DMS – RE 2017

The twenty-seven joint seminar

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

BOOK OF ABSTRACTS OF THE 27th JOINT SEMINAR

4 – 8 September, 2017
Kežmarské Žľaby

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DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

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Organized by

Slovak Expert Group of Solid State Chemistry and Physics
Czech and Slovak Association for Crystal Growth
Faculty of Chemical and Food Technology STU
Faculty of Materials Science and Technology STU in Trnava
Crystallographic Society
Slovak Society for Industrial Chemistry
Regional Committee of Czech and Slovak Crystallographers

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FOREWORD

The seminar “Development of Materials Science in Research and Education” is already the twenty seventh in the series started at Gabčíkovo in 1991 by the initiative of the Czech and Slovak Association for Crystal Growth and the Slovak Expert Group of Solid State Chemistry and Physics.

The objective of this meeting is to offer an opportunity to Czech and Slovak teachers and scientists as well as guests from other countries who are working in the field of Materials Science to present their recent results and experience and to exchange new ideas and information.

The scientific session will cover the following topics on materials science:

- Trends in development of materials research
- Education of materials science at the universities
- Information about the research programmes of individual institutions
- Information about equipment for preparation and characterization of materials
- Results of materials research

This workshop is aimed at creation of a stimulating atmosphere of cooperation and at the support of patient dissemination of scientific ideas and propagation of materials science in education.

Organizers

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ABSTRACTS

Nucleation and microstructure development in Cr-Mo-V tool steel during gas atomization

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Nucleation studies of undercooled metallic melts are of essential interest for the understanding of phase selection, growth kinetics and microstructure development during their rapid non-equilibrium solidification [1-6]. The paper deals with the modeling of nucleation processes and microstructure development in the hypoeutectic tool steel Ch12MF4 with the chemical composition of 2.37 % C, 12.06 % Cr, 1.2 % Mo, 4.0 % V and balance Fe [wt. %] in the process of nitrogen gas atomization.

Based on the classical theory of homogeneous nucleation, the nucleation temperature of molten rapidly cooled spherical particles from this alloy with diameter from 40 mm to 600 mm in the gas atomization process is calculated using various estimations of parameters influencing the nucleation process - the Gibbs free energy difference between solid and liquid phases and the solid/liquid interfacial energy. Results of numerical calculations are compared with thermodynamic calculations applying CALPHAD method, achieved experimental nucleation temperatures and microstructures developed in rapidly solidified powder particles from the investigated alloy [7].

The research has been supported by the Scientific Grant Agency of the Slovak Republic (VEGA) within the project No. 1/0811/14 and the project ITMS 26220120048 under the Research & Development Operational Programme funded by the ERDF.

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Doping study of SnS

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Thermoelectric (TE) materials are substances that show strong thermoelectric effects. These effects describe the link between temperature difference and difference of electric potential. Thus, these materials allow mutual transformation between thermal energy and electric energy. This fact can be utilized in waste heat power generation or green cooling technologies. Efficiency of a thermoelectric device is a function of the dimensionless figure of merit $ZT = \alpha^2\sigma T/\kappa$, where α, σ, T and κ are Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively. Recently, high TE performance has been reported in single crystals of SnSe [1] which has similar structure to SnS [2].

Aim of this work was to investigate the influence of Tl, P, F and Cl doping on thermoelectric properties of SnS in terms of enhancement of ZT. Hot-pressed polycrystalline samples with 0, 0.25, 0.5 and 1 % of the dopants as substituents in cation or anion sublattice of SnS were prepared. The samples were characterized by X-ray diffraction, electrical and thermal conductivity, Hall and Seebeck coefficient. These parameters were measured over a temperature range of 300-725 K. Figure of merit ZT was calculated from obtained data.

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Heterospinové komplexy na báze nositeľov spinov S = 1 a S = 1/2

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Magneticky aktívne koordinačné zlúčeniny sú v súčasnosti v dôsledku perspektívy lukratívnych aplikačných možností (kvantové počítače, pamäťové médiá, nové spôsoby chladenia) predmetom intenzívneho záujmu vedeckej komunity [1]. Aj keď jej aktuálna pozornosť sa prednostne orientuje na vyhľadávanie látok vykazujúcich vlastnosti jednomolekulových magnetov [1,2], predmetom záujmu sú aj iné systémy vykazujúce fyzikálne javy spojené s magnetizmom, napríklad alternujúce spinové reťazce tvorené spinmi S = 1 a S = 1/2. Takéto heterospinové systémy sa môžu chemicky realizovať látkami obsahujúcimi dva rôzne centrálne atómy s rozdielnymi hodnotami spinov (heterospinové komplexy), napríklad komplexmi na báze medi a niklu. Cu-Ni komplexy s ohľadom na oxidačné stavy centrálnych atómov a tvary ich koordinačných polyédrov sa môžu deliť do 4 základných skupín označených **d-d**, **d-p**, **p-d** a **p-p** (**d** = diamagnetický a **p** = paramagnetický centrálny atóm), pričom najzaujímavejšie sú zlúčeniny typu **p-p** s jednorozmernou kryštálovou štruktúrou ako modely alternujúcich spinových reťazcov [4,5]. Chemicky rovnakú kombináciu spinov je možné dosiahnuť aj kombináciou komplexov Ni(II) (S = 1) a organického radikálu so spinom S = 1/2, napr. anión-radikálu $\text{TCNQ}^{-}\cdot$ (TCNQ = tetrakyanidochinóndimetán) [6]. V rámci prednášky sa uvedú príklady pre jednotlivé typy Cu-Ni heterobimetalických komplexov ako aj komplexov Ni(II) s anión-radikálom $\text{TCNQ}^{-}\cdot$ vrátane dosiahnutých výsledkov.

Táto práca bola finančne podporená z grantov VEGA 1/0063/17 a APVV-0014-78.

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Spin crossover with thermal hysteresis in iron(III) complexes

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Novel iron(III) mononuclear complex [Fe(3,5-Cl-*salpet*)(NCSe)] with a pentadentate Schiff base ligand 3,5-Cl-*salpet* and $NCSe^-$ as a coligand exhibits a thermally induced cooperative spin crossover between 123 K (warming) and 99 K (cooling) with hysteresis width of 24 K. The other complexes of [Fe(3,5-X-*salpet*)(Y)] type with X = Cl^- or Br^- and Y = NCS^-, $NCSe^-$ and $N3^-$ are high-spin over the whole temperature region.

The magnetic data for the complex showing a thermally induced spin crossover was analyzed by using Ising-like model with vibrations (equivalent to the thermodynamic regular solution model) yielding the enthalpy ΔH and entropy ΔS of the spin transition along with the critical temperature $T_{1/2}$ and the solid-state cooperativeness Γ.

Slovak grant agencies (APVV-14-0078, VEGA 1/0522/14 and VEGA 1/0534/16) are acknowledged for the financial support.

