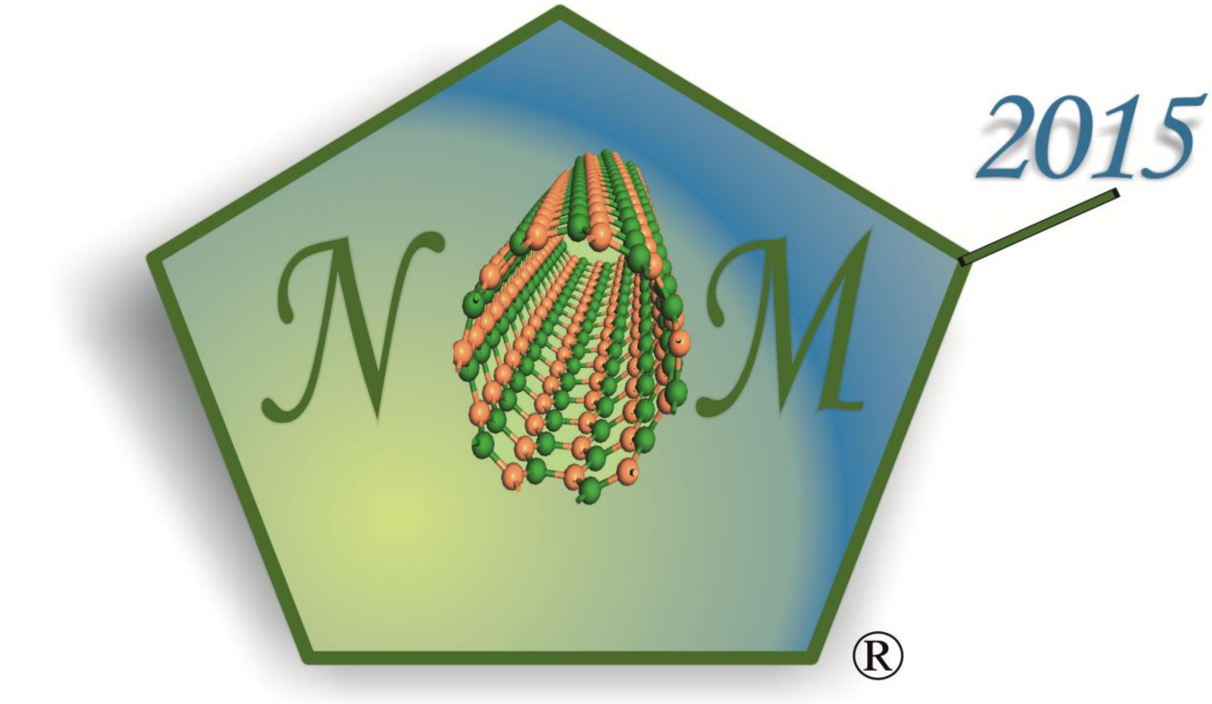
VŠB – Technical University of Ostrava

NanoOstrava 2015



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VŠB-TU Ostrava
May 18-21, 2015
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Dear Conference participants, Visitors and Colleagues,

We welcome you to the NanoOstrava 2015 - 4th 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 project IT4Innovations.

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 is organized in several sessions with plenary lectures focusing on important areas of Nanomaterials and Nanotechnologies.

1. Advanced materials, technology and characterization
2. Nanomaterials for medicine
3. Nanostructured materials in electronics and optics
4. Nanocarbons
5. Nanocomposites and nanofillers

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

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Welcome from NanoOstrava 2015 Organizing Committee Chair

On behalf of NanoOstrava 2015 Organizing Committee, it is my honour and pleasure to welcome you to the NanoOstrava 2015, 4th Nanomaterials and Nanotechnology Meeting organized at VŠB – Technical University of Ostrava campus. The conference is aimed to 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 part of Central Europe. Our University 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 100 papers from more than 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, NanoOstrava2015

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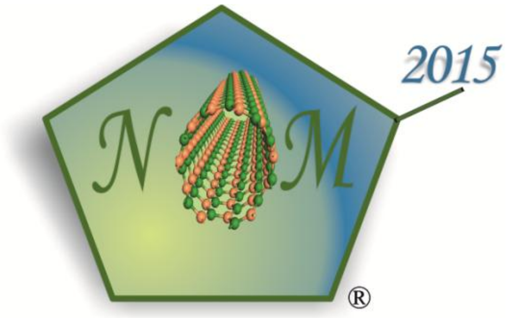
TOPIC 1

Advanced materials, technology and characterization

Chair: Pavla Čapková
Co-chair: Jonáš Tokarský

New trends in preparation of nanomaterials
Nanotechnology for energy generation and storage
Simulation and modeling for nanomaterials
Chemistry and physics of nanomaterials



Phyllosilicates – suitable scaffold for functional nanostructures

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Using a suitable scaffold for the design of functional nanostructures provides a double benefit: scaffold serves as the support for anchoring guest molecules and may also positively affect the properties of the guest substance. Phyllosilicates represent such a suitable scaffold thanks to their unique crystallochemical properties – layered structure, charged silicate layers (due to the isomorphic replacement of octahedral and tetrahedral cations).

Functional nanostructures can be formed by surface modification or by intercalation of layered phyllosilicate structure. There is also a wide variety of guest substances in various forms – nanoparticles [1], organic molecules, macromolecules - polymers, dendrimers etc. Currently, the wide use of nanostructures based on phyllosilicates includes sorbents [2], catalysts [3], photo-catalysts [4,5], antibacterial media [6,7], new pharmaceutical forms, biomedical use as a contrast agent for MRI (Magnetic resonance imaging) diagnostics of the gastrointestinal tract [8], photo- and electro-functional units [9,10], etc. Intercalation of phyllosilicates can be based either on ion exchange or ion-dipol interaction of neutral polar guest molecules [11], where the original interlayer cations remain in the interlayer space. A large part of potential applications of modified phyllosilicates does not require intercalation, but only surface modification. This concerns especially the photocatalytic and antibacterial materials and various optical functions.

The aim of this conference review is to provide brief summary of modified phyllosilicates with emphasis on cases where the silicate layers positively affect the properties of guest substances and brought a double benefit for practical use. This is the case of luminophores based on organic dye/montmorillonite nanocomposites [12] and conducting polymer/montmorillonite nanocomposites [13].

Acknowledgement

Results concerning the modified phyllosilicates for wide range of practical use have been supported by a series of grants from Czech Science Foundation, grants No: 205/99/0185; 205/05/ 2548; 205/08/0869; P108-11-1057.

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Keywords: phyllosilicates, nanocomposites, intercalates

Phase transitions in metastable compounds facilitated by microstructure defects

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Microstructures defects facilitate phase transformations in many materials. Frequently, the presence of microstructure defects influences also the stability of metastable phases. Some examples of such materials, which will be discussed in this contribution, are metastable oversaturated cubic solid solution of $Ti_{1-x}Al_xN$ and boron nitride.

The metastable face centred cubic (fcc) $Ti_{1-x}Al_xN$ is typically employed for production of hard refractory coatings, which are prepared in nanocrystalline form by using physical vapour deposition methods like magnetron sputtering or cathodic arc evaporation. At elevated temperatures (≥ 850°C), fcc-$Ti_{1-x}Al_xN$ decomposes into titanium-rich (Ti,Al)N and aluminium-rich (Al,Ti)N. This process is usually described as spinodal decomposition [1] that is followed by the transformation of the metastable (or high-pressure stable) fcc-AlN into the thermodynamically stable w-AlN with the wurtzitic crystal structure. However, the in situ high-temperature synchrotron diffraction experiments indicated that fcc-AlN and w-AlN form concurrently [2] during the thermodynamically driven and kinetically controlled segregation of TiN and AlN. Recently, we could show that this phase transition is facilitated by the presence of the stacking faults in fcc-(Al,Ti)N [3,4].

Boron nitride is known to exist in three modifications: h-BN, w-BN and c-BN. Graphitic boron nitride (h-BN) is frequently used as isolating material with low electrical conductivity, as crucible material with bad wett ability and with excellent temperature and thermo-shock stability, or as starting material for high-pressure and high-temperature synthesis of both super-hard cubic boron nitride with the sphalerite crystal structure (c-BN) and BN nanocomposites. Wurtzitic boron nitride is an intermediate phase, which emerges in some cases during the high-pressure and high-temperature synthesis of c-BN from h-BN. It was shown that the formation of partially coherent interfaces between c-BN, w-BN and h-BN increases the hardness of the BN nanocomposites beyond the hardness of c-BN [5]. As an essential factor determining the presence or absence of w-BN along the transformation path from h-BN to c-BN, the kind of dominant microstructure defects in starting h-BN was identified [6, 7]. In this talk, the typical microstructure defects in h-BN will be presented and their impact on the product of the high-pressure and high-temperature synthesis of the BN nanocomposites discussed. Furthermore, it will be shown how the microstructure defects can be recognised and quantified by X-ray diffraction methods.

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Keywords: Metastable phases, Microstructure defects, Titanium aluminum nitride, Boron nitride

Ultrafine grained Aluminium with long term stability of microstructure and properties at elevated temperatures

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The continuous effort in increasing energy efficiency of transport vehicles, building structures or energy conversion devices results in growing role of lightweight construction, which creates great challenge also for material science community. Light metals based on aluminium and magnesium are still hot candidates for this purpose thanks to their unique combination of low density, high strength, stiffness, fracture toughness and excellent corrosion resistance. There are still many possibilities to improve their properties, most of them are based on alloying followed by proper thermal treatment or by making composites. However there is usually a trade-off between strength, plasticity and corrosion resistance, where improvement of one property leads to reduction of another one. Moreover the use of standard strengthening approaches based on precipitation hardening is limited by low structural stability at elevated temperatures, due to favourable diffusion conditions and inevitable microstructural changes.

Most of these drawbacks can be avoided using alternative strengthening approaches based on proper tailoring of microstructure of light metals without excessive use of alloying elements or strengthening additives. The effect of different technological methods providing variable microstructures of the identical material on its mechanical properties will be presented. It will be particularly demonstrated on compacts made of ultrafine aluminium powder. Their microstructure usually includes a small portion of aluminium oxides coming from the surfaces of initial powders. Depending on processing route, the amorphous ~3 nm thick native Al_2O_3 layer either disrupts into separate nano-metric dispersions or remains as continuous 3D skeleton within final compact and substantially contributes to structure stabilization at elevated temperatures. The distribution and morphology of oxides and grain size (Fig.1) exhibit a decisive influence almost on all mechanical properties. Remarkable improvement of the material performance in many applications especially at elevated temperature up to 400°C can be thus achieved. Successful application cases including engine pistons of racing cars with excellent structural stability, stiffness and creep resistance will be presented.

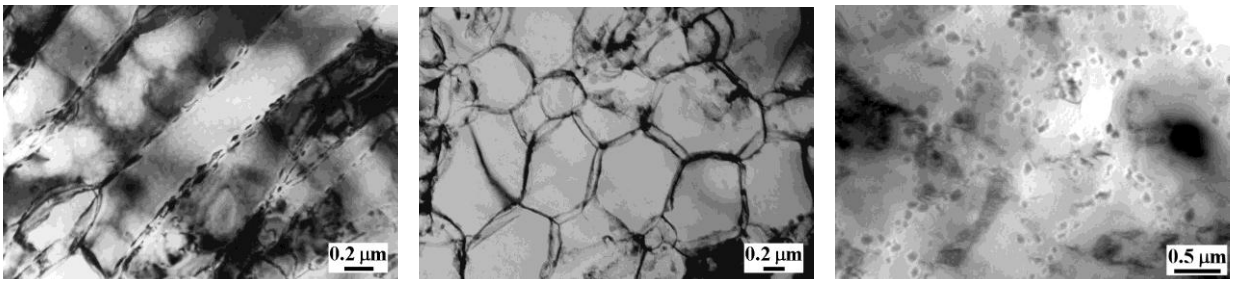

Fig. 1: Bright field TEM micrographs of ultrafine Al powders compacted using different technologies (from the left: ECAP, forging, hot isostatic pressing) revealing variable alumina morphologies.

Keywords: Ultrafine grained Aluminium, Creep, Nanoalumina, ECAP, HIP, Hot forging

3D nanostructured metallic materials prepared by rapid quenching

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Using planar flow casting from a single crucible with single, double or triple-nozzle technique a set of monolayer, bilayer and trilayer amorphous ribbons with different combinations of Fe, Co and Ni-based alloys has been prepared. Attention will be focused on structure and character of the interface between individual layers and its evolution with the transformation of the layers. Physical properties of the layered ribbon systems will be analyzed with respect to the effect of the layers interface and with the possibility of formation and application of such pseudobulk soft magnetic amorphous and nanocrystalline ribbons with enhanced thickness. Attempts to show the enhancement of properties by post processing treatment in electromagnetic fields and by shape-forming of ribbons will be presented.

Keywords: Rapid quenching, Glassy ribbon, Bilayer, Trilayer

Nanoporous molybdenum metallic films and their applications in catalysis

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It is well known that several materials, when are in nano- or well-ordered form, exhibit catalytic properties different from those of in bulk phase [1]. Gold nanoparticles [2], thin vanadium oxide layers [3] can be mentioned as examples which later gained industrial importance.

In this contribution we present the preparation of non-continuous MoO_2 films which were created by oxidation of nano-porous pure molybdenum films in a controlled atmosphere. The monoclinic phase MoO_2 particles with mean size lower than 10 nm exhibit 42% selectivity to propylene oxide.

Microstructure of PVD deposited metallic layers is described by Thornton diagram of film growth [4]. Detailed study of Thornton`s model for the deposition at low substrate temperature was published in 2003 by Petrov et al [5]. In this work there was shown the possibility to deposit non - continuous films with various aspect ratios of individual (consisting) metallic particles. By other words there is possibility to prepare non - continuous metallic film consisting of separated metallic needle-shape crystallites. The pores (voids) in such films extend through the entire thickness of the layer. This film morphology is very suitable for the subsequent oxidation needed for the creation of single phase MoO_2 films.

The dc magnetron sputtering was used for Mo deposition The discontinuity of Mo layers was achieved by the deposition at relatively high Ar pressure (approx. 0,1 Pa) and low substrate temperature (approx. -20 ^{0}C).By this procedure we obtain the nano-structured Mo non- continuous films.

The nano-morphology of all prepared films was controlled by in- plane and cross-sectional transmission electron microscopy.

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Keywords: nanoporous molybdenum films, catalysis

The Search for New Super- and Ultrahard Materials: Go Nano!

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Indentation hardness is the average pressure beneath the indenter under conditions of fully developed plasticity. Intrinsically super- ($H \geq 40$ GPa) and ultrahard ($H \geq 80$ GPa) materials attain high hardness due to their strong covalent bonds, three-dimensional bond network and electronic stability upon finite shear strain that occurs during plastic deformation, whereas extrinsically super- and ultrahard materials reach such hardness due to their nanostructure that impedes the plastic flow [1].

The recent search for intrinsically super- and ultrahard materials focused on those with high elastic moduli. However, elastic moduli describe only the reversible, elastic deformation upon small strain close to the equilibrium, whereas plastic deformation occurs in shear upon a large strain at atomic level, where the electronic structure may undergo instability. Therefore many solids with a high value of elastic moduli undergo, upon such shear, structural transformations to softer phases.

I shall discuss several examples of materials with high values of zero-pressure elastic moduli but relatively low hardness, such as C_3N_4, Re-, Os- and Ir- diborides [2], diamond and others in order to show that the most promising way towards the preparation of new super- and ultrahard materials is the design of nanocomposites consisting of a transition metal nitride and very thin interfacial silicon nitride. I shall focus on the recent progress in the understanding of the origin of ultrahardness in nc-TmN/a-Si_3N_4 nanocomposites (Tm = Ti, V, W, $(Ti_{1-x}Al_x)N$, $(Cr_{1-x}Al_x)N$ ...), in which 3-4 nm size TmN nanocrystals are “glued” together by about 1 monolayer (1 ML) thick SiN_x interface. A combined first-principles density functional theory (DFT) and quantum molecular dynamics (QMD) calculations of the stability and shear strength of the interface, Sachs averaging of the shear resistance of the interfaces of randomly oriented nanocrystals, pressure enhancement of the flow stress and the constraint factor calculated by non-linear Finite Element Modelling [3] show that these materials can reach hardness significantly larger than diamond [4], when correctly prepared and essentially free of impurities [5]. This finding will be supported by experimental results. The 1 ML thick SiN_x interface is strengthened by valence charge transfer, being stronger than bulk SiN_x crystal [6]. The results of recent investigations by means of first-principles DFT and QMD provide deep understanding of the experimental results obtained for a variety of nc-TmN/XY nanocomposites and heterostructures (XY=covalent compound forming the interfacial layer).

Finally, I shall briefly summarize the present industrial applications of the nanocomposite coatings on tools for machining, forming, injection moulding and the like, which have been pioneered by the Czech company SHM [7], and discuss the possibilities of further improvement of the presently available nanocomposites.

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Keywords: ultrahard materials, elastic moduli, nanocrystals

Multistep resonance energy transfer in complex systems based on organic dyes and layered silicate

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Förster resonance energy transfer (FRET) represents photophysical phenomenon playing a significant role in photosynthesis. It is the result of an electrostatic resonance coupling between different dye molecules of specific electronic properties. FRET does not require any direct chemical bonding between the molecules and is efficient to the distances of a few nanometers. It is likely that solar cells of future will be based on the components performing on a molecular scale and FRET would play a significant role in such devices.

This work was focused on a multistep FRET, mimicking thus a cascade character of the phenomenon occurring in photosynthesis systems in green plants. Laser dyes of xanthene and oxazine types with appropriate spectral properties to fit resonance conditions were selected. In preliminary experiments, hybrid materials based on colloidal systems of layered silicate saponite were investigated. The results helped to design the synthesis of thin solid films of dyes intercalated in saponite. The specimens were characterized with absorption spectroscopy and X-ray diffraction. FRET was described using steady-state and time-resolved fluorescence spectroscopy and fluorescence anisotropy.

Efficient multistep FRET between up to six different laser dyes was achieved in the most of the prepared specimens. The effects of the concentration of dye molecules intercalated in the films on RET efficiency and the role of the alkylammonium (AA) cations to suppress dye molecular aggregation were investigated. Emission from directly excited energy donor molecules was reduced in favor of the emission of energy acceptors. The presence of AA cations brought about to the reduction of dye molecular aggregation in the colloids, which was reflected in the increase of overall fluorescence. Linearly-polarized absorption spectroscopy helped to sensitively detect the formation of H-aggregates in the films. The enhanced presence of the aggregates was reflected in overall lower fluorescence yields. Results from fluorescence anisotropy measurements and time-resolved fluorescence spectroscopy confirmed occurrence of FRET and the efficiency of the phenomenon in respective samples.

The multicomponent materials based on layered silicate of saponite type and organic laser dyes are easy to be assembled and exhibit high yields for an excitation energy transfer and manipulation on a molecular level. Such materials have potential to be applied as components in future solar cells working on organic dyes photocomponents.

Acknowledgement
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Keywords: FRET, layered silicates, hybrid materials, fluorescent dyes

A mechanochemical approach for the synthesis of CaFe-layered double hydroxides

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In recent years, many methods have been developed and used in the synthesis of layered double hydroxides (LDHs). In the experimental work leading to this contribution, a relatively rarely used method, mechanochemistry that is, was investigated in the syntheses of Ca(II)Fe(III)-LDH samples. The syntheses were performed using a mixer mill.

The samples were prepared by using a two-step grinding procedure. The thus prepared samples were investigated by various structural characterization methods, such as X-ray diffractometry (XRD), thermogravimetry (TG/DTG), scanning electron microscopy (SEM) and energy dispersive X-ray analysis (EDX).

The goal was the optimization of the synthesis, therefore, various parameters were systematically changed in order to get phase-pure product. In the X-ray diffractograms of the grinded materials, the characteristic reflections of the LDHs were observed verifying that LDH structures were indeed formed under these circumstances. The samples, which proved to be phase-pure LDHs were investigated with further characterization methods. The TG measurements show the characteristic weight losses of the LDHs, SEM images and elemental maps obtained from SEM−EDX measurements proved that the morphology of the samples resembled the typical morphology of the LDHs, elemental maps show that Ca(II) and Fe(III) are present in the samples, and their distribution is uniform within the particles.

It may be concluded that using mechanochemical methods LDHs can indeed be synthesized, furthermore, with the correct selection of the reaction parameters even the synthesis of phase-pure LDHs can be achieved.

Acknowledgement
This work was supported by the NK106234 grant by the Science Fund of Hun-gary. The financial help is highly appreciated.

Keywords: Layered double hydroxides, mechanochemistry, structural characterization

Electrodeposition of Calcium Phosphate on EV31 Magnesium Alloy

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Magnesium is very important materials for many applications in transportation, electronic devices and in biomedical applications. It is an exceptionally lightweight metal. With a density of 1.74 g/cm³, magnesium is 1.6 and 4.5 times less dense than aluminum and steel, respectively. The unfortunate complication is that pure magnesium and its alloys can corrode too quickly in the common environments. Surface modification is an effective approach to solve this problem and improve the corrosion resistance of Mg alloy.

This contribution deals with evaluation of mechanism of dicalcium phosphate dihydrate (DCPD) layer creation on the extruded EV31 magnesium alloy. Process of DCPD creation was evaluated by potentiostatic method and described by light stereomicroscopy. The dicalcium phosphate dehydrate layer was electrochemically deposited in a solution containing 0.1M$Ca(NO_3)_2$, 0.06M$NH_4H_2PO_4$ and 10 mL/L of H_2O_2, at static controlled potential of -1.8 V against standard hydrogen electrode. Before electrodeposition of DCPD layer the surface of experimental material was pre-treated by grinding on 1200 emery paper.

Second goal of this contribution is evaluation of corrosion properties of EV31 magnesium alloy coated with calcium phosphate. The influence of the dicalcium phosphate dihydrate layer on the electrochemical characteristics of EV31 magnesium alloy was evaluated by potentiodynamic measurements and electrochemical impedance spectroscopy in 0.1MNaCl solution at a temperature of 22 ± 1 °C. Basic electrochemical characteristics – corrosion potential and corrosion current density were evaluated after 5 minutes of stabilization before potentiodynamic tests. Polarization resistance after longer immersion times up to 168 hours were obtained by electrochemical impedance spectroscopy. The obtained results were analyzed by the Tafel-extrapolation method (potentiodynamic curves) and equivalent circuit method (Nyquist diagrams).

Results show significant positive influence of deposited layer on the thermodynamic and kinetic corrosion properties and the improvement of short-time electrochemical behavior after deposition of DCPD layer.

Acknowledgement
The research was supported by the European Regional Development Fund and the Slovak state budget by the project "Research Centre of the University of Žilina" – ITMS 26220220183.

Keywords: EV31 magnesium alloy, dicalcium phosphate dehydrate, electrochemical properties, electrochemical impedance spectroscopy

Size-selected emissive nanocluster for boosting the performance of inverted organic solar cells

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In spite of the successful enhancement of the power-conversion efficiency (PCE) in organic bulk heterojunction solar cells by surface plasmon resonance (SPR), the incorporation of several tens of nm-sized (25–50 nm) metal nanoparticles (NPs) has some limitations to further enhancing the PCE due to concerns related to possibly transferring non-radiative energy and disturbing the interface morphology. Instead of tens of nm-sized metal NPs, here, we have incorporated dodecanethiol stabilized Au nanoclusters (Au:SR, R=the tail of thiolate) with sub-nm-sized Au38 cores on inverted bulk heterojunction (BHJ) solar cells. Although metal NPs less than 5 nm in size do not show any scattering or electric field enhancement of incident light by SPR effects, the incorporation of emissive Au:SR nanoclusters provided effects that were quite similar to those of tens of nm-sized plasmonic metal NPs. Due to effective energy transfer, based on the protoplasmonic fluorescence of Au:SR, the highest performing solar cells fabricated with Au:SR clusters yielded a PCE of 9.15%; this value represents an ~20% increase in the efficiency compared to solar cells without Au:SR nanoclusters.

Keywords: Au 38, Nanocluster, Energy transfer, Invertedorganic solar cell

Natural substances as substrates in metallic nanoparticles synthesis

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Synthesis methods, properties and stability of nanomaterials having an impact to an unlimited utilization of nanotechnology-based products, are the subject of extensive studies. Research conducted by our team is mainly focused on the silver nanoparticles (AgNPs), due to their attractive physical, chemical and optical properties applied in medicine, pharmacy, food production and packing, electronic, optic, chemical and textile industries where they play significant role as substrates for synthesis, catalytic materials, sensors, conductors, detergents or antimicrobial coatings.

There are many methods of silver nanoparticles synthesis and they can be divided into three main groups. The most widespread and most numerous are chemical methods that rely on use of suitably selected reducing agents and stabilizers. The second group are physicochemical methods use to obtain desired products microwaves, ultrasound, irradiation, templates or milling process. The third group are biochemical methods - relatively recently discovered - also known as biological. These methods using microorganisms, enzyme, plant or plant extracts to synthesis of nanoparticles.

The most widespread method of AgNPs production is wet synthesis, in particular, chemical reduction process, which involves the reduction of silver salt by a reducing agent in the presence of suitable stabilizer. The literature describes compounds commonly used in silver nanoparticles synthesis in chemical reduction processes, for example formaldehyde, sodium borohydride, sodium dodecylsulfate or ethylene glycol. However, nanosilver prepared using mentioned substances can have negative impact on the environment and accumulate in body of different organisms. Referring to the above, the best solution is the synthesis of silver nanoparticles using safe and non-toxic substrates which do not endanger human health and the environment.

The main aim of presented research was obtaining of monodispersive and stable silver nanoparticles suspension in a simple oxidation-reduction reaction between Arabic gum and silver nitrate in aqueous solution. The Arabic gum played double role – a reducer and stabilizing agent of final product. Based on the UV-Vis date can be concluded that all silver colloids exhibit absorbance in the visible region which proves the AgNPs formation. The BSE-SEM images and DLS measurements confirmed differences in size, size distribution, shape and capacity for aggregation depending g on the type and concentration of Arabic gum. The synthesized nanoparticles are found to be stable for several months, so they can be used for a long time after preparation.

Acknowledgement
This research was financed from the budget for education in the period 2013-2015, project IUVENTUS PLUS no. 0628/IP2/2013/72.

Keywords: metallic nanoparticles, AgNPs, chemical reduction method, natural substances

The importance of surfactant and its type on MoS_2 nanoparticles formation

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At the moment, the most successful and popular way to control and define the properties of functional nanosized materials is the initial stage of the synthesis, in which the specifically preset conditions determine the size, morphology, structure and composition of the desired nanoparticles. One of the controlling leverages is the use of different additives, such as surfactants and templates.

MoS_2 is widely used in many applications layered compound, one of the features of which is a variety of morphological characteristics. Here we present the synthesis of MoS_2 nanoparticles by hydrothermal method using micelle-forming agent as a vivid example of impact of various surfactants on the same material in the same conditions. To compare results, we took two different additive substances: cetyltrimethylammonium bromide which is a cationic surfactant and nonionic Triton X-100. In both cases all conditions and precursors were the same, pH = 7.8, the temperature of 220°C and time 24 hours. Obtained material samples were characterized by the methods of XRD, TEM, EDS and porosimetry.

According to XRD study, the patterns (Fig.1) of both samples are analogous that indicates the similarity of their structures. In particular, both materials are in the state close to X-ray amorphous. The broad peaks in the angle ranges of 33-36° and 57-59° confirmed the formation of disconnected 2H-MoS_2 layers.

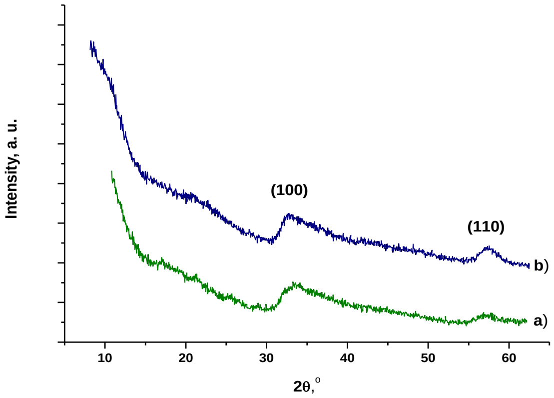

Fig.1: XRD patterns of MoS_2 synthesized using CTAB (a) and Triton X-100 (b).

But in the same time TEM images (Fig.2) show the evident divergence in samples morphology. Using cationic CTAB we obtained mostly spherical multilayer nanoparticles with average diameter 40-70 nm. In case of Triton X-100 the synthesized MoS_2 has a sponge-like morphology consisted of highly disordered nanosheets. The key of this result evidently is the interaction between $[MoS_4]^{2-}$ and surfactant units, created during synthesis process. In the first case, the electrostatic interaction between the $[MoS_4]^{2-}$ complexes and positively charged parts of surfactant molecules causes the multilayer spherical particles imitated the micelle form. In the second case, the cloud point phenomenon takes place inducing the surfactant-rich phases that inhibit the growth of the MoS_2 layers.

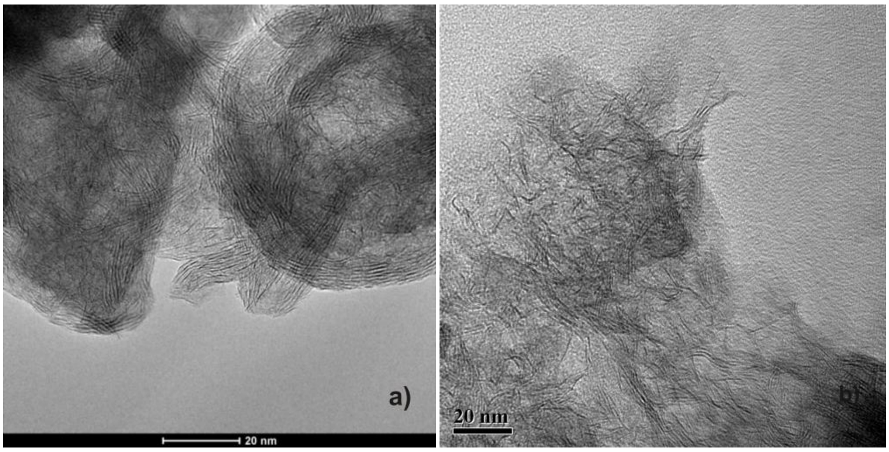

Fig.2: TEM images of MoS2 synthesized using CTAB (a) and Triton X-100 (b)

Keywords: Hydrothermal synthesis, Surfactant, Nanospheres, Nanosheets

Ab-initio calculation of exchange-interaction constants and optical properties of a monoclinic antiferromagnetic insulator $Cu(H_20)_2SO_4(en)$

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We report attempts to calculate from first principles exchange-interaction constants in $Cu(H_2O)_2SO_4$(en), en=$C_2H_8N_2$, antiferromagnetic insulating material displaying low-dimensional magnetism. We discuss influence of computational relaxation and used value of the Hubbard U parameter on the calculated constants. Further, we suggest a possible explanation of one phenomenon encountered during experimental optical studies of the material using Mueller ellipsometry.

