrMo4 used for manufacturing of car wheel hubs was considered in this study. Two sets of specimens (11 PCS each) were machined from a die forged wheel hub. One set was mechanically polished (marked NP – not peened) and the second one was severely shot peened with use of S170 peening medium(steel shots, ø = 425 μm), Almen intensity 15.6 A and coverage of 1000 % (this group is marked as SSP – severely shot peened). Severe plastic deformation created by shot peening treatment caused crystallite fragmentation of the surface layer. According to crystallite size measured in terms of XRD diffraction (X'Pert PRO diffractometer, Co radiation, diffraction angles from 45° to 130° (2θ), paralel plate collimator, crystallite size evaluated with TOPAS software according to all four diffraction lines {110, 200, 211, 220}), the crystallite size on the surface decreased from average value of 74 ± 3 nm for the NP specimen to 38 ± 4 nm for the SSP specimen. This surface layer has also different appearance under secondary electrons of scanning electron microscope (Figure 1).

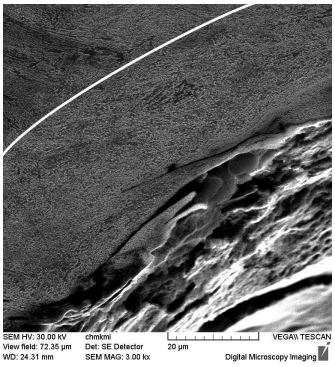


Fig. 1 Nanostructured surface layer (SEM).

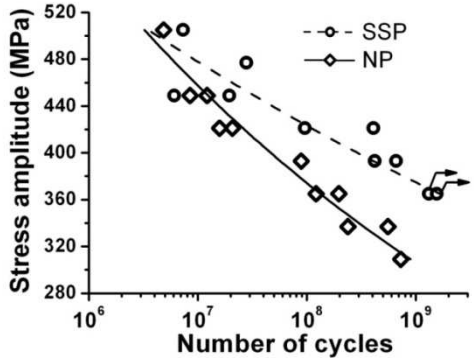


Fig. 2 S – N curves of NP and SSP specimens.

Fatigue test in the high and ultra-high cycle region were carried out with use of ultrasonic fatigue testing device with frequency f ≈ 20 kHz, tension – compression loading with stress ratio R = -1 and temperature of T = 20 ± 5 °C. Results are presented in form of S – N curves (dependence of the number of cycles to failure or run out on the stress amplitude, run – out specimens are marked by arrows). According to obtained results (Figure 2) it is obvious, that severe shot peening significantly increased the fatigue life of 50CrMo4 steel in the high and mainly in the ultra-high cycle region. However, for lower number of cycles than approximately $N = 4 \times 10^6$, severe shot peening seems to have a negative effect on the fatigue life.

Akcnowledgement:
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Keywords: high and ultra-high fatigue region, severe shot peening, nanostructured surface layer, 50CrMo4 steel, high frequency fatigue testing

Abrasive in brake friction composites

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Abrasives are one of groups utilized in brake friction materials and they play a critical role in friction and wear performance. Factors affecting friction coefficient (μ), wear rate, formation of friction layers and disc life as well as theoretical consideration related to abrasives were discussed in this research. The critical volume fraction of abrasives was experimentally determined and explained by a competitive relation between adhesion and abrasion friction mechanisms. Effect of particle size of abrasives on friction and wear performance can be explained by abrasion friction and wear model where two parameters, *r* (radius of abrasives) and *d* (depth of abrasives embedded into disc), are involved. The area of friction layers caused by abrasives including primary and secondary contact plateaus can be calculated by using an elliptical model. Formation of friction layers can be simulated by two- and three-dimensional cellular automata models.

Keywords: brake friction materials, friction and wear performance, friction layers, abrasives

One – and two-step resonance energy transfer between cyanine dyes in layered silicates colloidal systems

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RET is a phenomenon of radiationless transmission of excitation energy from donor to acceptor molecules (1). The objective of this work was to achieve an efficient resonance energy transfer (RET) between molecules of three different cyanine dyes on two-dimensional surface of layered silicate particles. The adsorption of dye cations on negatively charged surface of layered silicate was achieved via ion-exchange reaction. Concentration of adsorbed dye cations has to significantly increase to approach intermolecular distances of a few Å so that RET could be achieved. However, dye adsorption and concentration on the surface is often accompanied by molecular aggregation. Depending on the layer charge of silicate, various forms of dye assemblies can be formed, such as dimers and larger aggregates of H-, and J-type. The molecular aggregation is mostly undesirable process, because it leads to fluorescence quenching and the loss of photoactivity. One is able to suppress the molecular aggregation and, in the same way, to achieve remarkable yields of RET using an appropriate selection of reaction conditions and layered silicate with low layer charge density (2). In this study the cationic cyanine dyes were adsorbed on the surface of colloidal particles of layered silicate, synthetic saponite (Sumecton SA). Cyanine dyes represent interesting compounds due to a preferential formation of photoactive J-aggregates and lower occurrence of inactive H-aggregates (1). Single- and two-step RET were achieved between adsorbed molecules of cyanine dye cations (NK1, NK2, NK3). The cations of three different dyes played the role either of energy donor (NK1), or energy acceptor (NK3) or of both the donor and acceptor (NK2). The absorption spectroscopy did not detect large amounts of the molecular aggregates. Effects of various parameters on the efficiency of the RET process, in both the single- and two-step RET were analysed. RET efficiency and the effects of various parameters were similar to our previous results obtained by similar system with laser dyes (2).

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Keywords: Resonance energy transfer, layered silicates, cyanine dyes

ZnO and CuO/ vermiculite nanocomposites for medicine applications

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In recent years there are prepared many important nanomaterials for various usages. Very interesting materials are metal oxides such as cupric oxide and zinc oxide.
Nanoparticles of cupric oxide are used in optoelectronics, transformation of solar energy, magnetic storage medias, electronics, sensors, catalysis and/or batteries. It has got some advantages in comparison to other transitional metal oxides such as his structural stability, non-toxic and antibacterial properties. Nanoparticles of cupric oxide are prepared by different syntheses process such as solvothermal, sol-gel, mechanochemical methods or microwave irradiation. Antibacterial behavior of cupric oxide was investigated in recent years on bacteria Escherichia coli, Pseudomonas aeruginosa, Bacillus circulens, Staphylococcus aureus, Pseudokirchneriella subcapitata.
Nanoparticles of zinc oxide are very important nanomaterials also. Nanoparticles are chemically stable, no-toxic nanomaterials used in electronics, for photocatalysis as gas sensors, solar cells, in cosmetics and medicine as antibacterial nanomaterials. Zinc oxide nanoparticles are usually prepared by the sol-gel, hydrothermal and solvothermal, mechanochemical methods, thermal evaporation and/or microwave synthesis. Antibacterial behavior of zinc oxides nanoparticles was investigate in recent years on Escherichia coli, Acacia concinna, Pseudomonas, Saccharomyces cerevisiae, Vibrio fischeri or on Thamnocephalus platyurus.
Nanocomposites on the base of vermiculite/zinc and cupric oxides were prepared by the mechanochemical process. Structural differences of nanocomposites are depend on grow of oxides in interlayer spaces or on surface of vermiculite particles. Different concentration of zinc and cupric oxides on vermiculite particles were prepared after calcined on 150, 350 and 650 °C for 1,5 hour. Nanocomposites characters have been studied using scanning electron microscopy (SEM). Structural and phase analysis has been performed using X-ray diffraction (XRD) method. Antibacterial activities were tested on different bacterial strains.

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Keywords: antibacterial nanocomposites, ZnO, CuO, vermiculite

Clay/porphyrin based optical oxygen sensors

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The present study is related to the investigation of hybrid systems with incorporated metalloporphyrin molecules. These systems consist of two parts: a synthetic clay and metalloporphyrin molecules, suitable or the construction of perspectively efficient oxygen sensing, as well as the singlet oxygen production. Taking into account the complexity of these systems, the choice of suitable starting materials is of a crucial importance. As guest materials, metalloporphyrins containing heavy metals are usually utilized. These are known to be very efficient for the sensing applications because of "heavy atom effect". This effect promotes a spin-orbit coupling, resulting in the fact that almost all of the radiation from singlet excited state undergoes the inter system crossing, followed by the de-excitation via a triplet state. As a result, phosphorescence from these systems can be observed in a presence of an inert gas, e.g. nitrogen. However, in a presence of reactive oxygen the collisional quenching takes place, resulting in a diminish of phosphorescence. By changing the nitrogen-to-oxygen atmosphere and vice versa, one can study the behaviour of an "on-off" type sensing. These hybrid systems show interesting luminescent properties with the simultaneous singlet oxygen formation. Hence, they can be utilized as the efficient oxygen sensing materials, as well as the singlet oxygen producers.

