DMS – RE 2019

The twenty-nine joint seminar

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

BOOK OF ABSTRACTS OF THE 29th JOINT SEMINAR

2 – 6 September, 2019
Nová Lesná

DMS – RE 2019

The twenty-nine joint seminar

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
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FOREWORD

The seminar "Development of Materials Science in Research and Education" is already the twenty nineth 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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Monday, 2 September 2019

12:00 – 14:00 Registration
Location: Hotel Lounge

13:00 – 13:45 Lunch

14:00 – 14:10 Opening
Location: Lecture Hall

14:10 – 15:50 **Monday Session I**
Location: Lecture Hall
(chairperson: B. Papánková)

14:10 – 14:30: Maroš Martinkovič:
Utilization of stereology for the characterization of material microstructure

14:30 – 14:50: Martin Necpal:
A numerical simulation study of cold drawing tubes with internal rifling

14:50 – 15:10: Martin Sahul:
Deposition and characterization of Ti-Al-C-N coatings

15:10 – 15:30: Pavlína Ruleová:
The effect of transition metal - Mo on transport properties of Bi_2Se_3

15:30 – 15:50: Vladimír Kucek:
Thermoelectric properties of W-doped Bi_2Se_3 single crystals

15:50 – 16:20 **Cofee break**

16:20 – 17:40 **Monday Session II**

Location: Lecture Hall
(chairperson: M. Behúlová)

16:20 – 16:40: Zdeněk Remeš:
Optoelectronic properties of hydrogenated amorphous substoichiometric silicon carbide with low carbon content deposited on semitransparent ZnO

16:40 – 17:00: Peter Drobný:
Acoustic Emission Analysis of Hard Coatings Cracking during Indentation test.

17:00 – 17:20: Jan Strnad:
Possibilities of Creating a Ball Joint Mechanism by FDM Technology

17:20 – 17:40: Hüsnügül Yilmaz Atay:
Investigations of microstructure and mechanical properties of brass alloys produced by sand casting method at different temperatures

18:10 – 19:00 Dinner

19:30 – 22:00 Evening programme: Welcome party

Tuesday, 3 September 2019

08:00 – 8:50 Breakfast

09:00 – 10:00 **Tuesday Session I**

Location: Lecture Hall
(chairperson: M. Koman)

09:00 – 09:20: Marek Brezovan:
Study of dicarboxylatecobalt(II) complexes with succinic acid

09:20 – 09:40: Miroslava Puchoňová:
Study of cis and trans isomers of bis(ethylbenzimidazole)bis(benzoato)copper(II) complexes

09:40 – 10:00: Vladimír Kuchtanin:
New Ni(II) coordination compounds with aminomethyl and hydroxymethyl substitued benzimidazoles

10:00 – 10:30 Cofee break

10:30 – 11:30 **Tuesday Session II**

Location: Lecture Hall
(chairperson: V. Jorík)

10:30 – 10:50: Juraj Černák:
Use of selected computing tools for study of molecular and supramolecular structures of (not only) coordination compounds

10:50 – 11:10: L'ubor Dlháň:
Deposits of Magnetite in the Human Brain and Spleen

11:10 – 11:30: Marian Koman:
New complexes Fe(III) with mixed anion ligands

11:30 – 11:50: Zdeněk Potůček:
Photoluminescence of CVD graphene layers transferred onto SiO_2 coated silicon substrate

11:50 – 12:10: Jan Havlíček:
Transparent ceramics - preparation, properties and application

12:30 – 13:15 Lunch

14:00 – 16:00 **Tuesday Session III**

(chairperson: Ľ. Dlháň)

14:00 – 14:20: Zdeněk Kožíšek:
Model approaches to overall crystallization

14:20 – 14:40: Dušan Poštulka:
Microdefects in Czochralski single-crystal silicon

14:40 – 15:00: Jaromír Drápala:
Structural characteristics of TiNi alloys after thermal treatment

15:00 – 15:20: Stanislav Minárik:
On the Problem of Processing Data from a Cross-Sectional Image of Grained Structure

15:20 – 15:40: Paulína Babincová:
Morphological changes of the PVD coatings after isothermal annealing

15:40 – 16:00: Jan Krčil:
The comparison of two anodic oxidation methods on Ti-6Al-4V ELI

16:00 – 16:30 Cofee break

16:30 – 18:10 **Tuesday Session IV**

Location: Lecture Hall
(chairperson: J. Černák)

16:30 – 16:50: Jaroslava Maroszová:
Aluminum-from industry to modern medicine

16:50 – 17:10: Pavla Ryparová:
The effect of temperature to bacterial self healing processes for building materials

17:10 – 17:30: Vladimír Mára:
Analysis of Behavior of Fiber Composite During Loading Tests

17:30 – 17:50: Zuzana Štrbová:
Impact of phase composition on quality of ASN fertilizers

18:00 – 18:50 Dinner

Wednesday, 4 September 2019

08:00 – 8:50 Breakfast

09:00 – 17:00 Panel discussion and joint meeting of the Slovak expert group of solid state physics and CSACG

18:00 – 18:50 Dinner

Thursday, 5 September 2019

08:00 – 8:50 Breakfast

09:00 – 10:00 **Thursday Session I**

Location: Lecture Hall
(chairperson: Z. Kožíšek)

09:00 – 09:20: Ondřej Bílek:
Prediction and Modeling of Roughness in Ball End Milling with Tool-Surface Inclination

09:20 – 09:40: Milena Kubišová:
Study of Bending Resistance of Sandwich Structures

09:40 – 10:00: Milan Žaludek:
Fatigue Life of Thermoset Composite Materials

10:00 – 10:30 Cofee break

10:30 – 12:10 **Thursday Session II**

Location: Lecture Hall
(chairperson: J. Drápala)

10:30 – 10:50: Libuše Sýkorová:
Influence of Laser Cutting On Structural Changes in Metals

10:50 – 11:10: Jana Knedlová:
Influence of Optics on Depth of Engraved Surface

11:10 – 11:30: Radoslav Milde:
Construction of magnetorheological equipment for finishing of non-metallic materials

11:30 – 11:50: Viera Zatkalíková:
Detection of the resistance of austenitic stainless steels to the intergranular corrosion

11:50 – 12:10: Lenka Markovičová:
Change of physical-mechanical properties of LD-PE foils

12:30 – 13:20 Lunch

14:00 – 15:20 **Thursday Session III**

Location: Lecture Hall
(chairperson: M. Martinkovič)

14:00 – 14:20: Mária Behúlová:
Analysis of temperature and stress-strain fields during laser beam welding of a TRIP steel

14:20 – 14:40: Štefan Vrtiel:
Stress-strain analysis of hybrid connections using numerical simulation

14:40 – 15:00: Monika Losertová:
Influence of microstructure on fracture feature of Ti6Al4V alloy prepared by 3D printing

15:00 – 15:20: Jozef Dobrovodský:
Hydrogen depth profile measurement of WC thin films by ERDA and 1H(19F, $\alpha\gamma$)16O resonance NRA

15:20 – 15:50 Cofee break

19:00 – 23:00 Evening programme: Farewell party

Friday, 6 September 2019

08:00 – 8:50 Breakfast

10:00 – 11:00 Departure (individual)

ABSTRACTS

Morphological changes of the PVD coatings after isothermal annealing

Paulína Babincová, Martin Sahul, Peter Drobný, and Ľubomír Čaplovič

Slovak University of Technology, Faculty of Materials Science and Technology, Jána Bottu 25, Trnava, Slovakia

The main of this work is to investigate the impact of the isothermal annealing on the structure and morphological changes on the PVD hard coatings. Three different coatings based on the AlTiN system were deposited onto cemented carbide substrates containing 6 wt% of Co. Two coatings AlTiN/TiAlN and AlTiN/TiN with an initial thickness of 3 μm had a coarse-grained columnar structure with a chemically graded nanomultilayering consisting of alternating Ti-rich and Al-rich layers. In the case of the AlTiN/TiAlN coating, a total of 20 layers were applied. 10 layers had a thickness of 200nm (AlTiN) and 10 layers with a thickness of 100 nm (TiAlN). The same number of nanolayers was also retained for the AlTiN/TiN multilayer coating. The TiN layers were 100 nm thick. The third coating was a nanocomposite sandwich coating formed by a TiSiN adhesive layer (50nm), a functional nanocomposite AlTiSiN layer (2 μm) and a top functional TiSiN layer with a thickness of 1 μm. The coatings were prepared by cathodic arc evaporation using the LARC$^{\®}$technology. After deposition, the samples were annealed at high temperatures (700°C, 800°C, 900°C, 1000°C) for one hour in air. With X-ray diffraction and scanning electron microscopy, the morphology, structure and phase composition of coatings and oxide layers after annealing were evaluated.