Status of material analysis in the new STU Ion Beam Centre

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Status of material analysis in the new STU Ion Beam Centre

<p> Ion Beam Analysis (IBA) means analysis of surface layers of materials using the energetic ion beams. We consider ions in the energy range from hundreds of keV to tens of MeV The interaction of accelerated ions with atoms of hit sample leads to several physical phenomena. Depending on the layout and geometry of the experiment, and on which interaction product is detected, we can utilize a variety of ion beam based analytical methods. In some cases, it is also possible to determine the isotopic composition of the sample material.
IBA is an effective tool for investigation of the sample elemental (or in some cases isotopic) composition, to some extent also of the structure of the surface layers of materials. The typical diameter of analyzing ion beam - the lateral resolution is from 1 to 3 mm, the depth of analysis is from nm to about 20 μm. Depth resolution of few nm can be achieved at the sample surface region. Analytical sensitivity of doping elements and impurities ranges from a tenth of percent to the level of ppm, depending on the sample composition and on the use of a particular method.
IBA analytical methods at STU:
• **RBS - Rutherford Backscattering Spectrometry**
• channeling or RBS/C
• ERDA - Elastic Recoil Detection Analysis
• PIXE - Particle Induced X-ray Emission
• NRA - Nuclear Reaction Analyses
IBA analytical methods are quantitative, with an accuracy of typically 5 to 10 %, but also 1 % accuracy can be achieved. IBA is considered to be nondestructive and works also with insulating samples. Typical sample size is 10x10x0.5 mm.
Summary of the Ion Beam Analysis performed in the new STU Ion Beam Centre in Trnava [1] is presented. Examples of the most latest RBS, channeling, ERDA, PIXE and NRA analyses of nm to 20 μm surface layers of solids are given.

This work was supported by the European Regional Development Fund, Research and Development Operational Programme, project No. ITMS: 2622022079, the Slovak Grant Agency VEGA under contract No. 1/0219/16 and the Ministry of Education, Science, Research and Sport of the Slovak Republic under contract No. 003STU-2-3/2016.

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Contribution to the aluminum - tin - zinc ternary system

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The Sn - Zn - Al alloys are one of significant candidates in the proposal of alternative lead-free solders for higher temperature soldering. Our paper deals with the study of the aluminum - tin - zinc system. Twenty Sn - Zn - Al alloys altogether with six binary Sn - Zn alloys, were prepared and studied experimentally. The specimens were studied metallographically including the micro-hardness measurements, complete chemical analysis (ICP-AES, OES), X-ray micro-analysis of alloys by EDX or WDX including SEM (BSE) in order to determine the composition and identification of individual phases. Significant temperatures and enthalpies of phase transformations were determined by DTA.

Alloys were prepared experimentally from pure Sn, Zn and Al (melting and casting into graphite mould). The alloys were further studied after casting and after long-term homogenization annealing. Cast structure with dendritic formations was apparent from the metallographical study of Al - Sn - Zn alloys. It formed due to relatively high rates of the melt cooling. Zn precipitated primarily and its volume portion decreased with increasing Sn content.

DTA analysis of all the specimens was performed on the SETARAM SYSTEM 18^{TM} apparatus in high pure dynamical atmosphere of argon (> 6N). The analyses were carried out twice at the speed of heating as well as cooling 4 K/min. Temperatures and latent heats of corresponding phase transformations (liquidus, solidus, invariant reactions etc.) were obtained. The aluminum influences on the phase transformations temperatures. Resulting experimental data were compared with the data of known Sn - Zn binary system and Al - Sn - Zn ternary system and with the diagrams of other authors.

After long-term annealing of selected alloys in vacuum followed by quenching were carried out structural and chemical microanalyses of the present phases and their limit concentrations. The achieved results were compared with the thermodynamic modelling of the ternary Al - Sn - Zn system (computer programs THERMOCALC, MTDATA, PANDAT and database CALPHAD, COST). The diagram of the Al - Sn - Zn ternary system was given thermodynamically more precisely on the basis of our complex study [1].

This work was solved in the frame of the project COST Action MP0602 Advanced Solder Materials for High Temperature Application, and with the technical support of the project No. LO1203 Regional Materials Science and Technology Centre - Feasibility Program.

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Analysis of properties laser welded Trip steel sheets

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Both, the ecological production and operation of vehicles demand using such materials for deformation zones' structural parts, which show some specific properties and innovative technologies to process them. Specific requirements for functionality (strength, stiffness, deformation work, fatigue properties) are closely linked to processability (formability). In the paper are presented results for multiphase steel Trip RAK40/70 when welded by pulse solid-state fiber laser YLS-500. Based on microstructure analysis in the fusion zone and heat affected zone the welding parameters were optimised. The influence of laser welding on the strength and deformation properties was verified by characteristics of strength, stiffness and deformation work, as they were calculated from mechanical properties measured by tensile test and three-point bending test. The knowledge gathered in the field of laser welding influence on the strength and deformation properties of multiphase steel Trip RAK40/70 should help to designers when design the lightweight structural parts of the car body.

The authors are grateful for the support to project APVV-0273-12 "Supporting innovations of autobody components from the steel sheet blanks oriented to the safety, the ecology and the car weight reduction", as well as the project VEGA 2/0113/16 "Influence of laser welding parameters on structure and properties of welded joints of advanced steels for the automotive industry".

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Power density spectral analysis of ion-beam induced changes in surface morphology

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Ion irradiation, and particularly ion beam sputtering of surfaces results in the development of self-assembled nanostructures at certain irradiation conditions [1], [2]. If the ion beam direction is above a critical angle with respect to the target surface normal, ripple structures evolve perpendicular to the ion beam direction and at grazing incidence, the ripple structure gradually flips orientation from perpendicular to parallel. In case the substrate is irradiated at a temperature above its recrystallization temperature, the self-assembly of vacancies dominates the process, called reverse epitaxy [3].

We have investigated changes in surface morphology and possible pattern formation due to ion bombardment in a plasma immersion implantation (PIII) process. The surfaces of (100) Si monocrystalline samples were bombarded by 1 keV and 35 keV Ar ions generated by a RF plasma, accelerated by pulsing the bias voltage of the sample holder. The surface morphology was evaluated by Atomic force microscopy.

Surface morphology was further analysed using Fourier analysis. We are presenting results obtained by power density spectra estimate method.

This work was supported by the European Regional Development Fund, Research and Development Operational Programme, project No. ITMS: 2622022079 and the Ministry of Education, Science, Research and Sport of the Slovak Republic under contract No. 003STU-2-3/2016.

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Hydrogen treatment of titanium based alloys

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Room temperature workability of the alpha + beta titanium alloys that are used as biocompatible implants in biomedicine is difficult and forming must be performed at elevated temperatures. Thus, improving hot deformation behavior by decreasing flow stress and working temperature is essential challenge. Although hydrogen deteriorates mechanical properties of many engineering metallic materials at room temperature as well as at elevated temperatures, in case of Ti alloys the hydrogen can act as a temporary alloying element in special heat treatment technology, so-called the thermo-hydrogen treatment (THT) [1, 2]. Whereas the hydrogen works as beta stabilizer in Ti alloys, THT technology employs the reversible reaction of hydrogen with titanium in order to modify phase compositions, kinetics of phase transformations and evolution of metastable phases in titanium alloys [3]. THT technology shows beneficial effect in improving particular properties of alpha + beta Ti alloys. The effect of heat treatment on the microstructure and hot deformation behavior of Ti6Al4V and Ti24Nb alloys was investigated. Specimens of both alloys were heat treated in flowing hydrogen or argon gases and submitted to uniaxial compression tests at 750 °C on the Gleeble 3800 machine. The amount of hydrogen in specimens was measured by means of an analyzer LECO RH600. The microstructure study was performed before and after isothermal compression test on the specimens in hydrogenated and non-hydrogenated conditions. Comparing the results obtained for the non-hydrogenated and hydrogenated specimens it was found that hydrogen in Ti6Al4V alloy lowered the thermal deformation resistance, while in case of Ti24Nb alloy affected suppression of instabilities in true stress-true strain curves. The benefit effect of hydrogen on increasing formability of Ti24Nb at lower temperatures was not evident as it was observed in case of Ti6Al4V alloy.