Acknowledgements:
This work was supported by the Slovak Grant Agency for Science VEGA (No. 2/0107/13) and APVV (No. APVV-0291-11).

Keywords: porphyrin, clay, oxygen sensor, phosphorescence

The influence of ionic strength on stability photoactive composite TiO_2/kaolinite

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The article focuses on studying the influence of ionic strength on the stability of photoactive composite TiO_2/ kaolinite. Although TiO_2 is non-toxic material, it can be dangerous for environment and living organism if it occurs in the form of nanoparticles (NPs). The potential risk for environment could be prevented by fixing TiO_2 NPs on suitable carrier (for example clay minerals). Therefore, the photoactive composites TiO_2 NPs/kaolinite were prepared. Photoactive composite with the same content of photoactive TiO_2 was dried at 100°C or calcined at 600°C. Chemical composition of prepared sample was determined by using energy dispersive fluorescence spectrometer. The stability of photoactive composite was studied by leaching test. Material was leached in deionized water or in solutions with different NaCl concentrations. The leaching test was carried out in bath reactor with the solid: liquid phase ratio 1:10. The experiments were done at laboratory temperature for 24 hours. Conductivity and pH were measured immediately after separating the liquid phase by filtration. Dissolved elements were determined by atomic emission spectroscopy with inductively coupled plasma. The changes in composition of photoactive material were evaluated on the basis of dissolved elements in filtrates after leaching. The influence of ionic strength of extraction solution on structure was described.

Keywords: TiO_2/kaolinite, photoactive composite, stability

Resonance energy transfer in the systems based on layered silicates and laser dyes

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The main objective of present work was to prepare supramolecular systems in both colloidal and thin films that exhibit the process of resonance energy transfer (RET). The phenomenon of RET is a radiationless transmission of energy from donor molecules to acceptor molecules. If the molecules of two dyes with suitable spectral properties are in close proximity to each other (typically between 1 and 10 nm), RET can occur [1]. In general, the RET can be monitored as lowering of fluorescence emission from a donor molecules in favour of the increase of the fluorescence from the acceptor molecules. The intercalation and co-adsorption of cationic dyes into the two-dimensional space of layered silicates leads to the formation of various forms of dye assemblies. These aggregates can easily be distinguished by absorption spectroscopy. The main problem which occurred during the dye adsorption is the formation of non-fluorescent H-aggregates. In the first part, the colloidal systems based on synthetic saponite and adsorbed cations of rhodamine and oxazine dyes were prepared. The process of RET was studied using fluorescence spectroscopy. The cations of rhodamine played the role of molecular antennas absorbing green light. RET was detected as a quenching of light emission from rhodamine (580 nm) in favour of the red light luminescence from oxazine (635 nm). The second objective of study was to prepare thin films of saponite using a spin-coating method followed by the intercalation of the molecules of both the dyes in the films. Preparation of photoactive hybrid systems mainly in a solid state is a challenge due to the formation of non-fluorescent H-aggregates and a complete loss of fluorescence. This problem was solved by an appropriate modification of inorganic host with hydrophobic alkylammonium cations. The surfactant cations probably played an important role in preventing the dye molecular aggregation [2]. In this case, the energy transfer occurring in the solid film from R3B to Ox4 and ending with the radiation from the energy acceptor molecules (Ox4) was clearly proven.

Acknowledgements:
This work was supported by the Slovak Grant Agency for Science VEGA (No. 2/0107/13) and APVV (No. APVV-0291-11). This contribution is the result of the project implementation: Centre for materials, layers and systems for applications and chemical processes under extreme conditions - Stage II supported by the Research & Development Operational Programme funded by the ERDF.

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Keywords: energy transfer, laser dyes, fluorescence spectroscopy, layered silicates

Influence of flank wear on plastic deformation after turning via Barkhausen noise technique

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This paper deals with the stress and temperature induced microstructure transformations in a soft bearing steel 100Cr6 after turning operation. Investigation is carried out through a mechanical and thermal load of machined surface as well as micromagnetic technique based on Barkhausen noise. Evaluation of surface integrity via structure transformations, X - ray diffraction as well as microhardness inspection is carried out as well. A surface integrity is investigated with the respect to the variable tool wears and consequent mechanical and thermal loads applied on the inspected surfaces.

Different surface microstructures caused by the mechanical and associated thermal aspects of the surface formation are discussed and correlated with the parameters obtained from the measured Barkhausen emissions. Results of measurements indicate that rapid decrease of micromagnetic responses is associated with severe plastic deformation and corresponding increase in dislocation density. As soon as, the dislocation density attains the critical value over which the structure can not afford, near surface dynamic recovery occurs and Barkhausen noise parameters saturate.

Keywords: turning, Barkhausen noise, plastic deformation, structure transformation

Synthesis and Properties of Lamellar Aggregates of Globular Fullerite Nanoparticles

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This paper describes an alternative of microemulsion synthesis of globular nC_{60} nanoaggregates (cca 26 nm), which exhibit high colloidal stability in water without emulsifying surfactant additives (see Fig.1).

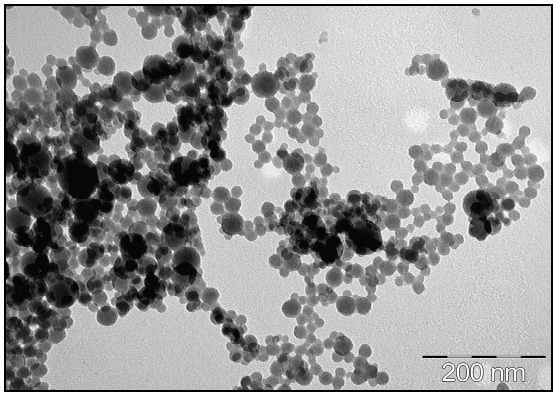


Fig. 1 The TEM micrograph of globular nanoparticles nC_{60} after the normal drying the dispersion on a TEM grid.

In the successive part of the technological process the dispersion was solidified by freezing and subjected to controlled sublimation under carefully selected conditions in a vacuum sublimation chamber. Applying the specific conditions during the vacuum freeze-drying we achieved the formation of large lamellar nC_{60} aggregates at the sublimation interface.

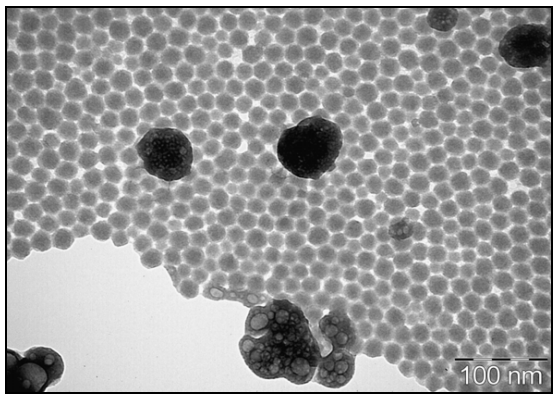


Fig. 2 The monolayer lamellar structure of globular nanoparticles nC_{60} self assembled by controlled vacuum freeze-drying.

An arrangement of such self-assembled nanoparticles (see Fig.2) in volume is very tight and the material exhibits a high specific surface area value and other unusual physical properties.

Keywords: nanoparticle, nanoaggregates, vacuum freeze-drying, lamellar nanostructures

A novel route for electrodeposition of CuCl and CuBr thin films and their conversion to textured porous CuO. Photoelectrochemical studies

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Here we report a novel route for electrodeposition of CuCl films on fluorine doped tin oxide (FTO) electrodes. The electrodeposition of CuCl was carried out in a two-electrode cell in the presence of Cu^{2+} and Cl^- ions. Detailed analysis confirmed that reduction of Cu^{2+} to Cu^+ happens at the vicinity of the FTO electrode, which in the presence of excess Cl^- ions favors the formation of insoluble CuCl phase. Due to the relatively low solubility product constant (K_{sp}) of CuCl in water which is in the order of $K_{sp}=1.9\times10^{-7}$ we were able to electrodeposit this material on FTO substrates.[1] The obtained CuCl films are dense and the film thickness is in the order of ~8 μm. This electrodeposition process also holds for the preparation of CuBr thin films. Annealing of the as-prepared CuCl and CuBr films at 380 °C, 420 °C, and 460 °C, in air, yielded CuO phase. Figure 1 shows SEM images taken from a representative CuO sample that was annealed at 460 °C. The obtained CuO film exhibit textured features with average grain sizes in the order of ~300 nm. Detailed X-ray diffraction (XRD) studies confirmed that complete transformation of CuCl to CuO phase happens at temperatures above 420 °C for 30 min (Fig. 1c).