After the heat-treatment at 800°C, cross-sectional and surface morphology images revealed, that an oxide layer has grown on top of all coatings. EDS analysis showed that the oxide layers on the multilayers coatings had a layered structure, which was found to be the consequence of the high diffusion rate of Al. The interface with the coatings was very rough. It was depleted of Al, which diffused to the upper surface of the oxide. The oxidation process of nanocomposite AlTiSiN/TiSiN coating started by forming an oxide layer of ternary Ti-Si-O at the interface. This system segregated into two phases of TiO_2 and SiO_2. The nanocomposite coating remained stable even after annealing at 1000 ° C. The surface of the multilayers was accompanied by a network of cracks at this temperature. An interesting phenomenon was also observed on the substrates itself during the annealing. As a result of oxidation, unprotected sides of the substrates expanded. Globular oxides based on tungsten and cobalt were also formed on the surface of the samples at the places where the coating was peeled off. The reasons for the differences are discussed.

This work was supported by the Project of VEGA Grant Agency of the Ministry of Education, Science, Research and Sport of the Slovak Republic and Slovak Academy of Sciences, No. 1/0540/19: "Research of possibilities of increasing the thermal and oxidation stability of Al-Ti-N based hard coatings" and also by the Slovak Research and Development Agency with grant number APVV-15-0168: "Research of modification of phase interfaces in the coating/substrate system to increase the adhesion of hard coatings".

Analysis of temperature and stress-strain fields during laser beam welding of a TRIP steel

Štefan Vrtiel and Mária Behúlová

Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, Ulica Jána Bottu č. 2781/25, 917 24 Trnava, Slovakia

Transformation Induced Plasticity (TRIP) steels belong to the group of Advanced High Strengh Steels (AHSS) that are characterized by good strength-strain combination and formability [1-3] required for special applications in the automotive industry [4]. The excellent combination of strength, ductility and formability of TRIP steels is achieved by a careful control of microstructure development in the process of their production [5-6]. The microstructure of multiphase TRIP steels typically consists of ferrite, carbide-free bainite and metastable retained austenite, which can be transformed into martensite by plastic deformation. Upon crash, this feature allows the TRIP steels to absorb more energy, ensuring greater passenger safety.

In the automotive industry, TRIP steels are mainly joined by resistance spot welding, laser or electron beam welding. Generally, the thermal cycle of a fusion welding process destroys the sophistically designed microstructure of these steels in fusion and heat-affected zones resulting in deterioration of mechanical properties of the weld. Negative consequences of the welding process can be eliminated using proper welding parameters [7-8].

The paper deals with numerical simulation and analysis of the temperature and stress-strain fields developed during the laser beam welding of a CMnSiNb TRIP steel sheets with the thickness of 2 mm. Simulation model takes into account non-linear temperature and phase dependent material properties. The heat input during the laser beam welding is modelled using the conical volumetric heat source. The optimal welding parameters for production of butt joints of CMnSiNb TRIP steel sheets using the TruDisk 4002 disc laser with the maximum power of 2 kW are designed.

The research has been supported by the Scientific Grant Agency of the Slovak Republic within the Projects VEGA No. 1/1010/16 and KEGA No. 029STU-4/2018.

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[2] Keller S, Kimchi M and Mooney P J 2017 Advanced High-Strenght Steels Application Guidelines Version 6.0. Available at: https://www.worldautosteel.org (Accessed 7.7.2019)

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[6] Kah P 2014 Adv Mat Res 849 pp 357-365

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[8] Pekovič M e al. 2018 Manufacturing Technology 181 pp. 84-89

Prediction and Modeling of Roughness in Ball End Milling with Tool-Surface Inclination

Ondřej Bílek, Milde Radoslav, Strnad Jan, Zaludek Milan, and Bednarik Martin

Tomas Bata University in Zlín, Faculty of Technology, Vavreckova 275, Zlin, Czech republic

The quality of finish milling of shaped surfaces is influenced by a number of input parameters. Current automated manufacturing systems allow adaptive adaptation to the local machining area. Despite all the advantages, these systems require a behavioral model, a prediction of the output of the input parameters. Many of the models currently in place summarize this paper, including contemporary published models and their functional dependencies; it also offers the application of milling with a ball-end cutter with an inclined tool axis or surface.

This work and the project is realized with the financial support of the internal grant of TBU in Zlín No. IGA/FT/2019/001 funded from the resources of specific university research.

Study of dicarboxylatecobalt(II) complexes with succinic acid

Marek Brezovan, Vladimír Kuchtanin, and Peter Segľa

Faculty of Chemical and Food Technology STU in Bratislava, Radlinského 9, Bratislava 812 37, Slovak Republic

Thesis deals with the study of spectral (infrared and electronic) and magnetic properties and the molecular and crystal structures of cobalt complexes with succinic acid. Reaction of Co^{II} salt, $Na_2suc{\cdot}6H_2O$ and corresponding benzimidazole derivate (1-H-benzimidazole - bzim, 2-methyl-1-H-benzimidazole - 2-mebzim, 2-ethylbenzimidazole - 2-etbzim, 2-hydroxy-methyl-1-H-benzimidazole - 2-CH_2OHbzim) or nicotinamide (nia) in a mixed solvent water/methanol (1:1) were prepared six new coordination compounds, [Co(μ_2-suc)(bzim)$_2$(H_2O)$_2$]$_n$ (**1**), [Co(μ_2-suc)(bzim)$_2$(MeOH)$_2$]$_n$ (**2**), [Co(μ_2-suc)(2-mebzim)$_2$(H_2O)$_2$]$_n$(**3**), [Co(2-CH_2OHbzim)$_2$ (H_2O)$_2$]·suc (**4**), [Co(μ_2-suc)(2-etbzim)$_2$]$_n$ (**5**) and [Co(μ_2-suc)(nia)$_2$(H_2O)$_2$]·2H_2O_n (**6**) of a different composition and molecular structure. Obtained coordination polymers were characterized by elemental analysis, mass spectroscopy, IR, Raman and electron spectroscopy and X-ray structural analysis. Dianions suc^{2-} are coordinated to central ion Co^{II} in bis(monodentate) bridging manner, leading thus to formation of polymeric chain.

Financial support was provided by: grant VEGA 1/0639/18, APVV-18-0016 a KEGA 017STU-4-2017.