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Study of the Niobium Phosphate glasses

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The phosphate glasses are intensively studied through several decades because of their potential technological applications due to some unique properties, i.e. low synthesis temperature, UV transmission or higher thermal expansion coefficient. They can be used in laser technologies, sealing waxes, as bioimplantates, composites and also storage of nuclear waste [1].

Binary phosphate glasses have relatively limited interval of chemical stability, because ultraphosphate glasses are hygroscopic and polyphosphate glasses can be prepared only in interval ~35-50 mol % P_2O_5. Their properties and chemical stability can be enhanced by adding modifying oxides, i.e. alkaline, alkaline earth, rare earth or transition metal oxides.

Niobium phosphate glasses were previously investigated [2] to obtain chemical resistant and thermal stable materials. However, in all previously studied compositions, PbO was added as a glass modifier; these glasses were very stable, and chemically resistant. The bridging oxygen is now bonded to Nb^{5+}, forming O-P-O-Nb-O- type chains. It was also shown that P-O type bonds are mostly found in terminal sites of the chain, while Nb-O bonds are located in the middle of the chains [3].

In this work were studied the 17 glass samples in four compositional lines - 1) xNb_2O_5-(50-x)ZnO-$50P_2O_5$ ($0 \leq x \leq 15$ mol %); 2) xNb_2O_5-50ZnO-(50-x)P_2O_5 ($0 \leq x \leq 15$ mol %), 3) xNb_2O_5-(50-3x)ZnO-(50+2x)P_2O_5 ($0 \leq x \leq 16{,}67$ mol %) and 4) xNb_2O_5-(50-2x)ZnO-(50+x)P_2O_5 ($0 \leq x \leq 25$ mol %). The substitution of Nb_2O_5 for ZnO in base matrix and its impact on the structure and thermal properties was studied. Glass transition temperature, temperature of softening and thermal expansion coefficient was measured. The structure was studied by Raman, NMR and ESR spectroscopies. The changes observed from thermal measurements indicates forming of the more rigid structure and interconnection of the phosphate chains with increasing content of the Nb_2O_5. The Raman spectra showed that the niobium is present as 6-coordinated into NbO_6 units in these glasses. It was also stated that those octahedra are linked through corners into the 3D structure.

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Discrepancy between crystal structure and magnetic properties of Ni (II) complexes synthetized with 4-methylpiperidine and tridentate Schiff base

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Slow magnetic relaxation and paramagnetism in a supposed dimer made of two square planar Ni(II) units, namely [Ni(L)(Me-*pip*)]$_2$ consisting of the tridentate Schiff-base ligand L and 4-methylpiperidine was observed. However, crystal structure of [Ni(L)(Me-*pip*)] solved by single crystal structural analysis approves that complex is a mononuclear entity. In such a case the complex would be square-planar and thus diamagnetic. In order to check the purity, crystalinity and identity of the bulk powder material a series of X-ray experiment was done: single-crystal structure determination at T = 100, 150, 200, 250, and 298 K; powder diffraction at the room temperature followed by LeBail refinement.

It was found that the simulated diffraction pattern from the single-crystal structure determination does not match the experimental diffraction pattern of the bulk powder sample. It was considered that this sample could be mixture of complex with already solved crystal structure and other yet unknown compound. Based on this observation, the syntheses with the same reactants at different experimental conditions were made. The products were evaluated with qualitative phase analysis and four different products were found. It has been shown that the mix of two of these products can form the already mentioned bulk sample. This work presents preliminary results of single crystal and powder structural analysis of the four samples and comparison of the crystal structures obtained from powder and single crystal analysis.

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The three new groups Mn(III) and Fe(III) dipicolinate complexes

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Dipicolinic acid (pyridine-2,6-dicarboxylic acid = H_2dipic) is known to be a major component of bacterial spores. The metal dipicolinate complexes are also used in environmentally friendly "green" catalysis. The most common include heterogeneous catalysis, oxidation reactions and degradation reactions of waste water. The chemistry of manganese and iron complexes has been investigated recently since these metals are present in a various biological redox systems including peroxidases, catalases, superoxide dismutases, dioxygenases and lipoxidases. In this lecture we report the structural characterization of a three new groups manganese(III) and iron(III) dipicolinate ionic complexes with three types of cations. The general formula of anions in these complexes is $[M(dipic)_2]^{-1}$ (M = Mn(III) and Fe(III)). Each of the dipic anions are coordinate to one central atom in a terdentate fashion manner, via two O atoms and the N atom (dipic = pyridine-2,6-dicarboxylate anion). The cations in these groups of complexes are 2-, 3- or 4-hydroxymethylpyridinium, 2- or 4-carbamoylpyridinium, 1,10-phenantrolin-1-ium, or 2-(pyridin-2-yl)pyridinium and theirs derivatives. Observed structural data are discussed and correlated with those of known Mn(II/III) and Fe(II/III) complexes found in Cambridge Crystallographic Data Base.

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Radiation Resistance of Glass Fiber Optic Cable

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The good experience with optical communication and its advantages in industrial applications have lead to introduction of optical communication technology into more conservative areas, such as the nuclear and aerospace industries. The number of optical cables in nuclear power plants has been increasing. Fiber optic cables are commonly used at nuclear power plants in I&C systems but they are usually used in mild environments, i.e. without radiation. Nevertheless, currently, the number of applications in harsh environments with radiation is increasing.

One of the most prevalent effects of radiation exposure is an increase of signal attenuation (signal loss). This is a result of fiber darkening due to radiation exposure and it plays a very important role in application of fiber optics in radiation environment. However, after the irradiation, the fiber optics go through a “recovery process” during which the optical properties improve again. As we discovered, this healing process can stop and switch its trend.

Test samples were kindly provided by GOC Co., Ltd (Fiber optic cable manufacturing company, Gwangju, Korea). This work was supported by the Grant Agency of the Czech Technical University in Prague, grant SGS 16/224/OHK3/3T/13. Special thanks to colleagues from VŠB (Technical University of Ostrava, Faculty of Electrical Engineering and Computer Science, Department of Telecommunications), for the initial cooperation and measurement.

Size distribution and growth rate of crystal nuclei near critical supercooling in small volumes

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Physical properties and structure of the newly forming material are often predetermined by the formation of nuclei from the supercooled (or supersaturated) parent phase. The phase transition is detected using optical measurements or thermal analysis methods when critical supercooling is determined. Analysis of the critical supercooling in various volumes enables to determine the stationary nucleation rate from so-called survivorship function [1]. However, it is not clear how many particles of various sizes is formed near the critical supercooling ΔT_C. The classical nucleation theory, which is applied for the determination of the stationary nucleation rate, underestimates the number of nuclei formed in Ni droplet. The size dependence of the interfacial energy of clusters has been taken into account to overcome this discrepancy [2].

Kinetic equations are numerically solved to determine the size distribution of crystal nuclei, F, formed in Ni droplets near ΔT_C supercooling. The maximum size of nuclei r_{max} was determined from F as a function of time and the growth rate of the largest particles $v = dr_{max}/dt$. In the sufficiently large volumes of the parent phase, the growth rate of particles v reaches some minimum value (at certain time when the critical clusters are formed) and then increases with time to the growth rate of the flat interface limit. In smaller volumes, only a certain maximum size of nuclei r_{max} is reached, which quickly increases with supercooling. In consequence of depletion of the parent phase, the growth of the largest particles is stopped in small volumes. The growth of nuclei occurs only when the number of critical nuclei is sufficiently high.