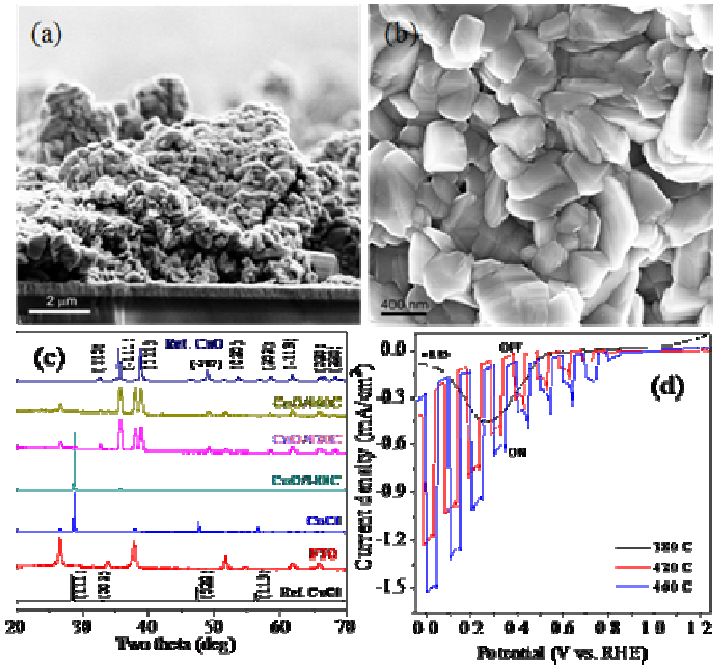


Fig. 1 SEM images of texture CuO films: (a) cross-section and (b) top view. The CuO film was annealed at 460°C for 30 min. (c) XRD spectra of the various phases and (b) chopped photocurrent density vs potential of the CuO films annealed at different temperatures and measured in 0.5 M Na_2SO_4 aqueous solvent (AM1.5, 100mW/cm^2).

Moreover, the obtained CuO films were tested for water splitting reaction in a three-electrode configuration cell. The highest obtained photocurrent density was in the order of ~1.5 mA/cm^2 at 0 V vs. reversible hydrogen electrode, RHE, for the sample annealed at 460 °C. We attributed this observed photocurrent responce to the water splitting reaction combined with photocorrosion which happens on the CuO electrode surface. Furthermore, the photoresponce of the CuO electrodes were also studied in the presence of I^-/I_3^- redox couple in propylene carbonate solution. The experiments in I^-/I_3^- redox couple confirmed that the photoresponce arises entirely from the photogenerated current in the CuO films. By employing I^-/I_3^- redox couple we conclude that the films are stable in non-aqueous solution. However, the stability of the CuO films greatly deteriorate in water due to photocorrosion. Future, research will be focused on stabilising the electrodes. The current method seems a promising way for preparation of textured porous CuO films for light harvesting applications.

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The surface properties of antibacterial nanomaterials

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Antibacterial nanomaterials have attracted significant attention in recent years. Advances in many specialty metal oxide and hydroxyapatite nanoparticles and their nanocomposites materials have made significant contribution to the development of modern health care industry and have improved the quality of human life. They are primarily used as bone substitutes in the biomedical industry due to their biocompatibility, low density, chemical stability, high wear resistance and mainly for their compositional similarity with the mineral phase of biological materials.

The surface modification of metal oxides and hydroxyapatite nanoparticles and their nanocomposites can change their behavior in the physiological solution and interaction with the tissue in vivo and adjust the release rate of ions and biological properties on the surface of materials. Especially nanocomposites materials with various morphologies and surface properties have been investigated as drug carriers for the delivery of a variety of pharmaceutical molecules because of their antibacterial, biocompatible, osteoconductive, nontoxic, and noninflammatory properties for various medical applications.

Zeta-potential is the most interesting surface property, which gives information about total surface charge. It can be exploited to assessing of physical stability of particle dispersion. Around charged particles in solution arises the electric double-layer, which is formed by ions from liquid medium. The zeta-potential is electrostatic potential which is measured between two internal layers of electric double layer. The quantification of zeta-potential are ordinarily performed by the following methods as electrophoresis (is measured the movement of charged particles in solution), eletroosmosis (measured is the particle transited time by micro-canal or capillary), streaming potential (the electric field is measured), sedimentation potential (is measured by electric field which arises when the solid is stationary and the liquid phase is moving around it). For describe the electrophoretic mobility is used the Henry's law or his approximations (Schmoluchowski or Huckel approximations).

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Keywords: Zeta-potential, surface properties, nanoparticles, nanocomposites

Iron-containing composite cathode materials

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The results of electrochemical research of delafossite $LiCo_{1-x}M_xO_2$ (M = Cr and Fe) synthesized solid solutions have been presented. $LiMn_{1/3}Cr_{1/3}Fe_{1/3}O_2$ has been synthesized and studied as well as the composite material $SrFe_{12}O_{19}$@$LiNiPO_4$ with dominating core@shell type distribution. Chronopotentiometry and CV methods were applied to study the opportunity to use them as positive electrode materials for lithium and lithium-ion batteries. The highest specific electrochemical capacity appeared in materials $LiCo_{1-x-y}Cr_xFe_yO_2$ and $LiMn_{1/3}Cr_{1/3}Fe_{1/3}O_2$ (220 and 270 mA·h/g) isostructural to $LiCoO_2$.

$LiCoO_2$ is currently widely used as cathode material for lithium-ion batteries. Its advantages are high operating voltage, power and thermal stability. Among its disadvantages high cost and cobalt toxicity as well as structural instability at lithium deintercalation can be mentioned. Partial cobalt substitution for manganese, chrome, nickel or iron within the structure $LiCoO_2$ allows to improve electrochemical performances. The main aim of the present research is to study electrochemical performances of the phases with delafossite structure when partial or even complete cobalt substitution for manganese, chrome or iron is applied. We also consider promising the synthesis and study of composite core@shell material electrochemical performances, i.e. the materials with dominating bulk distribution of electrochemically active phases. To determine the desired phase formation temperatures complex differential thermal analysis of the prepared precursors was carried. The synthesized sample electronic-microscopic study was performed with the microscope Zeiss Supra 25. The obtained sample electrochemical testing was carried out in two modes. Firstly, the chronopotentiostatic mode with stable charge-discharge current (C/10) using time relay and AKTAKOM AM-1118 multimeter was applied. Secondly we applied the cyclic VA mode using bipotentiostat PINE AFCB P1. Scan rate was 0.2-0.5 mV/s in the voltage range of 2.8-4.8 V. The experiment was carried out in three-electrode cell assembled in the glove box in dry (≈ 99 %) carbon dioxide. Metal lithium acted as a counter electrode and an electrode of reference. The positive electrode was assembled according to standard commonly used method [5].

After synthesis the obtained samples were studied with X-ray diffraction. It was found that the composition 8 has cubic $LiFeO_2$ structure, the composition 9 is a two-phase sample consisting of solid solutions based on cubic $LiFeO_2$ and layered $LiCoO_2$. The compositions 1, 2, 3, 4, 5, 6 are solid solutions isostructural to $LiCoO_2$ and 7 is $LiCoO_2$.

There have been synthesized in total 25 simples with water soluble compound method and then studied. Cobalt, iron, chrome nitrates and manganese acetate were solved in a small quantity of water, after that lithium carbonate was added to the solution obtained with constant stirring until fully dissolved. The final solution was evaporated at 120 °C until completely desiccated. Solid residue was homogenized mechanically and studied with XRD method. But the desired phases did not form. The results of electrochemical testing in chronopotentiostatic mode for some phases are given in the table 1.

The DTA and DTG method results allow us to state that the desired phases are formed at 800 - 850 °C. At DTG curve the mass stability is observed at 500 °C. According to thermal analysis results the synthesis was carried out for pressed tablets at 900 - 1000 °C for 1h.

Table 1. The results of electrochemical testing for some samples.