Use of selected computing tools for study of molecular and supramolecular structures of (not only) coordination compounds

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Full characterization of the molecular and supramolecular structure of the studied compound is one of the main goals of single crystal X-ray structure analysis. This characterization includes calculations of various geometric parameters as well as graphical drawing of the formed structures. Standard computing tool for calculation of (not only) geometric parameters is the program *PLATON* [1] while for drawing of illustrations program *DIAMOND* [2] is used in our laboratory. Recently, program *CrystalExplorer* [3] became very popular as it, as an advanced tool for study of the (supra)molecular structure, allows among others to calculate Hirshfeld surfaces; this allows to visualize the packing modes and intermolecular interactions in a new way. In addition, program *Mercury* [4] can be also used for advanced study of (supra)molecular structure as it offers visualization of closely related molecules (e.g. solvatomorphs) by structures overlay or to explore the crystal packing forces using statistical data of CSD using the Full Interaction Maps. The use and usefulness of these advanced computing tools will be illustrated on two polymorphs of the Co(III) complex with Salen-type Schiff base and two solvatomorphs of Ni(II) complex based on 2,2'-bipyridine and oxalato ligands.

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Deposits of Magnetite in the Human Brain and Spleen

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Samples extracted from the human spleen and from the human brain (*Globus Pallidus* region) after lyophilization were studied by means of SQUID magnetometry. The measured functions cover the temperature dependence of the magnetic susceptibility, the field dependence of the magnetization at low temperatures, the temperature dependence of the magnetization at zero and non-zero magnetic fields (ZFCM / FCM), as well as the hysteresis loops at several temperatures. The data obtained were analyzed by fitting on Curie's law as well as the Langevin function, thus obtaining a set of quantitative parameters characterizing the magnetic properties of the samples [1,2].

Spleen specimens have been found to contain a non-diagnosed ferritin that behaves as a superparamagnet below the irreversible temperature, similar to a spleen of bovine and a pure ferritin extracted from the horse spleen. However, other magnetoactive iron oxide deposits are also registered in the spleen sample. Significant anomalies due to excess iron oxides have been reported in subjects with haemosiderosis and hereditary spherocytosis, which are manifested by hysteresis even at the room temperature, confirming the presence of magnetite and/or maghemite.

Human brain samples were classified into three classes according to magnetoactivity: I - predominant diamagnetism, III - predominant para- or ferromagnetism, II - intermediate behavior. Low-temperature magnetic hysteresis was confirmed in all 20 samples, some surviving up to room temperature, confirming the presence of ferromagnetic magnetite or maghemite. In one sample (no. 20), a Verwey phase transition was observed, which is a fingerprint of magnetite. The collection of extracted magnetic parameters was subjected to in-depth statistical analysis by modern methods such as cluster analysis, principal component analysis, factor analysis, and paired correlation analysis. From these data, there is information about a mutual correlation or non-correlation of parameters characterizing the magnetic response of the samples. It has also been found that only the Curie constant and the remnant magnetization correlate significantly with the donor age.

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Hydrogen depth profile measurement of WC thin films by ERDA and 1H(19F, $\alpha\gamma$)16O resonance NRA

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Hydrogenated nanocomposite W-C:H coatings exhibit a wide range of mechanical and tribological properties, which are dependent on the content of carbon and hydrogen in coating layers. To optimize the process parameters of the W-C: H coatings prepared by the direct current magnetron sputtering (DCMS), by High Power Impulse Magnetron Sputtering (HiPIMS) and High Target Utilization Sputtering (HiTUS) techniques, it is necessary to measure the composition of the synthesized coatings. The composition and concentration depth profiles of the basic elements in W-C:H coatings were commonly measured by the Rutherford Backscattering Spectrometry (RBS) and Elastic Recoil Detection Analysis (ERDA) at the ion beam laboratory of the Slovak University of Technology in Bratislava (STU) at the Faculty of Materials Science and Technology in Trnava. Since the depth resolution of hydrogen ERDA measurements was limited, the nuclear reaction analysis (NRA) method, using ^{1}H(19F, $\alpha\gamma$)^{16}O resonance reaction was alternatively used to measure the hydrogen concentration profiles. The depth resolution of the NRA for hydrogen is better than that of ERDA, allowing details to be seen in variation in its concentration in surface areas coating. Examples of the hydrogen depth concentration profiles of selected W-C:H coatings obtained by ERDA and NRA measurements are presented.

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Structural characteristics of TiNi alloys after thermal treatment

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Shape memory alloys based on NiTi, commonly known as "Nitinols", are nowadays successfully used in different areas of the medicine, as for instance plates and nails in traumatology, vascular stents, surgery catheters, root canal instruments or orthodontic braces. Other properties, in addition to the shape memory behaviour, are also very good corrosion resistance, biocompatibility, advantageous strength/density ratio or high damping ability. The shape memory effects and superelastic behaviour of Ni-rich NiTi alloys, it means more than 50.6 at% Ni, are significantly dependent on microstructural modification provided through heat treatment. It is generally known that thermal treatment of Ni-rich NiTi alloys induces diffusion processes that lead to precipitation of different phases: metastable Ni_4Ti_3, metastable Ni_3Ti_2 or stable Ni_3Ti. Owing to an appropriate thermal regime the austenite-martensite transformation temperatures can be modified.

These and other microstructural changes can have a major impact on the martensitic transformation in NiTi alloys and, essentially, on the transformation temperatures. In addition, the precipitation of secondary phases can also contribute to a substantial increase in the strength of NiTi alloys. Another critical factor affecting the properties of these materials is the composition.

The experimental samples of NiTi alloy with 50.7 at% Ni were subjected to heat treatment. The thermal regimes consisted of aging treatment at 300, 350 and 400 °C for 30 minutes followed by air cooling. The microstructures before and after the heat treatment were observed by optical microscopy. The study was completed by microhardness measurement and X-ray analysis. The obtained results show that the aging temperatures led to microstructural and microhardness changes for the investigated alloy.

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Acoustic Emission Analysis of Hard Coatings Cracking during Indentation test.

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Hard coatings are widely used in industries where the good behaviours of surface play the main role in life cycle of machine components. The main material characteristic of coatings which determines behaviour of surface is Hardness. In the past, hardness of materials was considered to be the most important material property, which influence wear properties of coatings and value of maximal elastic tension needed for initiation of cracks. However, Adhesion of hard coatings depends on mechanical properties such as Young Modulus E, Hardness H and fracture toughness R. Initiation/Formation of fractures and their propagation in hard coatings is commonly investigated using indentation tests.

Basically, three main types of hard coatings cracks deposited on ductile substrate have been identified:

- circumferential cracks which appear at the periphery of plastic zone,
- channel cracks, which are initiated under big stress caused by contact between indenter and coating,
- radial cracks, which come from the middle of indentation imprint and propagate outside in the form of beams.

If the indentation loading force is high enough and the substrate is plastically deformed, the coatings start losing adhesion with surface and then delamination or spalling can occur.

Because of this type of damage, it is inevitable to find an appropriate method for diagnostics of hard coatings cracking. Hard coatings cracking and spalling generate the energy which propagates through the material in the form of elastic waves, the formation of which could be detected by an acoustic emission measuring device during instrumented indentation.

Creation of Hard coating crack during indentation is usually detected like a wide frequency AE signal. In this article, the initiation of cracks is investigated using data measured during indentation. The cracks formation/propagation and spalling in hard coatings during indentation were observed and quantified by using AE. AE frequency analysis calculated from signals measured during indentation were evaluated from recorded AE signals.