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Nickel(II) Schiff base complexes: Synthesis, reactivity,magnetic properties and catalytic activity

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Schiff base ligands have been extensively studied in coordination chemistry mainly due to their facile syntheses, easily tunable steric and electronic properties as well as good solubility in common solvents [1]. Transition metal complexes with Schiff bases, which contain oxygen and nitrogen as donor atoms are of particular interest, because of their ability to possess square-planar or octahedral stereochemistry [2].

The reaction of nickel(II) acetate with tridentate *O,N,O*-chelating Schiff base (L) lead to the distorted monomeric square planar [NiLB] complexes (where B are derivatives of pyridine, piperidine, imidazole or phosphine). Some [NiLB] complexes under study were tried for their catalytic activity in Kumada cross-coupling reactions.

Five new octahedral Ni(II) complexes, namely $[Ni(L)(CH)(MeOH)] \cdot MeOH$ and $[Ni(HL)_2(CH)] \cdot AcN$ (5), were synthetized from a *O,N,O*-chelating Schiff base (L), phenanthroline or bipyridine (CH) and nickel(II) acetate, using different solvents and their ratios (MeOH and/or acetone and acetonitrile). The hypothesis with positive and negative D parameter was tested with better fit for negative alternative and weak supramolecular antiferromagnetic coupling.

The complexes under study have been characterized by spectral methods (IR, UV-VIS and NMR spectroscopy) and single crystal X-ray analysis. Using different chelating ligands (aromatic or sterical aspects) leads to tri- or tetranuclear coordination compounds with octahedrally coordinated Ni(II) centres.

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Microstructure and mechanical properties of selective-laser-melted Ti6Al4V alloy

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The present work analyzes the problem of Ti6Al4V materials processed by selective laser melting (SLM) [1-4]. The samples were tensile and compression tested before and after heat treatment that consisted of solution annealing at 955 °C followed by water quenching and aging at 600 °C followed by air cooling. The microstructure and mechanical properties of SLM samples were evaluated before and after the heat treatment. The results showed that the samples exhibited high mechanical values even though they contained a relatively high porosity. The anisotropy of tensile and compressive strength was observed, which was related to the occurrence of voids. The causes of the porosity have been outlined. The brittle nature of failures of non-heat treated samples can be explained by synergy of martensite presence, microcracks and residual stress produced by SLM. The plastic properties of specimens were improved by means of heat treatment that led to the transformation of martensite to the lamellar structure composed of alpha + beta phases. The parameters affecting the preparing process as well as characteristics and mechanical properties of samples prepared by SLM were discussed.

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History and Present of the Department of Physics at VŠB-Technical University of Ostrava

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Department of Physics was founded as a school-wide department of VŠB-Technical University of Ostrava at the beginning of the year 2016. This Department was originally a historical part of the Mining-Geology Faculty, but has been connected to a more than one-hundred and twenty year tradition of physics education, previously in terms of the Mining Academy and today as VŠB-Technical University of Ostrava.

The Department of Physics guarantees its own study branch of Applied Physics in all three levels of study, it ensures the instruction of basic physics subjects for six technical faculties and further for the study programs Nanotechnology, Mechatronics, Applied Sciences and Technology and Computer Science. At the present time there are 21 staff members working at the Department, of which 17 are academic workers, 3 non-academic staff and 1 worker.

The scientific-research activity of the Department of Physics is oriented on the development of basic and applied research. It is presently focused on six specializations: applied nuclear physics, the progressive technology of material disturbance, optical diagnostics, optical spectroscopy, special materials and technology and the magnetic properties of materials, which corresponds to the personal and experimental equipment the Department of Physics has. Members of the Department are also active participants and proposers of scientific-research and educational projects and are also connected to projects, which are led at other working centres, for example,

• IT4Innovations excellence in science, MŠMT, LQ 1602

• Optical spectroscopy of Heusler compounds (HEUSPECTRO), 7. FRAMEWORK PROGRAMME OF THE EU (M. Curie), PIEF-GA-2009-254511

• Regional material technological research centre (RMTVC), OP VVI, Z.1.05/2.1.00/01.0040

In terms of scientific-research activities the Department has also developed close cooperation with local and foreign working centres. From the Czech Republic there are for example the Institute of Material Physics AVČR, v. v. i, Physics Institute CAS, v. v. i, and Palacky University in Olomouc, Jan Evangelista Purkyně University in Ústí nad Labem, Charles University, etc. Cooperating foreign institutes are for example: the Silesian University in Katowice (Polsko), the Slovak Academy of Science in Bratislava (Slovakia), Paris-Saclay University (France), Grenoble University (France) and Marie Curie-Sklodowska University in Lublin (Poland).

An important activity of the Department is also popularization activities, including a whole range of activities, oriented especially on co-operation with secondary schools or the promotion of physics studies at VŠB-TUO in our region, such as for example providing lectures, seminars and excursions or organizing Student Competitions. Some members of the Department are active members of the Ostrava branch of the Union of Czech Mathematicians and Physicists.

Rutherford Backscattering Spectrometry system in channeling regime

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This contribution deals with Rutherford Backscattering Spectrometry in channeling regime (RBS/C) which is an ion beam analysis for near surface layers of solids. The experiment is most often carried out using He^+ ions at energy typically around 2 MeV. The sample holder is attached a 4D goniometer. Channeling of high energy ions can be used to analyze the crystalline quality of the lattice, i.e. lattice disorder, substitutional or interstitial atom impurities present in the lattice etc. As the channelling experiment is preceded by at least 160 RBS spectra measurements, the manual preparation of hundreds of scripts, as well as manual evaluation of measured data is complex and time consuming. Hence, the automatization of this process is required in order to increase the efficiency [1].

The standard experimental set up for ion beam analysis (IBA) at ion beam laboratory in STU does not provide straightforward way for channeling spectra measurement [2].The 6 MV Tandetron which includes IBA system is computer operated and enables to run RBS measurements via the several successive scripts (batches). The control software written in MATLAB contains the preset parameters of the measurement and enables collecting of the measured data.

An example of channeling measurement prepared and evaluated by the software will be presented.

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UV radiation and change in properties of polymer composites

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Composites are used not only for their structural properties, but also for electrical, thermal, tribological, and environmental applications. Modern composite materials are usually optimized to achieve a particular balance of properties for a given range of applications. Composites typically have a fibre or particle phase that is stiffer and stronger than the continuous matrix phase. Many types of reinforcements have good thermal and electrical conductivity, a coefficient of thermal expansion that is less than the matrix, and or good wear resistance. The first level of classification of composites is usually made with respect to the matrix constituent. The major composite classes include organic-matrix composites (OMCs), metal-matrix composites (MMCs), and ceramic-matrix composite (CMCs). The term organic-matrix composite is generally assumed to include two classes of composites: polymer-matrix composites (PMCs) and carbon-matrix composites.