№	Composition	Molar weight	$C_{theor.}$, mA·h/g	Initial voltage, V	Voltage range, V
1	$LiCo_{1/3}Fe_{1/3}Cr_{1/3}O_2$	94.53	284	3.79	3.44-4.68
2	$LiCo_{0.65}Fe_{0.1}Cr_{0.25}O_2$	95.87	280	3.76	3.25-4.27
3	$LiCo_{0.25}Fe_{0.1}Cr_{0.65}O_2$	93.05	288	3.30	3.2-4.42
4	$LiCo_{0.2}Fe_{0.2}Cr_{0.6}O_2$	93.09	288	3.39	3.3-4.65
5	$LiCo_{0.1}Fe_{0.45}Cr_{0.45}O_2$	93.36	287	3.76	3.36-4.4
6	$LiCo_{0.1}Fe_{0.15}Cr_{0.75}O_2$	92.21	291	3.80	3.45-4.18
7	$LiCoO_2$	97.87	274	3.44	3.22-4.15
8	$LiCr_{1/3}Mn_{1/3}Fe_{1/3}O_2$	94.52	282	3.77	3.7-4.55
9	$LiNiPO_4$	161	166	3.33	2.5-4.5
10	$SrFe_{12}O_{19}$	1061.77	302.89	3.45	2.8-3.5
11	$SrFe_{12}O_{19}$@$LiNiPO_4$	251, 08	196, 29	3.34	2.86-4.41

It should be noted (table 1) that $SrFe_{12}O_{19}$@$LiNiPO_4$ composite electrochemical performances exceed the initial component performances of $LiNiPO_4$ and $SrFe_{12}O_{19}$.
The research results showed that $SrFe_{12}O_{19}$@$LiNiPO_4$ composite material as well as the phases based on $LiCo_{1-x-y}Cr_xFe_yO_2$ solid solutions isostructural to layered $LiCoO_2$ and $LiMn_{1/3}Cr_{1/3}Fe_{1/3}O_2$ are promising positive electrode materials for lithium and lithium-ion batteries.

Keywords: lithium-ion batteries, delafossit, solid solutions, composite

Study of a load sensor based on polyaniline/phyllosilicate matrix

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Present work deals with the preparation of kaolinite/TiO_2 nanocomposite matrix (KATI) coated with polyaniline (PANI) layer. The aim is to achieve the functional unit responding to the external mechanical pressure by changing the electrical conductivity. Pellets made of pure PANI and PANI/kaolinite composite were also prepared for the control comparison.

KATI matrix was prepared from kaolinite SAK47 (either dried or calcined at 600 °C) mixed with titanyl sulfate as a precursor of TiO_2 nanoparticles. Preparation of PANI/KATI and PANI/KLT composites was one-step process. The aniline sulfate and ammonium peroxodisulfate were added into water suspension of KATI or KLT matrices, respectively. PANI powder has been prepared by oxidative polymerization of the solution of aniline by ammonium peroxodisulfate in acidic environment (sulfuric acid). All materials prepared in powder form were pressed into pellets in LECO PR-36 hand press using the pressure 28 MPa at room temperature, without any lubrication and binder.

Electric current flowing through the pellet (in the direction of pressing) was measured in dependence on mechanical load. Twelve weights (124 g each) were used. Experiment started after loading the pellet with two weights (i.e. 248 g). In this loading part of measurement a pairs of additional weights were added at definite time intervals. After reaching the maximum load (1 488 g) the pairs of weights were again removed at the same time intervals in the unloading part of the measurement.

Idea of the load sensor lies not only in its ability to respond to external loads, but also in ability to respond to the same load identically, even for multiple repetitions. The measurement results showed that the pellets containing the calcined KLT exhibit stable response to the same load. The average differences between the values of current for the same number of weights both in loading and unloading part of measurement do not exceed 4.5 %. For PANI / KLT and pure PANI pellets the difference is 5.2 and 15 %, respectively.

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Keywords: polyaniline, kaolinite, TiO_2, conductivity, pellets

Effect of kaolinite exfoliation on the photocatalytic properties of kaolinite/TiO_2 composite

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It was shown that the composites kaolinite/TiO_2 (KATI) represent valuable material showing enhanced photodegradation activity. Fixing of the photoactive TiO_2 particles at the surface of kaolinite brings following advantages: i) diminishing of the possible negative environmental impact of TiO_2 nanoparticles, ii) enhanced photodegradation activity of TiO_2 related to the presence of kaolinite which serves as adsorbent of pollutants being degraded by TiO_2, iii) easier removing of the KATI photocatalysts after the photodegradation process by sedimentation and/or filtration, iv) positive effect of calcined KATI composites on mechanical properties, self cleaning properties and durability of building materials based on Portland cement binder.

In simplified way the kaolinite structure can be presented by layers composed of net Si tetrahedrons connected to net of Al octahedrons, the individual layers are separated by the interlayer space which consists of interlayer water. There are several ways making possible to decrease the size of kaolinite particles and these methods can be categorized to mechanical, mechano-chemical and chemical methods. Chemical methods based on intercalation of organic molecules into kaolinite interlayer are used for process of exfoliation/delamination of the kaolinite structure which leads to decrease in the size of the particles in z direction, in ideal situation the individual kaolinite layers can be obtained.

The present research is focused on the evaluation of the effect of delamination/exfoliation of kaolinite structure on the photodegradation activity of KATI composites. The exfoliation/delamination of kaolinite structure was achieved after its intercalation with urea followed by its removing during heat treatment. Chemically exfoliated kaolinite was used as a substrate for growing of the TiO_2 particles prepared using titanyl sulphate as TiO_2 precursor. TiO_2 content in KATI composites was determined using X-ray fluorescence spectroscopy, the morphology of the particles of KATI composite was studied using scanning electron microscopy and phase composition was studied by X-ray diffraction analysis. Photodegradation activity of prepared composites was evaluated by the means of photodegradation of model organic dye acid orange 7.

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Keywords: Kaolinite, Titanium Dioxide, Composite, Exfoliation, Photodegradation Activity

Nanocomposite of cement paste/graphene oxide - hydratation kinetics and early age response with AFM

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The application of nanomaterials in construction is a new alternative to enhance the mechanical properties of the traditional materials e.g cement mortars and concretes. One of the most intersting nanomaterial which still requires detailed investigation is graphene and and graphene oxide. Therefore, here we present study on hydrataion kinetics and early age mechanical response of the cement mortar modified with graphene on a nanoscale using atomic force microscopy (AFM). The kinetics of the hydratation process was investigated by means of calorimetry, Infrared (IR) and X-Ray diffraction (XRD) techniques. The morphology of the nanocomposite was revealed by scanning electron microscopy with EDX as its mode.

Keywords: graphene oxide, hydratation kinetics, mechanical properties, cement mortar

Mechano- and solvo-chemical methods for hydroxyapatite nanostructures preparation

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Nanomaterials are more and more becoming part of the human life. Hydroxyapatite (HAp, $Ca_{10}(PO_4)_6(OH)_2$) nanomaterials are among of the few materials that are classified as bioactive. The interest about HAp is focused to their mineral components being similar to bones and teeth of human body. HAp is characterized as osseointegration nano-material used in orthopedic, dental and maxillofacial applications. Hydroxyapatite may be employed in forms such as powders, layers, porous blocks and/or hybrid composites to fill bone defects or voids (e.g. dental applications).

HAp nanostructured materials can be produced from coral, seashell, eggshell and also from body fluids. HAp nanoparticles are in technical industries prepared by the precipitation and hydrolysis, refined solid state reactions, sol-gel syntheses, hydrothermal reactions and emulsion and microemulsion syntheses. During the past years are mechanochemical syntheses used for HAp nanocomposites and nanoceramics also.

The combinations of mechano- and solvo-chemical method have been successfully used for HAp nanoparticles and HAp/vermiculite nanocomposites preparation. The nanostructures have been obtained from calcium oxide (CaO) and anhydrous dicalcium phosphate ($CaHPO_4$) precursors. HAp nanostructures have been prepared with the respect to the control of the Ca/P molar ratio. HAp nanoparticles and nanocomposites have been defined using the particle size distribution (PSD) analysis. Character and shape have been studied using scanning electron microscopy (SEM). Structural and phase analysis has been performed using X-ray diffraction (XRD) method and infrared spectroscopy (FTIR).