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Transparent ceramics - preparation, properties and application

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Transparent ceramics is currently field of interest of many researchers. Materials prepared in the form of transparent ceramics have wide spectrum of potential applications like laser hosts, infrared windows, transparent armor or scintillation materials and bring new possibilities. Unfortunately, preparation of this materials is very difficult, using of sophisticated technologies (eq. HIP, vacuum sintering, SPS) and perfect technological procedure is necessary. This contribution summarizes basics of this field - theory, preparation process and methods, material properties and applications - and gives overview of current topics. Also work of our group in this field will be presented - namely powder precursor preparation of garnets (YAG, LuAG) and Lu_2O_3 and its sintering in SPS equipment.

Influence of Optics on Depth of Engraved Surface

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The paper focuses on laser cutting of polymer material PMMA . Specifically, the influence of optics on the depth of the engraved surface is investigated with the use of 1.5”; 2.5”; 4” focal length lenses. Commercial CO_2 laser ILS 3NM by firm Laser Tools &Technics Corp., Taiwan, was used for experimental machining.

New complexes Fe(III) with mixed anion ligands

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The chemistry of iron complexes is investigated recently since these is present in various biological redox systems including peroxidases, catalyses, superoxide dismutases, dioxygenases and lipoxidases. Pyridinecarboxylic acids are present in many natural products, such as alkaloids, vitamins and enzymes, so their metal complexes can be used as models in many research fields. The dicarboxylic acid analogue especially pyridine-2,6-dicarboxylic acid (dipicolinate acid) is one of the most suitable ligand systems for modeling potential metallopharmaceutical compounds because of its low toxicity, amphophilic nature and diverse biological activities. Anion NCS- as ligand may be bonded in complexes of eleven possible manners. In Cambridge Crystallographic Data Base are 997 crystal structure where NCS groups are bonded through nitrogen atom. But in Cambridge Crystallographic Data Base there is neither one structure that would include these two anionic ligands.

This contribution present black complexes of compositions $(cat)_2[Fe^{III}(\eta^3\text{-dipic})(NCS)_3]$ (cat = (H-qui)(**1**); (H-3-meiq)(**2**); (H2-4,4-bipy)(**3**), $(H\text{-3-meiq})_4[Fe^{III}(\eta^3\text{-dipic})(NCS)_3]_2$(**4**) and $(H\text{-2-pic})_2[Fe^{III}(\eta^3\text{-dipic})(H_2O)(NCS)_2]$(**5**) (H-qui = quinolinium; H-3-meiq = 3-methylisoquinolinium; H_2-4,4-bipy = 4,4-bipyridinium; H-2-pic = 2-picolinium) were prepared and studied by X-ray analyses. Each Fe(III) atom has pseudo-octahedral arrangement created by terdentate dipic - ^{1}O,^{2}N, ^{3}O ligand and three monodentate NCS ligands in complexes (**1** - **4**) and one H_2O plus two NCS ligands in (**5**). Each dipic - ^{1}O, ^{2}N, ^{3}O forms a pair of five-membered metallocyclic rings ($^1OC_2{}^2NC_2{}^3O$) with the mean value of O - Fe - N bite angles of 75,5^o. The inner coordination sphere FeO_2N_4 (**1** - **4**) and FeO_3N_3 (**5**) are unsymmetric, because one side is build up by terdentate dipic ligand and other one by three monodentate $(NCS)_3$ (**1** - **4**) or H_2O+$(NCS)_2$ (**5**) donor ligands.

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Model approaches to overall crystallization

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Thermal analysis (DTA, DSC, TGA) is the basic method detecting the temperature, heat flow or mass change when the phase transition occurs. During the crystallization, the heat of fusion is released and that is why the temperature change at crystallization is detected. An amount of released heat needs to be sufficiently high to influence temperature and thus this method detects the overall crystallization. Model approaches of the thermal analysis data are usually based on the Johnson-Mehl-Avrami-Kolmogorov (JMAK) model, when crystallization fraction $X(t) = V_c(t)/V_0 = 1 - exp[-V_{ex}(t)/V_0]$, where V_0 is the initial volume of the melt, $V_c(t)$ is the volume of the crystalline phase at time t and V_{ex} denotes so-called extended volume. JMAK model presumes that crystallization occurs by nucleation (homogeneous or heterogeneous) and successive growth. In consequence of crystallization, volume of the melt decreases with time as V_c increases, and to take into account this depletion is rather difficult and thus V_{ex}, which represents the volume of the crystalline phase if overlap among the growing nuclei is disregarded, was introduced. JMAK model is widely used in thermal analysis though model assumptions are not often fulfilled.

In this work aluminum (Al) crystallization was detected by simultaneous thermal analyzer Setaram Setsys Evolution 16 at isothermal conditions (multiple isotherms were studied). Obtained experimental data were analyzed by two methods: (I) JMAK model and (ii) numerical solution of the kinetic equations of homogeneous nucleation to determine the crystallization fractions of Al crystallization including melt depletion at crystallization. Comparison of these models enabled us to verify if the JMAK model approach was justified.

The comparison of two anodic oxidation methods on Ti-6Al-4V ELI

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The oxide layers on the surfaces of titanium alloys are important for corrosion resistance and bio-compatibility. The compatibility between the tissue, bone and the implant is realized through the properties of the implants stable oxide layer. This oxide layer is mostly consisting, in the case of titanium alloys, of titanium dioxide. This kind of layers can be prepared by various methods; the oxidizing process and its parameters strongly influencing the properties of a layer. Then the differences in the chemical composition, mechanical properties, structure etc are influencing, among others, the stability, adhesion and bio-comopatibility of a bio-implant.

The anodic oxidation of titanium alloys, in proper electrolyte and oxidizing conditions, can lead to creation of oxide layer with certain structure on its surface. This surface structure is characterized of pores which size is in range from tens to hundreds of nanometers. The structured surface can change the interaction of cells (and subsequently the tissue) with the implants surface.

In the case of this work the oxide layer was realized on the Ti-6Al-4V ELI specimens by the means of anodic oxidation. The oxidizing process was realized in two electrolytes: acidic (1M H_2SO_4) and basic (0,5 % NaOH) with voltages between 25 V and 100V, the current density was preset at about 50 mA/cm^2. The prepared anodic oxide layer was then characterized by the surface coloration, the change in surface roughness, the thickness and surface morphology of each oxide layer. The basic behaviour of oxide layer was observed by the submersion in the Hanks balanced salt solution (HBSS).

Study of Bending Resistance of Sandwich Structures

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Article deals with the study of the flexural limit state of sandwich structures based on fiberglass and polymeric foams. Whether geometrical and material parameters influence the resulting load-bearing capacity of these structures are studied experimentally using FEM models.

This study shows it is necessary to particular emphasis attention to the issue of flexural strength, the load capacity when of the walls designing sandwich shell products to avoid possible failures in the practical use of these types of structures. Subsequently, Horm's evaluation method is used to compare the experimental testing and the FEM model.

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Thermoelectric properties of W-doped Bi_2Se_3 single crystals

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There is currently a boom in a search for alternative power resources. One of the alternatives is the usage of the thermoelectric effect. Research on thermoelectric (TE) materials is thus a very active field of research. Efficiency of a TE material is expressed in terms of a so-called dimensionless figure of merit, ZT, where $ZT = \alpha^2\sigma T/\kappa$. In this formula, σ, α, T and κ are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively [1]. Next to the low thermal conductivity, the numerator $\alpha^2\sigma$ (so called power factor PF) needs to be high for a large TE performance.

Bi_2Se_3, which adopts the tetradymite structure, is one of the constituents of room-temperature thermoelectric (TE) materials. Recently we observed the extraordinary behavior of the Seebeck coefficient and carrier mobility leading to an enhanced power factor in the doped crystals in Cr-doped Bi_2Se_3 single crystals [2]. Considering to this fact we examine the influence of tungsten (as like chromium the transitive metal of 6^{th} group) doping on single crystals of bismuth selenide in terms of thermoelectric and transport properties.