Rheology and its experiments reveal information about the flow behaviour of liquids but also the deformation behaviour of solids, because it is the typical behaviour of polymers. Changes induced by the environment with degradation effect can be evaluated by rheological measurements which monitor changes in visco-elastic properties of the tested polymers. The fundamental of rheological characteristics is viscosity which defines the internal resistance of material against its creep generated by external forces. It is necessary to realize the dual character of majority of polymer materials from visco-elastic point of view. The action of external force on the ideal viscous material results in its deformation i.e. irreversible locomotion (movement) of macromolecules and after removal of the external force material retains its “new” shape. The action of external force on the ideal elastic material results in its deformation but after the removal of the external force, the material returns to its original shape. Polymers are generally characterized by the visco-elastic nature, which means that external forces cause partly permanent (viscosity element of polymer) and partly reversible (elastic element of polymer) deformation

The present article deals with monitoring the changes in the mechanical properties of composites with polymer matrix. The composite was formed from the PA matrix and glass fibers. The composite contains 10, 20 and 30 % (vol.) glass fibers. The mechanical properties were evaluated on samples of the composite before and after UV radiation on the sample. Light microscopy was evaluated distribution of glass fibers in the polymer matrix and the presence of cracks caused by UV radiation. By the rheological measurements the changes of visco-elastic properties (complex viscosity, moduli of elasticity and plasticity) were carried out after different times of exposition in UV box.

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Possibilities of estimation of grain deformation in polycrystalline materials

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Mechanical working of polycrystalline materials leads to deformation of grains affected by deformation. Amount of grain surface (S_V) and grain edge (L_V) per unit volume are presented as the parameters for deformation description. Direction of grain boundaries orientation caused by deformation is the same as direction of deformation. If deformation scheme is known (there are only three principal schemes of elementary bulk deformation), grain boundaries can be decomposed into isotropic, planar and linear oriented components. Saltykov stereology methods with oriented test lines were used in case of grain surface S_V – common boundary of two grains, respectively stereology methods with oriented test planes in case of grain edge L_V – common boundary of three grains [1]. On metallographic cuts total specific surface area S_V of grains and planar and linear oriented part of specific surface area $(S_V)_{OR}$ of grains are estimated. Degree of grain boundaries orientation O can be estimated as $(S_V)_{OR}$ to S_V ratio. Similar total specific line length L_V of grains edges and linear oriented part of specific line length $(L_V)_{OR}$ of grains edges can be estimated too. From these results analytical formulas relating structure parameters and strain in each position inside the bulk sample can be developed. One of the methods using idealized tetrakaidehadreon shape of grain (mathematical description of real state shape of grain is quite impossible) is based on dependence of the ratio of specific surface area of grain boundaries in deformed state S_V and undeformed state S_{V0} (respectively specific length of edge L_V and L_{V0}) [2]. The method requires knowledge of the parameter of structure in case of zero value of initial deformation, which is unknown in most of cases, it is not the same in the whole volume of pieces and it depends on grain size. Our conversion method was based on analysis of orientation – deformation relation of a grain. Dependence of strain on orientation O was derived from three basic equations – definition of deformation, definition of degree of orientation and invariability of volume (initial volume is equal volume after plastic deformation). The solution of the system includes one free parameter – grain size. Solution of the system of equations for used idealized grain shapes is independent on the initial dimension of grain – strain depends only on shape of grain and it does not depend on its dimension. Due to it the method enables estimation of local plastic deformation from estimation of microstructure anisotropy in arbitrary place of body with arbitrary state of initial deformation.

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Preparation of lithium niobate waveguiding structures

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Optical signal guiding is the discovery of the late 20th century and it has become a technological miracle for telecommunication technology. Nowadays, three wavelengths (830, 1300 and 1550 nm), so-called telecommunication windows, are used in the telecommunication technology. Waveguides are most often prepared in the form of optical fibers, but also as monocrystals and thin films. Because optical fibers show still undesirable attenuation the use of amplifiers is needed. Lithium niobate doped with Er^{3+} and Yb^{3+} can be used as an active waveguide in the amplification or switching in the 3rd telecommunication window (1530 nm).

My work presents an overview of the $LiNbO_3$ waveguiding structures preparation by various methods e.g. Czochralski process, ion implantation, LPE, PLD, PVD, CVD, etc. will be outlined. Then an alternative and cheaper sol-gel technique will be described as a suitable process for the preparation of multimode thin films.

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A Novel Approach to Quantitative Analysis of Local Plastic Deformation in Grained Structures

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Novel technique for identifying and quantification of local deformation phenomena in continuum model of grained solid structure is presented in this paper. We propose a method that combines deformation properties of structure with the changes of grains geometry deformed under the influence of local force. Experimental analyses of grains shapes subjected to a local force show a specific spatially oriented prolongation of grains in direction determined by applied force. However the volume of each grain is retained during the force application in case of plastic deformation. Character of individual grain prolongation depends on the initial shape of grain and direction of loading force. There is a definite relationship between the change in grain shape and nature of the driving deformation force. We contribute to the revealing of mentioned relationship because of we propose and analyse a method for quantification of the effect of grain shape modification on the basis of grain deformation.

Quantitative analysis of local deformation in grained structure can be realized in a perspective using mentioned method. Map of local deformation data in grained system can be constructed in this way and next the local deformation dynamics analysis can be performed. However precision of mentioned analysis must be proven by evaluating of its practical predictive performance in future.

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Design of welding parameters for the laser welding of thin stainless steel tubes using numerical simulation

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Nowadays, the laser technology is used in a wide spectrum of applications, especially in engineering, electronics, medicine, automotive, aeronautic or military industries [1]. In the field of mechanical engineering, laser technology in connection with the automation utilizing 5-axial movements reached the highest rise in the automotive industry [2-4]. Modelling and numerical simulation of laser welding processes has been exploited with many advantages for investigation of physical principles and complex phenomena connected with this joining technology [5-6]. The paper is focused on the use of numerical simulation for the analysis and design of parameters for circumferential laser welding of thin exhausting pipes from AISI 304 steel for automotive industry. Applying developed and experimentally verified simulation model for laser welding of pipes, the influence of welding parameters including the laser velocity from 30 mm/s to 60 mm/s and the laser power from 500 W to 1200 W on the temperature field and dimensions of fusion zone was investigated using the program code ANSYS. Based on obtained results, the process window for laser beam welding of pipes from the AISI 304 steel was predicted.

The research has been supported by the Scientific Grant Agency of the Slovak Republic (VEGA) within the project No. 1/1010/16 and the Programs to support excellent young researchers and research teams (NUM-LBW-FE/Al and 1347/PRO-MAT-ZVAR) of the STU Bratislava.

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The application of coordination chemistry principles to material synthesis

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Extensive studies of single-molecule magnets (SMMs) have evoked the emergence of a new research field: molecular spintronics, where SMMs are used as the core building blocks for recording, transport and sensing devices [1 - 3]. Typical SMMs comprise of organic molecules and 3*d* transition metal (TM) cores (especially Mn, Fe, and Co) and their electronic and magnetic properties can be conveniently tuned by selecting appropriate molecules or TM atoms [2, 3]. Coordination complexes of paramagnetic metal ions of the second and third transition series have attracted considerable interest due to strong spin - orbital interactions giving rise to a significant magnetic anisotropy. The study of paramagnetic compounds based on 4*d* and 5*d* transition metals is an emerging research topic in the field of molecular magnetism. An essential driving force for the interest in this area is the fact that heavier metal ions introduce important attributes to the physical properties of paramagnetic compounds.

The magnetic properties of the lanthanides are due to the electrons in the partial filled 4*f* shell. The magnetic properties of the first-row transition metals are due to the electrons in the partial filled 3*d* shell. There are two important differences between the 3*d* shell and the 4*f* shell. The first difference is that *d* electrons have much greater overlap with their neighboring atoms than *f* electrons do. This means that *d* bands are not as localized as *f* bands are. The second difference is that the spin-orbit coupling is much stronger in the lanthanides than in the 3*d* transition metals.