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Keywords: Hydroxyapatite, Nanocomposites, Nanoparticles, Preparation method, Particle characterization

Hybrid materials of clay minerals grafted with reactive fluorophores

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Hybrid materials based on clay minerals and fluorescent dyes have mostly been prepared by ion exchange reaction with cationic dyes. This work presents a novel type of hybrids with fluorophore units covalently attached to clay mineral particles. The anchoring of dye moieties was achieved via reaction of dye precursors bearing reactive ethoxysilane groups, which was based on the condensation with hydroxyl groups present on the surface of clay mineral particles. We have prepared two types of the materials. First type was based on the surface reaction of synthetic smectites, which were represented with laponite and fluorohectorite. The modification of smectite particles with fluorophore moieties was limited to the edges of the layers (the only sites on smectite surface having hydroxyl groups). Both the smectites were grafted with silanes bearing rhodamine or napthalimide groups. The hybrid products were characterized using UV-VIS and fluorescence spectroscopy in both the steady-state and time-resolved modes. Aggregation and fluorescence quenching were negligible. The absence of the adsorbed fluorophores at the surface of silicate particles were demonstrated by XRD. Optical heterogeneity of fluorohectorite-naphtalimide monolayer films was detected by confocal fluorescence microscopy and fluorescence lifetime imaging. The second type of materials was prepared by the reaction of silane bearing rhodamine moiety and kaolinite particles, pre-expanded with dimethylsulfoxide (DMSO). Since kaolinite is mineral with hydroxyl groups on the basals, a relatively large fraction of its surface could have been modified with the reactive dye. Successful modification of kaolinite interlayer spaces was proved by XRD measurement. Covalently bound dye groups were also resistant to a mild thermal treatment, which otherwise was able to expel co-adsorbed DMSO molecules. The hybrid material exhibited a relatively high fluorescence, comparable to the quantum yields having been reported for aqueous solutions of the dye precursor.

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Keywords: hybrid materials, dyes, fluorescence, silanes, grafting

Processing, microstructure and mechanical properties of PA1010/kaolinite nanocomposites

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A series of PA1010/kaolinite nanocomposites have been prepared by melt compounding with two kinds of intercalators, potassium acetate or urea. The blending components and conditions were explored to achieve optimal intercalating efficiency for the intercalators. After intercalation, the effects of intercalator's contents on mechanical properties, crystalline behavior and morphology of the PA1010/kaolinite/potassium acetate and PA1010/kaolinite/urea nanocomposites were studied systematically. The results showed that the tensile and impact strengths of the PA1010/kaolinite/potassium acetate and PA1010/kaolinite/urea nanocomposites significantly increase. Kaolinite acts as nucleating agent of PA1010, evidenced by the drop of crystalline temperature using DSC measurements. Both intercalated and exfoliated kaolinite disperses in PA1010 were analyzed by XDR, FTIR, SEM and TEM and simulated by theoretical models.

Keywords: polymer nanocomposites, PA1010, Kaolinite, intercalation

Two functions to aid in chemical identification of mineral/inorganic substances: First tests on the mineralogical system

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Whether their particles are in the nano-, micro-, or mega- range, crystalline inorganic compounds have specific stoichiometries that reflect crystal-structure constraints on the proportions of the elements present. Natural minerals are crystalline inorganic compounds (save a few exceptions) that have withstood the test of time.

However, a chemical analysis is often not sufficient to properly identify each such compound, particularly if no accompanying diffraction data or other physical properties are available. Basically, an analysis provides two pieces of information, (i) which elements are present (qualitative elemental composition) and (ii) the stoichiometry. Two functions were tested to represent these two aspects: First, logarithm of the sum of 2.0 exponentiated to the atomic number of the elements present

$$\log \Sigma_i (2.0^{at.no.[i]})$$

which is a function of the qualitative chemical composition. The second function is C.E. Shannon's (1948) information entropy

$$H = -\Sigma(p_i \ln p_i)$$

which reflects the stoichiometry of the compound (p_i are atomic fractions of the elements present, scaled so that $(p_i) = 1.0$).

The values of these functions were calculated for 4764 mineral end-member formulas (extracted from M.Ciriotti, 2012), as were other indicators for use in various statistics and plots. Conversely, program *PETROV* accepts an individual chemical composition (such as obtained on a microprobe) as input and searches among the 4764 minerals for those elemental compositions and stoichiometries that fall within the ranges specified by the user. The 'hits' represent identical, analogous, or related compounds to the one a researcher is dealing with. Provisions for treating incomplete chemical analyses are incorporated in the approach.

Keywords: mineral, chemical composition, information entropy

IR study of the octylammonium cations intercalation into montmorillonite

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Organically modified clay minerals are an attractive group of hybrid materials with wide potential in environmental protection and industry, e.g. as sorbents of organic pollutants from waste waters or as fillers in clay-polymer nanocomposites. While the intercalation of long chain alkylammonium cations into smectites is extensively studied, detailed investigation of octylammonium cations is reported seldom. The objective of the present work was to examine the effect of size and loading amount of dioctylammonium (2C8) and tetraoctylammonium (4C8) cations, isomers of frequently used surfactants with 1C16 and 2C16 hydrocarbon chains, on their arrangement within montmorillonite interlayers.

Less than 2 μm fraction of bentonite from Jelšový Potok (Slovakia) and dioctylammonium and tetraoctylammonium bromides were used for organo-montmorillonites preparation. The concentration of organic salts varied from 0.2 to 2.0 mmol.g^{-1} or between 20 % and 200 % of the cation exchange capacity of montmorillonite. The carbon analysis revealed gradual grow of the surfactant content with increasing amount used suggesting that in addition to organic cations the molecules of the 2C8 and 4C8 salts were co-adsorbed to montmorillonite interlayers and/or outer surfaces. The thickness of the organic phase depended on the cation size and its loading. The d_{001} value of 2C8-montmorillonite showed consecutive creation of monolayers, bilayers and paraffin arrangement at cation adsorbed amount 0.2-0.4 mmol.g^{-1}, 0.6-1.1 mmol.g^{-1}, and 1.4-1.7 mmol.g^{-1}, respectively. For 4C8-montmorillonite the paraffin configuration was detected at 1.0 mmol.g^{-1} intercalation. The infrared (IR) spectroscopy in the middle (MIR, 4000-400 cm^{-1}) and near (NIR, 8000-4000 cm^{-1}) regions was used for organo-montmorillonites characterization. With increasing content of the intercalated surfactants the intensity of CH stretching (νCH, 3000-2800 cm^{-1}) and the first overtones (2νCH, 5900-5500 cm^{-1}) bands increased. The νCH and 2νCH bands were also used to probe the ordering of the intercalated cations because their positions sensitively reflected the conformational changes of the hydrocarbon chains. With increasing amount of the 2C8 and 4C8 cations both bands were shifted to lower wavenumbers. While for 2C8 cation distinct change of the position appeared at 0.6 mmol.g^{-1}cation intercalation, continual changes were observed for 4C8 cation. Downward shift indicated increasing number of highly ordered (*all-trans*) conformers of alkyl chains. The NIR spectra of 2C8-montmorillonite revealed also pronounced modification of the first combination region of NH_2 groups. Samples with low cation content showed $(\nu+\delta)NH_2$ band at 4819 cm^{-1} due to free NH_2 groups. With rising 2C8 amount a new component corresponding to hydrogen-bonded NH_2 groups was observed near 4770 cm^{-1}. Its intensity gradually increased with cation loading while the intensity of the 4819 cm^{-1} band was reduced. A doublet with comparable intensities of both components was detected at 0.6 mmol.g^{-1} loading, i.e., for sample with bilayered arrangement of the alkyl chains. NIR spectrum of the montmorillonite containing the highest amount of 2C8 confirmed predominantly H-bonded NH_2 groups. These findings are of high importance for the preparation of organo-montmorillonite hybrids with less common surfactants not investigated in detail for clay-polymer nanocomposites utilization so far.