Keywords: ab-initio, exchange constants, antiferromagnetism, low-dimensional

A fast and easy protocol for the preparation of layered double hydroxides

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A novel method, the combination of mechanochemical and ultrasonic treatments, was developed for the production of ZnAl-layered double hydroxide (ZnAl-LDH).LDHs arelamellar, ionic solids composed of positively charged sheets and hydrated anions between layers. They can be expressed by the $[M(II)_{1-x}M(III)_x(OH)_2]^{x+}[A^{m-}_{x/m}\cdot nH_2O)]^{x-}$ formula, where M(II) and M(III) are di- and trivalent metal ions, respectively, x= M(III)/[M(II)+M(III)], and A^{m-} stands for the interlayer anions [1].

The method of synthesis consists of two main steps: the suitable metal salts were mechanically activated in a mixer mill first; then, the mixture with added water was irradiated with ultrasound in a thermostated (25 °C) ultrasonic bath. Several parameters of the synthesis were altered (duration of milling and ultrasonic stirring, concentration of hydroxide ions in the added solution),and their effects werefollowed and identified mainly by X-ray diffractometry (XRD).The efficiencies of ultrasonic mixing and mechanical stirring (magnetic stirrer was used) were also compared. As further tools for structural investigation,scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX), infrared spectroscopy (IR), thermal methods (TG−DTG) and specific surface area (BET) measurements were applied.

The X-ray diffractograms showed the typical reflections of ZnAl-LDH, and the infrared and thermogravimetric measurements also verified the presence of layered hydroxides. In the SEM images, the lamellar crystal forms, typical of LDHs, were seen, and the elemental maps from SEM−EDX measurements gave further evidence for the successful preparation. The comparison of the XRD patterns and thespecific surface areas revealed better crystallinity and higher surface area for the sample prepared by ultrasonic treatment than for the mechanically stirred one.

In conclusion, amechanochemical method complemented with eithermechanical or ultrasound stirring was used to produce ZnAl–LDHsamples. The parameters of the syntheses were varied to find the optimal conditions, and the efficiencies of the two stirring types in producing high-quality LDHs were compared.It was found that ultrasonic stirring decreased the necessary time of the crystallisation, and increased the value of specific surface area compared to the mechanical stirred sample. Additionally, this technique seems to be a simple way to intercalate organic anions of various complexities into LDHs.

Acknowledgement

This work was supported by the NK106234 grant by the Science Fund of Hungary. The financial help is highly appreciated.

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Keywords: ZnAl LDH, milling, ultrasound mixing, hydrotreatment

Aluminosilicate/graphene nanocomposite prepared from montmorillonite and polyaniline

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Very interesting discovery was made during research focused on phyllosilicate/polyaniline nanocomposites. Nanocomposite material containing graphene has been successfully prepared using simple three-step method. In the first step, layered silicate montmorillonite was intercalated with conducting polymer polyaniline. In the second step, montmorillonite/polyaniline nanocomposite in powder form was pressed into tablet using high pressure (400 MPa). Finally, in the third step, the tablet was calcined in an inert atmosphere at 1400°C. Although the temperature induced phase transformation of montmorillonite into mullite and cristobalite, layered structure remained unchanged and created suitable conditions for formation of graphene sheets from polyaniline chains intercalated into montmorillonite during the first step of the preparation process. Electrical conductivity of the resulting aluminosilicate/graphene nanocomposite increased dramatically from 0.03 to 693.41 S/m, i.e., the conductivity is 23000× higher in comparison with conductivity of uncalcined montmorillonite/polyaniline nanocomposite before calcination. Low cost of all starting materials (phyllosilicate montmorillonite and conducting polymer polyaniline) and the fact that furnace with appropriate volume allows us to prepare any amount of the nanocomposite are the main advantages of this preparation method.

Acknowledgement

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Keywords: graphene, aluminosilicate, electrical conductivity, polyaniline, calcination

Phase separation of semiflexible diblock copolymer melt: insight from mesoscale modelling

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In recent years, semiflexible diblock copolymers (SDBC) have attracted much attention due to self-assembly to plateau of well-ordered nanostructures. While technological application of SDBC strongly depends on equilibrium nanostructure, the theoretical understanding of their phase behaviour is essential to cost-effective production and design of tailor-made materials, stimuli-responsive materials, etc.In Fig 1a), the theory predicts that flexible AB diblock copolymer phase separates into lamellar (L), hexagonally packed cylinders (C), spherical (S, S_{cp}) and bicontinuous morphologies (G, O^{70}), where f is relative block length ratio and χ is Flory-Huggins interaction parameter. Phase behaviour of real DBC melt in Fig 1b) is in addition influenced also by polydispersity and semiflexibility of A and B block. Nevertheless, inclusion of semiflexibility into theoretical models is still a formidable task. Therefore mesoscale modelling can be used to obtain DBC conformations and thus obtain phase behaviour.

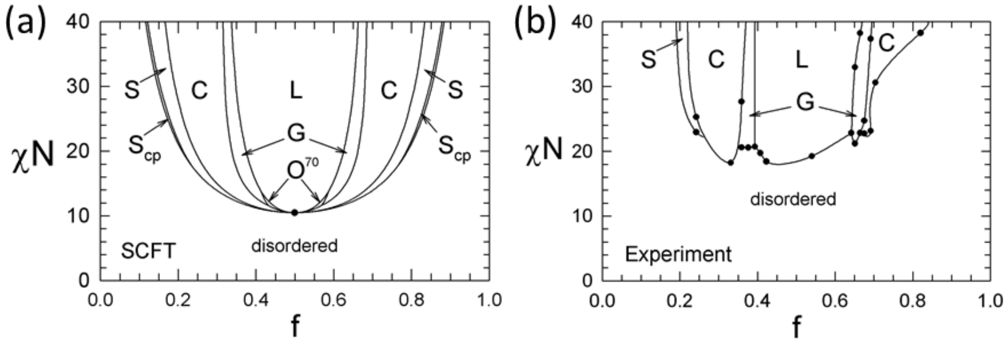

Fig. 1: (a) Phase behaviour of AB diblock copolymer: (a)theoretical phase diagram and (b) Poly (styrene)-poly (isoprene) real melt. Diagrams were reprinted with permission from *.S. Bates et al., Faraday Discuss. 98, 7 (1994)* and from *M.W. Matsen, Eur. Phys. J. E 30, 361 (2009).*

We employed Dissipative particle dynamics (DPD), well established mesoscopic method, to model phase behaviour of semiflexible diblock copolymer melt. Our AB diblock copolymer chain consist of $N = N_A + N_B$ segments connected by harmonic spring. Semiflexibility of the chain was modelled by changing the stiffness of the spring bond between A segments from $K_A=4$ (refer to fully flexible chain) up to $K_A=10$ (refer to semiflexible chain).

We observed that DBC with flexible blocks phase separates in agreement with theoretical model in Fig 1a). Asymmetry of phase diagram was also observed with increasing the K_A. Furthermore, we observed that bicontinuous morphologies were replaced by hexagonally packed cylinders, for K_A>8, in semiflexible block rich phase (f> 0.5) and by lamellar and perforated lamellar morphology in flexible block rich phase (f< 0.5). Finally, we observed that order-disorder transition was only slightly changed with increasing the stiffness K_A.

Keywords: self-assembly, semiflexible diblock copolymer, mesoscale modelling, phase diagram

Structure and properties of nylon 6 nanofiber textile prepared by *Nanospider* technology

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The structure of nanofibers prepared by *NANOSPIDER* technology i.e. the roller spinning is less studied compared to melt and/or capillary spinning, although this technology is industrially used and important for practice. This study is devoted to the structure, phase composition and surface properties of nylon 6 nanotextile prepared by *NANOSPIDER* technology. It is well known that nylon-6 is polymorphic, having the following crystal structures: (1) The α- form described by Brill [1] and Holmes et al. [2] and (2) the γ-form determined by Holmes et al. [2]. In electrospun nanofibers, both phases α and γ usually coexist together with amorphous phase and their volume fraction depends on the spinning conditions. There are many factors affecting the morphology and phase composition of nylon-6 nanofibers, anyway the phase composition always depends on the cooling rate. It is well known that α-phase with higher density needs longer crystallization time than γ-phase, which has more loosely packed chains. Phase composition, morphology and surface properties of nylon-6 nanofibers prepared by *Nanospider* technology have been studied in dependence on spinning distance using combination of X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), electrokinetic analysis and scanning electron and transmission electron microscopy (SEM, TEM).

Increasing electrode distance led to the increase of crystallinity, i.e. to a decrease of the amorphous phase content. Comparison of theoretical and experimental XRD intensities led to the identification of the texture type in fibers. The crystallographic direction ⟨010⟩, which is the direction of the molecular axis, is preferentially oriented in the fiber axis. *NANOSPIDER* technology provides different phase composition of nylon-6 nanofibers as compared with the melt spinning. The nylon-6 nanofibers prepared by NANOSPIDER technology consist predominantly of γ-phase for all electrode distances and the content of α-phase is lower than in fibers prepared by melt spinning. XRD analysis combined with XPS and TEM analysis led to the core-shell structure model of nylon-6 nanofibers, where α-phase is in the fiber core and fiber surface always consists of γ-phase, due to the more rapid cooling of surface region. Zeta potential and adhesion properties are significantly different for the face and reverse side of nanofiber textile adjacent to the spunbond, due to the interaction of positively charged amino-groups with polypropylene spunbond.

Acknowledgement

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Keywords: nylon-6 structure, nanospider, zeta potential, core-shell structure model

Photo-Catalytic activity of pure and doped CeO_2

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Nano-sized CeO_2 was prepared via hydrothermal method and three factors are handled (temperature, reaction time and material precursor). CeO_2 nano-particles were successfully doped with Sm_2O_3 and Gd_2O_3 nano-particles. The synthesized powders were characterized using X-ray diffraction (XRD), Raman Spectroscopy, transmission electron microscope (TEM) and field emission scanning electron microscope (FESEM). It was found that increasing reaction temperature from 120°C to 200°C leads to increase the crystallinity, particle sizes and more dispersal particles obtained. Also, by increasing the reaction time from 12 to 24 h the particle size was decreased, semispherical shape was appeared and dispersion of the particles was increased. The photo-catalytic activity of the prepared samples toward methylene blue (MB) degradation was studied. It was found that Gd_2O_3 doped CeO_2nano-particles have the best catalytic degradation effect on methylene blue dye under UV irradiation. The degradation pathways of methylene was followed using liquid chromatography (LC/MS).We found that, Gd doped CeO_2/UV-based photo-catalyst was simultaneously able to oxidize MB dye, with a complete mineralization of carbon and of nitrogen and sulfur heteroatoms into CO_2, NH_4, NO^{3-} and SO_4^{2-}.

Keywords: CeO_2; Doping; Gd_2O_3; Sm_2O_3; Photo-catalytic degradation; Methylene blue.

NiAl-Layered Double Hydroxide: Preparation, Characterization and Applications in photo-catalysis and Hydrogen Storage

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NiAl-Layered Double Hydroxide (NiAl-LDH), one of anionic functional layered materials, has been prepared by a simple co-precipitation process. X-ray diffraction patterns confirm the formation of the desired compounds of NiAl hydroxide single phase and the crystallite size was found to be about 4.6 nm. The morphology of the prepared samples was investigated using scanning electron microscopy and the layered structure was appeared under the transmission electron microscope. The thermal stability and the function groups of NiAl-LDH were investigated using thermal gravimetric analysis (TGA) and Fourier transform infrared (FTIR) respectively. NiAl-LDH was investigated as a photo-catalyst for the degradation of some toxic dyes such as toluidine blue and bromopyrogallol red. It shows good catalytic efficiency in visible light and even in dark. For the first time NiAl-LDH was used for hydrogen storage application. NiAl-LDH samples were exposed to 20 bar applied hydrogen pressure at room temperature, 100 and -193 ^{o}C. NiAl-LDH samples appear to have feasible hydrogen storage capacity. It was capable to adsorb0.1wt% at room temperature, 0.15wt% at 100^{o}C and storage capacity reached 0.3 wt% at -193 ^{o}C.

Keywords: NiAl-LDH; Preparation; Characterization; Photo-catalysis; Hydrogen Storage

Formation of Ca-Al containing layered double hydroxides and its solubility product determination in highly caustic solutions

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The formation and nature of solid phases in the $NaOH/NaAl(OH)_4/Ca(OH)_2$ system are very important and intensively investigated topics since the introduction of the Bayer process in the alumina industry [1-3].

Different types of calcium- and aluminium-containing solid phases, like $Ca(OH)_2$, $Ca_3Al_2(OH)_7$ (tricalcium aluminate) and layered double hydroxides (LDH), form highly alkaline solutions. The most populous group of LDHs is the family of hydrotalcite-like materials. Hydrotalcite itself can be found in Nature, and has the formula of $Mg_6Al_2(OH)_{16}CO_3 \cdot 4H_2O$. The calcium analogue of hydrotalcite is called hydrocalumite (HC) with the general formula of $[Ca_2Al(OH)_6]X \cdot nH_2O$, where X^- is a charge balancing monovalent anion. This is a stoichiometric LDH, where the Ca:Al ratio is always 2:1. In this work, the charge balancing monovalent ion is the OH^-, which is situated in the interlayer space. In these types of materials numerous anion could be intercalated into the interlayer region, and the basal distance of the intercalated material could be as large as 10 Å.

Firstly, our goal was to characterise the solid phases with XRD measurements in solutions containing $NaOH/NaAl(OH)_4/Ca(OH)_2$, as a function of time and temperature. The results showed that hydrocalumites with two different interlayer distances hydrocalumite were formed in this system, and tricalcium aluminate tended to form on changing the aluminate concentration and temperature in highly (up to 1 M) caustic solutions. A point in the aluminate concentration and temperature could be identified when the solid phase contained only $Ca(OH)_2$. After learning this result, experiments were performed to find the maximum aluminate concentrations at different temperatures and NaOH concentrations where the hydrocalumite just appeared in the diffractograms. From the result, the solubility product of the hydrocalumite could be calculated from the equation below:

$$L_{HC} = [Ca^{2+}]^2[NaAl(OH)_4]_{max}[OH^-]^3 \qquad (1)$$

It was found that the solubility product for the hydrocalumite was lgL = −11.1 ± 0.05.

Acknowledgement

The work leading to this contribution was financed by a grant (NK 106234) from the National Science Fund of Hungary. The support is highly appreciated.

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Keywords: layered double hydroxide, hydrocalumite, solubility product, caustic medium

Electrochemical polishing in the magnetic field

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In the paper there is described the work of the international scientific team on the subject influence of magnetic field during electropolishing on the surface layer after that treatment. There were observed mechanical (nanohardness and reduced Young's modulus) and electrochemical (corrosion resistance) properties as well as the amount chromium compounds to iron compounds ratio (XPS) and amount of hydrogen (SIMS) in the surface layer structure. The best results were observed after electropolishing with agitation created by the magnetic field (B $\approx$ 350 mT) at a current density 200 A/dm^2 and at electrolyte temperature 65±5 °C.

Keywords: electropolishing, magnetic field, XPS spectroscopy, nanoindetation

Molecular modeling of antibacterial clay nanocomposites

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Antibacterial nanocomposites based on active agents incorporated into environmentally friendly clays are promising materials in the area of controlled release. If the agent is attached to support matrix it can achieve prolonged antibacterial effect which is useful especially when the target cannot be treated by the agent continuously, as is for example the case of implants. Among many candidate matrices clay minerals exhibit excellent properties for this application because they have large surface area, good swelling properties and are environmentally stable. In previous works, various clay minerals including montmorillonite (MMT), kaolinite and vermiculite (VMT) were successfully used in preparation of organo-clay antibacterial nanocomposites. However, because variety of MMTs and VMTs exists, different kinds of these clays previously untested were used in this work in order to obtain complement results utilizable in further design of antibacterial nanocomposites. One of the key characteristics playing role in prolonged release is the amount of intercalated agent. However, it can be estimated only very roughly on the basis of X-ray analysis. Better information may be obtained when X-ray analysis is combined with molecular modeling. Such approach was utilized in this work where molecular modeling using Universal force field as implemented in Materials Studio modeling environment was performed and results of simulation were confronted with experimental data.

Interlayer structure of MMT and VMT was investigated using serie of models with different interlayer content of chlorhexidine diacetate (CA) ranging from 0.5 CEC to 1 CEC and 0.5 CEC to 2 CEC, respectively. Except the influence of CA on separation of layers the role of interlayer water content was also studied.

Obtained results indicate partial intercalation in the case of MMT while interlayer cations of VMT seem to be exchanged completely, taking into account the best agreement between simulated and experimental basal diffraction. Naturally, real samples are composed from variety of distinct phases which cannot be simulated directly. Nevertheless, the structure of main part of sample could be estimated and, therefore, amount of intercalated agent determined.

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) and by the Ministry of Education, Youth and Sports of Czech Republic SGS project no. SP2015/59. Dominik Hlaváč also thanks to the City of Ostrava, Czech Republic, for provision of scholarship in the academic year 2014/2015.

Keywords: antibacterial nanocomposites, clay minerals, molecular modeling, interlayer structure

Noble metal nanoring and nanodot array catalysts for electrocatalytic reactions

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In this work, nanoscale metal ring and dot array patterns were fabricated by direct transfer printing. Vertically aligned 1D carbon nanostructures with two different tip shapes were used as stamps: one had a carbon nanotubes (CNT) structure with the ring-featured tips and the other had a carbon nanopost (CNP) architecture with the dot-shaped tips. These nanostructure arrays were supported by hexagonally arranged porous channels of anodic aluminum oxide(AAO), and their tip shapes were controlled by adjusting the ion milling conditions during stamp fabrication. The metal nanoring and nanodot arrays were formed onto indium tin oxide (ITO) glass substrates by the printing protocol, and these ring and dot nanoarrays were applied for electrooxidation reactions, indicating that ourprinting methodology could establish the foundation of the printable catalyst system for a wide range of catalysis applications and provide the fundamental catalytic understanding arising from themorphological difference between the ring and dot components.

The printable nano-sized catalyst systems, made of metal rings and metal dots, were developed for the first time. The vertically aligned carbon-based nanostructures of the ring-shaped tips and the dot-featured tips were employed as the stamps to create the nanoscale ring and dot catalyst arrays. Importantly, the printed nanorings and nanodots were employed into the electrochemical oxidation reactions, which demonstrates catalytic properties caused from the morphology difference of the metal rings and metal dots. It is straightforward that our printing methodology can be highly versatile for fabricating diverse ring and dot arrays made of not only metals but also various organic and inorganic materials, indicating that the printable sub-100-nm ring and dot arrays could play an important role in comprehending the fundamental nature of dot and ring nanomaterials and thus incorporating them into suitable catalysis applications.

Keywords: Electrocatalyst, Fuel cell, Nanoring, Nanodot

Characterization of electron generating efficiency enhancement of microbial fuel cell system with Ti nano-particle as an electron acceptor by using scanning probe microscopy (SPM) analysis

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Microbial fuel cell(MFC) systems use electrochemically active biofilm which can exchange electron discharged from internal metabolic pathway into electrically conductive electrode as terminal electron acceptor and/or donor. Conventionally MFC has been applied to produce renewable energy such as electricity and hydrogen from various biodegradable organic materials, and biosensor for organic contaminant monitoring. We investigated the effect of Ti nano-particle on the electron generating efficient of MFC by deposition of nano-particles on the carbon paper electrode. Since the generated voltage and current from MFC are depend on the amount of microbes which are attached on the anode, a surface area and bioaffinity of electrode materials are important factor. By monitoring the voltage of MFC which employing Ti-nano-particle, we evaluated and compared performance enhancement with a case of general carbon paper anode. The Ti- nano-particles were dispersed in an acetone as a solvent by using sonication for 30 minutes and a various anode electrode such as carbon paper, Ni form plate and stainless steel mesh were dipped in the dispersed solution. An amount of attached Ti nano-particles on the surface of electrode were controlled by dipping duration. Also, an influence of nano-particle size and gap of inter-particle variation were investigated. The generated voltage and current from MFC have been monitored for about 14 days and they showed difference of electrical properties between various electrodes. To understand a mechanism of electron transport from alive microbe to conductive electrode, we need to observe an individual electrochemically active bacterium such as *Shewanella oneidensis* MR-1by using nano-probing technique. The electrical properties such like resistance and dielectric constant of microbes were analyzed by scanning probe microscopy(SPM) with conductive cantilever tip and nanowire of microbe which known as an electrical pathway to transmit an electron to the electrode were characterized with a various mode of SPM. To investigate an interaction between microbe and anode electrode with Ti nano-particle would be a clue for understanding of electron generation and transmission mechanism.

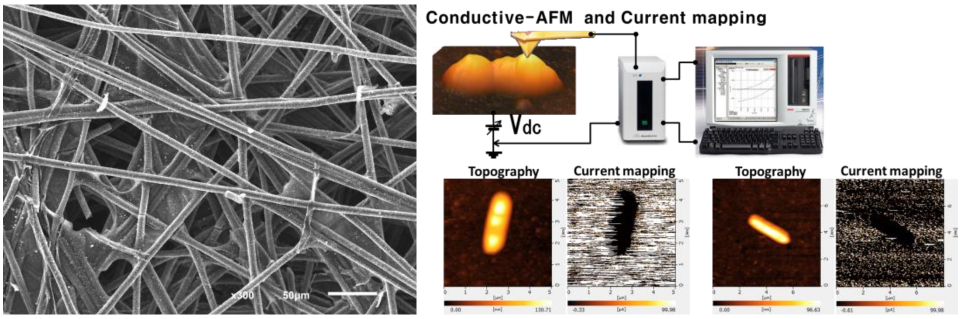

Fig. 1: SEM image of carbon electrode and schematic of conductive-AFM system.

Keywords: microbial fuel cell, scanning probe microscopy, Ti nanoparticle, carbon electrode

CO_2 responses based on pure and doped CeO_2 nanoparticles

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Pure and Gd-doped Cerium oxide (ceria) powders have been prepared via co-precipitation technique. The powder was found to be nano-sized particles in the range of 20-29 nm as transmission electron microscope analysis revealed. The powder also has been examined using X-ray diffraction and Raman spectroscopy to estimate the effect of Gd-doping on the properties of ceria. It was found that the particle size has been decreased by doping which indicates that the growth restriction rule of Gd in the ceria matrix. Also a small shift in the peak position accompanied with more broadening in Raman analysis. Finally the gas response of all powders has been tested for CO_2 gas in temperature range 200-400^oC, 50^o at a time. The powder sensitivity was found to be maximum at 250^oC for Gd-doped ceria where the pure powder maximum response is predicted to be beyond 400.

Keywords: CeO_2; Doping; Gd; CO_2 gas sensors;co-precipitation.

Modelling stress strain states of nanomaterials created by multiple plastic deformation

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The paper studies stress strain states of an aluminium alloy EN AW 6060 (AlMgSi 0.5) during the process of extrusion in order to identify changes in elasticity under pressure applied to the material by multiple plastic deformation. The results of indirect measurements (calculations based on direct measurements) of elastic modules are presented and compared and verified with predicted theoretical relationships. It can be said that when a sample of material with given geometric dimensions undergoes multiple plastic deformation, it is stressed in volume. Extrusion forces are directly measured depending on the length of sample, in particular when a equidistant step of the sample displacement is known. By indirect measurements, extrusion stress can be evaluated as a mechanical work applied to an extruded volume. If a user of the technology will evaluate the coefficient of extrusion forces for his specific device in the described manner and measure the extrusion stress for a given extrusion process, then he will be able to evaluate the modulus of elasticity using the ratio of the physical quantities. By means of a Poisson's ratio, it is also then possible to estimate the value of Young's modulus relatively very precisely, depending on a number of extrusions. The objective of this research consisted especially in the evaluation of the modulus of elasticity, and then the identification of the Young's modulus as accurate as possible after each extrusion, in particular through material relations between elastic modules.

Keywords: Direct channel of angular extrusion, Multiple plastic deformation, Modulus of elasticity, Young's modulus.

Synthesis and characterization of samarium oxide nanoparticles

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Lanthanide oxide nanoparticles have gained a lot of attention due to their diverse use for an application and from this reason it is very important to find a suitable method preparation that would be economically inexpensive and easy to implement.The article describes the preparation of samarium oxide nanoparticles (nano Sm_2O_3) via thermal decomposition of the complex formedby the selected default salt $Sm(NO_3)_3 \cdot 6\,H_2O$ and glycine. Decomposition of the complex occurred at about of (250 ± 10) °C. Ultra-fine white powder of samarium oxide nanoparticles was obtained due to this method. The resulting nanoparticles were characterized by X-ray powder diffraction analysis, which showed the samarium oxide nanoparticles to be with the crystallite size of 10.7 nm. Morphology of the samarium oxide nanoparticles was examined by scanning electron microscopy. The elemental composition of the product was confirmed by EDS analysis.

Keywords: Thermal decomposition, Nanoparticles, Samarium oxide, XRD

The sorption of aniline on organically modified bentonites

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Several samples of bentonites were modified by different types of 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-bentonites 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 bentonite samples. The simultaneous thermogravimetry and differential thermal analysis showed, that the organically modified bentonites generally exhibited better thermal stability indicated by higher values of temperatures related to dehydroxylation as well as the total melting process. The sorption properties of both the original and modified bentonites for aniline were studied. Modified bentonites showed higher sorption capacity for aniline compared with natural bentonites. Also the type of alkylammonium cation greatly influenced the rate of aniline sorption, the hexadecylpyridinium chloride appeared as the most effective one.

Acknowledgements
This work has been done in connection with project Institute of clean technologies for mining and utilization of raw materials for energy use - Sustainability program. Identification code: LO1406. Project is supported by the National Programme for Sustainability I (2013-2020) financed by the state budget of the Czech Republic.

Keywords: bentonites, alkylammonium cations, sorption, aniline

Experimental verification of theoretical efficiency of high gradient magnetic separation

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The article presents an experimental verification of magnetic separation efficiency using the theoretical model. Steady state, laminar flow and a spherical magnetic particle (paramagnetic or weakly ferromagnetic) was assumed in the model. The magnetic behavior of the liquid and influence of the steel wool is neglected. From the mathematical model we have estimate that separation efficiency is proportional to the square of the particle radius, inversely proportional to the velocity of the particles in liquid and directly proportional to the magnitude and the gradient of the magnetic field.

The measurement was carried out using two new laboratory magnetic separators constructed at the Department of Physics, VŠB - Technical University of Ostrava. These separators are mounted with two or four NdFeB permanent magnets symmetrically around a central separation cell. High magnetic field gradient (HMFG) inside of the separation cell is created using steel wool.

Three grain size fractions were prepared – coarse, medium and fine, mean particle size about 5 μm, 1.4 μm and 100 nm, respectively. Separation processes using both separators were following: prepared suspension was brought into the separator using the peristaltic pump after its homogenization by ultrasound in ultrasonic cleaner. The suspension further continued through the separation cell filled with steel wool to the collection vessel, where the separation process finished. In our case, the separation process for the every sample underwent five cycles.

The efficiency of the high gradient magnetic separation (HGMS) separation process was tested on a water suspension containing weakly magnetic Fe_2O_3 nano/micro-particles by the turbidimetry, i.e. measurement of intensity of scattered light. The correlation between the magnetic field magnitude and concentration ratio is depicted in the Fig. 1.

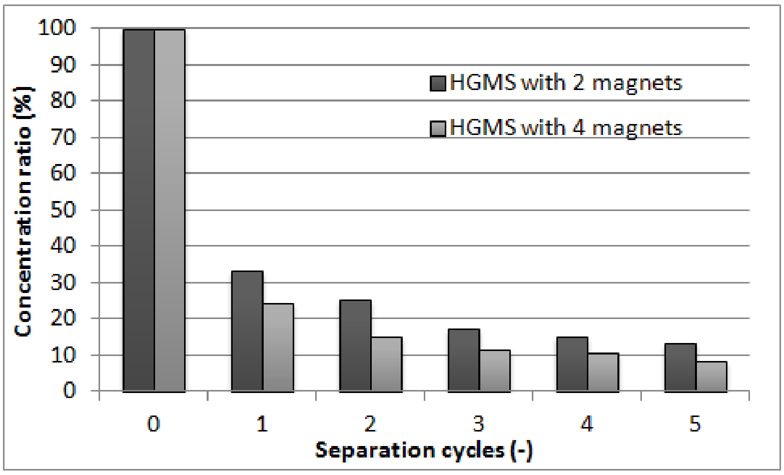

Fig. 1: Concentration ratio as a function of separation cycles in the separator with 2 or 4 permanent magnets.

Keywords: high gradient magnetic separation, permanent magnets, turbidimetry, separation efficiency

β-In_2S_3 nanoparticles synthesized via sonochemical and reflux method

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Nanosized indium sulfide, particular β-In_2S_3, has attracted significant interest due to its specific properties and prospective applications in the field of green energy and medicine. Several different techniques were used for the synthesis of β-In_2S_3 nanoparticles, including sonochemistry. To determine the effect of ultrasound and the phenomena of acoustic cavitation on the particles formation, β-In_2S_3 nanoparticles were synthesized by the reflux and sonochemistry method synthesis.

β-In_2S_3 nanoparticles have been prepared by sonochemical and the reflux method in aqueous solution from an equimolar ratio of indium salts ($In(NO_3)_3 \cdot xH_2O$ and $InCl_3$) and thioacetamide as sulfur source. For the sonochemical synthesis of β-In_2S_3, the samples were ultrasonic irradiated with high-intensity direct immersion ultrasonic probe under ambient air for 1h with no temperature control. By the facile reflux method, the samples were heated and refluxed at around 95 °C for 1h and stirring on a magnetic stirrer. The orange products were characterized by X-ray powder diffraction (XRD), transmission electron microscopy (TEM) and ultraviolet-visible (UV-vis) spectroscopy. The Scherrer equation was used to calculate the crystalline size.

With both synthesis techniques pure β-In_2S_3 nanoparticles were obtained. The smallest particles, approximately 8 nm, were estimated for the reaction with $In(NO_3)_3 \cdot xH_2O$ by reflux method. For the formation of β-In_2S_3 nanoparticles from indium salt and thioacetamide, the reaction temperature is important for the release of sulfur. Additionally, the reaction time, as viewed from the perspective of the beginning of the formation of particles, has a significant impact on the particle size. The effect of acoustic cavitation on the particle size cannot be confirmed.

Keywords: indium sulfide, nanoparticles, sonochemistry, reflux

Influence of different preparation methods on properties of ZnO nanoparticles

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In this work, semiconductor zinc oxide nanoparticles were synthesized via different methods and their optical and structure properties were discussed. The first method of ZnO nanoparticles preparation (ZnO(1)) was based on the thermal annealing of zinc acetate ($Zn(OAc)_2$) in a muffle oven at 350 °C. The second method of preparation (ZnO(2)) consisted of the precipitation of zinc hydroxide followed by its thermal annealing at 350 °C to obtain ZnO nanoparticles. Zinc hydroxide was prepared by the precipitation reaction between $Zn(OAc)_2$ and sodium hydroxide with the ratio $[OH^-]/[Zn^{2+}] = 3$. The third method (ZnO(3)) was similar to the second one with the difference that a UV lamp with the emission maximum wavelength of 254 nm was used during the precipitation reaction. In both cases, zinc hydroxide precipitates were obtained, filtered, washed several times with demineralized water in order to remove sodium acetate and annealed in the muffle oven at 350 °C as ZnO(1) samples.