The possibility of constructing single molecule magnets (SMMs) using a single lanthanide ion was first demonstrated experimentally on phthalocyaninato-lanthanide complexes having a double-decker structure [4]. The lanthanide complexes showing SMM behavior have significantly large axial magnetic anisotropy, which is given to the complexes by essentially different mechanism than those of the well-established 3*d* metal-cluster SMMs. In the 3*d* cluster SMM cases, the easy-axis-type magnetic anisotropy, which is represented by the negative zero-field-splitting constant D, is caused by the magnetic interactions among high-spin 3*d* metal ions in a molecule. In the lanthanide single-ionic SMM cases, on the other hand, such anisotropy is given by the ligand field (LF) in which the lanthanide ion is placed.

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Influence of additives on crystallization of blends based on polyactid acid

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Due to growing environmental problems resulting from the impact of the use of plastic materials is the current development of materials mainly focused on that ones, which are environmentally friendly. There is an increasing effort to replace conventional plastics for biodegradable ones. The food packaging industry requires the development of material which production is easy, readily available and cost effective. At the same time, consumers demand high quality food with long shelf-life and also they desire to see through the packaging to perceive the foodstuff aspect. However, compared to conventional plastics the physical and mechanical properties of biodergadable materials in food packaging has been limited and need to be modified. Improving their processability and properties is an important challenge to be afforded before using these materials on the market. One way to improve the properties of these materials is to prepare their blends [1]. The most common way of preparation of packaging materials is the injection moulding, where crystallization of material is very important. That is the reason the crystallization has become one of the most studied characteristics of biodegradable blends based on PLA / PHB. The work is a contribution to works that deal with the description of the structure of PLA / PHB blends, which have been modified by the addition of various types of additives, mainly nucleating agents and plasticizers [2].

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Preparation of Er:YbAG waveguides

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Synthetic garnets are very popular materials in optical and optoelectronic applications such as lasers and scintillators. Garnet structure is a suitable matrix for doping with optically active elements and it can therefore be used for the preparation of active optical planar waveguides. Depending on the application, dopants can be the cations of transition metals (for example Cr, Co, Mn) or rare earth metals. Erbium ion is nowadays one of the most often used activators. Garnets doped with trivalent erbium (Er^{3+}) can emit luminescence in visible and infrared light depending on the excitation energy. The problem of Er^{3+} is in a small effective cross-section. To solve this problem, Er^{3+} is co-doped with another cation, most often Yb^{3+}. The energy levels of Er^{3+} and Yb^{3+} are close enough for an efficient energy transfer.

The goal of this work was to prepare thin films of $(Yb_{1-x}Er_x)_3Al_5O_{12}$, (x = 0.005; 0.02; 0.1) where ytterbium is a part of the matrix and is therefore in close vicinity to every Er^{3+} ion. Fused silica and monocrystalline $SiO_2(0001)$ were used as substrates. Solutions for deposition of thin films were prepared from erbium acetate and ytterbium acetate together with aluminium chloride. As chelating agents, acetic acid and polyvinylpyrrolidone were used. Thin films were deposited by spin-coating and thermally decomposed and crystallized under two different atmosphere pressures. The phase composition of prepared samples was studied by XRD. The microstructure of the films was analysed by AFM and SEM methods. Optical properties were measured by m-line and photoluminescence spectroscopy.

All prepared films were single phase and their thickness was sufficient to guide an optical signal at 1552 nm. Crystallite size of the layers was around 100 nm and their surface roughness was in the order of units of nanometres. All prepared layers show photoluminescence of the Er^{3+} ions in the near infrared region ($^4I_{11/2} \rightarrow {}^4I_{15/2}$).

Energy Levels of Erbium Centers in $KTaO_3$:Er Crystals

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Potassium tantalate ($KTaO_3$) is promising material for wide range of applications due to exceptional properties that can be tailored by adding suitable impurities. However, proper understanding of the impurity-induced phenomena is largely limited by the lack of information on the microstructure and properties of impurity centers. Therefore, a study of optical absorption and photoluminescence of $KTaO_3$ crystals doped by erbium, one of the most used rare-earth laser active impurities, appears very attractive because of deepening knowledge of optically active impurity centers in highly polarizable ABO_3 perovskite-type crystals. $KTaO_3$ crystals possess a cubic inversion symmetric structure down to the lowest temperatures but they tend to impurity induced structural and ferroelectric phase transitions. In $KTaO_3$, Er^{3+} ions can be substituted in the dodecahedral K^+ sites and/or in the octahedral Ta^{5+} sites in the crystal fields of the cubic O_h symmetry. Necessary charge compensation can occur either locally lowering the symmetry of Er^{3+} center or non-locally preserving its O_h symmetry.

The absorption spectra of the blue tinted $KTaO_3$:Er (500 ppm) crystals recorded at 2, 77, and 300 K within the 350 - 650 nm spectral region revealed the structured absorption bands corresponding to f-f optical transitions from the $^4I_{15/2}$ ground state to the excited states of $Er^{3+}(4f^{11})$ ions. An analysis of the spectra proved in the studied crystals an existence of the "major" and less concentrated "minor" Er^{3+} centers that give rise to the observed intense and weak zero-phonon absorption lines, respectively. Moreover it allowed us to determine structure of energy levels for the $^4F_{9/2}$, $^4S_{3/2}$, $^2H_{11/2}$, $^4F_{7/2}$, $^4F_{5/2}$, $^2H_{9/2}$, and $^4G_{11/2}$ excited states of the "major" Er^{3+} center. The number of zero-phonon absorption lines of the "major" Er^{3+} center observed at 2 K exactly corresponds to that theoretically possible for f-f optical transitions of Er^{3+} ions in the crystal field of non-cubic symmetry. Comparison of the ionic radii of Er^{3+}, K^+, and Ta^{5+} ion indicates together with the n-type conductivity of $KTaO_3$:Er crystals that the "major" Er^{3+} centers are formed by Er^{3+} ions substituted for K^+ ions. The emission bands corresponding to the $^4S_{3/2} \longrightarrow {}^4I_{15/2}$, $^4F_{9/2} \longrightarrow {}^4I_{15/2}$, and $^4S_{3/2} \longrightarrow {}^4I_{13/2}$ transitions of Er^{3+} ions were found in the photoluminescence emission spectra taken on $KTaO_3$:Er crystals within the 350 - 860 nm spectral region at temperatures between 4.2 and 300 K. The number of zero-phonon lines detected at low temperatures within the emission bands of Er^{3+} ion photoluminescence exceeded that theoretically allowed for one type of Er^{3+} center. Besides, their relative intensities were dependent on excitation wavelength. Thus a study of low-temperature excitation spectra of Er^{3+} ion photoluminescence allowed us to separate zero-phonon emission lines corresponding to the "major" and "minor" Er^{3+} centers and to determine crystal field splitting of the ground state $^4I_{15/2}$ and of the first excited state $^4I_{13/2}$ for the "major" Er^{3+} centre at 4.2 K. The possible origin, symmetry and energy level structure of the "minor" Er^{3+} centers in $KTaO_3$:Er crystals is discussed too.