Keywords: organo-montmorillonite, surfactant loading, cations arrangement, near-IR spectroscopy

Structure, conductivity and optical properties of polyaniline thin films

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Polyaniline (PANI) thin films have been prepared according standard protocol using ammonium peroxodisulfate as the oxidizing agent and two different precursors: aniline sulphate and aniline hydrochloride. Polymerization was performed in aqueous suspension at room temperature under the constant stirring for 1 hour. PANI thin films have been deposited on glass substrate by chemical bath deposition method. (For more details see [1]). Thickness of PANI films has been controlled by the deposition time. Structure, conductivity and optical properties have been investigated in dependence on deposition time in order to monitor the development of structure and properties in early stages of crystallization and to optimize the technology with respect to maximum conductivity, maximum transmittance and maximum optical homogeneity. Structure and properties have been studied by the combination of following methods: atomic force microscopy, Raman and UV-VIS spectroscopy and transmittance mapping using spectrometer equipped with light collecting multimode optical fibers. Conductivity of the samples has been measured by static applied voltage in DC regime using linear copper electrodes (copper wire with a triangular cross-section). This special apparatus has been designed in order to eliminate the effect of structural inhomogeneity on the conductivity of PANI films. Results showed that PANI films prepared using aniline sulphate exhibit much higher conductivity and higher optical transparency than those prepared from aniline hydrochloride. These two different precursors exhibit different kinetics of polymerization reaction and consequently also different nanostructure. Unfortunately the increase of conductivity with the deposition time is accompanied by a decrease in optical homogeneity. The maximum conductivity for PANI films from aniline sulphate 1,8 S/cm for the deposition time ~ 20 min corresponds to the maximum optical inhomogeneity. Reasonable compromise has been found for the deposition time ~ 30 min with optimum optical homogeneity and still reasonable electrical conductivity ~ 1.5 S/cm.

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Keywords: Polyaniline, Thin film, Homogeneity, Transmittance, Conductivity

Antibacterial properties of chlorhexidine/urea/kaolinite nanocomposites

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The clay minerals in the kaolin group consist of dioctahedral 1:1 layer structures built from one tetrahedral silica sheet and one octahedral Gibbsite-like sheet (aluminium hydroxide sheet), which are linked by oxygen atoms. Kaolinite can be modified from its natural state by physical or chemical treatments to enhance the properties of the material. Compounds with bulky substituents are not intercalated, but many of them can be intercalated by displacement reactions since strong polar molecules can expand the basal spacing, which eventually leads to the rupture of the interlayer hydrogen bonds. For this purpose are used compounds like hydrazine, urea, formamide and dimethyl sulphoxide.

Clay minerals can be used to prepare new materials with ability to inhibit bacteria by loading them either with inorganic species with antibacterial properties such as Ag^{+}, Cu^{2+}, Zn^{2+} or with organic antibacterial agents. Antibacterial nanocomposites based on kaolinite aren't much explored.

This work deals with preparation of antibacterial kaolinite/urea/chlorhexidine nanocomposites. Two different techniques to expand basal space of kaolinite by urea were used. Firstly, mixture of kaolinite and solid urea was ground (mechanochemically intercalated) in planetary micro mill. Secondly, intercalation was made by mixing of kaolinite with aqueous urea solution. These two expanded kaolinites were treated with chlorhexidine diacetate, which is a bisbiguanide antiseptic and disinfectant with bactericidal or bacteriostatic behavior against a wide range of Gram-positive and Gram-negative bacteria. The structure of resultant organoclays were characterized by X-ray powder diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). The antibacterial activity of prepared organoclays against *S. aureus*, *E. faecalis*, *E. coli* and *P. aeruginosa* were evaluated by finding minimum inhibitory concentration. Both organoclays had considerable antibacterial effect at the lowest concentrations against *S. aureus*, *E. faecalis*, and *E. coli* after 1 day. Moreover, sample prepared under first way showed slightly better antibacterial activity after 180 minutes against *S. aureus*.

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Keywords: chlorhexidine, kaolinite, urea, antibacterial

Preparation of magnetic bentonite

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Magnetic materials are the research subject of many scientific teams in the world for many purposes (drug delivery, sorbents etc.) [1-4]. Magnetic materials based on magnetite (Fe_3O_4) or maghemite (γ-Fe_2O_3) are the most common.

This work deals with possibilities of preparation composite materials based on magnetite-bentonite which could be further used for example as sorption materials. Great advantage of these materials is possibility of separation by external magnetic field, instead of slow filtration.

Materials were prepared by co-precipitation of Fe(II) and Fe(III) from suspension containing also bentonite. Fe(III):Fe(II) ratio was 1:1 and 2:1. Fe:bentonite ratio was chosen 10% (w/w), 50% (w/w), 100% (w/w) and 200% (w/w) of iron on bentonite. Water solution of ammonia (concentration 2 mol/l) was used as a precipitation agent. Materials were washed 3 times by demineralized water and dried at 60 °C for 4 hours after precipitation. Samples were marked according to following template: MBxxx Y:Z, where xxx is Fe:bentonite ratio (10, 50, 100, 200 % of iron) and Y:Z is Fe(III):Fe(II) ratio.

Simple device for magnetic force measurement was made. Device measure decrease of weight of counterweight while sample (approx. 0.1 g) is exposed to constant external magnetic field. Values are then converted to attractive force - mN/g of material.

It was found out that material MB10 1:1 exhibits only very small magnetic effects (attractive force 1,01 mN/g). Another materials exhibit higher attractive forces with rule, that materials MBxxx 1:1 exhibit higher attractive forces than materials MBxxx 2:1. The highest force was measured at material MB200 1:1 (720 mN/g).

It is interesting that materials prepared with stoichiometric ratio for magnetite formation (2:1, Fe(III):Fe(II)) exhibit much lower attractive forces. This could be caused by preferential fast adsorption of Fe(II) on bentonite. This adsorbed ions then lack by precipitation and nonmagnetic Fe(III) oxides generate preferably. In the case of ratio 1:1 also take place adsorption of Fe(II), but it causes conversely approach to ideal ratio for magnetite formation.

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Keywords: Bentonite, Magnetite, Magnetic materials, Composite materials

Investigations of chiral structure in new smectogenic salicylaldimine liquid crystals

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Liquid crystals, having rod-like, disc-like and bent-core molecules, exhibit various types of physically anisotropic mesophases. These mesophases are characterized by different structure and space symmetry and display various types of physical properties.

The smectic C* mesophase has the chiral structure, is optically active system and displays optical birefringence. Chiral structure of the smectic C* mesophase is formed by the rod-like molecules, which have sizes as ~ 20 – 40 Å. Space structure of this liquid crystalline mesophase is characterized by the pitch of the smectic spiral. The pitch is fundamental parameter of chiral structure, is sufficiently sensitive to temperature and pressure, and determines the value of optical activity of this structure.

In this work we study, describe and try to interpret the textures and their temperature transformations in new salicylaldimine liquid crystals, synthesized by our group. Temperature dependences of the pitch of helical structure of the smectic C* mesophase have been also investigated for these materials. Investigations have been carried out in large temperature interval and especially in the region of the direct smectic C* – isotropic liquid and the reverse isotropic liquid – smectic C* phase transitions. The thermal hysteresis in the peach behavior is found for the salicylaldimines. Connection between value of the pitch and length of the alkyl chain of salicylaldinmine molecule was found.

Keywords: Liquid crystals, Smectic C mesophase, Chiral structure, Pitch of smectic spiral*

Thermal behaviour of organically modified clays

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The clay minerals were modified by two alkylammonium cations under sorption procedure. The X-ray powder diffraction and FT-IR spectroscopy were used to evaluate the intercalation process of organic cations into the clay structure. The organo-montmorillonites exhibited IR spectra giving evidence about sorption or intercalation of the alkylammonium cations. The enhancement of the basal spacing obtained by X-ray diffraction confirmed the intercalation process of cations into montmorillonite and vermiculite samples. Thermal behaviour of the modified clay minerals was investigated by simultaneous thermogravimetry and differential thermal analysis. The organically modified montmorillonites exhibited the higher values of temperatures related to the total melting. Also the temperatures of exotherm effects connected to recrystallization and transformation increased with the concentration of alkylammonium salts. The temperatures of dehydratation and dehydroxilation decreased with concentration of alkylammonium cations. Vermiculite samples showed generally reducing of their thermal stability.

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Keywords: clay minerals, alkylammonium cations, intercalation, thermal analysis

Molecular modeling of ZnS-CTA$^+$-MMT nanoparticles

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Zinc sulfide is a very good photocatalyst and semiconductor with wide direct band-gap energy of about 3.7 eV. ZnS nanoparticles were prepared by precipitation in aqueous dispersions of cationic surfactant cetyltrimethylammonium bromide (CTAB). The sphere radii of ZnS nanoparticles decreased from 4.5 nm to 2.2 nm in dependence on CTAB concentrations from 0.4 to 1.5 mmol L^{-1}. Above the concentration of 1.5 mmol L^{-1}, the radii were stabilized at R = 2.0 nm and increased up to R = 2.5 nm after 24 h.