The all prepared ZnO samples were analyzed and characterized by thermogravimetric analysis, X-ray diffraction, UV-Vis diffuse reflectance and photoluminescence spectroscopy, transmission electron microscopy and specific surface area and pore size measurements performed by the common BET method. Based on the obtained results, the different preparation methods were found to have an influence on size and oxygen lattice defects of the ZnO nanoparticles. The size of ZnO nanoparticles varied in from 14 nm to 89 nm. These defects are generally considered to play crucial role in electrical, optical and also photocatalytic properties of semiconductor materials. The photoluminescence spectroscopy is an easy way to recognize the defects in ZnO nanoparticles. Figure 1 shows the photoluminescence spectra of ZnO(1), ZnO(2) and ZnO(3) samples.

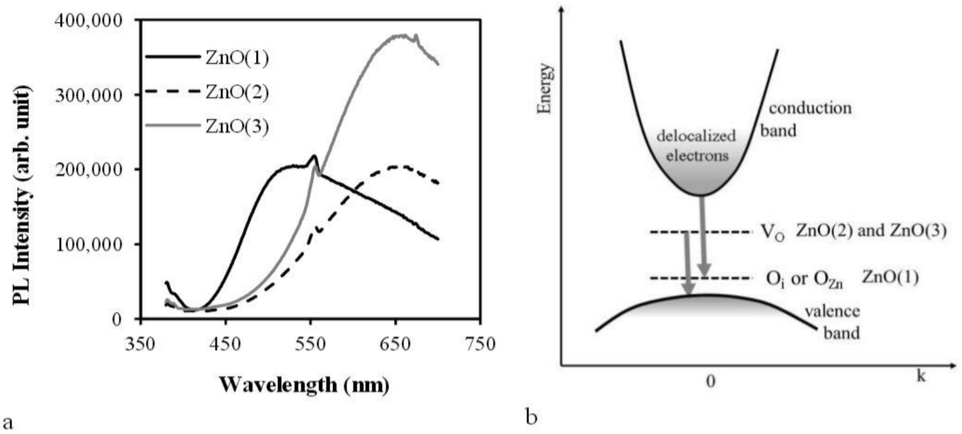

Fig. 1: (a) Photoluminescence spectra of ZnO nanoparticles, (b) Scheme of suggested most probable electron transitions responsible for measured PL maxima.

Keywords: Zinc oxide, Photoluminescence, UV irradiation, photocatalyst

Laser-induced chemistry in a mixture of nanoparticles in solution

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In the present study, laser irradiation of a mixture of gadolinium and silicon nanoparticles (NPs) produced by laser ablation in liquid was used for synthesis of binary gadolinium silicide NPs. Nanoscale compounds and alloys of gadolinium have promising biomedical applications due to the unique combination of high magnetization and superparamagnetic behaviour. For example, gadolinium-based NPs can be used as therapeutic agents in drug delivery, as contrast agents in magnetic resonance imaging (MRI) and magnetic resonance angiography (MRA), and as magnetic particles for the hyperthermia treatment of tumors.

The initial Gd and Si colloids were prepared by laser ablation in ethanol. Nd:YAG laser (LOTIS TII, LS2134D), operating in a double-pulse mode at 1064 nm (energy 80 mJ/pulse, repetition rate 10 Hz, pulse duration 10 ns) was used for ablation of the relevant target placed in the cell filled with liquid. After the preparation the colloids were mixed in the proportion corresponding to the atomic ratio Gd:Si=5:4 and subjected to laser irradiation by the second harmonic of the Nd:YAG laser (wavelength 532 nm) with fluences of 230 and 400 mJ/cm^2. The morphology and structure of the resulting NPs was analyzed by SAED, XRD, TEM and SEM techniques. To determine the temperature of the NPs, their thermal radiation spectra were fitted by a Planck curve, taking into account the emissivity function of the NPs and that the CCD detector counts the number of photons.

Gd and Si NPs prepared by laser ablation were near-spherical and rather small in size (5 nm for Si and 10 nm for Gd). However, Gd NPs formed aggregates with size more than 100 nm, while Si NPs were well-separated and had a narrow size distribution. Addition of silicon colloidal solution to the Gd colloid resulted in the drastic change of the morphology and structure of the prepared NPs: in addition to the small spherical particles, that mostly formed aggregates, large near-spherical particles with the diameter more than 70 nm and hollow NPs were formed. The change in the morphology after mixing of colloidal solutions can be the evidence of the chemical processes between the particles in solution. The analysis of the SAED patterns of the mixture samples proves that in the mixed colloid Gd_5Si_4 phase was formed. The order of mixing of the colloidal solutions was found to be the factor that influences the phase composition of the NPs in the mixture: the addition of silicon to gadolinium colloidal solution is more favourable for the formation of compound Gd_5Si_4 NPs. That is why the colloidal solution prepared using this order was further subjected to laser irradiation with the purpose of the controlled change of NPs composition.

Laser irradiation of the colloidal solutions resulted in a change in the morphology and phase composition of the NPs depending on the laser fluence. Laser treatment with fluence of 400 mJ/cm^2 resulted in the formation of orthorhombic GdSi phase while the major phase that constitutes NPs irradiated with fluence 230 mJ/cm^2 was Gd_5Si_4. So, laser ablation technique with a post-ablation irradiation of a mixture of as-prepared gadolinium and silicon colloidal solutions has been demonstrated to be a tool to prepare gadolinium silicides particles with sizes in the nanometric range. The synthesized particles exhibited the superparamagnetic behavior promising for their potential application in the method of magnetic hyperthermia treatment.

Keywords: Laser irradiation, nanoparticles, chemical interactions, gadolinium silicides

Different level of fluorescence at Raman spectroscopy of selected clay minerals

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Two specimens of kaolinite and four specimens of montmorillonite were used for this study. The specimens of kaolinite differ in rank of crystal lattice order; the specimens of montmorillonite differ mainly by interlayer cations. Elemental analysis, XRD analysis and thermal analysis were performed for detailed description of used samples. FT-Raman spectroscopy (excitation laser 1064 nm) and dispersive Raman spectroscopy (excitation lasers 532 nm and 780 nm) with microscopy (excitation laser 532 nm) were used for obtained Raman spectra of selected clay minerals. All spectra of kaolinite samples and almost all spectra of montmorillonite samples were significantly affected by fluorescence. Only one montmorillonite sample were affected by fluorescence only little or almost not. The most intensive was band at 145 cm^{-1} belonging to deformation vibration of AlO_6 octahedron in the spectra of kaolinite samples. The most intensive were bands at 96 cm^{-1} (vibration of interlayer cation), 200 cm^{-1} (deformation vibration of AlO_6 octahedron), 710 cm^{-1} (stretching vibration of SiO_4 tetrahedron), and 3620 cm^{-1} (stretching vibration of OH) in the spectra of montmorillonite samples.

Acknowledgements
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Keywords: Raman spectroscopy, fluorescence, clay minerals

SEM and EDS analysis of surface layer formed on titanium after plasma electrolytic oxidation in phosphoric acid with the addition of copper nitrate

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Plasma Electrolytic Oxidation (PEO), also know under the name Micro Arc Oxidation (MAO), is very often used to modify a surface layer on biomaterials such as titanium, tantalum, niobium and their alloys. The surface which is obtained after that process is more biocompatible than that after a standard electrochemical polishing. The obtained surface layer formed after PEO on pure titanium is porous and amorphous and consists mainly of phosphorus, oxygen and titanium atoms. The analysis shows that the thickness of PEO layer is about 1 μm (Fig. 1). The outer layer consists of phosphorus (16 wt %), titanium (41 wt %), oxygen (40 wt %) and copper (3 wt %) whereas the inner layer consists only of phosphorus (23 wt %), titanium (35 wt %) and oxygen (42 wt %).

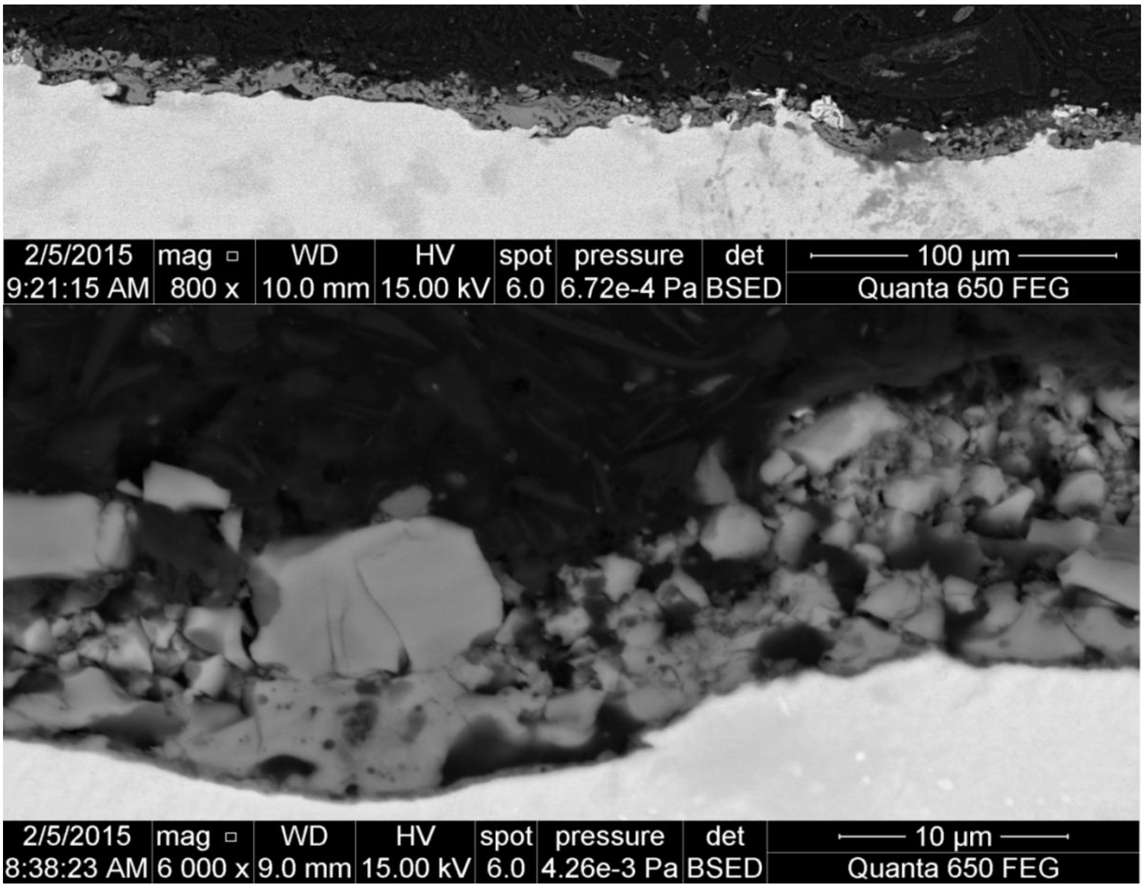

Fig.1: Cross section of surface layer formed on titanium after Plasma Electrolytic Oxidation at voltage of 450V and current density of 0.3 A/dm^2 in electrolyte containing of concentrated phosphoric acid within cooper nitrate

Keywords: SEM, EDS, Titanium, Plasma Electrolytic Oxidation

Interparticle magnetic interactions in the powder samples of magnetite and magnesium oxide mixtures

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In this paper magnetic properties and interparticle magnetic interactions of the powder mixtures consisting of a ferrimagnetic magnetite (middle particle size about 50 nm) and diamagnetic MgO (middle particle size about several μm) are presented. Mixtures with concentrations of Fe_3O_4 from 10 to 80 wt. % were prepared by two methods: ultrasonic homogenization and manual mechanical mixing. Homogenization was carried out in an ethanol solution in the ratio of one to one by rotation in the ultrasonic field and additional evaporation using a water pump. Finally, the powders were mechanically pressed in a specially developed device to produce the samples in form of the tablets with diameter of 10 mm.

An EV9 MicroSense vibrating sample magnetometer (VSM) was used for measurements of the virgin curves, magnetization loops, and isothermal remanence (IRM) and dc-demagnetization (DCD) curves. Magnetic interparticle interactions were investigated using the Henkel plots which were constructed in two ways. The first one includes interconnection between virgin and hysteresis curves, while the second one combines IRM and DCD curves.

Effect of the sample preparation on the shape of the Henkel plots ΔM (H) is demonstrated in Fig. 1. In this case the method of virgin and hysteresis curves was used. All samples exhibit negative dipolar interactions. Application of the ultrasonic homogenization method leads to the systematic dependence between concentration change of Fe_3O_4 and the minimum position of ΔM (see Fig. 1A). On the other hand, samples prepared by manual mechanical mixing exhibit different results (see Fig. 1B) due to not adequate homogenization leading to incorrect Henkel plots.

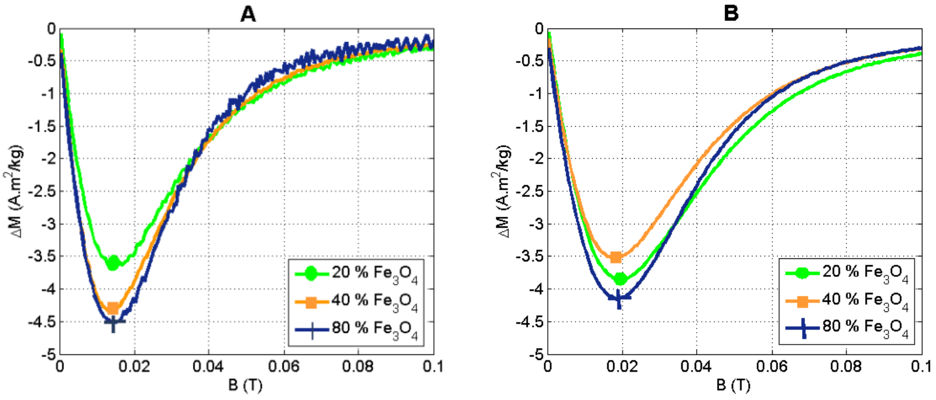


Fig. 1: Comparison of the Henkel plots for mixtures prepared by ultrasonic homogenization method (A) and manual mechanical mixing (B). ΔM is normalized relative to the weight of magnetite.

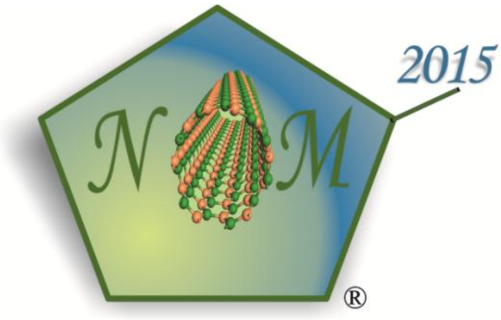
Keywords: Magnetite nanoparticles; vibrating sample magnetometer, Henkel plot; ultrasonic homogenization

TOPIC 2

Nanomaterials for medicine

Chair: Josef Jampílek
Co-chair: Daniela Plachá

Nanomaterials for drug delivery
Interactions with living organisms
Nanobiotechnologies & Nanomedicine



Polyamidoamine-based nanoparticles designed for drugs and protein drugs delivery systems lower case

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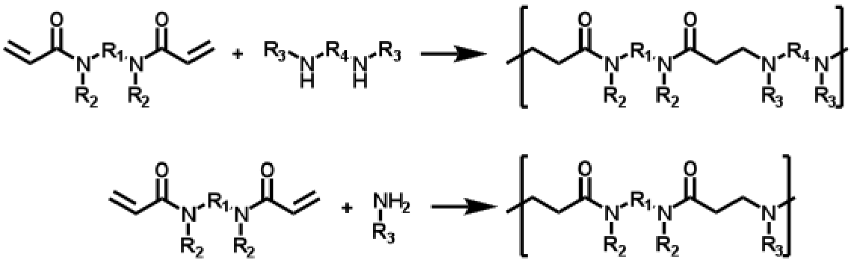
Polyamidoamines (PAAs) are a family of ionic polymers that can be designed to be biocompatible and degradable in the body fluids. They are prepared by Michael polyaddition of primary or secondary amines to bisacrylamides and carry amide- and *tert*-amine groups regularly arranged along the polymer chain:



The reaction is remarkably specific and takes place in water or alcohols, at low to moderate temperature and in most cases without added catalysts. Nearly all amines and bisacrylamides can be used as monomers. By employing functional monomers, a number of additional functions may be added, including peptide and sugar moieties.

PAAs are admirably suitable for producing nanoparticles to be tested for several biotechnological applications. In particular, the following items will be reported:
a) Thiol-containing PAAs and nanoparticulated thiocholesterol conjugates therefrom;
b) Nanoparticle-forming PAAs with hydrophobic pendants;
c) Nano-polyplexes of fully biocompatible PAAs with nucleic acids and their transfection ability;
d) Self-assembling optically active PAAs deriving from α-aminoacids;
e) Nanoparticles formation from PAA adducts with hydrophobic drugs, such as quinine-like antimalarial drugs;
f) Intrinsic antiviral activity of the same PAAs and their potential as nanoparticulated “solubilisers” of hydrophobic antiviral drugs;
g) Nanoparticulated Cyclodextrin-PAA conjugates as protein delivery systems.

Keywords: polyamidoamines, nanoparticles, protein delivery, antimalarial drug delivery

Extract solution of Reseda luteola yellow follower as a biocompatible agent to stabilize silver nanoparticles and their antimicrobial activity

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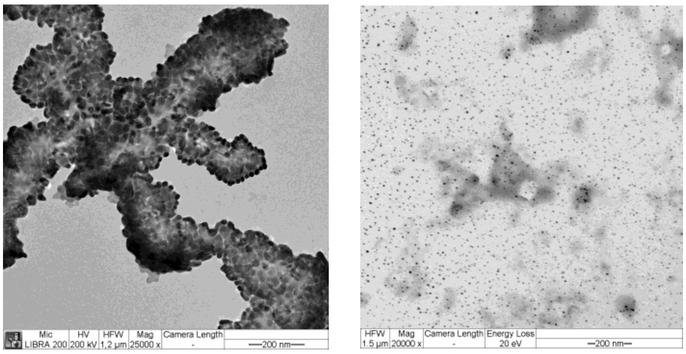
Many methods have been applied to synthesize silver nanoparticles, such as laser ablation, chemical reduction, photo-chemical or radiation-chemical reduction, metallic wire explosion, and sonochemical method. From a practical point of view, chemical reduction from aqueous solutions is the preferred approach to obtain nano-sized silver particles. Chemical reduction nanoparticle preparation basically relies on the chemical reduction of metal salts. Control over the growth of the primarily formed nanoclusters and their agglomeration is an important task and manages to use a variety of stabilizers, in the form of donor ligands, polymers, and surfactants. A number of chemicals have been used as protecting agents in the synthesis of AgNPs such as sodium citrate, CTAB (cetyl trimethyl ammonium bromide), SDS (sodium dodecyl sulfate), PVA (polyvinyl alcohol), PMVE (poly (methylvinylether)). However, the chemical stabilizers are toxic and will pollute the environment. Extensive efforts to more eco-friendly synthesis of nanoparticles have been directed toward using natural components as a stabilizer in the synthesis process such as gelatin, surfactin, starch and chitosan were reported to stabilize silver nanoparticles.

Here we demonstrate a clean method for stabilizing of AgNPs that exhibit antibacterial function. Nanoparticles have been prepared by a chemical reduction method from the aqueous solution of silver nitrate and extract of Reseda luteola yellow follower as a stabilizing agent in the presence of sodium borohydride as a reducing agent. The silver nanoparticles were characterized by dynamic light scattering (DLS), zeta-potential measurements, UV-Vis spectroscopy, and transmission electron microscopy (TEM). The antibacterial efficiency of AgNPs against *Escherichia coli* was investigated. In the presence of Reseda luteola yellow follower extract; the nanoparticles show stability at least for a week. Studies show that the synthesized AgNPs were stable at pH= 3-8 and temperature 25-85°C. Additionally, AgNPs exhibit antibacterial properties especially at the lowest amount of extract to silver ratio ($K_{Extract/Ag}$).



a b

Fig. 1: TEM images of synthesized AgNPs at different concentration of extract a) $K_{Extract/Ag}$=0 b) $K_{Extract/Ag}$= 1

Keywords: silver nanoparticles, Reseda luteola, antibacterial

SWATH-MS proteomics of tissue dissections: Towards analysis of a single cell

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The size and shape of proteins make them very similar to what we define as nanoparticles. Although proteins are different in nature than manmade synthetic nanoparticles, they can play many similar roles as synthetic particles. However, identification and quantification of protein changes in complex and dynamic biological systems with high accuracy, specificity and sensitivity is a demanding task. The complexity of this task is amplified by the fact that populations of cells which were thought to be homogeneous appear to be highly heterogeneous in their phenotype and more importantly their function(s). As technology develops, along with our ever increasing knowledge, the next step in the search of clues related to normal development and disease pathogenesis is analysis at the single cell level. OMICS technologies is a response to this demand and genotyping of single cells is now a reality. This, however, has been much more challenging for classifying proteins.Proteomics does not have the possibility of protein amplification and must rely on increasing the efficiency of sample preparations. Here we present our approachfor global proteomic quantitative profiling of small sections of mouse and humanized mouse brains.

Currently, the vast majority of proteomic quantifications are based on a mass-spectrometric bottom-up approach: multiple parameters acquired from instrumental analysis are assembled into one value of protein change. Recent advances in mass spectrometry has led to the development an emerging platform known as Sequential Window Acquisition of all Theoretical-Mass Spectra (SWATH-MS). Even though SWATH-MS is based on the principal of data-independent acquisition (DIA), data extraction from SWATH-MS analyses requires a reference library of spectra generated in data-dependant acquisition (DDA) mode.Thus libraries of spectra are necessary for protein identification while spectra acquired using SWATH-MS mode are used for quantification. A major goal of protein identification and quantification is being achieved by incorporating DDA and DIA approaches with SWATH-MS acquisition.

Many diseases are specific for humans only and study of the pathogenesis requires creation of specialized animal models. In recent years such models based on humanized mice have been created. These models provide a unique opportunity to have an insight into the function of human cells and proteins in the context of living tissue of model organism. The detection, characterization and measurement of manmade synthetic nanoparticles administered into such animals seems straightforward; however, sorting out the impact of proteins originating from different species is an additional challenge to precise and accurate quantification.

We explored whether proteins could be extracted and proteolytic peptides recovered from formalin fixed and paraffin embedded (FFPE) tissue samples. This is a significant step towards single cell proteomics with archived *ex vivo* materials of complex mouse-human chimeric tissues. We will present approach to SWATH-MS data analysis comparing acquisition performed on cell lysates and eight FFPE brain sections and challenges associated with this process. The overall scheme of data analysis is summarized in figure below.

Proposed method

Ion peak area $= x_{ijkl}$

↓

Remove ion outliers : Grubbs' test

↓

$$\text{Peak area for } j\text{th peptide} : x_{.jkl} = \frac{\sum_{i=1}^{n_{jkl}} x_{ijkl}}{n_{jkl}}$$

↓

$$\text{Peak area for } k\text{th protein} : x_{..kl} = \frac{\sum_{j=1}^{n_{kl}} x_{.jkl}}{n_{kl}}$$

Keywords: mass spectrometry, single cell analysis, proteins, SWATH-MS

Antibacterial activity of nanostructured composite materials under daylight irradiation

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During the past few years there has been a remarkable growth of research activities exploring properties and biomedical applications of nano-sized materials. Size, shape, size distribution, morphology, surface functionalization and stability of nanomaterials have an influence on resulting biological and other effects of nanomaterials.Due to the unnecessary overuse of antibiotics in the second half of the 20th century, mankind must face the incidence increase of resistant and/or multiresistant bacterial strains, which may significantly decrease the efficiency of current medical treatment, contribute to the development of various chronic diseases and even increase mortality. Therefore, a number of research groups all over the world are aiming to find and develop new antibacterial agents which could help to solve this persistent issue. Nanoparticles or nanomaterials could potentially represent the new medicines because no acquired bacterial resistance after application of nanomaterials has been observed yet. Fast, cheap and user-friendly method for the evaluation of antibacterial activity suitable for rapid screening of antibacterial potency of a single material among a number of developed nanomaterials needs to be designed. After this fast appreciation where the basic information about the antibacterial activity of the nanomaterial is obtained subsequently researchers can focus on some nanomaterials without wasting time and money with unpromising ones. With regard to the above mentioned, a modification of the standard microdilution method was designed and the antibacterial activity of photoactive composite kaolinite/nanoTiO_2 was evaluated under the daylight irradiation. It was found that the modification of standard microdilution method can be used for in vitro screening of antibacterial activity of photoactive nanocomposite materials. Therefore it was decided to further apply the modified evaluation method to other prepared nanocomposite materials. Next studies were focused on daylight induced antibacterial activity of ZnO/kaoline and kaoline/ZnO nanocomposite where the developed screening method was utilized for another nanocomposite material. Thanks to the developed method differences in the antibacterial activity among the nanocomposites can be compared and importance of the way of preparation or chosen matrix can be deduced.

Keywords: nanocomposites, antibacterial, S. aureus, SEM

Degradation of Warfare agents using bio-gold nanoparticles

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In this work the suspension of bio-gold nanoparticles synthesized by use of *Mallomonas kalinae* (MK) was prepared. Biosynthesized gold nanoparticles were characterized by transmission electron microscopy (TEM), atomic emission spectroscopy with inductively coupled plasma (ICP-AES) and X-ray diffraction (XRD). The cell suspension of MK contains crystalline gold nanoparticles with the diameter size from 7 nm to 14 nm.

Bio-gold nanoparticles and cellular debris of MK was used as a catalyst for hydrolysis of nerve agents Soman (GD) and VX. Degradation of nerve agents was observed by gas chromatography with the mass selective detector and solid phase extraction. The catalytic activity of gold nanoparticles for the degradation of nerve agents was compared with the hydrolysis in demineralised water and in the presence of pure MK cells.

The catalytic activity of the suspension may be supported by specific surface area of gold nanoparticles and also by silica matrix of MK. The siliceous algal structures are able to absorb GD and VX where active places with -OH groups are present. Degradation of warfare agents may also be supported by enzymes in cells [1]. The degradation of VX by pure biomass indicates that an enzyme-promoted hydrolysis may occur. In the presence of gold nanoparticles faster degradation of GD and VX in comparison to the control hydrolysis experiments was observed.

These are the first experiments using bio-gold nanoparticles immobilized on silica shells as the catalyst for degradation of warfare agents. The work will continue by modifying of the bio-gold suspension to increase its catalytic activity, for example preparation of bimetallic nanoparticles such as gold-iron or gold-zirconium [2, 3]. Other possibility could be the increase of pH values to alkaline area.

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Keywords: nanoparticles of gold, biosynthesis, degradation, Soman, VX

Overcoming blood-brain barrier using nanoparticles

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Although many agents have therapeutic potential for central nervous system (CNS) diseases, few of these agents have been clinically used because of the brain barriers. The blood–brain barrier (BBB) is the last, critical and serious obstacle for the permeation of drugs that require CNS action. The BBB represents a structure with complex cellular organization that separates the brain parenchyma from the systemic circulation. The structure of the BBB can be described as “bricks and mortar” model; it also acts as a metabolic barrier due to the presence of numerous enzymes. These enzymes can either metabolise potentially harmful drugs to CNS-inactive compounds or convert inactive drugs to their active CNS metabolites or degrade them into metabolites or substrates of specific efflux transporters.

All the above mentioned properties of the barrier result in strong selection of permeating drugs depending on their physicochemical properties, such as molecular weight, molecular volume, lipophilicity, ionisation state and/or their affinity to specific transporters (uptake/efflux transporters). The cellular organisation of the BBB and the presence of transmembrane proteins enable a selective regulation of the passage of molecules from the blood to the brain. Molecules present in the blood stream can reach the CNS by two different pathways, the paracellular pathway (through tight junctions) and the transcellular pathway (through endothelial cells). Molecules that reach the CNS via the transcellular pathway can diffuse passively, be actively transported by specific transporters or undergo endocytosis. To circumvent the BBB and allow an active CNS compound to reach its target, many strategies exist. They can be sorted with respect to the BBB as either invasive (direct injection into the cerebrospinal fluid or therapeutic opening of the BBB) or non-invasive such as the use of alternative routes of administration (e.g., nose-to-brain route, olfactory and trigeminal pathways to brain), inhibition of efflux transporters, chemical modification of drugs (prodrugs, bioprecursors) and encapsulation of drugs into nanocarriers (e.g., liposomes, polymeric nanoparticles, solid lipid nanoparticles).

Nanoparticles as drug carriers have also been extensively studied recently. Their uptake into the brain is hypothesised to occur via adsorptive transcytosis and receptor-mediated endocytosis. Particle size, surface affinity and stability in circulation are important factors influencing the brain distribution of colloidal particles. This contribution is focused on the current approaches to facilitate penetration across the BBB for enhancement of drug delivery to the CNS by means of various types of nanoparticles/nanocarriers.

Acknowledgement

This study was supported by GACR P304/11/2246.

Keywords: Blood–brain barrier, Drugs, Permeation, Nanoparticles

New bimetallic catalysts: synthesis and applications

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Over the past few years, a number of techniques have been developed for the production of nanosized metallic particles and their distribution on different carriers. The methods recently used, which are based on the “bottom-up” and the “top-down” approaches, still have some disadvantages, including broad nanoparticle size distributions and a tendency to aggregate or to form clumps.
During the lecture we will discuss general problems of nano bi- (poly) metallic synthesis and applications in catalysis.

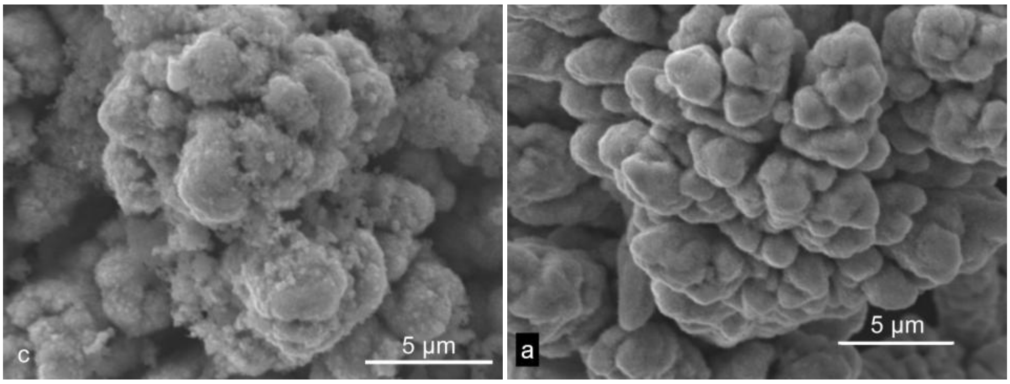

Fig. 1: Electrolytic Cu (a) and Nano-Pd in silica debris on the surface (b).