Modifications of Cu(3-Metylsalicylato)2(ronicol)2 moieties – synthesis and structure of 3-methylsalicylatocopper complexes with ronicol

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Copper complexes containing N-donor ligands are studied for many years from different points of view. For instance, the carboxylatocopper(II) complexes with ronicol form various structural motifs. [1,2] The study of preparation and properties of copper(II) complexes with derivatives of salicylic acid in presence of ronicol have resulted in four types of methylsalicylatocopper(II) complexes. The solid state complexes were characterized by spectral methods (infrared, electronic and EPR spectra) and by X-ray analyses.The complex $[Cu(3\text{-}Mesal)_2(ron)_2(H_2O)] \cdot H_2O$ (**1**) (3-Mesal$^-$ = 3-methylsalicylate, ron =ronicol) was obtained from mixture solvent water-acetonitrile. On the other hand, the using of pure acetonitrile solvent led to formation three compounds of formulae $[Cu(3\text{-}Mesal)_2(ron)_2]_x$ (**2**) (where x= 1 or n) with coordination environment $CuO_2N_2O'_2$. The laboratory temperature below 27 °C led to creation light blue polymeric compound (**2a**) which exhibits one dimensional chain. However, the increasing of the reaction temperature to 40 °C caused the formation of molecular complex $[Cu(3\text{-}Mesal)_2(ron)_2]$ (**2b**) of purple color. Another increasing of the temperature caused that the polymeric complex $[Cu(3\text{-}Mesal)_2(ron)_2]_n$ (**2c**) builds up the 2D supramolecular network. [3]

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Enhanced Thermoelectric Properties of Ge-doped n-type Bi_2O_2Se Ceramics

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Increasing global energy consumption and the negative environmental impacts of many current energy conversion technologies, such as the combustion of fossil fuels, has led to increased activity in developing alternative energy conversion technologies. Thermoelectric (TE) conversion of waste heat into electricity is one of them. The dimensionless figure of merit ZT is a measure of the applicability of a material [1]. $ZT = S^2\sigma T/\kappa$, where S is thermopower (Seebeck coefficient), σ is electrical conductivity, κ is thermal conductivity, and T is thermodynamic temperature. Accordingly, thermoelectric materials show high electrical conductivity, low thermal conductivity and high levels of thermopower simultaneously. Such materials are, however, rarely found because these three parameters cannot be controlled independently, as they are functions of the Fermi level (and other parameters) in conventional semiconductors.

Ceramic samples with the composition $Bi_{2-x}Ge_xO_2Se_{1,01}$ (x = 0, 0.05, 0.075 and 0.1) were synthesized by solid-state reaction and compacted using a hot-pressing technique. The prepared materials were characterized by XRD analysis, electron microscopy and measurements of electrical conductivity σ, Seebeck coefficient S, and thermal conductivity κ in the temperature range 300-780 K. Ge in the Bi_2O_2Se host structure led to an increase of the free electron concentration compared to pristine $Bi_2O_2Se_{1.01}$. The increase is explained in terms of the formation of point substitutional defects (donors) in the Bi sublattice - Ge_{Bi}^+, producing free electrons. As a result, we observe an increase in the lectrical conductivity and decrease in Seebeck coefficient while thermal conductivity changes slightly. The highest value of the dimensionless figure of merit $ZT = \sigma S^2T/\kappa$ reaches 0.25 for the composition $Bi_{1,95}Ge_{0,05}O_2Se_{1,01}$ at T=724 K, which is, to date, the highest ZT value reported for Bi_2O_2Se ceramics. Our results suggest that Bi_2O_2Se is still worth exploring.

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Influence of the dimensions of the sample on the measurements of Hall and Seebeck coefficient

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Measurements of Hall and Seebeck coefficient are essential for research of thermoelectric materials. The aim of this work was to investigate the influence of the dimensions of the sample on the measurements of these two coefficients. Two single crystals of well-known thermoelectric material Bi_2Se_3 were prepared. Samples of desired dimensions for our measurements were prepared with use of the electro-erosive cutter. We studied the influence of dimensions (shorting of the samples) and the influence of the shape (oblique cut) of the sample on the measurements. The statistical deviation between our measurements is about 10 %

We obtained interesting results in measurements of Hall coefficient and electrical conductivity in case of shorting of the sample. According to the theory the measurement becomes inaccurate if the ratio between length and width of the sample is smaller than 2 [1, 2, 3]. This is in contradiction with our results. From our measurements it follows that all of the measured values lie within the 10 % deviation even if the ratio between length and width of the sample is smaller than 2 (1.1). Greater deviation in the results was detected when the ratio was smaller than 1 (0.9). In this case the deviation of Hall constant was about 30 % and of the electrical conductivity about 15 %. In case of oblique cut of the sample our results changed dramatically (30 % in Hall coefficient and 15 % in electrical conductivity). The results of Seebeck coefficient showed no significant deviation in all types of measurements.

We also studied the influence of the measuring equipment, the stability of the samples and the attachment of current-introducing contacts (AquaDAG, Ni-paste, Ag-paste). The way of the attachment of the current-introducing contacts has in our temperature range (from the temperature of liquid nitrogen to 200 °C) and our experiment arrangement (alternating current) no influence on the measurement.

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Microstructure properties of Ti based alloys for processing of bulk metallic glasses

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Ti alloys having high strength-to-weight ratio, good corrosion resistance and biocompatibility are important materials applied in traumatology. Alpha and alpha-beta titanium alloys currently used in traumatology have the Young's modulus (105-110 GPa) much greater than that of human cortical bone (10-30 GPa) [1, 2]. Implants with higher stiffness than bone prevent the needed stress being transferred to adjacent bone that results in bone resorption around the implant and consequently to implant loosening. The alloys in glassy form show lower modulus of elasticity, better corrosion properties and higher strength comparing their crystalline form, which makes them promising candidates to serve as traumatology nails and plates.

Experimental work was focused on characterization of Ti based alloys for processing bulk metallic glasses: Ti60Nb15Zr10Si15, Ti65Ta10Zr10Si15 a Ti45Zr40Si15 (in at. percent). All the refractory metals used (Ti, Nb, Zr and Ta) prove no cytotoxicity and have important potential for alloying biocompatible materials [1, 2]. Doping by Si improves glass-formation parameters as well as the alloy densities [3, 4].

The titanium alloys doped by refractory metals and Si were prepared by plasma melting technology. Microstructure properties of the prepared alloys were determined using metallographic observation, microhardness measurement and EDX microanalysis. The microstructures of all three alloys were composed of intermetallic phases and eutectics characteristic for polycrystalline conditions.

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Microstructure evolution of heat treated NiTi alloy

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Superelastic behavior of off-stoichiometric NiTi alloys is significantly affected by microstructure changes that are provided by means of thermal treatment [1-3]. The temperatures of austenite-martensite transformation changed through appropriate thermal regime correspond to precipitation of Ti_3Ni_4, Ti_2Ni_3 or $TiNi_3$ [4-5]. The experimental samples of NiTi alloy with 55.85 wt. % Ni were submitted to thermal treatment and the microstructure before and after the treatment was observed. The heat regimes consisted of solution treatment at 600 °C for 1 hour followed by water quenching and of ageing at eight different temperatures (250, 270, 290, 300, 350, 400, 450 and 500 °C) for 30 minutes. Microstructures features studied by means of optical and scanning electron microscopies, EDX microanalysis and microhardness measurement, have shown that higher ageing temperatures led to an increase in microhardness and microstructure changes.