ZnS particles with radii 2.0 and 2.5 nm were used for calculations and were surrounded with various amounts of CTA^+ cations. In most cases minimization pushed CTAs further from ZnS surface but all stayed in perpendicular positions with respect to ZnS surface. This arrangement is strongly preferred with respect to other positions of CTA^+. Simulations show that at the higher CTAB concentrations, ZnS nanoparticles were surrounded by CTA^+ bilayers forming positively charged micelles with the diameter of 10 nm.

Wurtzite and sphalerite nanoparticles with R = 2.0 nm and 2.5 nm covered by a monolayer or a bilayer arrangement of CTA^+ were both modeled with and without water surrounding. Calculated sublimation energies confirmed that the bilayer arrangement of CTA^+ on the ZnS nanoparticles was preferred before the monolayer one[1].

Positively charged micelles of ZnS with CTA^+ bilayers and ZnS nanoparticles were placed into the interlayer space of montmorillonite and mutual interactions were compared. Molecular simulations confirm slightly stronger interactions among montmorillonite layer and ZnS with CTA^+ bilayers. Intercalation of modified ZnS nanoparticles was not confirmed experimentally. Sorption of them on the MMT surface is probably preferred. Molecular simulations were applied in Material Studio modeling environment.

Reference:

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Keywords: simulations, zinc sulfide, cetyltrimethyammonium bromide, montmorillonite

Infrared investigation of organo-montmorillonites prepared from *n*-alkylammonium surfactants

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The intercalation of organic guest species into clay minerals, especially montmorillonites, is the excellent way of fabricating organic-inorganic hybrid materials. Montmorillonites provide attractive features due to their large surface area, ion exchange and adsorption properties, and swelling behaviour. A significant reason for their modification by organocations is oriented to their application as fillers in polymers. The objective of this study was to investigate the effect of the alkyl chain length on the arrangement of intercalated surfactants.

Theorgano-montmorilloniteswere prepared from a sodium-saturated < 2 μm fraction of bentonite Jelšový Potok (Slovakia) and alkylammonium cations with increasing length of alkyl chain from trimethylhexylammonium (C6) to trimethyloctadecylammonium (C18).The content of intercalated cation, reported in % of the cation exchange capacity (CEC) of Na-montmorillonite, increased from about 90 % CEC for C6-C10 to 102 % CEC for C18.The XRD pattern showed almost the same basal spacing (~1.4 nm) for montmorillonite saturated with relatively small cations (C6, C8 and C10)suggesting a monolayer arrangement. With further increase of the alkyl chain length the d_{001} values graduallyincreased from 1.7 nm (C12) through 1.8 nm (C14), 1.9 nm (C16) to 2.1 nm (C18) indicating consecutive transition from monolayers to bilayers and paraffin arrangement of surfactants.The conformation of alkyl chains was examined by IR spectroscopy in the middle (MIR) and near (NIR) regions. While it is well established that the positions of fundamentalCH_2 stretching bands are very sensitive to the ordering of carbon chains, the changes of the vibrational modes of methylene groups appearing in the NIR region were not studied in this regard.The MIR spectrum of C6 showed the asymmetric ($\nu_{as}CH_2$) and symmetric ($\nu_s CH_2$) stretching bandsat 2930 cm^{-1} and 2861 cm^{-1}, respectively.With the increase of the alkyl chain length the bands were shifted to lower wavenumbers, i.e. to 2925 and 2851 cm^{-1} for C18,indicating that the number of disordered (*gauche*) conformers decreased in favour of more ordered (*all-trans*) conformers. The NIR spectra of organo-montmorillonites showed the first overtone (2ν) and combination($\nu+\delta$)bands of CH_3, $CH_2$and OH groups. A broad complex band in the7073-7075 cm^{-1}regioncontained overlappingcontributions of 2νOH of structural OH groups and H_2O molecules. The intense peak assigned to ($\nu+\delta$)H_2O is gradually shifted from 5254 cm^{-1} (C6) to 5262 cm^{-1}(C18) due to decreasing strength of hydrogen bonds between water molecules, number of which decreased with the length of the alkyl chain. The complex band observed in the 6100-5600 cm^{-1} region was related to 2νCH vibrations of CH_3 and CH_2 groups. The integrated intensity of this band, reflecting the amount of organic phase in the sample, gradually increased with the size of surfactant. The position of the most intensive component in this region related to $2\nu_{as}CH_2$ was shifted with the increasing length of the alkyl chain from 5812 cm^{-1} for C6 to 5783 $cm^{-1}$for C18suggesting that the alkyl chains adopted more ordered structure. The magnitude of the $2\nu_{as}CH_2$ shift was clearly higher than observed in the MIR region for CH_2 stretching modes which benefit the utilization of the NIR spectroscopy for probing the conformation of alkyl chains.

Keywords: montmorillonite, n-alkylammonium surfactants, cations arrangement, XRD analysis, IR spectroscopy

Clay modified with magnetic nanoparticles as a filler for polymer composites

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Recently, magnetic particles have gained a great potential in medical applications. Currently they may be used in several domains of medicine like therapy, e.g., in magnetic hyperthermia or drug targeting, diagnosis as a MRI contrasts and also for cells separation. Moreover such materials are considered for future applications in regeneration medicine and tissue engineering, particularly as components of nanocomposites based on biodegradable and bioresorbable polymer matrixes.

One of the most serious issues related to magnetic nanoparticles is their agglomeration while using as a filler in polymeric matrices. To avoid agglomeration several techniques are available. In polymer nanocomposites good dispersion of fillers is especially required to assure relevant mechanical and biological parameters of manufactured materials.

Bentonies comprising as a major component montmorillonite, are widely use as nanofillers in polymer composites. These nanocomposites exhibit better mechanical properties and also lower gas permeability in comparison to pure polymer materials. Serious disadvantage of bentonies used in polymer nanocomposites is incompatibility of hydrophilic clay to hydrophobic polymers matrixes. Therefore, an initial modification of clay is indispensable for assuring good dispersion in a polymer matrix.

The objects of this study were polymer nanocomposites made of biodegradable polymer, i.e., polycaprolactone, containing 0,5 and 2 wt% amount of montomorillonite clay modified with magnetic particles. Such a modification alters hydrophilic character of montmorillonite and enables a better dispersion of magnetic nanoparticles. In our experiments nanopowder composition MMT/magnetic particles was prepared. Magnetic particles were obtained by co-precipitation process made in well dispersed montmorillonite suspension. Subsequently, nanopowder was filtered and dried in vacuum for 24 hours. Polymer nanocomposites were prepared by the polymer casting method.

The manufactured nanopowder was characterized by X-Ray Diffraction Spectroscopy (XRD). The magnetic properties, both nanopowder and polymer nanocomposites, were determined with the use of Vibrating Sample Magnetometer (VSM). Contact angle, surface energy and mechanical properties of the obtained samples were also evaluated. Additionally, microscopic observations were performed.

Keywords: polymer nanocomposites, magnetic particles, montmorillonite

Utilization of Diffuse reflectance spectroscopy in the characterization of photocatalysts

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Diffuse reflectance spectroscopy (DSR) is a powerful technique to distinguish the presence of various types of metal-species present in solid catalysts and to determine the absorption edge of photocatalysts.

UV–Vis diffuse reflectance spectra of samples were recorded using GBS CINTRA 303 spectrometer equipped with a diffuse reflectance attachment with a spectralon-coated integrating sphere against spectralon reference. The reflectances were recalculated to the absorption using the Schuster–Kubelka–Munk equation, $F(R\infty) = (1-R\infty)2/2R\infty$, where $R\infty$ is the diffuse reflectance from a semi-infinite layer. Absorption edge was estimated by extrapolating the decreasing portion of the spectrum to the abscissa at zero absorption.

In general, photoinduced electrons (e^-) and positive holes (h^+) are produced from TiO_2 under the irradiation of UV light ($\lambda < 380$ nm) because this has an energy larger than the band gap (3.2 eV) of TiO_2. The photon flux necessary to initiate these processes can be supplied by sunlight or lamps.

For example, in the case of Ag-TiO_2 catalysts, the radiation with the shorter wavelength of 254 nm was significantly more effective for CO_2photoreduction than the 365 nm radiation, which was expected to be better from the Ag/TiO_2 band gap (2.74 eV) [1]. The yield of methane and methanol increase when modifying the TiO_2 with silver is mainly caused by more effective electron hole pair generation due to shift of absorption edge towards visible light in case of random dissipation of Ag atoms into TiO_2 crystals [2].