The series of $Bi_{2-x}W_xSe_3$ single crystalline samples with varying values of x (for x = 0 - 0,035) was prepared by the self-flux method. The phase purity of the products was verified by X-ray diffraction. The samples were then characterized by the measurement of electrical conductivity, the Hall coefficient and the Seebeck coefficient over a temperature range of 100 - 475 K. We discuss the influence of W substitution on the free carrier concentration and the thermoelectric performance. All of the samples demonstrate n -type conductivity. The results further showed low solubility of tungsten in bismuth selenide ($x \leq 0{,}005$) as well as decreased value of power factor suggesting that tungsten doping of bismuth selenide is contrary to chromium doping not promising in regard to thermoelectric applications.

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New Ni(II) coordination compounds with aminomethyl and hydroxymethyl substitued benzimidazoles

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In 1872, Hobrecker reported the first benzimidazole synthesis and over the years of active research, benzimidazole and its derivatives have evolved as important structure in coordination chemistry. The main features of benzimidazoles are the basic character, high stability, facile synthesis and its capability to form hydrogen bonds. Therefore presented study demonstrates preparation and characterization of Ni(II) coordination compounds with aminomethyl and hydroxymethyl substituted benzimidazoles.

The 2-hydroxymethylbenzimidazole (H_2L) and 2-aminomethylbenzimidazole dihydrochloride ($H_2L{\cdot}2HCl$) ligands were prepared by a modified Phillips method which involves condensation of o-phenylenediamine with glycolic acid or glycine. Coordination of prepared ligands to nickel(II) ions afforded new mononuclear complexes with octahedral stereochemistry of central atom, as well as new tetranuclear complexes depending on the counter anion.

Finally our study shows that 2-hydroxymethylbenzimidazole and 2-aminomethylbenzimidazole are typical chelating ligands. Prepared types of coordination compounds depends on used anions. Obtained complexes were characterized by IR and UV-VIS spectroscopy and suitable crystals were characterized by RTG structure analysis.

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Influence of microstructure on fracture feature of Ti6Al4V alloy prepared by 3D printing

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Today, most of traumatology or orthopedic implants are produced from Ti6Al4V alloy that possesses high corrosion resistance and favorable mechanical properties. The Young modulus that is the critical parameter to avoid stress shielding in healing process, is in the case of Ti6Al4V implants produced by conventional method still high comparing modulus of human bone [1]. Biomechanical compatibility of Ti6Al4V can be improved using advanced producing methods, as for example selective laser melting. However, the material prepared by this method can display some defects [2] and different fracture behavior.

In this work, the Ti6Al4V specimens produced by selective laser melting were mechanically tested in non-heat treated condition and fracture surface feature was compared with this one of the material prepared using conventional casting and forging. The results of the fractography observation for both types of the samples were explained on the base of the microstructure analysis. The fracture surface of selective laser melted specimens showed more brittle feature that was in relation with the microstructure composed almost fully of martensite as opposed to conventionally prepared alloy with (α+ β) bimodal microstructure and more ductile character of fracture surfaces.

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Analysis of Behavior of Fiber Composite During Loading Tests

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Acoustic emission is a physical phenomenon at which arises release of energy due to the stimulation by external or internal stress. The defects present in the material act as AE source that generates elastic stress waves. Propagating waves can be detected on the materials surface by mounted piezoelectric sensors and recorded as waveform. Formation or spread of damage processes can be determined by analyzing either the waveform or its parameters. Operating conditions (fatigue, impact, static overload) can lead to reduction of materials properties and collapse of the structure. Since acoustic emission is a non-destructive method it can be used to monitor the condition of components and thus prevent its catastrophic failure.

The unidirectional glass fiber reinforced polymer matrix composite (GFRP) was inspected with usage of acoustic emission during the static loading tests. For better detection and identification of damage processes 90° and 0° orientation testing specimens were manufactured and for each type of orientation tensile and three-point bend test was performed.

The data obtained from mechanical testing were correlated with selected acoustic emission parameters and based on the results the damage mechanisms were determined and for that purpose, the absolute energy, counts, events and peak frequency were chosen. Further investigation was done by converting the time domain of waveform recorded in different location to frequency by a Short-time Fourier transform (ST-FFT). Failure mechanisms were inspected by light microscopy and for more detailed analysis the scanning electron microscopy (SEM) was used.

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Change of physical-mechanical properties of LD-PE foils

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LD-PE (low density polyethylene) is a flexible material with relatively low thermal and chemical resistance and impact resistance. At room temperature it is insoluble in most organic solvents. Its resistance to strong oxidizing acids is low. At higher temperatures it is more susceptible to attack by aromatic and chlorinated hydrocarbons. The use of LD-PE must allow for cracking and subsequent propagation of cracks in the material. LD-PE is mostly used for the production of plastic bags, foils, packaging materials for bulk goods such as building materials, tubing, bottles, washing powder bags, soil, fertilizers, detergent bottles, fabric softeners and shampoos. It has long been used as an insulating material. LD-PE is produced by blowing shrinkable film. The films themselves are colorless, odorless and tasteless. Polymer production is always associated with post-use recovery. Recycling is a growing challenge in the world because material waste is a major environmental and social problem for humanity and nature. PE and PET products are the most recycled plastic due to the short life of packaging materials. A wide range of new products can be produced from plastic waste, so plastic waste must be collected and recycled.

The experiment is based on real issues in the recycling of plastic waste in a world that is increasingly up to date. Refillcase is also coming up with the solution to the problem of plastic waste produced in all industries and its recycling. The technology is to produce returnable plastic bottles that can be used up to 50 times. LD-PE film is applied to the plastic bottles before filling with a specific medium. After the contents of the bottle have been consumed, the LD-PE film is stripped and thrown into the compost where the material is naturally distributed, thereby avoiding additional plastic waste or recycling the film. The film used is melted into granulate, processed and used for other applications. Subsequently, a new recyclable film is applied to the bottles used and the process is repeated. Changes in the properties of LD-PE films applied to these returnable bottles have been evaluated by several tests. The following tests were performed on the LD-PE films: tensile test, water absorption test and melting point determination. The tests were performed on unused LD-PE films (N) and on used LD-PE films (P), which were filled with the medium for 3 months - medium. The fill media was chosen from commonly available goods. Unused films were filled with disinfectant (S), detergent (SR) and Coca-Cola (C). Based on the tensile test results, the tensile strength increased in the longitudinal direction of the material. The highest value was recorded for the foil exposed in the disinfectant. The melting point of the LD-PE foil is in the range of 100 - 115 ^{o}C, which corresponds to the table values of the melting point of PE.

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Aluminum-from industry to modern medicine

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Aluminum is the third most widespread element in the Earth's crust after oxygen and silicon, and the first abundant metal. For a long time, aluminum was considered as a non-toxic element, which has found its prevalent use in industrial production, materials, but also in the food, cosmetic and pharmaceutical industries [1]. Despite its rich application in various sectors of life, aluminum is not a biogenic metal and has no biological function in living organisms. However, nowadays it is wildly known that aluminum affects more than 200 different biological reactions [2]. The increased exposure of this metal is related to the level of exposure of organisms. An increasing number of scholarly articles and studies links the occurrence of aluminum and its salts in organisms with various diseases of a predominantly neurodegenerative nature, such as Alzheimer's disease, Parkinson's disease, dementia, encephalopathy and the like, appear. The hypothesis, that aluminum is a high risk factor for the development of these diseases has led to a sharp reduction, sometimes even a ban, on the use of aluminum cutlery and cooking utensils in the seventies. Despite these factors, aluminum is used as part of many drugs. Vaccination, one of the main pillars of contemporary medicine, has come into controversy between its proponents and opponents. Aluminum, as one of the essential components of vaccines, is also the subject of these expert polemics. Its main task is to strengthen the body's immune response. Although aluminum has been used as an adjuvant for more than 80 years, its mechanism of action in the human body and its neurotoxicity are still not sufficiently understood. Furthermore the way in which aluminum enters the body is very important. While the body absorbs only 0,3% of aluminum by the oral route [3], when injected intramuscularly (inoculation), the absorbability is almost 100% [4]. Where does non-excluded aluminum end? Does it have a cumulative and synergistic effect? Do we have enough information of aluminum neurotoxicity? The present paper attempts to bring the knowledge of aluminum from the industrial field through to the chemistry and biochemistry of aluminum up to modern medicine.