To minimize synthetic problems, we have recently developed a novel, innovative method for the formation of bimetallic catalysts [1-3]. We have prepared a variety of such catalysts that appeared to be highly efficient in a variety of reactions from Sonogashira coupling to glycerol oxidation. Our recent interests include especially ammonia cracking, where Nano-Pd on Ni appeared to be an interesting bimetallic combination. This method provides here interesting capabilities for the potential production of industrial catalysts including relatively low-cost Ni, e.g., in the form of wire meshes, provides not only a catalytic moiety but also a flexible catalyst support. This discovery is significant because hydrogen production from ammonia appears to be a difficult problem. Ammonia decomposition is a complex process that proceeds through stepwise dehydrogenation (NH_3 - $H \rightarrow NH_2$ - $H \rightarrow NH$ – $H \rightarrow N$) and yields H and N, which recombine to H_2 and N_2, respectively.

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Acknowledgement
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Keywords: Nanocatalysis, Sonogashira coupling, ammonia cracking, glicerol oxidation

PLGA-g-PVP amphiphilic bioactive and biocompatible copolymers for fabrication of nanostructured materials

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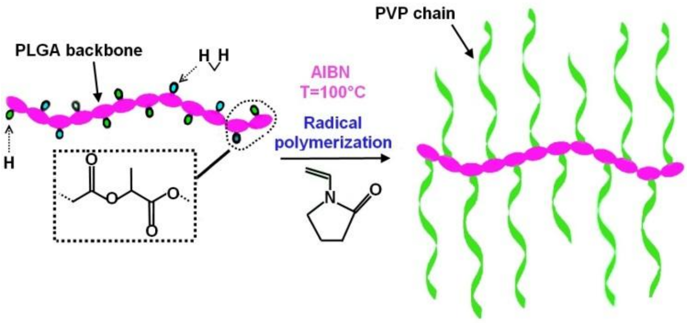
The aim of this work is to present a one-pot synthetic process leading to poly(lactide-co-glycolide)-g-poly(vinylpyrrolidone) (PLGA-g-PVP) copolymers consisting of high molecular weight PLGA carrying oligomeric PVP side chains. The title copolymers were prepared by chain transfer radical polymerization of N-vinylpyrrolidone in the presence of 50:50 PLGA, acting as polymeric chain transfer agent in the absence of solvents.



All copolymers were characterized by ^{1}H-NMR (400 MHz), FT-IR, SEC, MALDI-TOF, DSC, TGA and DLS techniques. PLGA is a lipophilic biodegradable polymer, whereas PVP is hydrophilic, biocompatible and also bioeliminable for molecular weights < 40.000. Both polymers have been approved for human use by the U.S. Food and Drug Administration, therefore the PLGA-g-PVP copolymers are eligible for medical applications. The water-soluble PVP portion imparts amphiphilicity to the otherwise hydrophobic PLGA, thus modifying its behavior in aqueous systems. In particular, PLGA-g-PVP samples spontaneously form nanoparticles when dispersed in water. In addition, PLGA-g-PVP samples, when used as additives, dramatically improved wettability of hydrophobic materials, as for instance polyesters, processed as nanofibers and intended for applications involving contact with the body fluids.

Procedures were established to fractionate the PLGA-g-PVP copolymers by selective precipitation and fractions analyzed. Four main fractions with different PLGA/PVP compositions were obtained, containing no residual homopolymers. Both fractions and unfractionated copolymers were used to obtain nanoparticles using different methods. In particular, the solvent evaporation method, gave nanoparticles acetone/water mixtures. For comparison purpose, the same procedure was followed with plain PLGA, PLGA/PVP- and PLGA/PLGA-g-PVP blends. The resultant nano-suspensions were characterized at different times by DLS for their size and z-potential. Nanoparticles obtained from PLGA/PLGA-g-PVP blends turned to be the best performing systems in terms of dimensions and suspension stability.

These nanoparticles, besides being suitable as carriers for hydrophobic drugs, for instance antimalarial drugs, compared with plain PLGA are expected to display better compliance many drugs known to interact with PVP.

Keywords: PLGA, poly-N.vinylpyrrolidone, nanoparticles

Nanoseparations in biosciences

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Nowadays analysis at nanoscale demands development and application of ultrasensitive techniques capable of identification and quantitation of minute amounts of complex, biological samples. Together with mass spectrometry, such approach comprise of an efficient tool for a thorough analysis of biomolecules, such as peptides, proteins, metabolites, isolated from living organisms (cells, tissues, body fluids). One of the spectacular applications of such approaches are proteomics and metabolomics.

Due to the minute amounts of biological material at femto/at tomolar level, and ultra small volumes, far below microliter, these methods bear many technical difficulties and a good experience of the operators is highly advisable to be able to deal with system diagnosis and small volume handling. An attractive "nanoscale" system is certainly of strong interest among researchers, but potential benefits should not obscure a basic rule that a combination of several experimental techniques adds their features but also adds all their individual problems, with few extra as a bonus.

The lecture will focus on the nano/micro scale sample handling techniques, frequently applied in biomedical analysis, including capillary LC/MS, multidimensional LC/MS, electrochemical simulation of metabolites), including practical applications.

Acknowledgement
This work was supported by the "META" grant 5/EuroNanoMed/2012.

Keywords: nanoseparations, proteomics, metabolomics

Novel one-step synthesis of silver nanoparticles using plant extract

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Nanotechnology as science about producing structures, devices and systems with one dimension between 1 and 100 nm. In our research plant extracts obtained from different kind of plant were applied for green synthesis of silver nanoparticles. The selected plant was extracted in Soxhlet apparatus, using water as solvent.

We use *Rhodiolarosea L., Zingiberofficinale* and *Betula L.*

All chemicals were of reagent grade and used without further purification. Silver nitrate, was purchased from POCh (Poland), poly-N-vinyl pyrolidone (PVP) was purchased from Sigma Aldrich.

The SEM image was obtained on a JEOL JSM 7500F with BSE detector (*Back Scaterred Electrons*). A drop of the sample solution was allowed to dry on a copper holder coated with chromium film.

Dynamic light-scattering measurements were performed in a Malvern Zetasizer Nano ZS apparatus (Malvern Instruments, Milan, Italy) at 25 ºC and started 2 min after the cuvette was placed in the DLS apparatus to allow the temperature to equilibrate. Measurements were carried out 24 h after the preparation of the suspensions.

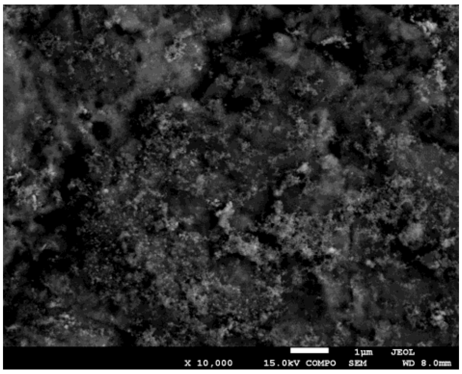

Image 2. SEM-BSE image of silver nanoparticles obtained at room temperature (Rhodiolarosea L.)

The mean diameter of silver particles prepared by our team reaches a 1,50 ± 0,43nm. After synthesis size distribution was narrow, however there was a few aggregates, but big cluster were not formed. Image 1 presents size distribution of AgNPs obtained at 10˚C determined by the DLS technique. The formation of silver nanoparticles was investigated by scanning electron microscopic images, given in Image 2. The silver nanoparticles are regularly, without a significant diversity of particle size and shape, however during preparation to SEM investigations particles formed agglomerates with irregular shapes. The silver nanoparticles were mostly spherical.

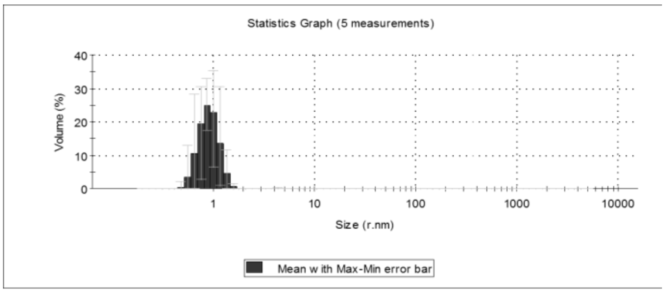

Image 1. Size distribution of AgNPs obtained at room temperature (Rhodiolarosea L.)

Acknowledgement

The authors would like to thank The Ministry Science and Higher Education (Grant no:0628/IP2/2013/72) for providing financial support to this project.

Keywords: plant extract, silver nanoparticles, DLS, SEM

Preparation of submicron particles and nanoparticles of biologically active compounds using supercritical fluid

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This research is aimed on a preparation of submicron particles and nanoparticles of biologically active compounds with using commercially available device destined for supercritical fluid extractions. Methods for utilization of supercritical CO_2 with and without addition of modifier were used. Prepared products were characterized by using SEM and particle size distribution methods.

Most of drugs are only slightly soluble in the circulatory system of the human body. This fact decreases efficiency of their utilization, thus new ways how to increase drugs' solubility are investigated. One way is to reduce their particle size. This leads to increase in specific surface area and to increase the reactivity and solubility. Conventional techniques such as crushing or grinding usually do not guarantee a narrow particle size distribution, which is required in pharmaceuticals. Application of supercritical fluids, especially of supercritical CO_2(scCO_2) or supercritical water (scH_2O), is very convenient method for the preparation of submicron particles or nanoparticles of pharmaceuticals. The method enables the preparation of particles in a narrow size distribution and at the same time they do not leave any unwanted residues of solvents or other chemicals.

The stimulant caffeine and two commercially available drugs cimetidine and hydrochlorothiazide were used as precursors. The caffeine was used as a model compound for application of the easiest method using scCO_2 – the method of rapid expansion of supercritical solution. The other compounds were chosen because they are insoluble in scCO_2, thus it was necessary to use preparation method in which scCO_2 is used as an anti-solvent. The aim was. 1)to prepare nanoparticle drugs in the narrowest distribution range of sizes and 2) to determine the conditions under which the particle size distribution is the narrowest and particle size is the lowest. Only pressure and temperature values were combined in various ways with respect to compounds properties and time length of the processes. The products were characterized with using SEM and particle size distribution analyses. Changes in the particle size were observed in the SEM images of modified drugs prepared at different pressures, temperatures and times. The drug size was reduced to size range from nm to several μm. The results were supported by particle size distribution analyses.

Acknowledgements
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Keywords: biologically active substances, supercritical fluid, Spe-ed SFE 4, nanoparticles

Hybrid materials based on luminescent alkaloid berberine and saponite

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Hybrid materials including natural bioactive substances attract much attention due to their unique properties and potential applications. Berberine (Berb) represents an alkaloid produced in the cells of specific plants. It is cationic, photoactive and luminescent dye, which changes its properties upon the illumination with UV or visible light.

Hybrid materials based on synthetic layered silicate saponite (Sap) and Berb were investigated from two viewpoints: photochemical properties and antibacterial effectiveness. Photoactivity of the hybrid materials were investigated by means of absorption and fluorescence spectroscopy. There were some slight differences between the spectral properties of the dye in solution, in the colloidal dispersions with Sap and intercalated in thin films of the hybrid material. However, no significant molecular aggregation was observed for the systems with relatively low concentrations which is very important for photophysical properties of the dye. The results of X-ray diffraction and linearly-polarized absorption spectroscopy of the hybrid films helped to design molecular arrangement of the dye cations intercalated in Sap films. Berb cations were oriented flat with respect to the plane of Sap, forming a single molecular layer. This orientation is in agreement with charge distribution in the molecule and enables efficient electrostatic bonding with negatively charged Sap surface.

Experiments with Gram-positive bacterium *Staphylococcus aureus* was evaluated by the cell survival (CS) tests. Samples of the hybrid colloids were illuminated with blue laser (445 nm, 500 mW, 100s) or cold white LED light (electric power 100 W, 5 h) and compared to the identical specimens cultivated under dark conditions. Results proved antimicrobial properties of the Berb/Sap colloid (1 mmol/g) reducing CS to 22 and 35 % for the samples illuminated with laser and LED lights, respectively. Bacteria grown in the presence of Berb solution of the same dye concentration (10^{-4} mol L^{-1}) exhibited higher CS; 77 and 84% for laser and LED light, respectively. The samples that were not illuminated grew up to 98% compared to the control sample without Berb (100%). Presented results indicate perspectives of similar hybrid materials incorporating natural bioactive substances in hybrid materials.

Acknowledgements
This work was supported by the Slovak Research and Development Agency under the contract No. APVV-0291-11, Grant Agency VEGA (2/0107/13, 1/0943/13), and grant UK/16/2014.

Keywords: berberine, cationic dyes, layered silicates, hybrid materials, Staphylococcus aureus, antibacterial properties

Hepatotoxicity and cardiotoxicity of mitoxantrone, vitamin C and anacardic acid liposomal formulation

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Our recent data shown that AA (anacardic acid) when added to liposomal formulation increase the number of surviving normal cells (NHDF-normal human dermal fibroblasts) in a manner dependent on incubation time and concentrations of liposomes with AA in the medium. Whereas the opposite effect its seen in the case of cancer cells (A375, Hs294T- melanoma cell lines). These results suggest that anacardic acid has dual mechanism of action due to type of cells.

The aim of this project is verification of anacardic acid and vitamin C ability to protection HepG2 cells (human liver hepatocellular carcinoma cell line) and H9C2 (rat heart myoblast cell line) against mitoxantrone– the compound with previously proven a hepatotoxic and cardiotoxic activity.

We examined the viability of both type of cell lines treated with mitoxantrone loaded liposomes with and without anacardic acid and vitamin C, also we checked the level of released LDH (lactate dehydrogenase) from cells. It is of medical significance, because it is released during tissue damage. LDH is found extensively in body tissues, such as blood cells and heart muscle.

One of proven mechanizm mitoxantrone toxicity is ROS (reactive oxygen species) production. We determined the level of ROS by measuring the total peroxidation of cells bilayers - TBRS method. We examined also the physiological and morphological state of cells after treatment with liposomes.

Our results indicate that anacardic acid and vitamin C have protective effect on heart muscle cells and liver cells against mitoxantrone toxicity. However this effect is observed only in liposomal formulations with 5 and 10% molar ratio of AA. Increased amount of anacardic acid makes higher toxicity towards both types of examined cell lines. These results suggest that is some ratio of anacardic acid and vitamin C we can observe synergistic protective effect against mitoxantrone mediated cell damage.

Keywords: mitoxantrone, hepatotoxicity, anacardic acid, cardiotoxicity

The study of heat shock protein Hsp70 and its meaning for medical aims

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Heat shock proteins are a class of proteins capable of correcting the spatial structure of the damaged polypeptides (i.e. have chaperone activity), transporting polypeptide molecules to destinations in the cell and contribute to the degradation of irreversibly damaged protein macromolecules. Inducible Hsp70 protein is representative of the family of heat shock proteins with a molecular weight of about 70 kDa. Heat shock proteins are required in all cell processes of its vital functions, including adaptation to a huge number of cytotoxic factors, such as xenobiotic and natural origin. Hsp70 is a first protein called chaperone. The function of chaperones in the cell is that they bind to newly synthesized or damaged polypeptides and help them to take their native conformation; chaperones are also involved in the delivery of proteins to certain organelles. Hsp70 is one of the members of the family of heat shock proteins, for which the chaperone mechanismis well studiedby now. Through this mechanism, Hsp70 has a dual role: it corrects the structure of newly synthesized or damaged polypeptides or promotes a degradation of "incorrigible" proteins in the proteasome. With the chaperone activity are related to many functions of Hsp70 in the cell and outside - protective and immunomodulating. Despite the huge number of studies on various aspects of the functioning of Hsp70, there are still many issues, which are fundamentally important. Although Hsp70 is inducible, that implies a keen increase of its expression in response to stress, its synthesis in human cells, although at a low level, occurs under normal conditions. It should be noted that in different tissues and cells of an organism the expressing degree of Hsp70 is different. For example, it is very high in the heart tissue, and very low (and is not initiated in response to stress) in some types of neurons in the brain. The expression level of Hsp70 is high in tumors, especially malignant. In connection with this, a number of questions arises. What are the consequences of high Hsp70 expression level in tumor cells? It is not clear how the nerve cells are protected from adverse factors, for example, from a formation of insoluble protein aggregates in the brain nerve cells at some hereditary neurodegenerative diseases (like Alzheimer’s and Parkinson’s diseases) and in the brain cells of elderly people. Several years ago, there appeared some data that Hsp70, previously considered as an exceptionally cytoplasmic protein, can be located in the extracellular space, in human biological fluids. Because of the above features, the protein Hsp70 is of considerable interest for the new therapeutic technologies development. The aim of this study was the selection of heat shock protein Hsp70, as wellas the study of its structure. Expression system was chosen, which allows to express soluble recombinant heat shock protein Hsp70 in large quantities; cloning of the gene from mammalian cells to E.coli cells and a creation of a bacterial strain producing the heat shock protein Hsp70; the selection of conditions and optimization of methods for isolation and purification of heat shock protein Hsp70; identification of the obtained recombinant heat shock protein Hsp70 by Western blot analysis; a preliminary study of the structure of heat shock protein Hsp70 by small-angle X-ray scattering (SAXS).

Keywords: heat shock protein, chaperone, neurodegenerative diseases

Application of microbial and plant extracellular metabolites in nanostructure fabrication

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The aim of this work is to evaluate application of microbial and plant extracts and extracellular metabolites in nanoparticle synthesis, while using "green chemistry principles" for technological applications.

In hypegenic zone of sub-aquatic and anaerobic environment, specific interactions between organic and inorganic components take place, including biological synthesis of inorganic nanoparticles. This established new biotechnological discipline called bionanotechnology. Its main principle is inspired by 2D and 3D biological (evolutional) structure formation and natural bio-geochemical processes. Bacterial, algal, fungal and plant extracts pose unique immobilization potential. At their presence, mobile metal species transform into stable, non-reactive, and non-soluble nano-forms. This transformation process includes reduction, conversion, and catalytic alteration mechanisms. Nucleation is usually initiated by enzymatic oxidation or reduction of dissolved metal, its accumulation and sorption by the outer membrane, and bonding to peptides and proteins, followed by efflux and precipitation. This decreases metal distribution, mobilization, bioavailability and potential toxicity, as well as affects its distribution and speciation. Biological crystallization of inorganic materials applying "green chemistry principles" poses notable technological and industrial advantages. Formation and development of nanoparticles can be presented by two different methodological principles - "top-down" and "bottom-up". There is some evidence that technological and scientific innovation is more interested in application of bottom-up mechanism which is based on self-assemblage or precise (2D linear or 3D structural) coordination of atoms and molecular building blocks. Therefore, biological components, enzymes and other biomolecules play a key role in nucleation and fabrication of "new" thermodynamically stable crystalline phases. Application of relative stable materials, kept in the nanoparticle size distribution, provides many technological advantages due to their unique physical, chemical, optical, and magnetic properties. Biological nanostructures, nanomaterials, nanocomposites, and bionano templates have considerable influence on medical, pharmaceutical, textile, electrotechnical, biotechnological and other industries. Due to these reasons potential is still not depleted in environmental and agricultural disciplines. Implementation of various microbial biomolecules and plant tissues in nanoparticle generation underlines the significance of biotransformation specificity and non-toxicity.

Keywords: Biogeochemistry, bionanotechnology, microorganisms, plants, technology application

Anticancer activity of the novel liposomal formulation of the curcumin against human cancer cell lines

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BACKGOUND: The purpose of this study is to design a stable liposomal formulation for the anticancer drug Curcumin. Curcumin is a food chemical presents in turmeric (Curcuma longa) that has pharmacological activity to suppress carcinogenesis and inhibits multiple singling pathways. The poor aqueous solubility and low bioavailability of curcumin restrict its clinical activity; however, a liposomal formulation of curcumin was developed to improve drug delivery for cancer treatment.

METHODS: Curcumin was encapsulated in a liposomal delivery system. The liposomal curcumin was characterized in terms of basic parameters; as, the size, encapsulation efficiency and stability. The cytotoxicity was assessed using two different cell lines, human pancreatic human cell line (AsPC-1) and adenocarcinomic human alveolar basal epithelial cells (A549). Two methods of liposome preparations were used, the first one was applying 100 mM Glycine pH 6.4 and the second one was applying 300mM ammonioum ascorbate pH 4.0.

RESULTS: The encapsulation efficiency was>90% for a drug-to-lipid molar ratio of up to 0.1 for both formulations. The results showed liposomal curcumin which prepared with Vitamin C had a higher cytotoxicity toward AsPC-1 compared to liposomal curcumin hydrated with Glycine buffer. As for, A549 cell line, liposomal curcumin prepared with Glycine buffer had a higher cytotoxicity compared to curcumin prepared with Vit C.

CONCOLUTIONS: The formulation combing of two natural products (Vitamin C and Curcumin) showed a promising results in terms of cytotoxicity toward pancreatic cancer**.**

Keywords: Liposome, Curcumin, Vitamin C, Cytotoxicity

Phytosynthesis of gold nanoparticles using medicinal plants

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The aim of this work was to perform preliminary experiments with phytosynthesis of gold nanoparticles (GNPs) by reducing chloroauric acid ($HAuCl_4$) with two different medicinal plants – linden and coltsfoot. Phytosynthesis of nanoparticles is eco-friendly and cost-effective [1]. On the other hand the medicinal plants may have important influence of human health.

Leachates from each plant were mixed with $HAuCl_4$ (1mM) in ratio 1:1. The interaction of reducing compounds contained in plants with aqueous salt promoted the precipitation of metallic nanoparticles. Moreover, the plant extracts contain reducing agents and compounds with stabilizing effect on the GNPs. Generally the duration of phytosynthesis depends on the plant species. The 1st color changes of suspension containing coltsfood with $HAuCl_4$ were observed after 24 h. In the case of linden gold nanoparticles were synthesized very quickly – in the course of few minutes.

The formation of GNPs was tracked visually and their characterization was performed using light microscopy and transmission electron microscopy (TEM).

The gold nanoparticles obtained by these phytosynthesis could potentially be used in different biological and medical applications [1].

Reference

[1] Husen, A. a K. S. Siddiqi. Phytosynthesis of nanoparticles: concept, controversy and application. *Nanoscale Research Letters*. 2014, vol. 9.

Keywords: phytosynthesis, gold nanoparticles, medicinal plants, linden, coltsfoot

Bioactive calcium phosphates of natural origin

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This work presented method of obtaining hydroxyapatite from trabecular and cortical animal bones. Bones are firstly deproteinised and defatted via acidic hydrolysis process of pork bones. Hydroxyapatite was received in calcining process in two stages at rotary kiln. Bone sludge and calcining products were characterized with X-ray diffraction method (XRD); Fourier transformed infrared spectroscopy (FT-IR) and scanning electron microscopy (SEM-EDS). Calcium was determined with titration whereas phosphorus was determined with the spectrophotometric method. Content of microelements were determined by the ICP-MS method. In all the products hydroxyapatite was the only one crystalline phase indicated. FT-IR spectra confirmed that the whole organic substances were removed during calcining process. Calcium and phosphorus contents was 38% and 18%, respectively that was responded to molar ratio Ca/P of nonstoichiometric hydroxyapatite.

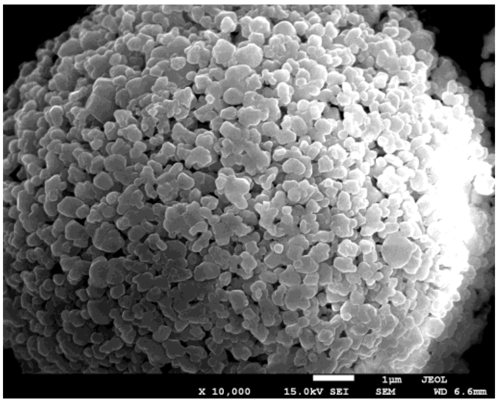

Fig. 1. SEM image of natural hydroxyapatite extracted from trabecular bone.

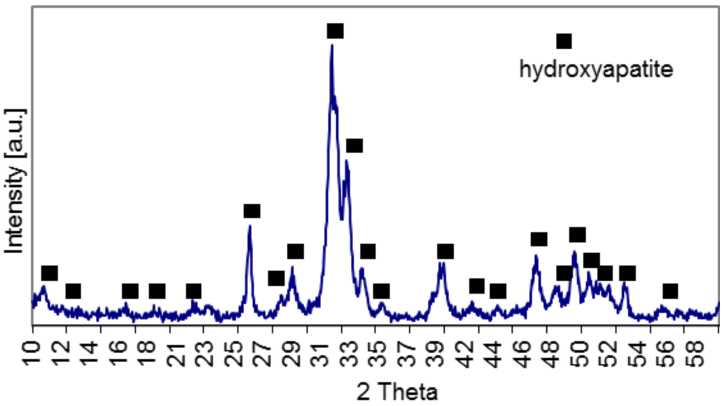

Fig. 2. XRD pattenr on natural origin hydroxyapatite

Investigations in physiological fluids were realized. The aim of tests was to evaluate chemical durability of natural origin materials. In tests Ringer solution, artificial saliva and SBF - Simulated Body Fluid were applied.

Acknowledgement

The authors would like to thank the The National Centre for Research and Development (Grant no: LIDER//037/481/L-5/13/NCBR/2014) for providing financial support to this project.

Keywords: calcium phosphates, hydroxyapatite, bone tissue, biomaterial

Preparation and properties of ZnO/vermiculite nanocomposite modified by the chlorhexidine

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In the last few years, the organic-inorganic nanocomposite materials have drawn tremendous attention to the field of nanomaterial science because of their multiple applications. The primary focusis on the ability to obtain control of the nanoscale structures via innovative synthetic approaches. The final properties of nanocomposite materials depend not only on the properties of their individual parents, but also on their morphology and interfacial characteristics. The general class of organic-inorganic nanocomposites may also be of relevance to issues of antibacterial materials in which layered nanocomposites represent an extreme case of a composite in which interface interactions between the two phases are maximized. As for the carriers, clay minerals have proven to be the best possible host for organic molecules, due to their layered structure. Nanocomposite materials on the base of zinc oxide and chlorhexidine nanoparticles as fillers in layered structures are widely known as a chemical antiseptic and antibacterial agent. Extremely effective in destroying gram-negative and gram-positive organisms. Chlorhexidine nanoparticles as organic phase can be prepared in different concentrations as a part of a solution or as an ingredient in antibacterial products.

This work deals with nanocomposites based on vermiculite/ZnO/chlorhexidine prepared by mechanochemical activation followed by intercalation. Vermiculite has been used as inert matrix especially for its ability to expand its volume and accept huge chlorhexidine molecules into its crystal structure.Character and shape of nanocomposite particles 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).

Acknowledgements

This work was supported by the project No. SP2015/18 - Functional gradient nanostructured materials and CZ.1.05/1.1.00/02.0070 – IT4 Innovations Centre of Excellence project.

Keywords: chlorhexidine, zinc oxide, vermiculite, nanocomposite particles.

Preparation of bioactive wound dressings based on chitosan of bee origin

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Bioactive wound dressings are the most modern generation of dressing materials, which are decisively different from traditional dressings. They maintain appropriate healing environment, interact directly with the healing process, act as a protective form a barrier against microorganisms, do not adhere to the wound and do not move - they remain in the place of application, and they also reduce the frequency of changing the dressing. In addition, they do not cause allergic reactions and toxic effects.

Hydrogel dressings are a mixture of natural and synthetic polymers, and contain about 75% water. Hydrogels, which are biocompatible and biodegradable, play a very important role in biomedical, pharmaceutical and tissue engineering. Biomedicine is a branch of medicine that combines the achievements of biological sciences, chemistry and biotechnology in the context of human health and diseases. In contrast, tissue engineering uses medical knowledge and materials engineering methods in order to achieve functional replacements of damaged tissues and organs.

The bioactive wound dressings were to obtain Beetosan® - chitosan from exoskeletons (armours) of bees. Typically extraction of chitin from armour of the bees is carried out in the following manner: dead bees are crushed, then proteins and calcium carbide are removed chemically. Enzymatic deacetylation of chitin is an interesting alternative to the chemical process. Thin and soft bees' armours are well suited for the mild conditions of the process, which generates significantly less waste than conventional chemical process. Enzymatic modification also allows to carry out the process under controlled conditions, which would enable the production of Beetosan with a predetermined degree of acetylation.In chemical terms, chitin has a structure similar to cellulose, however, it contains *N*-acetyl-D-glucose-2-amine units, which form long polymeric chains joined with β-1,4-glycosidic bonds. Chitosan, on the other hand, is a derivative of chitin and is formed in the reaction of N-deacylation (Fig. 1).

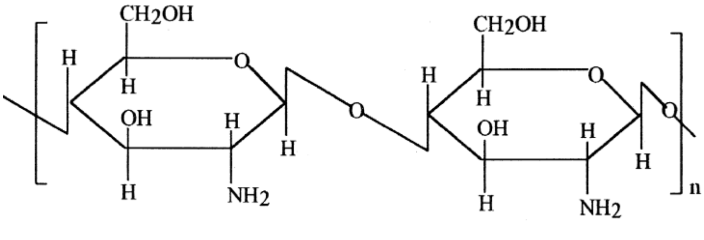

Fig. 1: Chitosan structure.

Acknowledgement
The authors would like to thank the The National Centre for Research and Development (Grant no: LIDER/033/697/L-5/13/NCBR/2014) for providing financial support to this project.

Keywords: Beetosan, Chitosan, Wound dressings, Hydrogel

Characterization of cimetidine nanoparticles for solubility test

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Cimetidine (1-cyano-2-methyl-3-(2-{[4-methyl-1*H*-imidazol-5-yl)methyl]sulfanyl}ethyl)guanidine) is a histamine H2-receptor antagonist that inhibits stomach acid production. It was used as a gastroprotective drug, butis no longer used in medicine;however it is aconvenient model compound due to its physicochemical properties. Cimetidine belongs to the Biopharmaceutical Classification System (BCS) Class III. Although itsaqueous solubility determined in the pH range 1–8 at 37 °C is only approximately6 mg/mL, by means of *in vivo* experiments the permeability rate-limiting properties of cimetidine drug products wereconfirmed, i.e. similar results as for other BCS Class III drug substances were obtained.

This study was designed to improve and increase aqueous solubility of cimetidine via preparation of nanoparticles, usingevaporative precipitation into aqueous solution.Acetone was chosen as a polar solvent that was more preferable for a number of prepared nanoparticles in comparison with the non-polar solvent used in the study. Cimetidine was solved in acetone, and 1% concentration was prepared. Water solution of macrogol 6000 was used as an excipient in 5% concentration. These two solutions were mixed together for 15 minutes, and then an ultrasound bath was used for elimination of acetone.All the preparednanoparticles were characterized by dynamic light scattering,zeta potential, scanning electron microscopy and FT-MIR spectroscopy.

Acknowledgements
This study was supported by GACR P304/11/2246, by the European Regional Development Fund in the IT4Innovations Centre of Excellence (CZ.1.05/1.1.00/02.0070), project Ministry of Education, Youth and Sport of Czech Republic SP2015/56 and also by the Slovak Research and Development Agency Grant No. APVV-0516-12.