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Keywords: Diffuse reflectance spectroscopy, TiO_2, adsorption edge

Pressurized and supercritical fluids as a tool for preparation of nanostructured materials

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Up to the present numerous chemical and chemico-physical approaches for preparation of nanostructured materials have been developed. Considering only the chemical ways, it can be stated that in the final step of most preparations the calcination (thermal treatment) commonly above 350 °C is used in order to remove used organics and/or precursors and to obtain nanocrystalline form of materials. Although this step leads to the required crystallization of material, on the other hand it is accompanied by the sintering of nanoparticles, especially at increased calcination temperature. Such a thermal treatment finally results in materials with markedly lowered specific surface area, total pore volume and porosity which may in final cause the decrease of catalytic performance of developed materials.

Concerning more advanced processing in the final step of preparation such as the supercritical carbon dioxide drying, it solves the problem from the view of preserving the porous structure, however, does not lead to crystallization of material. In this case the required crystallization is also commonly reached by subsequent thermal treatment.

Within this contribution the advanced processing opening up the possibility to prepare crystalline metal oxides with markedly improved properties of porous structure will be presented. Various modifications of this processing, based on the utilization of combination of pressurized and supercritical fluids, will be introduced. The impact of individual processing parameters in the relationship to textural and structural properties will be discussed.

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Keywords: pressurized solvent, supercritical carbon dioxide drying, nanostructure, metal oxide

Nanoparticles and their application in enzymatic chiral transformations for drug development

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During last decade, new drug candidates being introduced into pharmaceutical industry are chiral. Only one enantiomer-(R)/(S) exhibit the desired biological activity and the other enantiomer may exhibit undesired side effect, thereby making chiral purity an important parameter. Biocatalytic processes are useful methods for the production of such chiral intermediates. Nanotechnology is technology that deals with nano-meter sized objects as revolutionize the chemical, biotechnology industries and biomedical fields. One of the most important aspects of this field is the preparation and development of nanomaterials, such as nanoparticles. Nanostructured materials with various shape, composition and structure, and modified surface have generated interest as biocatalyst supports. Major aim of the work was development of the system for immobilization of alcohol dehydrogenases (ADHs) and cofactor (NAD(P)H) on nano-sized particles for production of enantiopure alcohols with high yield. Studies were performed using NADH-dependent ketoreductases and alcohol dehydrogenase from horse liver, and NADPH-dependent alcohol dehydrogenase from *Thermoanaerobiumbrockii*. Substrate dependent regeneration of the cofactors was done by 2-propanol which is oxidized by the ADH while the cofactor is reduced. Here, 1-(*p*-methoxyphenyl)-propan-2-one and 7-hydroxy-2-tetralone were used as substrates. Immobilization of ADHs on amino, epoxy, thiol and carboxyl groups modified (i) silica, (ii) gold and (iii) silver nanoparticles, through (i) physical and (ii) covalent adsorptions, were studied. Finally, activity, stability and structure of immobilized ADHs were analyzed using ECD, fluorescent and FTIR techniques. Experiments implied for (i) high affinity of the nanoparticles to enzymes and cofactors, (ii) extensively loss of initial enzyme activity (to 40-50%) and (iii) partial/fully loss of secondary and tertiary structures. Immobilization process influenced significantly the reaction rate, purity and stereoselectivity of immobilized enzymes in aqueous environment. (i) Silver and gold nanoparticle-enzyme preparations synthesized alcohols without loss in productivity and optical purity. (ii) Silica supported-enzyme showed high affinity to the substrate, and stereoselectivity of immobilized enzyme was switched.

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Keywords: nanoparticle, alcohol dehydrogenase, immobilization, enantioselectivity, chiral switch

Aquatic toxicity tests of nanomaterials

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The toxicity of nanoparticles for aquatic organisms is strongly affected by nature of particles (chemical composition, mean size and size distribution, shape, surface charge and chemistry, crystal structure) and by character of aquatic environment (pH, ionic strength, density, presence of surfactants and dissolved organic matter). Agglomeration (or aggregation) of nanoparticles fundamentally changes their features and consequently the way, how these particles interact with organisms. Behavior of nanoparticles in liquid media has to be taken into consideration, when we try to interpret results of particular eco-toxicity tests. The influence of parameters, which accelerates/decelerates the agglomeration of nanoparticles in aquatic environment, is desirable to reduce by appropriate modification of testing procedure.

Our approach is based on application of classical eco-toxicity tests prescribed by OECD guidelines (for example OECD guideline 212 - Fish, Short-term Toxicity Test on Embryo and Sac-fry Stages)originally designed for testing of soluble chemicals. In case of nanomaterials, parameters of a liquid media (composition, ionic strength - conductivity, viscosity - density) are optimized with respect to the agglomeration rate and maximal size of agglomerates is controlled by frequency of liquid media changing. The described modification of the test procedure allows us to obtain monotonicdose-response curves, which are not affected by different agglomeration rate in colloids with different concentration of tested nanoparticles. Limitation of such approach lies in its high labor intensity. The automation of some critical steps of the suggested procedure could be a solution of the problem.

Acknowledgment:
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Keywords: Aquatic toxicity, fish embryo, nanoparticles, agglomerates, physicochemical characterization

XPS Depth Profiling of Nano-Layered Polymeric Materials with a Combined Monatomic and Gas Cluster Ion Source

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A detailed understanding of surface and interface chemistry is critical to the successful production and operation of multilayer devices and materials with advanced coatings. It has been proven over the years that X-ray photoelectron spectroscopy, with its high surface sensitivity and chemical state specificity, is an ideal tool for the evaluation of surface and thin film composition. XPS depth profiling gives the analyst a method for measuring chemical variations from the surface of a sample through to the bulk, and facilitates characterisation of complex chemistries that may occur at interfaces.

Recent advances in ion source design have seen the introduction of noble gas cluster ion beams for depth profiling applications, which allow materials that are unstable under monatomic ion bombardment to be analysed. This presentation will focus on depth profiling data sets that have been acquired with such a source. A range of applications will be covered from the preparation of clean non-reduced oxide surfaces to composition profiling of organic thin film devices.

Nanosuspension Characterisation: Application of NTA to Bionanomaterials

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Here we demonstrate the novel developments of the Nanoparticle Tracking Analysis (NTA) technique that sizes nanoparticles in suspension, based on their Brownian motion. Unlike classical light scattering techniques, NTA allows nanoparticles to be sized on a particle-by-particle basis. This results in a higher resolution particle size distribution and therefore a better understanding of aggregation than ensemble methods (such as dynamic light scattering, DLS) and it also yields directly a count/concentration measurement.

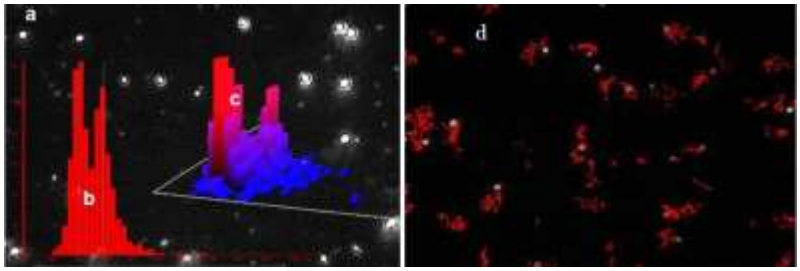


Fig. 1 above shows a mixture of 200nm and 300nm particles; a) still image, overlaid with b) particle size distribution, c) Number v. relative intensity v. diameter plot and d) An image showing only some (for clarity) Brownian motion trajectories analysed.

The light scattering properties of nanomaterial can also be used to distinguish between sub-populations within the same sample using the refractive index of nanomaterial. When used in fluorescence mode particles can be further differentiated and characterised within complex biological suspensions.

Further information on the material can be obtained through the NTA zeta mode. Applying an electric field across the scattering volume allows nanoparticle electrophoresis to be determined providing information on electrostatic repulsion and therefore colloidal stability of the sample.

This technique has been extensively applied to the measurement of a wide range of nanomaterials such as exosomes, viruses and VLPs, liposomes, protein aggregates, bacteria as well as a range of engineered nanoparticles for their use as drug delivery nanoparticles. Examples of the characterisation of several of this will be discussed highlighting the crucial parameters in each case (be it size distribution, concentration, fluorescence or some other parameter) along with research showing the necessary steps that have been taken to optimize such measurements.

Keywords: characterisation, nanoparticles, NTA, analysis

APPENDIX

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