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Numerical simulation of laser beam welding using 3D conical heat source model: affect of model geometry on dimensions of fusion zone

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Numerical simulation of welding processes has been a major topic in welding research for several years. The results of numerical simulations can be used to explain complex phenomena involved to welding processes and investigate the influence of welding parameters on the quality of weld joints. Numerical simulation is widely applied for optimization of welding parameters [1-4].

The paper deals with the modeling and numerical simulation of temperature fields by laser beam welding of two sheets from AISI 302 steel with the thickness of 4 mm using the FEM code ANSYS. To model the heat input to the weld, the conical volumetric heat source [5] was applied. The influence of geometrical characteristics of 3D conical model on the temperature distribution in welded components and the dimensions of fusion zone were investigated. For the verification of the developed simulation model, the butt weld joints were prepared using the TruDisk 4002 disk laser with different welding parameters. The computed shapes of fusion zones were compared with the macrostructures of produced weld joints. The obtained results will be applied for the calibration of a heat source for the following optimization of laser welding processes.

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Corrosion behavior of electropolished AISI 316L austenitic biomaterial in physiological solution

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Currently, austenitic stainless steels are one of three metallic biomaterials used in the manufacture of implants. Coronary stents, fracture fixation plates and screws, spinal implant devices, aneurysm clips, temporary fixation devices, dentistry and surgical instruments are the most common medical applications of austenitic biomaterials. Compared to titanium alloys and chromium-cobalt alloys, the advantages of stainless steels are suitable mechanical properties (strength, mechanical workability), low cost and acceptable corrosion resistance. Due to the protective passive surface film, stainless steels are resistant to the uniform corrosion, but possibility of local pitting or crevice corrosion have to be taken into account in an internal human body environment. The quality of surface, which depends on used mechanical and chemical surface treatment, plays the major role in the biocompatibility and corrosion resistance of austenitic implants.

Polished smooth surfaces are strictly required especially for surgical and dentistry instruments, ophthalmic devices, coronary stents, fracture fixation plates and screws. According to studies of many authors, bright smooth surfaces have markedly higher corrosion resistance and also provide increased resistance to micro-organisms that have less chance of getting caught than those with higher roughness. For the above mentioned biomedical applications, mechanical and electrochemical polishing of austenitic steels is commonly combined with pickling (acid cleaning), ultrasonic cleaning and chemical passivation. There are various polishing processes commonly used to obtain a smooth material surface. Traditional mechanical polishing may result in deformed layer and residual stresses on the treated surface. Electropolishing is an electrochemical surface finishing process to enhance high surface brightness (mirror finish) with very low surface roughness ($R_a < 2\ \mu$m), without residual surface tensions and with improved corrosion resistance.

The paper deals with corrosion resistance of AISI 316L stainless steel, which is the most widely used Cr-Ni-Mo austenitic biomaterial. Corrosion behavior of five various surfaces (original without additional mechanical and chemical treatment, electropolished, ground + electropolished, pickled + electropolished, ground + pickled + electropolished) are evaluated on the bases of cyclic potentiodynamic polarization tests performed in physiological solution at the temperature of 37 ± 0.5 °C. Obtained potentiodynamic curves are characterized, compared and analyzed for determination of electrochemical characteristics. After tests, the surfaces are checked by optical microscope observation.

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Ordered nanoporous material: properties and perspectives of applications

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Nanoporous materials, based on porous coordination polymers (Metal-organic frameworks, MOFs) or periodic nanoporous silicas (PNS) prepared by self-assembly of surfactant molecules have attracted considerable scientific interest in recent years. These materials are structurally well ordered with very well-defined pore sizes and exhibit unique physico-chemical properties determined by their high surface area, large pore volume, and the possibility of their modifications. These properties make MOFs and PNS suitable for applications in the fields of catalysis, adsorption, magnetism, or as drug delivery systems. The aim of the lecture is to give an overview of current trends and perspectives in the research of above mentioned classes of nanoporous materials.

The lecture will focus on four areas. In the first part, synthesis strategy and unique structural features of MOFs and PNS will be presented, including their topology and possibility of modification. The second part of the lecture will be dedicated to the use of nanoporous materials for sorption and separation technologically relevant gases. Very highly porous MOFs and PNS offer a variety of chemical compositions and structural architectures that are suitable for the adsorption and storage of gases like hydrogen and carbon dioxide [1, 2]. Third part of the lecture will focus on the use of nanoporous materials as drug delivery systems. PNS materials possess favourable chemical properties, high porosity, stability and biocompatibility and thus are very promissing in drug delivery [3]. Final part of the lecture will be devoted to magnetic properties of MOFs and composite PNS, containing magnetic nanoparticles. The pehnomena like magnetocaloric effect and superparamagnetism will be presented [4].

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Modifikovaná mezopórovitá silika ako nosič pre naproxen a jej adsorpčné a desorpčné charakteristiky: vplyv povrchovej funkcionalizácie

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Veľké množstvo nesteroidných protizápalových liečiv má jednu spoločnú vlastnosť a tou je ich nízka rozpustnosť vo vode. To vedie k početným vedľajším účinkom od nevoľnosti až po tvorbu žalúdočných vredov. Možnosť izolovať liečivo od okolitého prostredia až do momentu jeho uvoľnenia v mieste účinku, resp. zvýšenie jeho rozpustnosti, účinnosti, prípadne postupnosti uvoľňovania s cieľom dosiahnuť nižšiu frekvenciu dávok je intenzívne študované už niekoľko rokov. V tomto príspevku opisujeme vplyv modifikácie povrchu mezopórovitého oxidu kremičitého SBA-15 na adsorpciu a desorpciu naproxénu ako nesteroidného protizápalového liečiva (NSAID). Mezopórovitá silika (MPS) bola modifikovaná 3-aminopropylovými, metylovými, fenylovými a cyklohexylovými skupinami využitím metódy graftingu. Naproxen bol adsorbovaný na pripravené MPS z etanolových roztokov s využitím metódy odparovania rozpúšťadla. Uvoľňovanie sa uskutočňovalo do prostredia tlmivého roztoku pri pH 2 a do fyziologického roztoku pri pH 7,4. Čistá SBA-15 ako aj modifikované SBA-15 s naproxenom boli charakterizované použitím početných fyzikálno-chemických techník, ako je adsorpcia / desorpcia dusíka pri 77 K, termogravimetrická analýza (TG), Zeta potenciál, infračervená spektroskopia s fourierovou transformáciou(FT-IR) a elementárna analýza. Množstvo naproxénu uvoľneného z pórov mezopórovitých matríc do roztokov bolo stanovené vysokoúčinnou kvapalinovou chromatografiou (HPLC). Ukázalo sa, že povrchová modifikácia SBA-15 má vplyv na adsorpčné a desorpčné charakteristiky naproxénu. Pri SBA-15 modifikovanej pomocou objemnejších a hydrofóbnejších ligandov (cyklohexyl-, fenyl-) pozorujeme, že sa do pórov MPS podarilo uzavrieť len veľmi malé množstvá naproxénu. Taktiež uvoľňovanie naproxénu do dvoch prostredí o rôznej hodnote pH ukazuje, že väčšie množstvo naproxénu sa uvoľnilo do prostredia fyziologického roztoku s pH 7,4 ako do prostredia s pH 2. Tento rozdiel možno vysvetliť prirodzene slabokyslím charakterom naproxénu.

Realizácia tohto experimentu je podporovaná Agentúrou na podporu výskumu a vývoja APVV-15-0520, Bratislava, Slovenská republika.

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