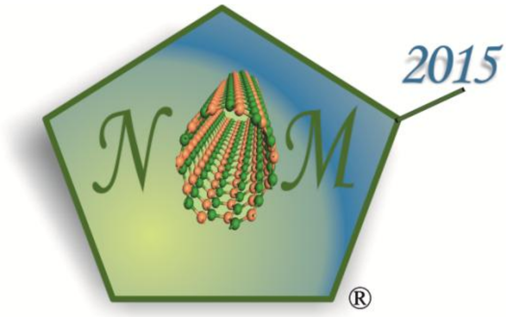
Keywords: Cimetidine, Nanoparticles, Solubility, Precipitation

TOPIC 3

Nanostructure materials in electronics and optics

Chair: Michael Cada
Co-chair: Ivo Vávra

Nanotechnology for electronic devices
Optoelectronics and magnetooptics
Numerical modeling methods and simulation



Plasmonics in Semiconductors

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Interactions of electromagnetic waves with charge particles have been investigated for many decades. Examples include propagation of radio waves in ionosphere (plasma medium) or discharge phenomena in vacuum tubes. In recent decades interest has focused on interactions with free electrons in metals. Collective behavior/oscillations of free electrons existing in metals in huge concentrations have been studied by describing the electron gas as some sort of a charged liquid whereby, as a result, electromagnetic waves can travel possessing a longitudinal component.

A great deal of quality interesting results has been reported on existence of surface plasmons and surface Plasmon polaritons occurring at an interface between a metal and a dielectric. Numerous applications of these plasmonic effects have been demonstrated experimentally, such as chemical or biological sensing, signal processing, super-resolution imaging, lasing, and many others. Plasmonics is thus an exciting field of research and applications development due to its unique characteristics in terms of localizing and controlling light properties.

Semiconductors are the most versatile materials known that enable one to literally tailor their electrical and optical properties to achieve desired functionalities. Doping is one of the technological processes that makes semiconductors very attractive and, indeed, successful in implementing a large variety of devices, circuits, and systems. Heavily doped semiconductors have proven to be an interesting alternative to metals as the levels of free carrier concentration can approach the ones in metals to within a couple of orders of magnitude.

In this invited presentation our work on theoretical and experimental studies of plasmonic effects in heavily doped semiconductors will be reviewed. A complete dispersion equation will be described showing some new interesting features that do not exist in metals. Experimental results on GaAs and InP will be presented in the view of confirming the theoretical conclusions. A novel experimental method for determining important semiconductor parameters such as, for example, the effective mass, will be proposed.

Keywords: plasmonics, semiconductors

Electrical Spin-Injection in Hybrid – III-V Heterostructures for Circularly Polarized-Light Emission in spin-LEDs and Lasers

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I will present fundamentals and experiments of electrical spin-injection in Hybrid – III-V heterojunctions (spin-LED, 1/2 VECSELs) designed for circularly-polarized light emission. In a first part, the key physical mechanisms and issues to obtain an efficient spin-injection into a III-V semiconductor with the focus on the need of inserting a thin (oxide) tunnel-barrier at the ferromagnet/semiconductor interface to circumvent the impedance mismatch problem will be presented. I will review our latest experiments that rely on Hanle and Inverted Hanle effect to probe the spin-accumulation generated in the semiconductor at the interface with our CoFeB/MgO tunnel barrier. This out-of-equilibrium spin-accumulation and associated spin-current are responsible for the emission of a large circularly-polarized light (70%)in spin-Light Emitting Diode structures as observed by spin-resolved Electroluminescence studies. In the end, I will present some concepts and first realization and operations performed on a III-V 1/2 spin-VECSELs laser composed of an external cavity designed for circularly-polarized coherent light emission.

Keywords: heterostructures, circularly polarized light emission, spin LEDs, lasers

Investigations of the magnetic proximity effect in non-magnetic/ferromagnetic bilayers by x-ray resonant magnetic reflectivity for spin caloritronic applications

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Platin is often used to detect spin currents in an adjacent magnetic film nowadays using the inverse spin Hall effect. But unfortunately, parasitic charge based effects can be induced due to spin polarization in Pt generated by the magnetic proximity effect, if Pt is adjacent to a ferromagnetic material. For example, in spin caloritronics the anomalous Nernst effect can contribute to the thermal generation of spin currents (spin Seebeck effect), when an out-of-plane temperature gradient is applied in magnetic thin films. We propose to use magnetooptic techniques like x-ray resonant magnetic reflectivity (XRMR) to investigate the spin polarization at the interface to a feromagnetic material to identify or exclude magnetic proximity effects in these nanostructures. XRMR is interface sensitive and, therefore, mainly independent from the Pt thickness, which makes it preferable over standard x-ray magnetic circular dichroism techniques. In my talk, I will introduce the strongly rising field of spin caloritronics. I will explain the thermal spin current generation (spin Seebeck effect) and the interface-sensitive techique XRMR for spin polarization detection.

Keywords: X-ray resonant magnetic reflectivity, spin caloritronics

Nano Particle Effects on Magneto Optic Ferrite Thin Films for Variable MUX/DEMUX Applications in Optical Communications

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It has been observed that the deflection of optical beam due to magnetic field variation or frequency variation is quite limited. In real world we would like to have a MUX/DEMUX with large number of channels where any incoming wavelength can be connected to any output point, in other words making a variable MUX/DEMUX. Larger deflections can be achieved by using array of magneto optic ferrite thin film components. For a practical MUX/DEMUX with a desired deflection for sending signals to any of the output fibers, it may be necessary to use several single stages to form a two dimensional array, as illustrated in Figure 1. In order to get total deflection from N stages it is considered that the incident angle for each successive stage is the deflection angle from the previous stage. The deflection angle (δ_D) is equal to the average of the refraction angle between the left and right polarization beams (θ^- and θ^+) with respect to a reference. The difference between the two angles being (δ), which is the deflection angle between left and right polarized beams as shown in Figure 2. The main advantage of this large deflection is that we do not require separate MUX/DEMUX for smaller number channels .i.e a 64 channel MUX/DEMUX can be easily used for 4, 8, 16, 32, or 48 channels as required. This would reduce the cost of the component and entire communications link where these components are used in larger numbers. Recently researchers have started exploring the effects on nano particle doping on materials. Researchers are seeing that adding lower refractive index nano particle dopants will lower the refractive index of the material, and adding high refractive index dopants will increase the refractive index. Lowering the refractive index of the magneto optic material will increase the deflections achieved in a single stage and a two-dimensional array configuration. As a result adding nano particles to thin film magneto optic materials will increase the total deflections achieved. This paper will look at the effects on Gold (Au) nano particle dopants at various volumes in a thin film Nickel (Ni) magneto optic material.

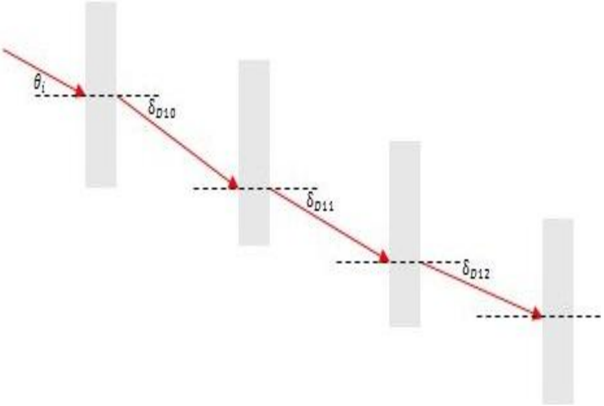

Fig: 2: Four Stage 2D Array

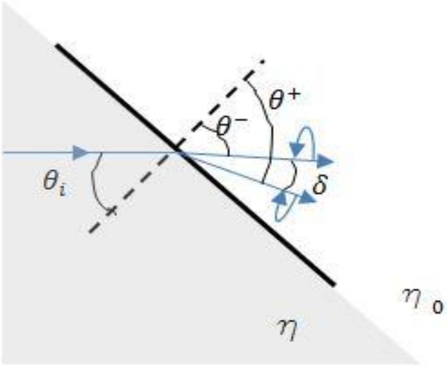

Fig. 3: Double Refraction at Faraday Medium

Keywords: MUX/DMUX, Nano Particles, Magneto Optic, Refractive Index

The semiconductors for nanoplasmonics

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Plasmonics is a research area merging the fields of optics and nanoelectronics by confining light with relatively large free-space wavelength to the nanometer scales. The most important challenges for nanoplasmonics include the delivery of energy to the nanoscale, the control of the local fields and manipulation with confined energy.

The negative permittivity, which is an essential property of any plasmonic material, typically originates from oscillations of free charges while the losses that reduce the performance of plasmonic devices arise from electron-electron and electron-phonon interactions and from scattering due to the lattice defects. Some metals (such as aluminum, copper, gold or silver) can be used at optical frequencies due to an enormous concentration of free electrons, their applicability in the THz and telecommunication frequencies is limited by the electron scattering frequency that is about two orders of magnitude lower than metal plasma frequency. Moreover there is a low energy confinement when the light frequency is small compared with the plasma frequency of the material. It is believed that it is possible to use a nanostructured material with reduced effective plasma frequency, but our simulations show that the useful plasmonic frequency band cannot be shifted by this method. It seems that the best material for specific purpose would be that with appropriate plasma frequency and damping.

This contribution is devoted to the possibilities of using semiconductors as plasmonic materials. The advantage of using semiconductors is the possibility of tuning the semiconductor properties by changing the composition and doping of a given material. The inhomogeneous structures with interesting properties may be prepared.

The conventional semiconductors are interesting by the low scattering frequency which arise mainly from electron- thermal phonon interactions and is under 1 THz at the room temperature. The disadvantage is the need for very strong doping in order to achieve a sufficiently high plasma frequency. The scattering of electrons on the ionised impurities become the dominant damping mechanism increasing the losses significantly. On the other hand, the optical phonons in the heteropolar semiconductors provide significant negative contribution to the permittivity with very low damping. This effect can be effectively used at frequencies near 10 THz.

Acknowledgements

This research is supported by IT4Innovations Centre of Excellence project, reg. no. CZ.1.05/1.1.00/02.0070, Regional Centre of Excellence reg. no. CZ.1.05/2.1.00/01.0040, New creative teams in priorities of scientific research. (CZ.1.07/2.3.00/30.0055). This work was supported by Natural Sciences and Engineering Council of Canada (NSERC) and its Collaborative Research and Training Experience (CREATE) Advanced Science in Photonics and Innovative Research in Engineering (ASPIRE) Program.

Keywords: Plasmonics, Semiconductors, Plasmonic materials, Surface plasmon resonance, Terahertz frequency band

Hyperbolic metamaterial interface: propagation of surface waves

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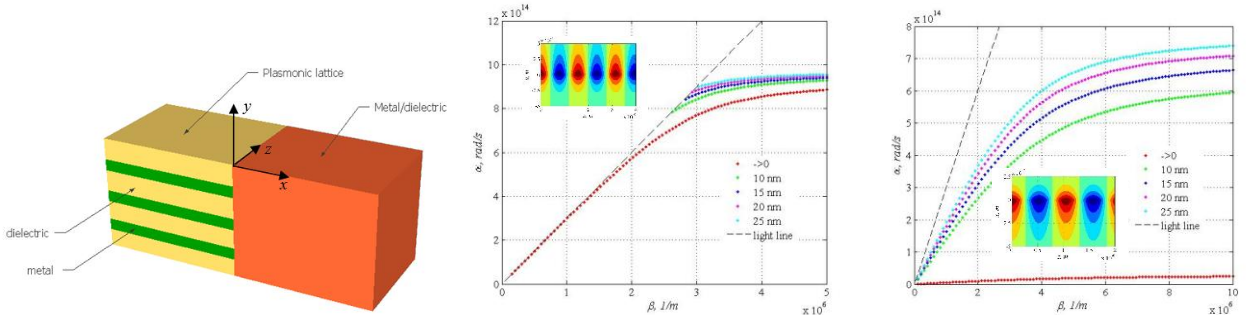
We analyze surface-wave propagation on a single interface between an isotropic media and a multilayered hyperbolic metamaterial [1, 2] (Fig. 1 (a)). The structure dispersion is discussed for various cases of a hyperbolic metamaterial. It is demonstrated that the frequency range of surface waves can be strongly influenced by varying the thickness of dielectric sheets. It is also shown that this frequency range can be broadened by decreasing the thickness of the dielectric in the metal-dielectric compound or by replacing the isotropic media with a metal.

Consider a single interface between isotropic media and a hyperbolic metamaterial (Fig. 1 (a)). It should be mentioned that the former one is fabricated by alternating layers of a metal and a conventional dielectric. The dispersion relation for the proposed structure is as follows [3]:

$$\omega^2(\varepsilon_1-\varepsilon_2)+\beta^2c^2\left(\frac{\varepsilon_2}{\varepsilon_1}-\frac{\varepsilon_1}{\varepsilon_2}\right)=0 \qquad (1)$$

Here, $\omega$is the angular frequency, ε_1 – permittivity of isotropic media, ε_2 – permittivity of multi-layered hyperbolic metamaterial, β– longitudinal propagation constant, c – speed of light.



(a) (b) (c)

Fig. 1: (a) The investigated structure consisting of an infinite multi-layered hyperbolic metamaterial ($x<0$) and an isotropic material ($x>0$). Dispersion curves of TM modes at a metamaterial/air (b) and at a metamaterial/metal (c) interfaces for different widths ofthe dielectric layer are shown.

Fig.1 (b) shows the dispersion of surface wavesat metamaterial/air interface. As can be seen from Fig. 1 (b), the frequency range for surface waves can be controlled by the fill factors of the air and metal sheets in the multi-layered hyperbolic metamaterial. However, in this case the frequency range for the surface wave existence is narrow. Thus, we shall leave the geometry unchanged but assume that instead of an interface between a metamaterial and air we will be dealing with an interface between a metamaterial and a metal. Doing so, we can extend the frequency range for the surface wave existence. The dispersion curves for the modified structure are presented in Fig. 1 (c).

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Keywords: hyperbolic metamaterial, interface, dispersion, surface wave.

Bloch-point velocity in square ferromagnetic nanowires – temperature-aware micromagnetic simulations

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We simulate a magnetic-field-driven Bloch-point motion in an elongated soft magnetic prism. The prism has a rectangular cross-section; we evaluate different square edge in the range from ca. 30 nm to ca. 60 nm. The sample is quasi-infinite, we realize it in a way suggested by Porter and Donahue [1].

The simulation is done within the OOMMF framework [2] with an extension we have developed recently to account for temperature effects [3]. This is a continuum micromagnetic approach where the well-known Landau-Lifshitz-Gilbert equation (LLG; valid for zero temperature) is replaced by the recently proposed Landau-Lifshitz-Bloch equation [4]. We perform test simulations in zero temperature (solving the LLG equation) and for temperatures in the range from the room temperature till the Curie temperature (870 K in our case).

Chosen sample size imposes magnetization to be parallel to the long edge of the prism. Initial condition is a head-to-head domain wall (DW) in the center of the sample. For considered sample size the domain wall has a vortex-shape with a Bloch point in the very center. Constant magnetic field is applied to move the DW. We simulate the most stable case, where highest mobilities can be achieved: a right-handed chirality vortex DW.

We extend the latest work of Andreas *et al.*, where the DW speed in circular rods is evaluated [5]. We test in that way the suggestion that Bloch-point mobility drops down with the increase of temperature [6].

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Keywords: Micromagnetism, Numerical simulations, Nanoscience, Domain walls

Terahertz spectroscopy of magneto-optic hexaferrites

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Magneto-optically active materials are crucial for construction of the nonreciprocal optical components. With increasing interest in terahertz wave guiding applications it is important to find suitable material for realization of the terahertz optical isolator. In our paper is proposed method for measurement of the optical functions and evaluation of the magneto-optical properties of solids in terahertz spectral range as combination of polarimetry methods with terahertz time domain spectroscopy. The first part is dedicated to evaluation of used apparatus. Used optical components are measured by terahertz time domain spectroscopy and their terahertz optical properties are determined as mathematical models using matrix notation. Then the method and configuration for measurement of the magneto-optical properties is explained. In the second part, the method itself is applied on $SrFe_{12}O_{19}$ and $BaFe_{12}O_{19}$hexaferrite samples which are partially transparent in the lower terahertz range and observe resonance in magnetic permeability around 60 GHz. Results show how suitable are used optical components in our configuration for the experiment and proposed method for measurement of magneto-optical effect. Obtained terahertz spectra of the samples and their suitability for design of the terahertz optical isolator is discussed.

Keywords: Terahertz spectroscopy, Optical properties, Magneto-optics, Hexaferrite

Application of the Poisson-Nernst-Planck theory to nanofluidic systems

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The concept of electro diffusion based on the Nernst−Planck equations for ionic fluxes coupled to the Poisson equation expressing the relation between the gradient of the electric field and the charge density (hence usually referred to as the NPP or PNP theory) is widely used as a useful theoretical tool for description and modeling of various phenomena and processes in both living and nonliving systems.

We present an application of the time-dependent PNP approach to study transient behavior of a simple ion channel containing a uni-uni-valent electrolyte solution, subject to a sudden electric potential jump across the channel (voltage clamp). In a typical calculation, diffusion coefficients of the cation and anion were set to 1×10^{-6} and 5×10^{-7} $\mathrm{cm}^2\ \mathrm{s}^{-1}$, respectively, at the temperature 293 K. Value of the relative permittivity $\varepsilon_r = 80$ corresponding to water was used. The channel length was usually 10 nm and size of the potential step was normally set to +100 mV. Standard boundary concentrations for the electrolyte were 50 and 500 mM for the left and right channel end, respectively. Calculated spatiotemporal profiles of the ionic concentrations and electric potential (Fig. 1) show that two principal exponential processes can be distinguished in the electro diffusion kinetics, in agreement with original Planck's predictions.

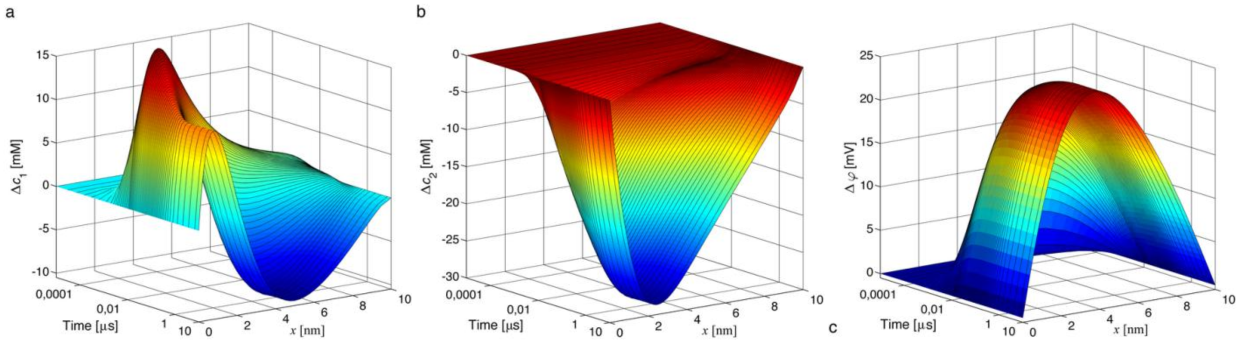

Fig. 1: Spatiotemporal profiles of the ionic difference concentrations ((a) for cation, (b) for anion) and the difference electric potential (c). The standard set of parameter values, as described in the text, was used in the calculation.

The presented results provide additional information about the classical voltage-clamp problem and offer further physical insights into the mechanism of electrodiffusion. The used numerical technique is directly applicable to other systems, such as synthetic nanopores, nanofluidic channels, and nanopipettes. More information can be found in Valent et al. (2013) *J. Phys. Chem. B* **117**, 14283.

Acknowledgements

This work was supported by the Slovak Research and Development Agency under the contract No. APVV-0291-11 and by the agency VEGA (grant No. 1/0633/15).

Keywords: Nanofluidic Channel, Ion Transport, Electrodiffusion, PNP theory

The interface nonplanarity investigated by the surface plasmon resonance imaging

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Surface plasmon resonance imaging (SPRi) sensors realize highly sensitive, real-time, quantitative, label-free, high-throughput biological interaction monitoring and the binding profiles from multi-analytes. Further provide the binding kinetic parameters between different biomolecules. With such a sensitive method it is very important to point the need for planarity and homogeneity of the entire biochip for a correct output data.

This paperis based on experimental SPRi data from our a commercial device GenOptics SPRI-Lab+ measured at biochip with Kretschmann configuration. Analyzing the raw data in the form of 2D images offers new possibilities for the evaluation of the issue. Initial processing of the calibration data shows significant variations in the fundamental properties across the active layer of the biochip. Here we focus on the spatial distribution of the resonance angle for each point in an image, see Fig. 1., in order to analyze possible reasons for observed drift in the horizontal direction.

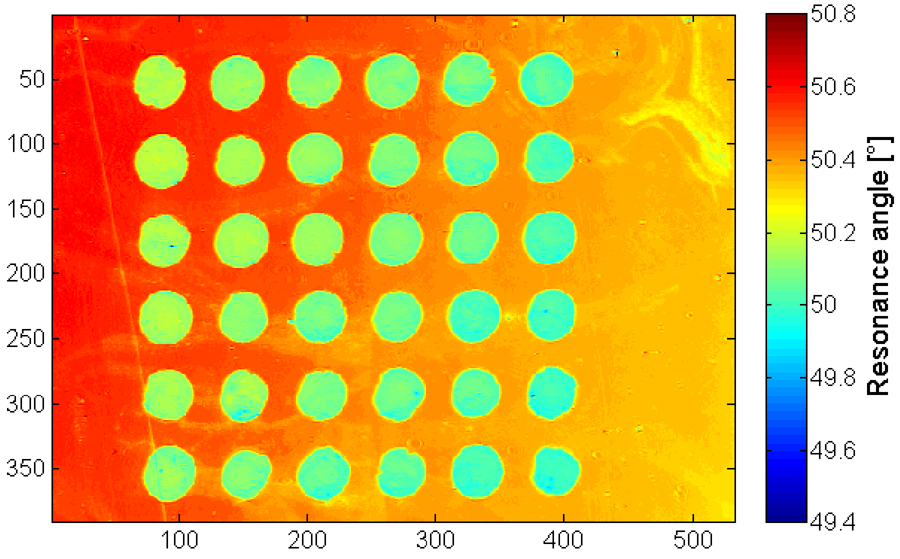

Fig. 1:The spatial distribution of the Surface plasmon polariton resonance angle.

Keywords: Surface plasmon resonance imaging (SPRi), biochip, microchip analysis, image processing, Kretschmann configuration

Mueller matrix ellipsometry: analysis of systematic errors in sample rotation data

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The Mueller matrix spectroscopic ellipsometry is a powerful optical method for characterization of the optical properties of anisotropic samples. The analysis of optical data measured for different angular rotation angles of the sample is the straightforward approach to obtain complex permittivity tensor of the anisotropic material. In this paper we analyze and model systematic errors in the rotation data caused by amisalignment of the normal of the sample surface with respect to the plane of the incident light. Presented developed model describes systematic variation of the angle of incidence and inclination of the sample surface with respect to the plane of the incidence. In the first step we fit our model to rotation data measured on calibration sample of 25nm thick SiO_2 layer of Si waver. Since the reference sample is isotropic and optical functions of $SiO_2$and Si are well known, only theSiO_2andparameters of model describing systematic errors are fitted. In the next step we characterize optical function of uniaxial rutile crystal. In the analysis we describe process of determination of the optical function from the Mueller matric data measured for different angular rotation of the rutile sample. In the next step the model describing optical functions is further extended with the model describing systematic errors. By the fitting the final model if optimized. Obtained optical functions from model with and without assumption of systematic errors are compared.

Keywords: Mueller matrix, ellipsometry, spectroscopy, uniaxial anisotropy.

Spectra of second order permittivity coefficients in cubic Fe, Co and Ni emerging from symmetry arguments

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Using ab-initio calculations, we determine spectra of the second-order magneto-optical permittivity coefficients ($2G_{44}$, G_{11}-G_{12}) for ferromagnetic bcc Fe, fcc Ni and fcc Co. Those second-order magneto-optical permittivity coefficients provide phenomenological description of all second-order magneto-transport effect (and its anisotropy), such as anisotropy magnetoresistance, quadratic magneto-optical Kerr effect, X-ray magnetic linear dichroism, magneto-reflectivity, etc. depending on the investigation technique and the energy of the probing photon (zero photon energy means dc). The calculations of the conductivity/permittivity tensor elements are done at general magnetic orientation with respect to the crystal axis. Then, dependence of the ab-initio permittivity elements on general magnetization orientation is compared with expected dependences from phenomenological model including coefficients $2G_{44}$, G_{11}-G_{12} based on symmetry arguments. In our best knowledge, those are the first time calculated spectra of the quadratic magneto-optical tensor elements G.

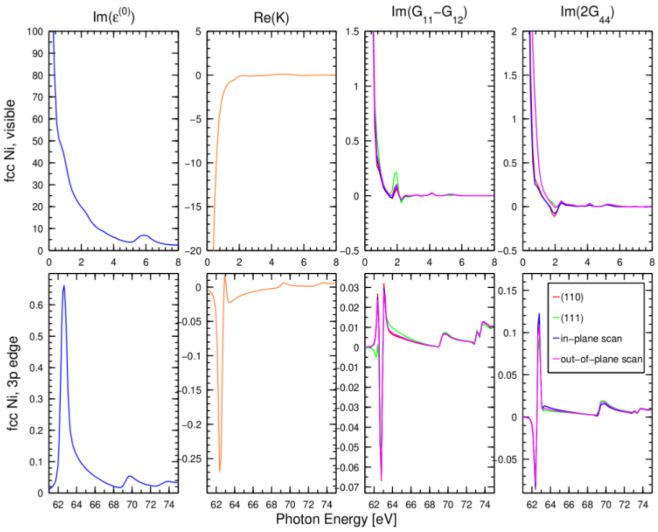

Fig 1: absorption part of optical constants of fcc Ni up to second order in magnetization: Im($\varepsilon^{(0)}$): diagonal optical constants, Re(K): linear magento-optical constant, Im($2G_{44}$) and Im(G_{11}-G_{12}): second order magneto-optical constants.

Acknowledgements

Financial support of the EU project Nanotechnology– the basis for international cooperation project (CZ.1.07/2.3.00/20.0074) and GAČR 13-30397S is greatly acknowledged.

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Keywords: Magneto-optical Kerr effect, effects quadratic in magnetization, DFT calculations

Magneto-resistive properties of the composites (1-x)La0.7Sr0.3MnO3/x(GeO2, Sb2O3)

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Strontium-lanthanum manganite La0.7Sr0.3MnO3 (LSMO) is ferromagnetic (FM), with high spin polarization of electrons. LSMO Curie temperature is 360 K that noticeably surpasses room temperature (TR). Because of these qualities of LSMO forms a basis of ceramic composites having a considerable magneto-resistive effect (MR) at room temperature. This fact is of interest for practical use.

The interface FM/oxide influences the MR effect. Therefore we synthesized and investigated ceramic composites based on LSMO. In these composites we used oxides GeO2, Sb2O3 with various ratio as the second component, that corresponds formula (1-x)La0.7Sr0.3MnO3 – x(GeO2, Sb2O3). In samples of composites the oxides are the isolating barriers between LSMO particles.

Thickness of barriers lies in the range 0, 1 – 1 μm that excludes tunneling of electrons between granules, but does not suppress the MR effect. The largest MR effect value (15 % in the field of 20 kOe) is obtained in investigated composites for samples with 90 % of LSMO and 10 % of GeO2.

The results of work are discussed assuming that LSMO is an effective spin filter of electrons and oxides have different conditions of carriers transport through thick barriers and different properties of the FM/oxide interface.

Keywords: magneto-resistive effect, composite, barriers, spin filter

Investigation of cerium titanates from first principles

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Cerium titanate structures offer broad range of technological applications because of their optical and catalytic properties. Cerium titanate can form various phases, which depend on the oxidation state of cerium. In $CeTiO_4$ and $CeTi_2O_6$ compounds cerium is in the oxidation state Ce^{4+}. We have investigated electronic structure of these compounds as well as CeO_2 using ab-initio calculations. For $CeTiO_4$we considered both orthorhombic and monoclinic phases. Furthermore, the influence of pressure applied to Ce titanate phases on various properties was revealed. Electronic structure, thermodynamical and optical properties were calculated using the single-electron framework of density functional theory employed in VASP code [1,2]. For the exchange-correlation term the generalized gradient approximation was considered [3].

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Keywords: Cerium, Titanates, Ab-initio

Modeling of Mueller matrix response from diffracting structures

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Mueller matrix ellipsometry becomes frequently used technique to characterize thin films, multilayers, nanostructures, and also more complex diffracting surfaces. Polarimetric study of new-generation solar cells with textured surfaces requires development of new modeling methods including phenomena as depolarization or s-p mode conversion. One of the effective modeling methods is to calculation the diffracted far field using diffraction integrals.

The main target of this paper is to propose a method to model ellipsometric and polarimetric response from an arbitrary diffracting element. We approximate the structure with the locally smooth piecewise surface with small surface curvature. The model neglect shadowing effect. The model is based on calculation of the complex amplitudes using the Fresnel-Kirchhoff diffraction integral of electromagnetic field near the surface. The surface can consist of arbitrary materials described by the complex refractive index or an arbitrary multilayer structure. The theory is demonstrated on reflection from a silicon with silicon oxide layer in the form of the square, circle, and triangular curved near edges.

Keywords: Mueller matrix, Ellipsometry, Diffraction, Scalar diffraction theory

Aniline- montmorillonit plasma deposited thin films composites

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Aniline (polyaniline) is one of the highly pursued conducting polymers owing to its high electrical conductivity, interesting optical properties and excellent environmental stability. In suitably doped form, its applicability as hole-injecting electrode in electroluminescent devices is one of the areas of research in the field of polymer optoelectronics. Its composites with many other materials are also being pursued for optoelectronic applications. Polyaniline can be prepared in bulk form using chemical oxidative polymerization or in thin film form using plasma polymerization technique, electrochemical deposition, spin coating or solution casting. One of the negative aspects of polyaniline is its comparatively low mechanical strength, which limits its applications to some extent.

The composites were prepared from Aniline vapors in assistance of a plasma discharge. The vacuum chamber was evacuated by diffusion pump with rotary pump to less than $1x10^{-3}$ Pa before the deposition. Aniline was placed in a glass vessel and connected to chamber over a precise needle valve for a flow control. The aniline was before used in the vessel evacuated during a freezing to solid state by LN2.

The plasma discharge was in a capacitive plan-parallel configuration. A powered electrode was on RF 13.56 MHz voltage. A matching network was set to minimalize a reflected power back to generator; it was reflected less than 1W. The connection between the matching network and the electrode was made from a short cupper belt. The total process pressure was monitored by MKS Baratron and the gas flow of main discharge gas Argon was controlled by MKS flow controller.

The MMT powder was separated to fractions by multistep centrifugation process in water based solution. Then the fractions were immobilized on microscopy glass slides by a spin casting process. The dry glass slides were placed on RF powered electrode in the chamber.