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Utilization of stereology for the characterization of material microstructure

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All materials consist of a lot of the same or different atoms. The properties of this system depend on its composition, macro and microstructure. The material structure is formed during production, treatment and utilisation of the material. The importance of microstructure in the control of properties of materials (metals, alloys and other materials too) is well recognised. There is necessary to specify and control microstructure in quantitative terms. It means to carry out a measurement on the two dimensional plane of a metallographic cut (quantitative metallography) and the magnitudes of the microstructural features in the three dimensional material (stereology).

Characterization of material microstructure consists of:

Structural types and its main characteristics - definition and characteristic of microparticles**,** types of structures, single phase and multiphase structures, isometric and oriented structures.

Quantitative parameters of the structures - definition and material application of volume fraction, specific surface area, specific line length per area, specific line length per volume, orientation of structure, shape of microparticles, number of particles per unit volume, mean value and particle size distribution, distance between particles.

Measurement and calculation - direct reconstruction, statistic reconstruction, derivation of basic stereology equations, measurement using the line coincidence method and oriented line method, measurement of point fraction, line fraction and area fraction, accuracy of measurement, methods for obtaining of spatial size distribution of particles from the size distribution of their planar section (area, diameter or chords).

The utilization of sterology metallography allow very simple and effective experimental estimation for the characterization of material microstructure.

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Construction of magnetorheological equipment for finishing of non-metallic materials

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Abstract. The paper deals with nano-finishing processes and nano-finishing processes in the presence of an external magnetic field. There is a construction of magnetorheological equipment for finishing of non-metallic materials and subsequent verification of functionality on the change in micro-roughness of the PA-6 material.

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On the Problem of Processing Data from a Cross-Sectional Image of Grained Structure

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The anisotropy of a grained structure is a consequence of non-uniform distribution of spatial orientation of grains. Conventional stereological methods allow determine spatial distribution of grain orientation from lines distribution observed on structure cross sections. The distribution of grain‘s surface orientation in space is determined by measuring the total length of cross sections on a cutting plane. In this paper, we indicate partial but significant problem of stereology. A rectangular model of grained structure is considered. Then the kernel function, which connects the probability density function (distribution) of lengths of rectangles intersections visible on observation planes with size of rectangles sides, is calculated.

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A numerical simulation study of cold drawing tubes with internal rifling

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A steel tube drawing process is a cold forming method to reduce the tube dimension and improve the surface quality simultaneously. The profiles and shape of drawing tools are key factors to achieve the requirements of tube geometric precision and surface quality. Production of multi-rifled seamless steel tubes by cold draw process using multi-rifled mandrel is quite a new technology. The important characteristic of the tube drawing process, unlike the tube with internal rifling, is the corner filling which influences the dimension accuracy of the internal shape of the tube. In order to ensure the reliability of the forming process and to achieve the desired product quality, FEM computer simulation and modeling are used to design forming tools and determination of forming process parameters [1,2] . A number of FEM applications are used in the manufacturing industry. DEFORM developed by Scientific Forming Technologies Corporation is an engineering software that enables designers to analyze me tal forming, heat treatment, machining and joining processes on the computer rather than the shop floor using trial and error [3]. In this study, the possibility of using DEFORM 3D FEM software for exploring the design and analysis of cold drawing processes of internal riffling tubes is discussed [4]. Investigation stress-strain state of forming material, load-stroke for forming tools and other software options will be introduced.

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Microdefects in Czochralski single-crystal silicon

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Microdefects can corrupt manufacturing of devices in active layer under wafer surface. One of examples could be bulk microdefect oxygen precipitate, which can corrupt TIGBT manufacturing. Many researchers and technicians from semiconductor industry preciously describe microdefects in boron doped silicon single-crystals in last decades. We have done complex investigation of microdefect distribution focused on heavily N-type doped Czochralski (CZ) single-crystal silicon.

Bulk microdefects (BMD) in heavily N-type doped CZ silicon wafers after two-step annealing at temperatures 750 °C/8 h + 1050 °C/16 h has been investigated. Samples were etched in selective etchant for delineation of microdefects. We observed radial and axial distribution of bulk microdefects in silicon CZ crystals. We found possible correlation between bulk microdefects distribution and oxygen concentration distribution. Bulk microdefects distribution was compared with resistivity, pulling rate and COP defect distribution also, but without any correlation.

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Photoluminescence of CVD graphene layers transferred onto SiO_2 coated silicon substrate

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Graphene composed of sp^2 bonded carbon atoms arranged in a two-dimensional honeycomb lattice structure is the thinnest and strongest ever known material with fascinating and exotic properties. Moreover, graphene is semiconductor attractive for application in various electronic devices due to outstanding transport properties such as high electron mobility and conductivity. However, owing to the zero bandgap width an observation of efficient photoluminescence on the high-quality graphene samples requires tuning the graphene electron band structure either by doping with various functional groups or by reducing the size of a graphene sheet down to a nanometer scale because isolated graphene clusters may have large bandgaps due to the finite number of atoms in the clusters. Graphene functionalized by fluorine, oxygen, nitrogen, or hydrogen is highly promising material for advanced optoelectronic applications. Functionalization of graphene by plasma treatment is one of the facile ways to tune the graphene properties and doping level without using wet chemicals in order to it becomes an applicable luminescent material.

We studied photoluminescence properties of the monolayer and bilayer graphene samples at room temperature in the spectral range from 350 to 850 nm. Graphene was grown by the CVD method at 1020°C on copper foil using a mixture of methane and hydrogen. The synthesized graphene was transferred one time or two times onto silicon substrate coated with 300 nm thick SiO_2 film in the case of monolayer and bilayer samples, respectively. Then the samples were exposed to oxygen or nitrogen plasma at room temperature. Photoluminescence of as-transferred and oxygen plasma treated samples mainly originated from substrate for both graphene monolayers and bilayers. On the other hand, the nitrogen plasma treated bilayer graphene sample exhibited in contrast to the monolayer sample exposed to the same plasma treatment additional efficient photoluminescence in the UV-green-red spectral region that under excitation at 250 nm consisted of three emission bands peaking near 390, 470, and 620 nm. The origin of this efficient photoluminescence discovered on the nitrogen plasma treated bilayer graphene will be discussed.