The plasma discharges under various conditions were investigated by Hiden EQP mass spectrometer. The plasma shield oscillations typical for RF plasma were detected, the energy distribution functions show that aniline main ion with mass 93amu is mainly ionized in bulk plasma and the ionization probability in RF sheath is low. The aniline fragment 66 amu has energy lower than the main Aniline ion therefore the most probable event in the plasma sheath is fragmentation of Aniline. The keep the Aniline properties the fragmentation has to be minimalized.

The luminescence properties of the samples were investigated and correlated to other properties of the coating obtained from XPS, XRD and FTIR.

The Aniline/MMT composites were prepared of the glass slides and the properties were investigated. The influence of the plasma discharge on the coatings itself and the aniline molecules was investigated.

Keywords: RF plasma, plasma diagnostics, aniline, montmorillonit, luminescence

Characteristics of the Bi_2S_3 nanowire surface promoted properties

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The semiconducting nanowires have demonstrated a great application potential in numerous electronic and optoelectronic devices. Current available growth methods can provide a high quality, homogenous nanowires with well-defined electronic properties. Even though the nanowires possess a remarkable structural quality and reproducibility, surface dependent processes of the nanowire as interaction with gaseous molecules can change their pristine characteristics. For example, transition from an n- to p- type characteristics due to the strong nanowire surface adsorption effects has been demonstrated [1]. Detailed studies are required to broaden the understanding of the nanowire's surface impact to the overall transport characteristics.

In this work, surface-defined transport properties of the nanowires formed from one of the first discovered photoconductors - bismuth sulphide [2] are studied. Combining the resistive sensing and the characteristics of the photoconductivity, one could evaluate the surface properties of the nanowires. The Bi_2S_3 nanowires were grown inside the pores of the anodized aluminum oxide (AAO) membranes. In order to access the individual nanowires, a selective etching was applied to the AAO and liberated nanowires were transferred onto the substrates. The contact electrodes were fabricated using electron beam lithography. The resistive sensing measurements were performed in a lab-designed system with the control of both temperature and relative humidity/concentration of oxygen in inert carrier gas of gaseous environment. The spectral response measurements were performed under a low power illumination with wavelengths ranged from 500 up to900 nm and at constant bias applied to the sample.

The Bi_2S_3nanowires are found to exhibit a response to the different relative humidity levels in inert atmosphere. Determined response has nonlinear characteristics caused by the presence of the pre-adsorbed oxygen on the surface of the Bi_2S_3 nanowires and different relative humidity levels modulating the overall charge transport characteristics [3].The spectral response of photoconductivity of the individual nanowires unveilsa distinctive behavior which is attributed to the charge carriers with different photoexcitation energies. Combining the characteristics of the individual nanowire and of the nanowires surrounded by the insulating AAO membrane, the impact and contribution of surface and under-surface layers of the nanowires to photoconductivity were identified [4].

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Keywords: Nanowire, Bismuth sulphide, resistive sensing, photoconductivity

Magnetic and optic properties of $NdFeO_3$ and $NdMnO_3$ under pressure – theory and experiment

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We present results of our studies of orthomanganite $NdMnO_3$ and orthoferrite $NdFeO_3$ done both experimentally and theoretically.

For the experimental approach, we use Raman spectroscopy to observe optically active phonons in the range from ca. 90 cm^{-1} to ca. 500 cm^{-1}. Our samples are grown using the vertical floating zone method. Diamond anvil cell is used to apply pressures up to 11 GPa [1]. Magnetic structure is analyzed with a neutron powder diffractometer.

For theoretical calculations, we use the VASP (Vienna *Ab-initio* Simulation Package) package, a plane-wave pseudopotential code, to perform spin-polarized calculations including the spin-orbit interaction. General gradient-corrected exchange–correlation functionals parameterized by Perdew-Burke-Ernzerhof and a plane-wave cut-off of 600 eV are used.

To calculate phonons, a direct method approach is utilized. A supercell 2×2×2 is created and atoms within are displaced. Resulting Hellmann–Feynman forces are used to calculate force constants within the harmonic approximation. We use the PHONOPY program [2]. Lattice vibrations are assigned as Raman-active modes according to the group theory.

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Keywords: Antiferromagnetism, Phonons, Density functional theory, Orthoferrites

Investigations of optical absorption of photonic nanostructures featuring inversed pyramid profiles

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This paper represents a numerical investigation on optical absorptance of omni directional nanograting structures using the rigorous coupled-wave analysis method. The results have shown that an inversed pyramid grating structure made of tungsten provides a promising solution for thermophotovoltaic emitters/absorbers due to its highly optical absorptance in the wavelength range from 0.6 to 1.72 μm and insensitivity to angle of incidence. The proposed structure constructed on a grating layer with a low and high filling ratio in the grating region is easily manufactured using current fabrication techniques. In addition, the physical origin of absorptance enhancement is also demonstrated by plotting magnetic and time-average energy Poynting vector distributions and verifying with analytic solutions. Further, this study may pave the way to apply optical extraordinary absorptance enhancement underlying photonic nanostructures for energy harvesting devices.

Keywords: Gratings, Thermal Emission, Subwavelength Structures, Nanostructures

Symmetry of nonlinear magneto-optic effects

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Nonlinear magneto-optic effects as second-harmonic generation are used for investigation of magnetism at ferromagnetic interfaces. Selective sensitivity to magnetic surfaces and interfaces is related to the breaking of space-inversion symmetry on them. Particular sensitivity of MO-SHG to vicinal surfaces, antiferromagnetic domains, surfaces with atomic steps, and buried magnetic interfaces has been demonstrated. Related phenomena of parametric down-conversion and generation of photon pairs, which up to now have gained less attention than they would deserve. The nonlinear MO processes are promising both from theoretical point of view (nonlinear MO spectroscopy, polarization entanglement and potential applications (switching of the generated photon pairs by fast magnetization processes, symmetry detection by polarization analysis).

In this paper, the nonlinear properties of magneto-optic materials are described using the nonlinear magneto-optic tensor. We calculate the symmetry of the tensor for the basic symmetry groups, particularly low symmetry materials at general crystal orientations. Three basic magneto-optic configurations are distinguished – polar, longitudinal, and transversal. We expect that due to the symmetry arguments, the nonlinear MO response will be induced even in structures without standard nonlinear optical activity.

Keywords: Magneto-optics, Nonlinear susceptibility, Crystal symmetry, Permittivity tensor

Morphology of porous silicon with vertical nanowires

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We suggest a new method for the description of complex structure of nanocluster semiconductor films on the base of theory of dynamical chaos. We use this approach because of the fact that dynamical chaos can be characterized by a statistical characteristic similar to characteristics of stochastic processes. So, the aim of our work is description of dynamical chaos with alternated and fractal structure close to structure of nanostructured films.

For the description of chaotic oscillations with characteristics corresponding to criteria of self-organization we use our own new equation for fractal evolution of a measure (additive value) [1, 2]. According to this approach, distribution of electrons, holes and impurities in nanostructured semiconductor can be described as

$$\boldsymbol{X_{k,i+1}} = \left(\frac{1}{C_k} + \sum_{k=1}^{3}\mu_{k.i}\right)\left|\frac{X_{k,i}}{X_{k,0}}\right|^{-\frac{1}{\gamma_k}}, \qquad \boldsymbol{\mu_{k,i+1}} = \left(\frac{1}{C_k} + \sum_{k=1}^{3}\mu_{k.i}\right)\left|\frac{X_{k,i}}{X_{k,0}}\right|^{-\frac{1}{\gamma_k}-1} \qquad (1)$$

where $k = (1, 2, 3) \equiv (n, p, a)$, (n, p, a) describe distribution of electrons, holes and impurities correspondently, C_k is precision factor of resolution, k is difference between fractal and topological dimensions, $X_{k,0}$ is equilibrium concentration of electrons, holes and impurities, μ is sign function.

For obtaining three-dimensional models of surfaces of thin films we use algorithm for reconstruction of dynamic chaos on the base of one-dimensional sequence of data [3].

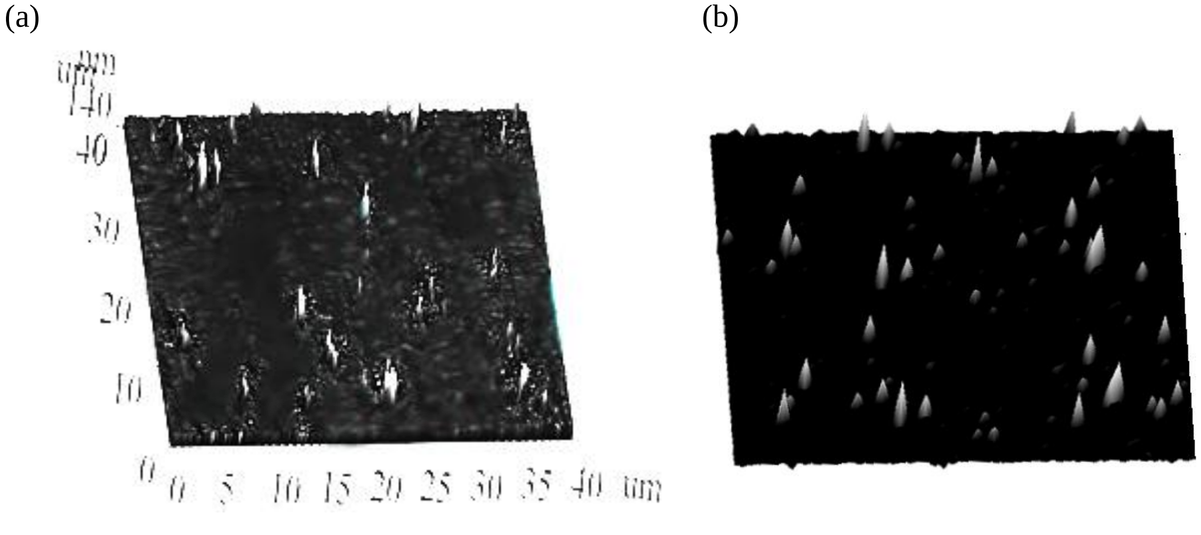

Figure 2.Quantum nanowires of porous silicon at an initial stage of growth.

Experimental data (a), results of numeric analyses (b).

$C_n = C_p = C_a = 0.999$, $\mu = -1$, $\gamma_n = \gamma_p = \gamma_a = 3.806$, $n_0 = p_0 = 0.25$, $a_0 = 1.30$.

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Keywords: porous silicon, dynamical chaos, quantum nanowire, nanostructured film.

Electrical properties of nanoscale silicon wires

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Silicon nanowires (SiNWs) have been attracting considerable attention because they have various applications in nanoelectronics, optoelectronics, and sensor devices. In our study silicon nanowires were grown by metal-assisted chemical etching process. We used boron doped *p*-type crystalline silicon with concentration of carrier 10^{15} cm^{-3}as an initial substrate. Thickness of the substrate is300 microns, crystallographic direction is (100),value of surface resistance of the substrate is 10 $\Omega\cdot mm^2$. We suggest a theory for the description of electrical conductivity of nanoscale semiconductor wires. We take into account the fact that SiNWs have nonlinear vibrational properties, and because of the fact they form groups considered as fractal structures. Electric potential of these structures can be described as non-linear fractal measures. Our theoretical results lead us to a conclusion that current-voltage characteristics of quantum wires have a hysteresis shape with oscillations (Figure 1 a).

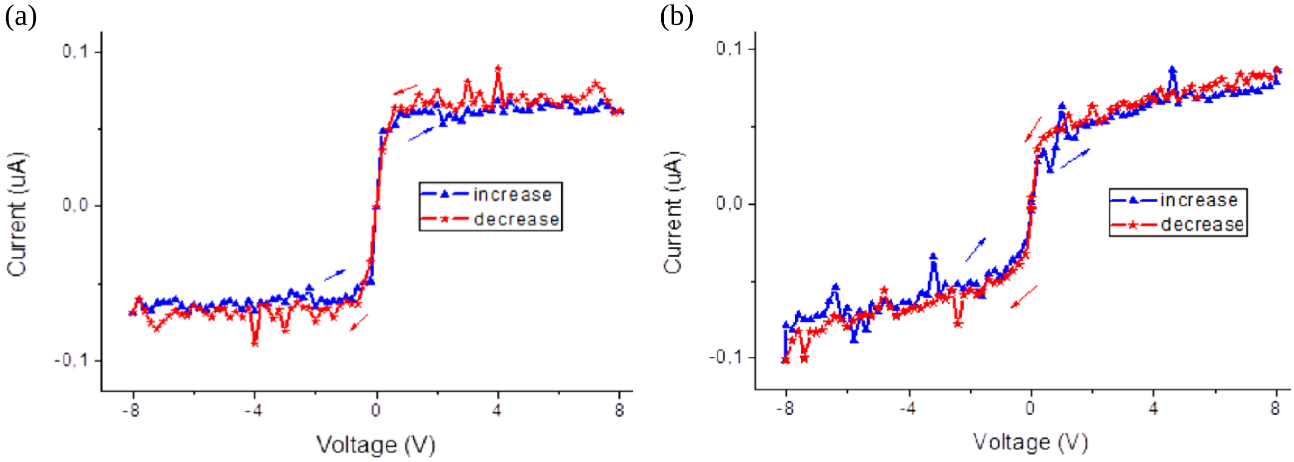

Figure 1 - Theoretical (a) and experimental (b) current-voltage characteristics of SiNWs.

Electrical conductivity of nanoscale silicon wires depends on capacity of internal fractal clusters and ratio between the de Broglie wavelength of electrons and lateral size of wires. Scattering potential is considered as a non-linear fractal measure defined by value of external voltage.

Existence of fractal structures is the reason for appearance of multi-barrier tunneling effects in nanoscale wires in homogeneous material (silicon).For this reason, the current-voltage characteristics of silicon nanowires have areas with negative differential resistance. These are as characterized by hysteretic type of curves(Figure 1 b).

The obtained results can be applied for further perfection of technology of memory electronic circuits, nanoelectronics and optoelectronics.

Keywords: silicon, quantum wires, tunneling effect, non-linear fractal.

Electrodiffusion dynamics simulation of ionic transport in a nanochannel

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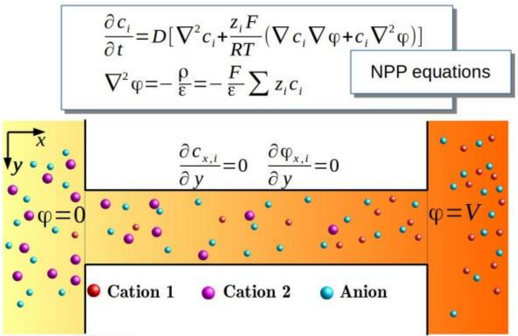
Electrodiffusion is a transport process that is involved in many biological pathways such as transmission of the electric nerve impulses or muscle contraction. One description of electrodiffusion is based on the Nernst-Planck-Poisson (NPP) theory. Current developments in computer power and numerical algorithms allow for solving full time-dependent NPP equations without approximations such as the electroneutrality or constant field assumptions [1,2]. Presented calculations were performed using the method of lines implemented in the VLUGR2 solver [3].



$$\frac{\partial c_i}{\partial t}=D[\nabla^2 c_i+\frac{z_i F}{RT}(\nabla c_i \nabla \varphi + c_i \nabla^2 \varphi)]$$

$$\nabla^2 \varphi = -\frac{\rho}{\varepsilon} = -\frac{F}{\varepsilon}\sum z_i c_i$$

Initial conditions:

$c_{0,cation\ 1}=50\,mM$, $c_{L,cation\ 1}=500\,mM$, $D_{cation\ 1}=13.10^{-5}\,cm^2 s^{-1}$
$c_{0,cation\ 2}=500\,mM$, $c_{L,cation\ 2}=50\,mM$, $D_{cation\ 2}=10^{-6}\,cm^2 s^{-1}$
$c_{L,anion}=550\,mM$, $c_{0,anion}=550\,mM$, $D_{anion}=5.10^{-7}\,cm^2 s^{-1}$

$V=100\,mV$, $L=10\,nM$, $T=293\,K$, $\varepsilon_r=80$

Temporal profiles of the ionic concentration and electric potential changes of the system with two cations and one anion (see figure) after potential jump exhibit three exponential phases and oscillations of potential. In the first phase (~1 ns) the concentration of the cation 1 is increasing and for the other ions is not changing. Then in the second phase (~50 ns) the concentration of the cation 1 and the anion is increasing whereas the concentration of the cation 2 and the potential is decreasing. Finally in the third phase the concentration of all ions is decreasing and the potential is increasing to it's original value. The steady state is reached after ~500 ns. The faradaic and displacement currents were calculated by an *a posteriori differentiation* of the solution profiles obtained from the previous step. The analysis of the time evolution of the total current density shows that the displacement current constitutes a significant part of it. Despite of the absence of an electric double layer in our model, an asymmetric current-voltage characteristics known as ion current rectification (ICR) was observed. Decomposition of the faradaic current to the individual contributions of the ions in the steady-state showed that the channel is selective to the cation 1 in a positive direction of external potential.

Simulations revealed interesting nonlinear dynamics of ionic transport. The used numerical approach can be readily extended to models in 2D or 3D and implemented to models of biological processes or other systems, such as synthetic nanopores, nanofluidic channels and nanopipettes.

Acknowledgement

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Keywords: Electrodiffusion, Ion channel, Time-dependent Nernst-Planck-Poisson equations, Ionic current rectification

Quadratic magnetooptic spectroscopy of bcc Fe and Co_2MnSi thin films

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The magnetooptic Kerr effect (MOKE) is a well known physical phenomena that enables detailed characterization of magnetic material properties. However, quadratic MOKE (QMOKE) is not well understood yet. Hence, QMOKE anisotropy measurements [1] or QMOKE spectroscopy are methods convenient for investigations of the magnetooptic effect quadratic in magnetization. Within the materials having a cubic crystal symmetry, any dependence of the permittivity elements on the direction of the magnetization (within the second order in magnetization) can be expressed by two, generally complex parameters G_{11}-G_{12} and $2G_{44}$[2]. We present here QMOKE spectra of those parameters for the bcc Fe and the Co_2MnSi Heusler alloy thin films as a novel spectroscopic approach revealing detailed magnetooptic information within the second order effects in magnetization. Both materials exhibit change of the QMOKE spectra with change of the crystallographic structure, which is achieved by post annealing at different temperatures.

Keywords: Magnetooptic Kerr effect, Quadratic magneto optic Kerr effect, spectroscopy, Heusler alloys.

Ab-initio study of cerium-doped anatase and brookite phases

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TiO_2 is a well-known catalyst [1]. There is a number of ways how to improve its efficiency in visible-light spectrum further. One way is to create oxygen vacancies or Ti^{3+} defects. Another way how to induce visible-light photoactivity is by doping by lanthanides. Here we consider cerium doped TiO_2 in the anatase and brookite phases. Our results were obtained using ab-initio calculations. The electronic structure and thermodynamical properties (enthalpy of formation) of Ce doped TiO_2 phases were investigated under pressure as motivated by experimental studies at VSB-TUO. Two valences, i.e. Ce^{3+}/Ce^{4+} were considered. The calculations were performed using the VASP code [2,3] and the generalized gradient approximation [4] was used to account for exchange-correlation effects. The thermodynamical stability with respect to the Ce concentration and Ce valence states are revealed in both anatase and brookite phases.

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Keywords: Anatase, Brookite, Cerium, Ab-initio

Optimization of spin injection and detection in lateral nanostructures by geometrical means

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Lateral spin devices are an important concept in nowadays all-metallic spintronic devices. One of the key problems is to obtain large spin injection and detection efficiency. Several concepts has been envisaged, such as to use half-metallic ferromagnetic electrodes or spin-polarized interface barriers. Within this work, we suggest an alternative way of the optimization of spin devices (namely optimization of spin current density, spin current and spin accumulation), based on optimization of the geometry (dimensions) of the device, jointly with optimization of the interface resistance.

Keywords: spin-polarized current, lateral spin-valve structure, Py/Cu, interface resistance

An *ab initio* study of the phonon vibrations of Co_3O_4

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Co_3O_4 belongs among the catalyst for N_2O decomposition. Since this reaction has oxidation-reduction mechanism, the electronic properties of Co_3O_4 represent important feature. Electronic structure and lattice dynamics, i.e. atomic vibrations were calculated using first-principles calculations. We determined Raman and infra-red frequencies of the phonon modes. Our results were calculated using single electron framework within the density functional theory. The general gradient approximation as parametrized by Perdew-Burke-Ernzerhof [1] was used for the electronic exchange correlation. To obtain the correct description of the insulating behaviour the Hubbard U technique was used. The anti-ferromagnetic ordering and spin-orbit interaction were also considered. For the lattice vibrations calculations Phonopy package was used [2]. The dependences of the band gap, infra-red and Raman frequencies on the Coulomb interaction (Hubbard U) were revealed. Calculated results are compared with experimental data measured at the VSB-TU Ostrava.

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Keywords: Cobalt spinel, Co_3O_4 catalyst, phonons, ab initio calculations

TOPIC 4

Nanocarbons

Chair: Mark H. Rümmeli
Co-chair: Grażyna Simha Martynková

Carbon nanocomposites and sorbents
Nanocarbons structure and properties
Methods for characterization and preparation of nanocarbons

Exploitation of reducible and irreducible oxides for graphitization process and their potential applications

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The catalytic potential of metal catalysts, in particular transition metals, is well known. Indeed, they are frequently used in the synthesis of nanomaterials. For example graphene growth is usually fabricated over copper. However, despite the success of metal catalysts sometimes this can be a disadvantage. In potential applications of graphene a transfer from a metal substrates is required, but this can introduce defects in the graphene structure and additional impurities. Therefore sometimes it is preferable to synthesize such materials directly over oxide supports *e.g.* for electronic applications, for avoiding these problems.

In this talk a variety of synthesis approaches for 0D, 1D and 2D synthesis over oxides along with their characterization will be presented. Structures like graphitic shells (0D), carbon nanotubes/fibers (1D) and graphene (2D) are discussed using synthesis routes such as chemical vapor deposition (CVD) and carbothermal reduction. The potential for these materials to be used in applications for electronic, energy and bio-medical applications is also discussed.

Keywords: graphitization, oxide catalyst, carbothermal reduction

Electron driven in situ transmission electron microscopy of nanostructures

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Contemporary aberration corrected transmission electron microscopes (TEM) offer new insight into nanomaterials. This is because many materials are highly electron beam sensitive to the electron acceleration voltages typically used in uncorrected systems (e.g. 300 or 200 kV). The introduction of aberration correction allows one to work at reduced voltages where damage is often significantly reduced while still allowing near atomic or atomic resolution. None-the-less, despite the reduction in electron-beam sample interactions, they do still exist and can be usefully exploited to drive reactions inside a TEM. In this talk a variety of in situ reactions driven by the electrons from the imaging beam are presented for a variety of nanomaterials.

It is also possible, with the use of a specialized sample holder, to drive electrons through a specimen (e.g. an electrical current). Dynamic reactions can also occur under electrical bias which can also be captured and investigated in situ. Various bias driven reactions are also presented.

In summary, these exciting studies show only a small part of the tremendous potential of in situ TEM to both characterize and study nanomaterials in a broader sense.

Keywords: transmission electron microscopy, nanostrucutres

Oxidation of carbon nanotubes

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Carbon nanotubes (CNTs) are in recognition of scientific community for almost 25 years. They are known for their unique physicochemical and electronic properties. During these years, methods of their production and characterization vastly improved and many new applications were developed in almost every aspect of our daily lives.

This work isfocused on the characterization and evaluation of oxidative treatments used to modify CNTs and comparison of pristine and modified materials. The goal is to propose suitable methods for purification, oxidation and evaluation. Samples were analyzed using TEM, Raman spectroscopy, FTIR spectroscopy, phase carbon analysis. Electronic structures of CNTs are also analyzed using DFTB (Density Functional based Tight Binding) method and CASTEP program. Demonstration of oxidation impact on electronic structure is also included.

Acknowledgements
This work was funded by the MSMT project SP2015/55 and the European Regional Development Fund in the IT4Innovations Centre of Excellence (CZ.1.05/1.1.00/02.0070).

Keywords: CNTs, Oxidation, Carbon, Nanotubes, Evaluation, Modeling, DFTB, CASTEP

Study of carbon-silver nanocomposite

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The application of carbon for various nanocomposites is often decided for the reason of interesting properties of carbon and moreover the nanocarbons.

Combining two inorganic particles in the nanocomposite can bring unpredictable compatibility issues. Metals and carbons are known to be difficult to give homogenous compact composite.

One of the options how to improve the compatibility of carbon and metal is homogenization by grinding in ball mill. This process is preparing not only fine powder with narrow distribution of particles (Fig.1) but also can initialize the nucleation of curved carbon structures.

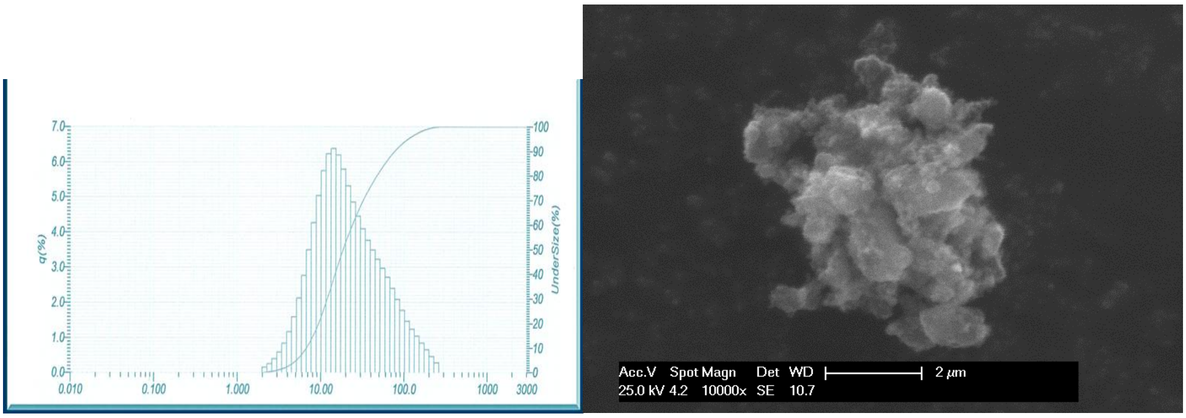

Fig. 1:a) Particle size distribution; b) Scanning electron microscopy image of the ground particles G Ag 100.

Graphite powder (median 40mm) ground for 100h in WC ball mill. Addition of silver powder (median 10 mm) to original graphite powder in 5 wt.%. Annealing of ground powder was performed in inert atmosphere of nitrogen at 1300°C for 2h.

Ground graphite for 120h and after 1300°C heat treatment exhibited new structural features.

Molecular modeling of exposed energetically favorable position of curved graphite bilayer studying interaction with silver.

Acknowledgement

This research has been funded by the European Regional Development Fund in the IT4Innovations Centre of Excellence (CZ.1.05/1.1.00/02.0070).

Keywords: nanocarbons, silver, structure, molecular interaction modeling

Wear behaviour of Al-Ni/CNT composite produced by powder metallurgy

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In recent years, much attention has been focused on aluminium-based metal matrix composites (MMCs) and because of the potential for weight savings in many applications. However, many researchers have observed a critical load above which the composite wears at an equal, and sometimes substantially greater, rate than the monolith [1]. It has been a steadily increasing interest in the development of carbon nanotubes reinforced composites. The motive is to transfer the exceptional mechanical and physical properties of carbon nanotubes to the bulk engineering materials [2].

A nickel chloride solution, consisting of 45 g/L $NiCl_2.6H_2O$, 100 g/L $C_6H_5Na_3O_7.5_{1/2}H_2O$, 50 g/L NH_4Cl, 8 g/L NaH_2PO_2O and 1 g/L aluminium particles in suspension, were used to produce Al-Ni core-shell composites. The core-shell Al/Ni particles and different amount MWCNTs (1, 5, 10 wt. %) were charged in bowl and mechanicallly milled for 2 h at 200 rpm to produce Al-Ni/MWCNT composites. For mechanical milling process, 80 ml stainless steel bowl and 5 mm stainless steel balls were used and ball to powder weight ratio was chosen 10:1. The resulting mixtures were cold pressed to determine mechanical and tribological properties. The cold pressed samples were sintered at 600^oC along 2 hours. The surface morphology of composites, after and before wear tests were characterized using with a scanning electron microscopy (SEM). The chemical composition of the composites carried out with X-ray diffractometry (XRD). The microhardness was observed using a Vicker's microhardness indenter. The wear tests were carried out using by a circular motion ball-on disk apparatus at a constant load. Differential scanning calorimetric (DSC) analyses were used in a purified argon atmosphere to investigate the reaction of conditions of the MWCNT and Al-Ni composites. The effect of the amount of MWCNT was investigated on the tribological and mechanical properties of the composites.

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Keywords: aluminium based metal composite, carbon nanotubes, tribological and mechanical properties

Processing of products prepared by joint oxidation of graphite and fullerene C_{60} with the aim to obtain suitable forms for separation of hazardous compounds

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Graphene oxide represents an interesting material enabling variety of chemical transformation due to its reactive oxygen groups. This paper describes preparation, characterization and modification of compounds based on graphene oxide (GO). Joint oxidation of graphite and fullerene C_{60} was performed to prepare hybrid GO-C_{60} compounds. The aqueous GO-C_{60} suspension has the ability to form fine films, their morphology and modification were studied here. Further, we focused on freeze-drying of prepared products with the aim to obtain lamellar fibres. Reduction of hybridGO-C_{60} compounds using ascorbic acid as an environmentally friendly reducing agent is also mentioned herein. Considering notable adsorption and separation capacity ofGOwe suppose possible usage of GO based materials in protective equipment.

Keywords: fullerene C_{60}, graphene oxide, fibre, freeze-drying

Synthesis of cable-like composite based on CNT and anodic titania

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In this work we present a novel approach to fabrication of cable-like structure of CNT@TiO_2-NT composites. The TiO_2 nanotubes array was prepared by electrochemical process in which a titanium sheet was anodized in a fluoride-containing electrolyte. CNTs inside the double-walled titania nanotubes were grown by CVD technique using embedded Ni as a catalyst. Composite structure of highly ordered TiO_2-nanotubes and embedded CNT with large specific surface area and enhanced electrical conductivity is potentially very promising material for many applications.

At present, nanostructured titania attracts significant attention due to the broad application potential in different fields, such as photocatalysis, solar energy conversion, electronic and optical devices, supercapacitors, ultrasensors etc. Unique properties of the material originate from its ability to form the charge carriers under the influence of the light. These carriers participate in heterogeneous red-ox reactions at the TiO_2 surface. A way to improve the efficiency of electron transfer to the active layer is the embedding of conductive CNTs into the titanium dioxide tubular structure for charge separation and decreasing the recombination rate of photogenerated electron-hole pairs. Thus, the aim of the present study is to develop a synthesis technique for cable-like (tube-in-tube) structures composed of tubular titanium dioxide layer with carbon nanotubes inside.