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Study of cis and trans isomers of bis(ethylbenzimidazole)bis(benzoato)copper(II) complexes

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Copper complexes containing N-donor ligands are studied for many years from different points of view. It is well known that benzimidazole derivatives possess a variety of therapeutic uses including antioxidant, antiinflammatory, antifungal and antibacterial properties [1-3]. Therefore, our attention is focused on study of copper(II) complexes with benzimidazole derivatives, specifically with 2-ethylbenzimidazole (2-Etbzim). Cambridge crystallographic database provides only few examples with this N-donor ligand with various central atom of transition metals what offer us the possibility for further studies. Preparation of Cu(II) compounds with derivatives of benzoic acid (XBz=methylbenzoate and methoxybenzoate anions) and 2-Etbzim have resulted in six monomeric methyl- and methoxybenzoatocopper(II) complexes with formulae $[Cu(XBz)_2(2\text{-}Etbzim)_2]$. The change of reaction conditions led to formation of cis and trans isomers. In presence of 4-methyl- and 4-methoxybenzoic acid only cis-$[Cu(XBz)_2(2\text{-}Etbzim)_2]$ isomers were formed. On the other hand, trans-$[Cu(XBz)_2(2\text{-}Etbzim)_2]$ was prepared with 2-methyl- and 2-methoxybenzoate anion in primary coordination sphere. By the change of reaction conditions with using of 3-methyl- or 3-methoxybenzoate anion, both isomers were prepared. Complex molecules of cis-$[Cu(XBz)_2(2\text{-}Etbzim)_2]$ are linked by hydrogen bond creating 2D supramolecular network. However, in trans-isomer different hydrogen bond motifs led to creation of 1D supramolecular chains. The solid-state complexes were characterized by spectral methods (infrared, electronic and EPR spectra) and by X-ray analyses.

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Optoelectronic properties of hydrogenated amorphous substoichiometric silicon carbide with low carbon content deposited on semi-transparent ZnO

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Zinc oxide and silicon carbide have interesting physical properties such as a large band gap and related optical transparency, large exciton binding energy, high thermal conductivity and tunable electrical conductivity [1-5]. We have shown recently that CH_4 added to SiH_4/H_2 prevents Si crystallization and hydrogen effusion in the hydrogenated amorphous substoichiometric silicon carbide (a-$Si_{1-x}C_x$:H) deposited at elevated deposition temperature 450°C. Here we study the optoelectronic properties of a-$Si_{1-x}C_x$:H deposited on semi-transparent ZnO electrode using otical absorption spectroscopy PDS (photothermal deflection spectroscopy), Fourier Transform Infrared Spectroscopy (FTIR), photoluminescence and electroluminescence spectroscopy. The infrared absorbance spectra confirm low carbon content x up to 0.1 in a-$Si_{1-x}C_x$:H for SiH_4/CH_4 ratio 1:3. The increasing CH_4 decreases the growth rate of a-$Si_{1-x}C_x$:H, increases x and lattice disorder and broadens the band gap. It follows from the ideality factor $n = 2$ that the diode current-voltage characteristics are dominated by the generation-recombination current for small voltages $0 < U < 0.5$ V. The forward currents at $U > 0.5$ V are dominated by the surface recombination and serial resistivity**.** The reverse dark currents at $U < -0.5$ V are dominated by the premature junction breakdown related to the edge effects due to the small diode area. The photoluminescence and electroluminescence appears below the band gap at room temperature.

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The effect of transition metal - Mo on transport properties of Bi_2Se_3

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Bi_2Se_3, which adopts the tetradymite structure, is a component of n-type legs of thermoelectric (TE) couples used in solid state coolers or generators having the dimensionless figure of merit $ZT \leq 1$ ($ZT = \sigma S^2 T/\kappa$, where σ is electrical conductivity, S is the Seebeck coefficient, κ is thermal conductivity, and T is thermodynamic temperature) in the range around room temperature [1]. In last decade, number of papers has been published showing that some TE materials of tetradymite structure (p-type) form diluted magnetic semiconductors (DMS) if they are doped with some transition metals [2]. Recently, it has been shown that these materials are bulk topological insulators (TI) [3]. Bi_2Se_3 is degenerate semiconductor due to a high concentration of native defects that produce large concentration of free carriers [4]. Selenium vacancies are the dominant defects, they produce a doping on the order 10^{19} cm^{-3}. Such a high concentration of free carriers affects the exploration and potential usage of this material as topological insulator. Further, n-type conductivity prevents potential carrier induced ferromagnetism in Bi_2Se_3 based DMS [5].

This work is focused on study of the effect of transition metal doping on transport properties of bismuth selenide. Single-crystalline samples were prepared in set of composition: $Bi_{2-x}Mo_xSe_3$, where x=0-0,05. Samples were characterized by the X-ray diffraction analysis, measurement of electrical conductivity σ, Hall coefficient R_H and Seebeck coefficient S. System $Bi_{2-x}Mo_xSe_3$shows remarkable material features and interesting thermoelectric properties.

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The effect of temperature to bacterial self healing processes for building materials

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The concrete is the most widely used construction material worldwide for its high compressive strength and good durability. The degradation of this material begins instantly after application in construction. The first degradation signs are change of chemical composition and cracking. The cracks are gates for water-soluble substances inlet. Many methods are developed for repairing concrete construction. They are divided in two groups: man-induced and self-healing.

The self-healing methods are spontaneous or bacterial induced. The bacterial induced calcitation for repairing of cracks is the topic of this article. The chosen bacteria are from group which is adapted for growth in high pH which is encountered in concrete, and they can create calcite. We used three bacteria *Sporosarcina pasteurii, Bacillus cohnii, Bacillus pseudofirmus* and we carried out a study of the influence of temperature. Our previous experiment proved that bacteria in spores (*Bacillus pseudofirmus*) were able to survive the temperatures in the range from -20°C to 140°C. This experiment extends the study to determine the effect of temperature on the change in growth activity and amount of calcite formed. The bacterial activity was measured as the change of absorbance. The value of created calcite was measured by standard analytic methods.

The experiment was performed for optimal temperature (30°C) and lower temperature (10°C) and it used the suitable broth for calcitation. The results showed that beginning of metabolism activity was shifted by 40 to 50 hours. Only *Bacillus cohnii* showed different results because its metabolic activity was nearly zero at 10°C.

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Deposition and characterization of Ti-Al-C-N coatings

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Titanium-aluminium based carbonitrides (Ti,Al)(C,N) hard coatings are characterized by excellent tribological behaviour in metal cutting and polymer forming contacts. In the present work, Ti-Al-C-N coatings were deposited on cemented carbides (WC-10 wt.% Co) substrates by lateral rotating cathodes (LARC$^{\®}$) process using Platit π^{80}+DLC deposition unit. The effect of C2H2/N2 gas flows ratio on element concentration, deposition rate, microstructure, cross-sectional morphology, hardness and tribological properties of the coatings was studied. Following analytical techniques, namely: scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDS), laser scanning confocal microscopy (LSCM), X-ray diffraction analysis (XRD), nanoindentation (NI) and tribological measurements were used for Ti-Al-C-N coatings evaluation.

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Impact of phase composition on quality of ASN fertilizers

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Ammonium Sulphate Nitrate (ASN) based fertilizers are very efficient fertilizers in modern agriculture. Designed to provide targeted nutrition and high yields, they combine the extended availability of Ammoniacal (NH_4) and rapid effect of Nitrate Nitrogen (NO_3) with the multiple agricultural benefits of Sulphur. Most of these products have some tendency to form agglomerates (caking) and dust during storage in a bulk of hundreds to thousands of tons. The severity of quality deterioration can be influenced by a number of factors, such as phase composition, moisture content, particle structure, mechanical strength, hygroscopic properties, product temperature, ambient conditions, storage time and pressure [1].

ASN fertilizer is mainly a combination of the double salts 3DASA ($(NH_4)_5(NO_3)_3SO_4$) and 2DASA ($(NH_4)_4(NO_3)_2SO_4$) [2]. It is known that presence of these mixed salts has a strong impact on the quality of fertilizer. Seeing that X-ray Powder Diffraction Analysis (XRDA) is commonly used to control the quality of industrially produced fertilizers, a new X-ray method has been developed. This new method is based on the determination of the ratio of the integral intensities of the diffraction lines of the 3DASA and 2DASA components. The ratio obtained by line profile analysis provides an effective screening test of the quality of fertilizer immediately after production. In accordance with ratio value it is possible to estimate quality changes of product during long-term storage.