The fabrication process for the CNT@TiO_2-NT composite material had three main stages. The first step was to create an array of nanotubular titania by electrolysis of 120 μm thickness Ti sheet in fluoride-containing solution based on ethylene glycol and glycerol. The next step was to deposit 5 nm layer of Ni with the Quorum Technologies Q150T ES magnetron sputtering machine. Finally, CNTs were grown on the Ni@TiO_2-NT array by the catalytic pyrolysis of ethanol at 600 ^{o}C and under the 12 kPa gas atmosphere. The surface and cleavage morphology of synthesized samples was then examined by Carl Zeiss SIGMA VP scanning electron microscope (SEM).

SEM images analysis confirmed that the entire surface of the anodized TiO_2 was covered by CNTs with average diameter of about 20 nm and length >0.5 μm. Examination of cracks and chippings on synthesized samples have showed that heating of microtubular TiO_2 layer of 4 μm thickness during the CNTs growing process has led to the appearance of concentric double-walled TiO_2 nanotubes with 80 and 250 nm diameters. CNTs were formed inside the double-walled TiO_2 tubes what resulted in tube-in-tube or cable-like structures. Prospective applications of synthesized structures for fabrication of solar cells elements were discussed.

Keywords: cable-like, composite, carbon, titania nanotubes.

Systems for the synthesis of carbon nanotubes dedicated for cancer cell thermal ablation

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One of the most promising areas for carbon nanotubes application is medicine. One of the most devastating diseases where nanotechnology can be applied is cancer. Worldwide research can be divided into two main groups: diagnostics and treatment. It may be used as carriers of slowly released drug. There are also several studies on the use of electromagnetic waves to destroy cancer cells by the carbon nanotubes (CNTs). Several techniques can be used for CNTs synthesis. In our work we use arc-discharge method, microwave plasma-assisted chemical vapor deposition (MPCVD) and hybrid physico-chemical vapor deposition (HPCVD).

In our arc discharge system the plasma reactor works with low pressure of He (up to 0,5 atm). The electric arc burns between two graphite rods. Temperature of the arc leads to vaporization of the anode. Vapors of carbon moves from the anode to the cathode and form cathode deposit with carbon nanotubes. However, carbon nanotubes can also be collected from the reactor walls. This method is suitable for production of multiwall nanotubes (MWNTs) with very high purity and single wall nanotubes (SWNTs) with yield up to 90%. Disadvantage is that SWNTs tend to be short with random sizes and directions.

In MPCVD system the plasma is generated in a waveguide connected to a microwave generator. As a source of carbon usually hydrocarbons such as acetylene, ethylene etc. are used. As a catalyst pentacarbonyl or ferroceneis applied. The microwave plasma is used for activation of the reagents.Then containing carbon and ferromagnetic elements plasma flux go to the quartz tube. The additional resistance heating can be applied to increase the reaction effectiveness and efficiency. CNTs nucleation occurs on the quartz tube walls. It is also possible to use a substrates to improve carbon nanotubes growth. Catalysts enhances the rate of reaction and, what is more important, enable ferromagnetic atoms attachment to the carbon nanotubes.

HPCVD system involves both chemical decomposition of carbon containing gases and vaporization of solid or liquid source of catalyst. In this system a tube furnace with three zones of heating is applied. A mixture of working and carbon containing gases go through the quartz tube placed inside the furnace. As a catalyst ferrocene vapors can be used. Catalyst is placed in the first zone of furnace and is initially preheated. It leads to vaporization of iron elements. Ferromagnetic CNTs may be collected in the third zone either from the quartz tube walls or on the substrates.

There are just a few systems to production of carbon nanotubes with magnetic properties. These nanotubes, purified and functionalized, can be used as a nanoheaters in RF electromagnetic field for thermal ablation.

Acknowledgment

Scientific work has been financed from the budget for science in the years 2013-2015 as a research project.

Keywords: carbon nanotubes, thermal ablation, arc discharge, CVD

Influence of metal elements on carbon plasma jet during arc discharge synthesis of carbon nanotubes

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Arc discharge is one of the most common method of carbon nanotubes synthesis. In this method the synthesis process occurs in a low pressure neutral atmosphere. In this case graphite carbon electrodes are used as a source of carbon. The high temperature of the electric arc plasma leads to carbon evaporation from the anode and deposition on the relatively cold cathode. The product consists of different carbon molecules – soot, amorphous carbon, fullerenes, and multiwall carbon nanotubes (MWNT's). In the case of catalysts application metals such as Ni, Y, Fe etc. are introduced into the system. Presence of catalysts determine single wall nanotubes (SWNT's) formation.

Catalysts significantly change plasma parameters such as electron density, thermal and electrical conductivity, effective ionization potential and in effect plasma temperature and carbon molecules structure. The carbon nanotubes growth occurs in environment composed on ions of gas (e.g. He, Ar), ions of carbon, multi-atom molecules, neutral gas particles, ions of catalyst, neutral catalyst particles and electrons. The aim of this work is establishing the influence of additional metal on plasma jet parameters affecting carbon nanotubes synthesis. It was noticed that morphology of the product depends on the carbon plasma composition.

Metal arc plasma consists of atoms, ions and electrons. Helium or argon has been used as a working gas. It was assumed that unbounded metal occurs in the inert atmosphere and that multiple ionization below 5000 K is negligible.The presence of catalyst resulted in higher average temperature than carbon arc. The reason of higher temperature of the arc channel with catalysts vapors is more complex and may results from much higher thermal conductivity.

Calculations of plasma composition were carried out for mixture of metal in inert gas. Different compositions of metal plasma have been considered to establish correlation between metal density and electron amounts. The results clearly show the strong influence of impurities in the plasma on the temperature and electrical properties. The lowest temperature and the highest resistance occurred in the case of the arc burning only in the neutral gas. The highest temperature occurred for the arc containing only copper vapours. Higher temperature cause a higher degree of ionization of gas affecting the reduction of its resistance.

It was noticed that the minimum metal content in the plasma arc determines the essential properties of the plasma. Addition of catalysts such as iron – changes the effective ionization potential, plasma composition, electro density, and in effect – temperature of the plasma. This fact affect the carbon nanotubes synthesis efficiency.

Acknowledgement
Scientific work was financed from the budget for science in years 2010-2014 as a research project.

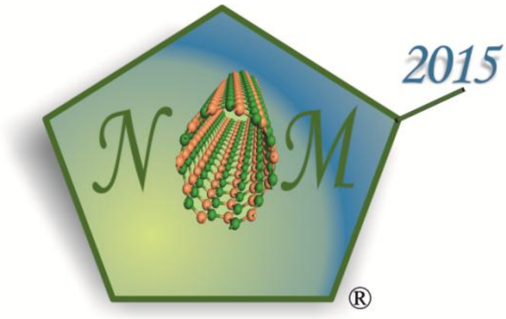
Keywords: carbon nanotubes, plasma jet, electric arc

TOPIC 5

Nanocomposites and nanofillers

Chair: Dušan Kimmer
Co-chair: Marta Valášková

Polymeric composites
Natural nanofillers for composites
Nanostructures and nanoparticle based materials
Nanoceramics and nanoporous materials
Methods for characterization and preparation



Synthesis of azide−CaAl-LDH nanocomposite by an improved mechanochemical procedure

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In layered double hydroxides (LDHs), charge-balancing anions located between the layers can be relatively easily exchanged to, e.g. anions of various complexities. The intercalation of several such anions has been published in the last decades; however, to this date, azide anions (N_3^-) were not among them. Indeed, the conventional synthesis techniques, most often applied to LDHs, led to explosive metalazides instead of layered hydroxides. During our experimental work leading to this contribution, we have improved the mechanochemical among it suitable for the synthesis of azide-intercalated LDHs avoiding the formation of hazardous materials. This is communicated in the followings applying azide−CaAl-LDH as the example.

The azide−CaAl-LDH composite was prepared from their hydroxide constituents *via* mechanochemical activation. Then, NaN_3 solution was added and the suspension was magnetically stirred in a thermostated glass vessel. The synthesis parameters, like the concentration of azide anions, the applied temperature, the ratio of metalhydroxides and the duration of mechanical stirring, were altered systematically.

The composite samples obtained were structurally characterized by X-ray diffractometry (XRD), scanning electron microscopy (SEM), energy dispersive X-ray analysis (EDX),infrared (IR) spectroscopy and thermal methods (TG−DTG).

In all cases, X-ray diffractograms revealed the formation of layered structure. SEM, EDX, TG−DTG and IR measurements provided with further proofs for the successful preparation of the LDH and the intercalation of the azide anion. Through varying the synthesis parameters, we were able to find optimal conditions for the production of high-quality azide−CaAl-LDH composite.

To sum up, an improved technique was developed for the simple and safe synthesis of azide−CaAl-LDH composite, which seems to be a promising material for the synthesis of triazols in the interlayer space of the LDH.

Acknowledgement
This work was supported by the NK106234 grant by the Science Fund of Hungary. The financial help is highly appreciated.

Keywords: CaAl-LDH, azide composite, hydrotreatment, XRD

PPI nano dendrimer functionalized polypropylene nonwoven: fast removal of acid dye from aqueous media

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Dendrimers are highly branched, star-shaped macromolecules with nanometre-scale dimensions having an exterior with several functional surface groups. The goal of this study was to stabilize polypropylene imine dendrimer on the surface of polypropylene nonwoven to achieve a filter layer with the ability of fast and highly efficient removal of anionic compounds from wastewater. In this regard, polypropylene nonwoven was grafted with acrylic acid using plasma technology to produce a functional surface rich of carboxylic acid groups on the nonwoven layer. The next step was the grafting of second generation PPI dendrimers on the functionalized surface through a pad-dry-cure process. The surface characteristics of raw, plasma treated, acrylic acid functionalized and dendrimer grafted fibers were analyzed using ATR-FTIR, FESEM, AFM, XPS and EDS techniques. The results confirmed the desired reactions and grafting of the dendrimer on the surface of the nonwoven.

Regarding the broad possible applications of the prepared product including: drug delivery and release, dye and ion removal, nanoparticles synthesis, antibacterial etc. the ability of the dendrimer grafted nonwoven for removal of cationic and anionic dyes was studied. The functionalized nonwoven showed excellent ability for the removal of acid dyes from water compared with previously studied procedures. More than 99% of the dyes were removed in the first 5 minutes (Fig. 1).

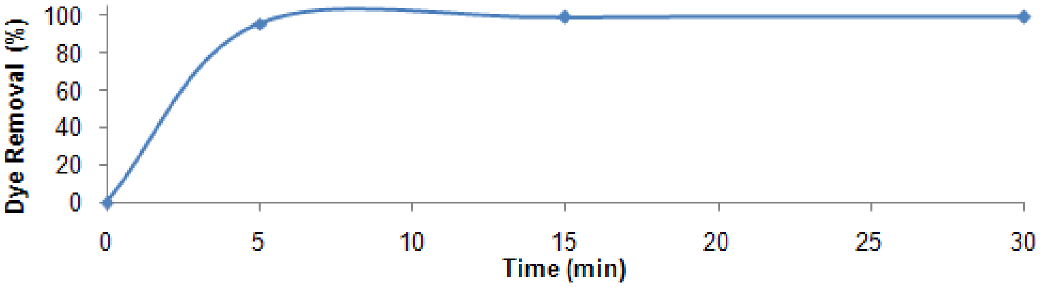

Fig. 1: Effect of time on acid dye removal at pH=3.

Keywords: Plasma, Dendrimer, Polypropylene, Dye Removal

Electrospinning for filter media and nanostructured composites

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The presentation summarizes the ways of several exploitations of polymeric nanofibers in various industrial spheres.

In case of application in air filtration the nanostructures prepared from nanofibres exhibit excellent filtration efficiency first of all in separation of ultrafine particles from the polluted air. Strong interception of influenza virus on the surface of nanofibres has been proved.

Application of nanostructured materials for waste water filtration requests additional filter reinforcing, rather poor mechanical properties of nanofibres being the reason. Ways of membrane reinforcing and influence of selected variables affecting membrane filtration properties will be discussed too.

Electrospinning process has been also used for the preparation of nanostructured materials based on nanoparticles of aluminosilicate fillers and polymeric nanofibers aimed to maximize distribution of filler in polymeric matrix and size of material active surface. Characterization by means of melt strength has been used to prove material costs and extrusion process energy savings in comparison of PE nanoaluminosilicate composite with polymer alloys based on PE and expansive branched PE.

Keywords: Nanofibres - filtration - ultrafine particles - influenza virus interception - liquid microfiltration - membrane reinforcing - dispergation of nanoparticles in nanofibres - composites

Design of fully eco-friendly brake friction composites

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Fully eco-friendly brake friction composites are defined as the debris released during braking is non-toxic to health and less impact to environment. Therefore, those raw materials from nature either biomass or minerals are critical issues to develop. Three kinds of non-toxic raw materials are researched in this study. (1) Micro- and nano-fibrils from bio-degradative natural fibers such as jute, flax and sisal are prepared to replace non-biodegrative organic aramid pulp and metallic steel wool. (2) Walnut shell particulates with chemical composition of lignin are chemically treated so as to enhance their thermal stability and to replace stibnite, which is toxic and clam shells with chemical composition of $CaCO_3$ are used as space filler. (3) Lignin resin prepared from nut shells is used as matrix to replace phenolic resin, which is non-biodegrative. By using above new ingredients and addition of non-toxic mineral basalt fiber as reinforcement, mineral zircon as abrasive and bio-crosslinking agent lysine based diisocyanate (LDI), fully eco-friendly brake friction composites are designed.

Keywords: brake friction composites, friction and wear performance, biomass

Theoretical and experimental selection of solvent for fabrication of electrospun PVP nanofibers

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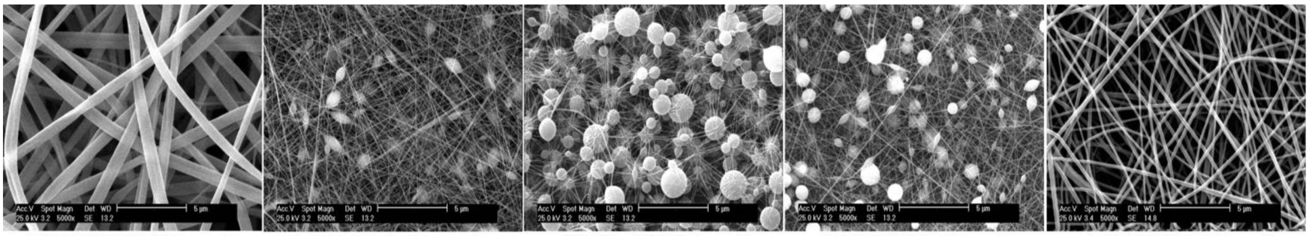
In this research, the effects of solvents and their properties on electrospinnability of the polyvinylpyrrolidone (PVP) solutions and the morphological appearance of the electrospun PVP nanofibers were investigated qualitatively by means of a scanning electron microscope (SEM). The issue of solvent suitability for electrospinning of PVP is a complex issue. Considerable efforts have been made on developing suitable solvents and solvent systems for electrospinnable PVP solutions. The spinnability of a polymer solution has been explained only by solution properties observation and it is usually mentioned that good solvents for a particular polymer were employed. Hansen solubility theory was found to be a useful tool for the prediction of suitable solvent for PVP nanofibers fabrication via the electrospinning process. For this aim, we employed various solvents with the purpose of determining the most suitable one for obtaining the lowest diameter with highest uniformity PVP nanofibers. The five solvents used were ethanol (EtOH), propanol (PrOH), chloroform ($CHCl_3$), N-methyl-2-pyrrolidone (NMP), and N,N-dimethylformamide (DMF). The Hansen solubility parameters of the PVP calculated by Van Krevelen method were δ_d=15.5, δ_p=11.7, and δ_h=7.2 $MPa^{0.5}$. Therefore, the dissolving power of the solvents for PVP was in the order of DMF> NMP>> $CHCl_3$> PrOH> EtOH. Figure 1 displays SEM photographs and corresponding fiber diameter distribution of the electrospun PVP nanofibers. By using PrOH, $CHCl_3$ and NMP, electrospun nanofibers average diameter was very low, but beads formations were observed. Only PVP solutions in EtOH, and DMF could produce continuous fibers with high enough productivity, while the PVP solutions in PrOH, $CHCl_3$, and NMP could not presented satisfied spinnability. Regarding to the obtained Hansen theory and experimental results, the PVP nanofiber uniformity obtained from PVP/DMF solution system was higher than other solvent systems leading to narrowest fiber diameter distribution. Finally, it has been demonstrated that with appropriate solvent the PVP nanofiber diameter distribution and formation of beads can be controlled with Hansen theory.



EtOH (932±202 nm) PrOH (134±31 nm) $CHCl_3$ (78±24 nm) NMP (109±28 nm) DMF (224±35 nm)

Fig. 1: SEM photographs of electrospun nanofibers from PVP solutions with various solvents.

Keywords: Polyvinylpyrrolidone, Nanofibers, Dissolving, Hansen theory, Morphology

CO oxidation catalyzed by bio-Au/SiO_2 composite

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Currently it is know that gold nanoparticles are catalytically active. There are a lot of possible ways how to prepare such gold-based catalysts, for example impregnation, coprecipitation, precipitation-deposition [1]. This work is focused on biosynthesis as alternative method of preparing similar materials. Biosynthetically prepared Au/SiO_2 nanocomposits were tested as catalysts for CO oxidation.

There was used algae strain *Diadesmis gallica* (DG) and $HAuCl_4$ as precursor of gold. Two samples were prepared by similar way, difference was only in the temperature, which was 5°C and 25°C. Both prepared Au/SiO_2 composites were characterized by TEM, XRPD, IR spectroscopy and ICP-AES. Average size of prepared gold nanoparticles was 16 nm (5°C) and 19 nm (25°C). After calcination (450°C, 4h) and activation (300°C in He) their catalytic activity in CO oxidation was observed in defined conditions (temperatures 30 – 270°C, atmospheric pressure, sample amount 0,1 g, overall flow of gas 100 ml/min and incoming mixture 2500 ppm CO + 2 mol% O_2 in He). The amount of CO was analysed using gas chromatograph with thermal conductivity detector. Surprisingly, catalytic activity of both samples was roughly the same – approximately 60% at 270°C. Size of gold nanoparticles was increased to 28 nm after catalysis. Slight aggregation was caused probably due to weak immobilization and stabilization of gold nanoparticles on SiO_2 surface.

The catalytic activity may be increased by modification through reductive oxide, namely by magnetic modification by iron oxide, this was already successfully tested at similar sample of bionanocomposite before [2].

References

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[2] Kratošová G. et al. In book: *Green biosynthesis of nanoparticles: Mechanisms and application*, chapter 5, p. 61-78. CABI Publishing, UK 2014.

Keywords: biosynthesis, gold nanoparticles, Au/SiO_2 composite, CO oxidation

Direct electrochemical synthesis of tin oxide nanoparticles on polypyrrole coated porous copper substrates

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Tin oxide can be used in Li-ion batteries, gas sensors and catalysts. The size of semiconducting metal oxide nanoparticles drastically affects their properties. Different methods have been developed to synthesize tin oxide nanoparticles such as high energy ball milling, homogeneous precipitation, sonochemical methods, etc. However, there is limited number of reports for the electrochemical synthesis of these nanoparticles. In the present work, tin oxide nanoparticles have been electrochemically synthesized in a layer-by-layer array. The synthesis was done from a solution of tin (II) chloride, directly on polypyrrole coated porous copper electrodes. The prepared electrodes showed electrocatalytic performance for methanol oxidation process.

The copper sheets, saturated calomel electrode, SCE, and platinum plate were used as working, reference and counter electrodes, respectively. Firstly a layer of Cu/Zn alloy was deposited on copper sheets. The alloy was then immersed in 3%w/v HCl solution for 30 minutes. A porous copper electrode was formed. It was then immersed in a solution of 0.1M distilled pyrrole monomers, 0.1M oxalic acid and 0.31M dodecyl benzene sulfonic acid. A constant current of +4.00 mA/cm^2 was applied for 1000 s, to the working electrode, and black PPy film was synthesized as second layer. Finally, a layer of tin oxide nanoparticles was electrochemically synthesized. A 25 mM solution of tin (II) chloride, $SnCl_2$, was used at different pH values. The solution was treated with an ultrasound probe for 1 hour before electrosynthesis. The PPy coated porous copper electrodes, Cu/PPy, were used as working electrodes. The synthesis was performed galvanostatically by applying different current densities between 2.00 and 8.00 mA/cm^2 for 70 s. Scanning electron microscopy, SEM, energy dispersive X-ray, EDX, spectroscopy and X-ray diffraction, XRD, were used for surface morphological and analytical studies. SEM results showed that the nanoparticles with average diameters of 20-30 nm have been formed on PPy film (Figure 1).

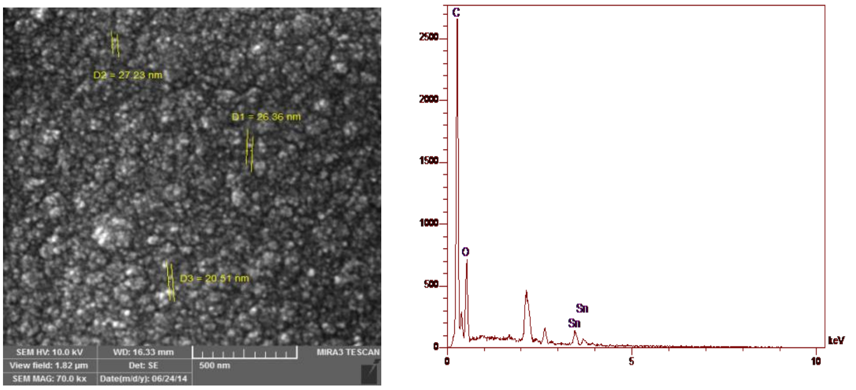

Fig. 1: The SEM image and EDX analysis of synthesized tin oxide nanoparticles on the surface of polypyrrole coated porous copper electrode.

Keywords: Tin oxide, Nanoparticles, Electrochemical synthesis, Polypyrrole

Antibacterial polypropylene/Ag-kaolinite, preparation and characterization

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Kaolinite (KA) belongs to layered silicates which structure consists from one tetrahedral and one octahedral sheet forming the type of layer 1:1.Kaolinite has no layer charge because the central cations in tetrahedra (Si^{4+}) and octahedra (Al^{3+}) are not substituted by the other cations. The structural properties make kaolinites difficult for modification to be used as a carrier of metal nanoparticles or clay nanofiller to polymers. Therefore, prior activation of its structure by mechanical or chemical procedures or their combination is often required.

Two structural types of kaolinites (KA1, KA2) prepared as nanofillers AgKA to polypropylene (PP) matrix were modified by formamide, ammonium bromide, benzoylperoxide and vinylacetate monomer and then treated with silver nitrate solution. Mixtures of PP with nanofillers, prepared by melt compounding technique, were pressed into thin plates. Content of silver was determined via X-ray fluorescence analysis.Structure properties of prepared powder AgKA materials and PP/AgKA composites were studied by X-ray diffraction analysis, infrared spectroscopy, scanning electron microscopy (SEM) and the specific surface area measurement. Figure 1 shows morphology of AgKA1 nanofiller with elemental map of silver.

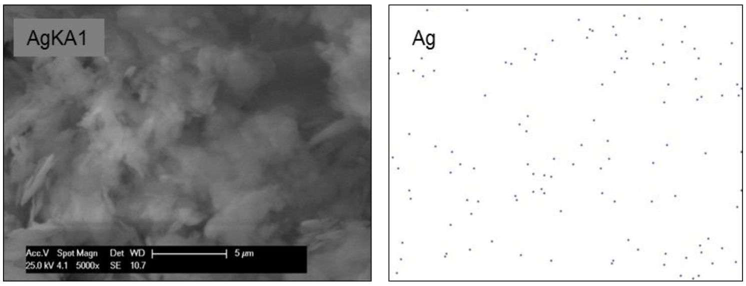

Fig. 1: SEM image and elemental map of silver on the surface of sample AgKA1. The scanned area on Ag map corresponds to the surface on image.

Antibacterial properties of PP/AgKA composites were tested on two different bacterial strains: Gram-positive *Enterococcus faecalis* and Gram-negative *Pseudomonas aeruginosa*. Surfaces of PP/AgKA composites showed good antibacterial effect against both tested bacteria. The results showed improving effect to inhibit the bacterial growth with increasing content of AgKA nanofillers in PP.

Acknowledgements

This work was supported by the Ministry of Education, Youth and Sport of Czech Republic (project no. SP2015/59), and IT4 Innovations Centre of Excellence(project reg.no.cz.1.05/1.1.00/02.0070).

Keywords: Kaolinite, Silver nanoparticles, Polypropylene, Antibacterial activity

Preparation of antibacterial polyethylene/inorgano-organo-vermiculite hybrid material

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In presented study, clay mineral vermiculite (VT) was modified by organic surfactant hexadecyltrimethyl ammonium bromide (orgVT). Subsequently, the samples VT and orgVT were treated with cerium chloride solution and pillaring aluminum chloride solution. Prepared materials were used as VT nanofillers to the polyethylene (PE) matrix. The composites ofPE with modified VT nanofillers were prepared by melt compounding technique, and pressed into thin plates for further analysis.

The morphology of powder VT nanofillers was observed by scanning electron microscopy. Content of inorganic and organic components in the samples was determined by X-ray fluorescence analysis and total organic carbon measurement. The structure properties of powder VT nanofillers and PE composites were studied by X-ray diffraction analysis (XRD).

The XRD patterns of powder VT nanofillers confirmed intercalation of organic surfactant and inorganic cations into the VT interlayer space.

Antibacterial activity of powder VT nanofillers and surfaces of PE composite plates was tested on different bacterial strains: 1) Gram-negative, represented by bacteria *Escherichia coli*, *2)* Gram-positive, represented by bacteria *Staphylococcus aureus*, and3) yeast, represented by *Candida albicans*.

The results from antibacterial tests show that powder VT nanofillers inhibited growth of tested bacteria already after 0.5 h of action and the effect was stable throughout the test period.

The surfaces of prepared PE composite plates showed good antibacterial effect against S*taphylococcus aureus* and *Candida albicans*.

Acknowledgement

This work was supported by Ministry of Education, Youth and Sport of Czech Republic (project no. SP2015/59),and IT4 Innovations Centre of Excellence (project reg.no.cz.1.05/1.1.00/02.0070).

Keywords: Vermiculite nanofiller, Polyethylene, Composite, Antibacterial activity

Evaluation of texture surface of composite material based on WPC after using machining technology

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The paper focused on evaluating the effect of changes in technological parameters within a turning process (rate of feed f and spindle revolutions *n*) on micro-geometric characteristics of the surface of an inhomogeneous composite material. In addition to the standard parameters used for evaluating the quality of machined surface – *Ra* (arithmetic mean deviation of roughness profile) and *Rz* (maximum height of roughness profile), or their ratio *Ra/Rz*, the contribution also deals with parameters highly sensitive to the presence of isolated protrusions and depressions – skewness *Rsk* and kurtosis *Rku*. By means of the two applied parameters, differences between obtained readings from a profilometer occur (when assessing the surface at 3 points of specimen machined under constant conditions). An analysis and interpretation of the results from surface texture of 2D parameters is very important for the future use of surface generated by turning technology. Its specifying description correlated with mechanical and technological parameters gives a comprehensive view of changes in conditions of feed rate and speed in relation to the generated surface texture.

Keywords: inhomogeneous material, surface texture, micro-geometric characteristics, turning technology

Effect of polymer matrix on gas separation in mixed-matrix membranes containing Cu-MOFs

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One way to satisfy the demand of polymeric membrane materials with high permselectivity for gas separation is the preparation of mixed matrix membranes (MMM) by the incorporation of nano-sized fillers such as silica, zeolite, metal organic frameworks (MOFs) into polymer matrixes.

In this presentation, we consider the use of new Cu-MOFs with high CO_2 selectivity as the dispersed component in MMMs and see the effect of gas separation performance using different matrix. High CO_2-selective frameworks, Cu-metal-organic frameworks (Cu-MOFs)[$\{Cu_2(Glu)_2(\mu$-bpa$)\}\bullet(CH_3CN)]_n$(Glu = glutarate, bpa = 1,2-bis(4-pyridyl)ethane) were synthesized and determined from the gas adsorption selectivity that can be used as carriers for CO_2.The choice of matrix polymer is also important; we fabricated MMMs using amorphous poly(2-ethyl-2-oxazoline) (POZ) and semicrystallinepoly(amide-6-*b*-ethylene oxide) (PEBAX®MH 1657) as a polymeric matrix and confirmed the effect of matrix on gas separation.

CO_2permeance of MOF-PEBAX 1657 MMM loaded 4.8% Cu-MOF was 13.12 GPU (1 GPU=1×10^{-6} $cm^3(STP)(cm^2 scmHg)^{-1}$) and CO_2/N_2 selectivity was 52.75 which are higher than those of the pristine PEBAX®MH 1657 (The CO_2permeance and CO_2/N_2 selectivity are 1.36 GPU and 12.51, respectively) and CO_2 permeance of MOF-POZ MMM loaded 7.2% Cu-MOF was 0.69 GPU and CO_2/N_2 selectivity was 33.76 which are also higher than those of the pristine POZ (The CO_2permeance and CO_2/N_2 selectivity are 0.58 GPU and 1.06, respectively). Improvement in the CO_2/N_2 selectivity of the membranes was achieved via both high adsorption selectivity of CO_2 over N_2 by the Cu-MOFs, and the morphological changes of the matrix due to the presence of Cu-MOFs. When comparing matrix polymer, the addition of CO_2 selective Cu-MOF carrier provides the synergic gas separation effect on PEBAX 1657 than POZ matrix.

Changes of the morphology of PEBAX 1657 and POZ with the addition of Cu-MOF were investigated by X-ray diffraction pattern and it was found that the permselectivity depends on the d-spacing change of the MMM with the addition of Cu-MOFs.

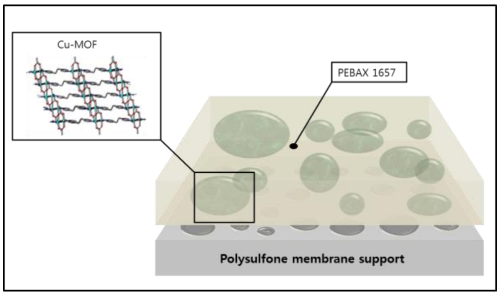

Fig. 1: Model of MMM containing Cu-MOFs.

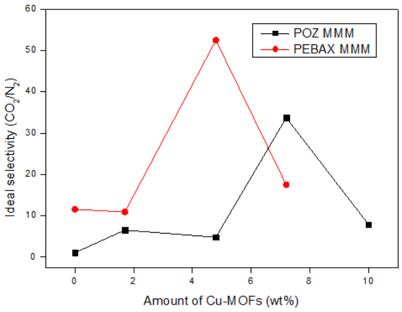

Fig. 2: CO_2/N_2 selectivity of MMMs that contain different amounts of Cu-MOFs in different matrix.

Keywords: Mixed matrix membrane, CO_2 separation, Metal organic framework, Poly(amide-6-b-ethylene oxide)

Kinetic studies of strontium ions sorption from aqueous solution

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Isotopes of strontium are one of the most abundant radioactive pollutants in aqueous effluents. The chemical properties of strontium-90 are similar to calcium, so when entering the human body, strontium-90 can easily replace calcium and cause leukemia, anemia, genetic changes and other diseases. Water solutions containing strontium could be harmful to the environment (especially soil and water systems). Moreover, as a result of chemical reactions, the water-insoluble strontium compounds could become water-soluble. Currently, various methods have been developed and applied to remove the Sr^{2+} ions from aqueous solutions, such as chemical precipitation, evaporation, ion exchange adsorption, and ion flotation. Adsorption on the mineral surfaces, based on the distribution of soluble components between aqueous solutions and solids, is the most effective method of pollutants removal from waste water.

The present study describes the effect of initial Sr^{2+} ions in solution on adsorption kinetics using the montmorillonite as sorbent. The model solution of Sr^{2+} ions was prepared from $Sr(NO_3)_2$. Experiments were carried out with various initial concentrations of Sr^{2+} ions at laboratory temperature. Concentrations of Sr^{2+} and other dissolved ions in filtrate were determined using atomic emission spectroscopy with inductively coupled plasma. The kinetic data were fitted using the pseudo-first and pseudo-second kinetic models. The coefficient of determination was used to describe the best corresponding model. The kinetic studies showed that the adsorption process was quite rapid and that the equilibrium capacity was achieved within 30 min; experimental kinetic data were found to be well fitted with pseudo-second-order kinetic model. The kinetic rate constant and equilibrium amount of absorbed Sr^{2+} ions were calculated as well, the kinetic rate constant was negatively affected with increasing initial concentration of Sr^{2+} ions (see Fig. 1).

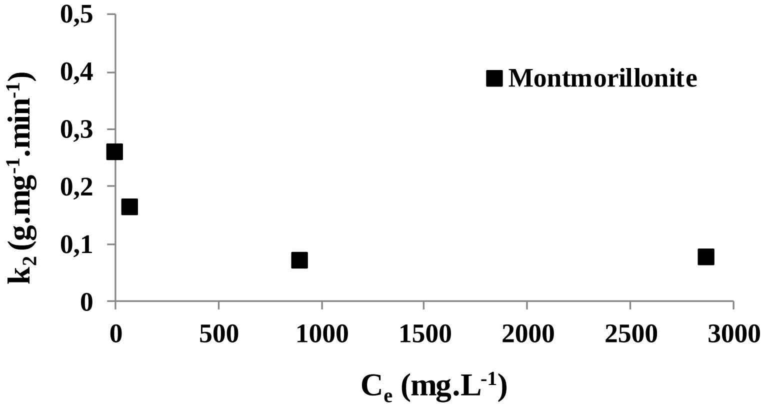

Fig. 1: Effect of varying initial Sr^{2+} ions concentration in solution on kinetic rate constant.

Acknowledgement
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Keywords: Strontium, Montmorillonite, Adsorption kinetic

Structural properties of ceria nanoparticles on vermiculite and ceramic matrices

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Clay mineral matrices and metal oxides are of current interest because of their high thermal stability, surface area, and catalytic and adsorption properties. For example, catalysts based on ceria (cerium oxide, CeO_2) are widely used as efficient systems for oxidation of CO in the atmosphere. The application of clay mineral vermiculite in preceramic mixtures with talc and kaolin contributed to the acquisition of a new type of the cordierite ceramics [1]. Cordierite with 10 wt% of CeO_2 was recommended as a suitable catalytic convertor for purification of exhaust gases [2]. Vermiculite (Ver) matrices carrying the nanoparticles CeO_2 (Ver/CeO_2) were firstly used as precursor for production of the photocatalytic cordierite/CeO_2 ceramics [3]. Despite the small content of active CeO_2 component (3 - 10 wt%), the ceramics exhibited a similar or even a higher activity in decomposition of N_2O in comparison with the commercial TiO_2 catalyst Evonik P25 [3].

This work presents the structural characteristics of the Ver/CeO_2 and cordierite/CeO_2 ceramics obtained by using X-ray powder diffraction (XRD), scanning and transmission electron microscopy (SEM and TEM), and photocatalytic activity on N_2O decomposition. Figure 1a shows the pore size distributions of vermiculite without and with CeO_2 (Ver and Ver/CeO_2), figure 1b the nanoparticles of ceria in Ver/CeO_2, which are attached to the silicate layers.

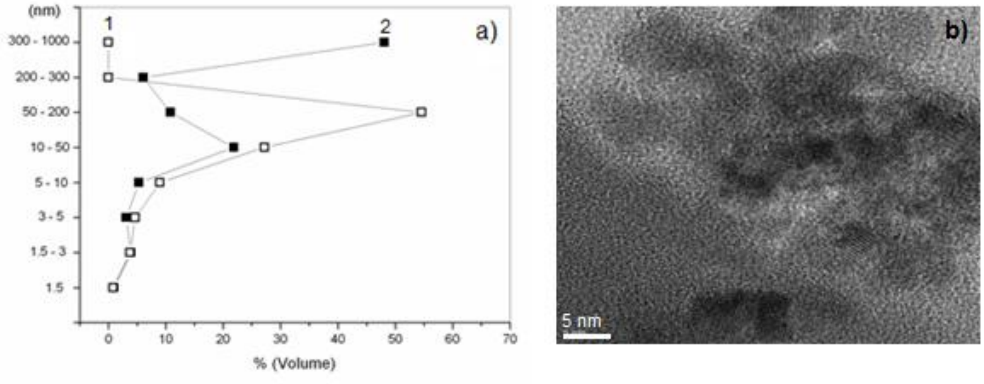

Fig. 1: a) Pore size distributions of Ver (1) and Ver/CeO_2 (2); b) Clusters of single-crystalline CeO_2 nanoparticles attached to the surface of vermiculite (HRTEM).

Acknowledgement
This work was supported by the IT4Innovations Centre of Excellence (project reg. no.cz.1.05/1.1.00/02.0070).

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Keywords: *Silicate layer matrix, Cordierite ceramics, Ceria nanoparticles, Precipitation, Structural analysis, Photocatalytic* N_2O *decomposition.*

Carbon nanotubes reinforced cement pastes – influence on mechanical properties and microstructure

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It seems that the term nanotechnology has been appearing almost everywhere for the last decade or so. This young field of study is offering a potential to revolutionize many industries. From facial cosmetic products to space shuttle's heat shields, the unique properties of nanomaterials come from single aspect – nanoscale. Due to their extremely small dimensions, nanoparticles behave more according to the laws of quantum physics than then laws of classical physics. Thanks to this, nanoparticles of electrically insulating element could conduct electricity, inert substance can behave as catalyst and gold will be bright red instead of yellowish.

The possibility of dramatic improvement in both physical and mechanical properties and maybe even obtaining of brand new ones is obviously very tempting for building materials such as concrete. Imagine that you could take away its negative properties (e.g. low tensile strength and high carbon footprint) and boost the positive ones. This could lead to the new generation of ultra-high performance concretes that would for example allow reduction of the dimensions of structural elements, which would lead to further economic and environmental benefits.

There is a whole range of cement-friendly nanoparticles and the ones that are gaining a lot of attention lately are carbon nanotubes (CNT). Looking like hollow tubes with diameter of several to tens of nanometers and length of several to hundreds of micrometers, these nanoparticles brings new opportunities as well as obstacles. On the journey from laboratory to factory we have to find ways to reliably overcome these obstacles. Besides possible toxicity and economic availability, there is a problem with effective dispergation. Due to the enormous specific surface of CNT (or nanoparticles in general), they tend to agglomerate to form clusters up to hundreds of micrometers in diameter. These must be efficiently deagglomerated and stabilized with cement compatible surfactants.

In this paper, the physical phenomenon known as cavitation is used in order to disentangle the bundles of CNT. Specifically the cavitation was induced by the passage of high frequency acoustic signal through aqueous medium, i.e. ultrasonication. Three different doses of CNT were used – 0,001 %, 0,0025 % and 0,005 % by weight of cement, with the lowest dose being recommended by the supplier.

Although the dispersion efficiency is best observed on mechanical properties of the nanocomposite, it is at least practical to be able to measure it before adding CNT suspension to, in our case, cement paste. For this purpose the spectroscopic methods, based on observation and measurement of the interaction of electromagnetic radiation with matter, as well as microscopic methods were used. Tensile and compressive strength of hardened cement pastes was determined in the age of 7 and 28 days. The remaining fractions of the samples were then observed using a scanning electron microscope (SEM) in order to investigate possible changes in the microstructure of cement stone.

Understanding of the dispersion and stabilization of suspensions of nanoparticles must be given a great deal of attention and effort. New generation of nanoparticles modified high performance concrete with reduced economic and environmental burden depends on it.

Keywords: carbon nanotubes, cement, dispergation, surfactant, reinforcement

Clay composite fillers in polymer matrix

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The study compares different clay polymer composites. Polymer matrix was made from polyamide 1010 (PA1010) and different clays and clay composites served as filler. The clay content in the polymer clay composites varied from 0 to 8 wt.% in 5 steps. Clay composites were prepared from kaolinite and montmorillonite clays combined with either titanium dioxide (TiO_2) or zinc oxide (ZnO). The samples were characterized by scanning electron microscopy (SEM), atomic force microscopy (AFM) and X-ray diffraction analysis (XRD). Tensile strength, Martens hardness and surface roughness were further determined. Tensile strength was improved with the addition of the clay filler but the Martens hardness decreased. The tensile strength was highest for the sample containing 4 wt.% of MSTi65 (montmorillonite (50 wt.%) + TiO_2 (50 wt.%) calcined at 600°C) filler, contrary the lowest tensile strength was for sample containing 2 wt.% of KATi65 (kaolinite (50 wt.%) + TiO_2 (50 wt.%) calcined at 600°C). Martens hardness was highest for pure PA1010 and lowest for sample containing 5 wt.% of ZinKa55 (kaolinite (50 wt.%) + ZnO (50 wt.%) calcined at 500°C) filler.

Acknowledgements

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Keywords: polyamide 1010, montmorillonite, kaolinite, composite, characterization

Synthesis and characterization of nanosilver-doped hydroxyapatite

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Being the main inorganic constitution of hard tissues (bone and teeth), calcium phosphates have been attractive in medical and dental applications in hard tissue repair. Hydroxyapatite ceramics have attracted attention since it may be possible to use them as an alternative to autogenous free bone grafting because of their excellent osteoconductive and bioactive properties. Furthermore, one of obstacles of all types of surgery is postoperative complications consisting mainly inflammation at the surgical site. This also applies to implantable materials where the inflammation after surgery at the site of operation can occur for reasons other than implant rejection.

In order to minimize the problem of infections it is possibility to improve calcium phosphates materials by introducing the silver exhibiting antibacterial and antifungal properties. The antibacterial activity against a wide variety species of microorganisms are described in the literature. Silver nanoparticles operate not only antimicrobial against bacteria, viruses and fungi, but also stimulates the number of living cells such as lymphocytes, fibroblasts, osteoblasts to increased activity. The presence of nanoparticles provides bactericidal properties of materials which significantly reduces the risk of postoperative infection.

The main aim of this work was to synthesis and physicochemical characterization of synthetic calcium phosphateswith hydroxyapatite structure with nanosilver inclusions. Two types of hydroxyapatite with different morphology and different physicochemical properties were obtained by co-precipitation method from water solutions using various reaction conditions. As a result, powders containing different amounts of silver in monophasic HAp without significant morphological changes were obtained. Incorporation of Ag into HAp material upgrades its quality – to have the capacity to maintain the sterility of the implanted material during the time of the adaptation of a foreign body and the process of wound healing. Evaluation of the surface properties of the materials obtained after immersion in simulated body fluids confirms the formation of new apatite layers. It is the most desirable feature of materials intended for implantation, and it proves their bioactivity.

It can be concluded that development of methods for the preparation of bioactive, metal-modified hydroxyapatite can be an important step towards creating a new generation of bioactive materials for applications in medicine and dentistry.

Acknowledgements
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Keywords: biomaterials, hydroxyapatite, silver nanoparticles, modification

Sorption properties of organovermiculites

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Vermiculite is well-known material from group of phylosilicates nowadays used for sorbents preparation. They are known to be very efficient sorbents of organic compounds, especially polycyclic aromatic hydrocarbons, in their modified forms. There are only few studies about their treatment after utilization. Thus, the goal of this work is to propose ways of disposing them after the application or to develop efficient regeneration procedure.

This work includes characterization of sorption properties of vermiculites modified with organic compound such as HDP and HDTMA. Sorption efficiencies were studied against phenol- ammonia water into which modified vermiculites were added. The obtained results showed increased levels of organic compounds in phase carbon, XRD, FTIR and SEM analyses. Consequently, the saturated sorbents were subjected to two desorption methods: 1) extraction with solvent – dichloromethane, acetone, hexane and 2) thermal treatment.

After the desorption processes the phase carbon analyses, XRD, FTIR and SEM analyses were performed to study not only desorption efficiency but also changes in structures of the treated organovermiculites. Ecotoxicity tests were performed on sorbed and desorbed samples as well to predict a possibility of organovermiculite disposal in future.

Acknowledgements
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Keywords: Vermiculite, Modified, Sorption, Desorption

MCM-41/PSF membranes for natural gas purification

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CO_2 represent one of the most important contaminants in gases as N_2, CH_4 and H_2 (including biohydrogen). Other contaminants like H_2O, H_2S and N_2 are also present in natural gas that influencing the quality of gas. In several regions from Romania (such as Timisioara, Deva, Hunedoara), the concentrations of carbon dioxide in natural gas are not so high compared to other countries, the gas chromatography analysis confirming concentrations between 0.1%-1.5 vol.%.

In gas purification processes the polymeric membranes have received significant attention, having several advantages including low capital and operating costs, high efficiency, simple operation compared to conventional purification techniques such as cryogenic distillation, adsorption and absorption or combinations of these. One of the most common amorphous glassy polymers used for gas membrane separation is the polysulfone (PSF). It presents a rigid and high-strength structure and offers a better transport performance for specific gas permeation mixtures than rubbery polymers.

In this work mesoporous silica/PSF composite membranes for CO_2 removal in CH_4 were prepared by incorporating silica particles (MCM-41) in the solvent (chloroform) in a proportion of 90/10 wt% solvent/MCM-41-polymer mixture. PSF was then added, and the whole mixture was magnetically stirred for 24 h, including five intervals of sonication for 10 min The membrane were cast on flat glass plates, and subsequently left overnight, partially closed to slow down the natural evaporation of solvent under ambient conditions. Prior, the MCM-41 was prepared. The as-made composite membranes were characterized by X-ray diffraction (XRD)/thermogravimetric analysis (TGA). The XRD patterns of MCM-41 obtained in laboratory were consistent with the typical XRD patterns for MCM-41 structure, highlighting that mesoporous ordered silica materials were obtained.

Keywords: PSF membranes, MCM-41, natural gas contaminants

Sorption properties of magnetic titanium dioxide composite

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The water pollution originating from industrial activities affects the environment and health of the population significantly. Adsorption is one of the most efficient methods of pollutants (both inorganic and organic) removal from aquatic solutions. It is therefore in the constant interest of researchers to develop new sorbents that could connect more useful properties. The titanium dioxide particles seem to be such a material because they possess both photocatalytic and sorption properties.

Presented article is focused on the verification of the sorption properties of magnetically modified TiO_2 particles prepared by diverse processes. Novel sorbent based on various TiO_2 particles was prepared. Batch adsorption techniques were used to study the effect (a) of the contact time of adsorbate with sorbent (b) type of TiO_2 particles (c) content of iron oxide nano- and micro-particles on the adsorption process. Surface of the materials before and after sorption was examined by electron microscopy and specific surface area was determined. The adsorbate concentration in solution after sorption was determined by AES-ICP. The stability of magnetic TiO_2 particles was studied by determination of the Fe concentration in solution after the sorption process using AAS-FA. The measured results were described by distribution coefficient, adsorption efficiency and both pseudo-first and pseudo-second kinetic model. The coefficient of determination was used to describe the best corresponding kinetic model. The results of Pb^{2+} ions adsorption from aqueous solution on magnetic TiO_2 were compared with adsorption on non-magnetic TiO_2 particles.

The results show that the adsorption process and the kinetic rate constant of Pb^{2+}ions adsorption were significantly positively affected by the presence of magnetic iron oxides on TiO_2 particles surface. While the non-magnetic TiO_2 particles did not adsorb the Pb^{2+} ions at all, the adsorption using the magnetic materials was quite rapid and the kinetic rate constant was dependent on the initial concentration of Pb^{2+} in the aqueous solution. Contrary to the previously published results where different type of TiO_2 particles was applied, the kinetics was fitted by the pseudo-first kinetic model. Magnetic iron oxides content in the used material was not affected by the adsorption process and the material can be thus deemed as stable. Overall, the results show that the TiO_2 particles magnetically modified with iron oxide nano- and micro-particles can be used as an efficient sorbent of Pb^{2+} ions from aqueous solutions.

Acknowledgements
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Keywords: titanium dioxide, sorption, lead, sorption kinetic

Effects of Rheological Properties on Polyvinylpyrolidone Nanofiber Morphology

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Rheological properties, especially solution viscosity influences nanofibers formation with electrospinning process. Solutions with high viscosity cannot be ejected from the spinneret whereas solutions with low viscosity do not manufacture nanofibers. In this research, the relationship between the rheological properties of polyvinylpyrrolidone (PVP) solutions and the morphology of their electrospun fibers was established. The viscosity, surface tension, and electrical conductivity of PVP in N,N-dimethylformamide (DMF) and ethanol were measured in the various concentration range. Measurement of the solution viscosity of the PVP/DMF and PVP/ethanol to the polymer concentration used in this study and subsequent fit to a power law relationship showed that $\eta \propto C^{2.96}$ and $\eta \propto C^{2.91}$ for DMF and ethanol solvent, respectively. Electrospinning of PVP solutions was carried out under controlled parameters. To obtain uniform and bead-free PVP nanofibers, it was evident that the minimum solution concentration must be chosen at 12 and 8 wt% in DMF and ethanol solvent, respectively. Uniform PVP nanofibers without beads were obtained from electrospinning of PVP/DMF solutions only in the range of 12-20 wt% concentration were obtained. The PVP/DMF solutions were found to fabricate a sufficient capacity of fibers to form a uniform nanofibers mat. But, ethanol solvent could be considered as a good solvent for PVP to produce electrospun nanofiber with wide diameter distribution, it is suitable for microfiber production. A power law model between viscosity and PVP solution concentration was established with exponents of 2.69 and 2.62 for DMF and ethanol, respectively. In addition, the average diameter of the electrospun PVP/DMF and PVP/ethanol solutions is related to the solution viscosity through a power law model at an exponent of 0.91 and 0.90 for DMF and ethanol solvent, respectively.

Keywords: Polyvinylpyrrolidone, Nanofibers, Rheological properties, Morphology, Power law

Sorption of Cd^{2+} on clay mineral/hydroxyapatite nanocomposites

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Clay minerals, montmorillonite (Mt) and vermiculite (Ver), are natural materials with wide range of usage. In this study, natural Mt and Ver, and monoionic sodium form of Mt and Ver were used. The surfaces of these clay minerals were utilized as substrate for in situ preparation of hydroxyapatite (HAp). Nanocomposites of clay mineral/HAp were investigated as sorbents of cadmium cations (Cd^{2+}).Two different processes of sorption were compared – 1) dynamic (shaking movement)or 2) static (maintaining the solutions containing $Cd^{2+}$with sorbents for 24h in constant conditions).
Sorption capacity of pure clay minerals, nanocomposites of clay mineral/HAp and pure Hap were compared. The samples were characterized using atomic absorption spectrometry (AAS), X-ray powder diffraction (XRD) and scanning electron microscopy (SEM).
The results show that nanocomposites of clay mineral/HAp have higher sorption capacity than pure clays. Comparison of sorption techniques reveals small differences between sorption on Mt clay and its composites. On the other hand, sorption on pure Ver shows lower sorption capacity during dynamic process than at static process. Pure clay minerals have been found aworse sorbents than a pure hydroxyapatite.

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Keywords: Clay minerals, Hydroxyapatite, Nanocomposite, Sorption

Structural properties of the cordierite ceramic particles

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Cordierite ceramics has been known for many years. Until these days, it was used as traditional technical ceramic materials. For example for refractory materials, heat and sound insulators, heaters, microwave sorbents, plumbing equipment etc. With technological development is more interesting and becoming rediscovered material. Especially, with the structure modification by the nano-structured fillers we expect its advanced use in technological practice.

Traditionally, the precursors of the cordierite ceramics consist of a mixture of aluminum oxide and clay minerals such as vermiculite, talc and kaolinite. The mixture is traditionally heat treated at temperatures higher than 1250 °C. In these paper we were used the nanoparticles of zinc oxide, copper oxideand cobalt oxideas three types of functional nano-structured fillers. The three modified mixtures were heat treated at 1300 ° C for 1 hour and then were milled in the planetary ball mill for 15 minutesfor cordierite ceramic particles preparation.

The morphology of cordierite ceramic particleswas studied using scanning electron microscopy (SEM), structural changes were monitored using X-ray diffraction (XRD) and X-ray fluorescence microscopy analysis.The particle size distribution and specific surface area were characterized also.

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Keywords: cordierite ceramic particles, nanofillers ZnO, CuO and CoO.

Phosphate removal using non-modified and magnetically modified montmorillonite

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Phosphorus compounds spreading from households and industry into waste water pose **a threat to** environment because just a small number of sewage treatment plants are able to effectively remove phosphorus compounds. An increasing amount of this element in water causes growth of algae and cyanobacteria and leads to eutrofication which affects negatively the quality of water resources; thus, it is necessary to prevent the phosphorus spread into waste water. Biological precipitation, ion exchange, electrocoagulation and processes using adsorbents all are up to date technologies. Regarding adsorption utilisation, the sorbents have large specific surface, high efficiency and there is a vast amount of types of sorbents available. Recently, active carbon, hydroxyapatite and aluminium oxide were widely used as sorbents for removal of various types of contaminants. Increasing number of studies deal with phosphate adsorption on clay minerals as e.g. kaolinite, bentonite and montmorillonite due to their large interlayer space, surface properties and overall environmental friendliness.

Presented study was focused on phosphate sorption on sodium montmorillonite and its magnetically modified form (using iron oxide). The chemical composition and specific surface area of both non-magnetic and magnetic montmorillonite were determined. Adsorption studies were carried out using the batch technique in a wide range of phosphate concentrations (1-1000 mg P/L) to obtain the equilibrium data. Model solutions of waste water were prepared using Na_3PO_4. Phosphate concentrations were determined by UV/VIS spectrometer and the determined concentration was verified by optical emission spectrometer with inductively coupled plasma. The efficiency of sorption and effect of sorbent dose in phosphate solution were evaluated. Obtained experimental equilibrium data were fitted by the Langmuir and Freundlich isotherm models using non-linear regression. The coefficient of determination and residual sum of squares were used to describe the best corresponding model calculated. The calculated parameters show that the Langmuir model fitted experimental data better in the case of both types of montmorillonite samples. The results show that efficiency increased with increasing amount of sorbent and that the maximum efficiency was 98 % when 5 g of adsorbent was applied to 50 ml of solution. The maximum adsorption capacity of the non-modified and magnetically modified sorbent calculated using the Langmuir adsorption model were the same (10.4 mg of P per gram of sorbent). That means presence of the magnetic iron oxides did not affect the adsorption capacity of sorbents while it allows the magnetic separation of the used sorbent after its application.

Acknowledgements

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Keywords: Adsorption, Magnetically modified montmorillonite, Phosphate

Electrical conductivity of PANI, PANI/kaolinite/titanium dioxide and PANI/montmorillonite pressed tablets – study of load sensor

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Polyaniline (PANI) is one of the widely studied conducting polymers due to its light weight, low cost, excellent environmental stability and reversible acid-base switching of its electrical conductivity. Composites based on PANI are often used as sensors for different purposes. Present work is focused on testing the pellets pressed from pure PANI powder and two composites (PANI/kaolinite/TiO_2 and PANI/montmorillonite) as load sensors. Our aim is to obtain a new functional unit able to respond to external mechanical pressure by changing the electrical conductivity. Pellets were pressed at ambient conditions using pressure 28 MPa. No binders were used and piston was not oiled. Electrical current flowing through the pellets was recorded in dependence on external mechanical pressure. Small weights were gradually added on the top of the pellet (i.e., external pressure ranged from 0 to 36768 Pa) during the “loading part” of one experimental cycle. During the “unloading part” of the cycle the weights were gradually removed. The stability of response was determined as a proportion of instantaneous electrical current (for actual load) and maximum (measured at maximum load) electrical current. It was found that pellets pressed from PANI/kaolinite/TiO_2 and PANI/montmorillonite composites exhibit more stable responses to increasing and decreasing load than pellets pressed from pure PANI powder.

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Keywords: polyaniline, phyllosilicate, titanium dioxide, electrical conductivity, load sensor

Polyaspartic acid as a component of polymer - ceramic composites for biomedical applications

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Polyaspartic acid (PAA), biodegradable and a non-toxic, is an interesting polymer material suitable for various applications such as industrial, agricultural and medical application. The biodegradability and environmentally friendly nature of polyaspartic acid makes it potential material to replace many non-biodegradable polymers in use. Polyaspartic acid from a chemical point of view, belongs to the group of polyamino acid. PAA may exist in four isomeric forms – α,β and L,D isomers.

PAAis a promising water-soluble, biologically inert, hygroscopic and water soluble. Over the30 days about 85% of PAA is degrade with the releases of amino acids, carbon dioxide, ammonia and carbonyl compounds as a products of degradation. Due to properties of polyaspartic acid and its copolymers have been widely used in medicine and pharmacy to obtain implants, surgical sutures and screws. PAA polymer is widely use as a temporary artificial skin substitutes in the treatment of burns and cover against tissue adhesion or as scaffolds for tissue culture. More recently, polyaspartic acid and its copolymers play an important role in drug delivery system as drug carrier which allows for a controlled release of the drug to prolong its activities in the patient's body.

Polyaspartic acid has also ability to control and modify the biomineralization process - can inhibit crystal nucleation and growth as well as change the morphology of the new formed crystals of calcium carbonate, calcium sulfate, calcium oxalate, calcium phosphate, and barium sulfate salts. When the PAA are immobilized by cross-linking to a structural framework such as collagen or chitin they can promote nucleation and the growth of crystals.

The role of the additive – polyaspartic acids in composites is to stimulate nucleation at a certain time or location in the case of biologically controlled mineralization of bone. Although the mechanism remains unclear, it was concluded that PAA asa nucleating agent and growth mediator has crucial role for biomineralization of hydroxyapatite.

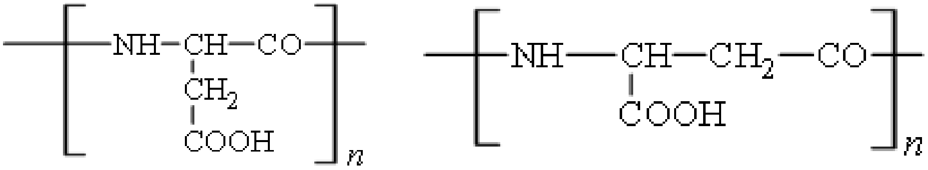

Fig. 1: Poly(α-aspartic) acid (left) and poly(β-aspartic) acid (right) structure.

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Keywords: Polyaspartic acid, Composites, Biomineralization, Biodegradation

The application of the scanning spreading resistance microscopy for the measurement of the surface electrical properties of nanocomposites

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Scanning spreading resistance microscopy (SSRM) is a new technique applied to investigate local surface electrical properties of conductive materials, electrical devices, etc., in the nanoscale. Present work aims to demonstrate the SSRM method on two types of electrically conductive nanocomposites – polypropylene/graphite (PP/graphite) and polyaniline/montmorillonite (PANI/MMT). PP/graphite nanocomposite was prepared via blending granulated PP with maleic anhydride grafted polypropylene (MAH-g-PP) and natural graphite, and subsequently modified by thermal treatment at temperature 170 °C for 1 hour and UV irradiation for 1 and 24 hours. The changes in the surface conductivity were compared for pristine and modified samples. In addition to the SSRM measurement, AFM analysis was performed in order to investigate the changes in surface roughness. It was found that the modifications induced the changes in surface roughness causing decrease in the surface conductivity. The PANI/MMT nanocomposite thin film was prepared by in-situ polymerization on the glass substrate and studied both by SSRM and AFM methods. Results of the SSRM (local current maps) and AFM (morphology of the surface) measurements were compared in order to localize the conductive and nonconductive components or areas of the nanocomposites. With the respect to the nature of sample the measurement results of SSRM depended mainly on the choice of the probe with appropriate stiffness of the cantilever, the type of the conductive tip and the value of the bias voltage applied between to the tip and the sample surface.

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Keyword: Scanning spreading resistance microscopy, conductivity, nanocomposites, atomic force microscopy

Electrical conductivity of polyaniline/montmorillonite nanocomposite films

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A simple method of time-controlled chemical deposition was used to prepare polyaniline/montmorillonite (PANI/MMT) thin films on various substrates at different temperatures. The aim of this work is to optimize the substrate choice and preparation temperature in order to achieve the highest conductivity of thin films.

For preparation of thin films anilinium sulfate was used as a precursor and ammonium peroxydisulfate as an oxidizing agent. The thin film was formed when these two solution were mixed with a desirable amount of MMT in presence of a substrate. All substrates were washed with detergent, rinsed with distilled water and ethanol and dried prior to use. To avoid double-side coating, one of the side of the substrate was covered with scotch tape. As a substrate microscope slides, silica glass slides and plastic foil were used. The preparation of thin films was carried out at two temperatures, 10°C and 20°C. The polymerization at 10°C was realized in a temperature controlling water bath set to 10°C and the polymerization at 20°C was carried out at 20°C.

A homemade apparatus was utilized to determine the specific electrical conductivity of prepared thin films. During the measurement constant voltage of 1 V in the DC regime was used, the distance between Cu-electrodes was 3 mm at all times. Prior to use, Cu-electrodes were treated with abrasive paste to avoid negative effects of impurities. A final value of electric current was received as an average of 300 values that were obtained during a 42 seconds-long measurement. Specific electrical conductivity was then calculated from achieved value of electric current.

The measurement results showed that the optimal temperature for preparation of PANI/MMT thin films is 20°C. Samples prepared at 20°C exhibited higher specific electrical conductivity than samples prepared at 10°C. Plastic foil was proven to be the most suitable substrate in order to obtain the highest specific electrical conductivity of the PANI/MMT thin layer. The surface of plastic foil has better adhesion than microscope slides or silica glass slides. Therefore, the PANI/MMT thin film is more easily formed on this substrate.

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Keywords: polyaniline, montmorillonite, conductivity, thin films

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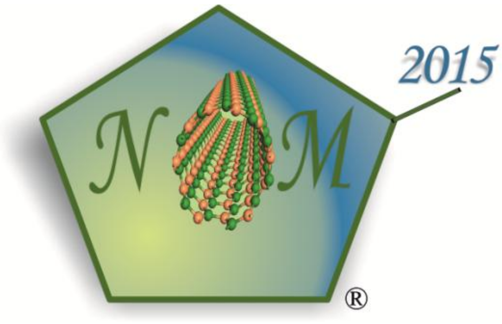

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