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Possibilities of Creating a Ball Joint Mechanism by FDM Technology

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The article deals with additive manufacturing technologies especially with ability to create reports on FDM 3D printers. These assemblies are non-disambiguable. Therefore, it is important to choose the optimal magnitude of the deviation between the walls so that the mechanism has the required mobility. These deviations are examined in several materials with different rheological properties. Finally, the dependence of the magnitude of the variance between the walls and the thickness of the layer for the given materials is shown. The result is the recommendation of modelling and printing parameters.

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Influence of Laser Cutting On Structural Changes in Metals

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The current level of engineering production requires that applied materials meet the most demanding criteria, whether in terms of longevity, wear or economic. We have to deal with the high demands on the processing of these materials by the application of unconventional technologies, as conventional machining methods often no longer meet the requirements for speed and quality of processing. Laser technology is undoubtedly at the forefront of these technologies. However, one of the drawbacks of the laser is the thermal impact of the workpiece due to the concentrated energy of the radiation and the resulting structural changes in the material, which may affect the physical properties of the material and, consequently, the product. The present paper deals with the issue of laser machining of metallic materials with a focus on the possibility of formation and assessment of structural changes as a result of the absorption of thermal radiation. Due to the thermal conductivity of the metals, the high temperature at the cutting point extends further into the material. The highest temperature is reached by the area closest to the cutting joint, which is why subsequent cooling leads to the most significant changes, with the possible formation of a martensitic, bainitic or pearlitic structure just in the vicinity of the cutting edge.

For a detailed assessment of the heat-affected zone, experimental machining of selected technical materials was carried out and, based on hardness measurements; this area was further statistically evaluated. The published article addresses the fundamental problem of whether similarity can be found between different types of laser-machined materials.

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Stress-strain analysis of hybrid connections using numerical simulation

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Technical calculations can be considered a fundamental and integral part of the design process. The application of various calculation procedures and analyses leads to the design of safe and reliable technical equipment and structures that perform the required functions. The computer simulations and analysis based mainly on the finite element method have a leading position in predicting the stress-strain state arising in the designed construction due to the applied load.

Connections between components of technical structures or equipment are very important parts and must be given due consideration. These joints may be demountable or dismountable. Problem of stress-strain state of hybrid dismountable connection is analyzed in this paper. Presented hybrid connection is formed by the combination of the pressed fit connection and welded connection. For the application of such hybrid joints, dimensional parameters and material properties of the individual joints are important. Key parameters that affect the stress-strain state and strength of this type of connections are mainly the overlap size of the pressed fit connection as well as the type and geometric parameters of the weld connection. In the framework of computer simulations and analyses, the effects of different size of overlap of pressed fit connection and various design solutions of weld connection on the load capacity of hybrid connection under loading are investigated. The results and new knowledge resulting from these analyses are applicable in the design of similar types of connections in technical equipment and structures.

The research has been supported by the Scientific Grant Agency of the Slovak Republic within the project VEGA No. 1/1010/16 and KEGA No. 029STU-4/2018.

Investigations of microstructure and mechanical properties of brass alloys produced by sand casting method at different temperatures

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Brass, alloy of copper and zinc, of historical and enduring importance because of its hardness and workability such that ancient metalworkers around the Mediterranean Sea were able to melt copper with zinc to make this metal alloy as early as 3000 B.C. Brass is stronger and harder than copper. The amount of copper varies between 55% and 95% by weight depending on the type of brass and its intended use. It is easy to form into various shapes, a good conductor of heat, and generally resistant to corrosion from salt water. It can be used to make pipes and tubes, weather-stripping and other architectural trim pieces, screws, radiators, musical instruments, and cartridge casings for firearms.

The manufacturing process involves combining the appropriate raw materials into a molten metal, which is allowed to solidify. The shape and properties of the solidified metal are then altered through a series of carefully controlled operations to produce the desired brass alloy. Temperature used in the process is one of the parameter to affect the product properties. In this study, the brass alloys were produced by sand casting method at different temperatures. Structural and mechanical properties were observed. Optical microscope, XRD and SEM-EDS tests were performed for microstructure and phase analysis of the material. Charpy impact test and tensile test applied to consider the mechanical properties of the samples. As a main purpose of this study, the results were evaluated and then the optimum temperature for the brass material production was determined.

Fatigue Life of Thermoset Composite Materials

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This article deals with the lifetime of laminated materials produced by different production technologies (hand lamination technology, vacuum bagging technology and pre-preg technology with curing in oven) during cyclic repeated bending stress. Like tested materials were chosen composite systems with epoxy matrix and carbon reinforcement (Kordcarbon CC200T, epoxy resin with trade name L285) and second composite epoxy system with glass reinforcement (quadraaxial glass fabric, named Saertex Q-E-820, epoxy resin Biresin CR 82 and third pre-preg systems (unidirectional pre-preg, trade name Deltapreg VV430U-DT860W-39% and prepreg system with glass fabric VV320P_DT806R-37%). Fatigue tests were performed by cyclic bending loads during a three-point arrangement on a universal servo-hydraulic testing machine INSTRON 8871. Experimentally was determined number of cycles to fracture of the material at 90% and 80% of the maximum breaking load.

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Detection of the resistance of austenitic stainless steels to the intergranular corrosion

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Intergranular corrosion is the special form of a local corrosion, which can occur in many alloy systems when the corrosion rate of the grain-boundary areas is higher than that of the grains interiors. This localized attack is very dangerous because the surface damage of the material is usually easily overlooked but it often leads to the dislodgment of individual grains and to the intensive negative influence on the mechanical properties. Intergranular corrosion is very typical corrosion attack in austenitic stainless steels. In common oxidizing environments these steels have good corrosion resistance due to the formation of passive protective surface film. However, under the action of aggressive halide ions, local breakdown of passivity occurs, causing pitting corrosion. The susceptibility of the austenitic stainless steels to the intergranular corrosion is connected with their exposition in the temperature range of 500 - 800 °C ("critical temperatures") and with consequent slow cooling in the air which leads to the precipitation of $M_{23}C_6$ chromium-rich carbides on the grain boundaries. The precipitation of chromium carbides consumes the main alloying element - chromium from a narrow band along the grain boundary and this makes the zone anodic to the unaffected grains. If the chromium content near the grain boundaries drops under the passivity limit (11.5 wt. %), the steel becomes to be sensitized and susceptible to the intergranular corrosion in aggressive environments. The chromium depleted zone becomes the preferential path for corrosion attack or crack propagation if under tensile stress.

The sensitization temperature range is often encountered during isothermal heat treatment, slow cooling from the solution annealing temperature, improper heat treatment in the heat affected zone of the welds or weld joints or hot working of the material. Degree of the sensitization is influenced by the factors such as the steel chemical composition, grain size, degree of strain, or temperature and time of isothermal annealing.

This contribution deals with the susceptibility of three austenitic stainless steels (AISI 304, AISI 316L, AISI 316Ti) to the intergranular corrosion. Both "as received" and improperly heat-treated specimens (sensitization for 10 hours at 650 °C and consequent cooling in the air) were tested by ASTM A262 standard method, A and E practices. Optical microscopy and SEM analysis were used for assessment of the obtained results. According to performed experiments all three steels in "as received" state showed high resistance to intergranular corrosion. After improper heat treatment AISI 304 stainless steel reflected the lowest resistance and AISI 3016Ti stainless steel the highest resistance to the intergranular corrosion.

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