DMSRE 2022

31st joint seminar

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

BOOK OF ABSTRACTS OF THE 31st JOINT SEMINAR

5 – 8 September 2022
Nová Lesná

DMSRE 2022

31st joint seminar

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

Hotel Eufória, Nová Lesná, 5 – 9 September 2022

Organized by

Slovak Expert Group of Solid State Chemistry and Physics
Czechoslovak Association for Crystal Growth

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FOREWORD

The seminar "Development of Materials Science in Research and Education" is already the thirst fist 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

CONTENTS

PROGRAM

Monday, 5 September 2022

12:00 – 14:00 Registration
Location: Lecture Hall

13:00 – 13:45 Lunch

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

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

14:10 – 14:30: Martin Necpal:
A Statistical Approach in the FEM Simulation Analysis of Geometrical Product Specification during the Cold Tube Drawing Process

14:30 – 14:50: Eva Babalová:
3D FEM thermal transient model for optimization of laser cutting parameters for stainless steel plate.

14:50 – 15:10: Eva Labašová:
Comparison of reliability functions of simple mixed four-element systems

15:10 – 15:10: Rastislav Ďuriš:
A comparison of the optical and strain gauge methods for evaluating tensile test

15:10 – 15:30: Milan Nad':
Modification of the stiffness properties of beam structures filled with aluminum foam.

15:50 – 16:20 Coffee break

16:20 – 17:40 **Monday Session II**

Location: Lecture Hall
(chairperson: Z. Kožíšek)

16:20 – 16:40: Václav Doležal:
Dielectric properties of calcium and europium copper titanate ceramics prepared by a sol-gel method

16:40 – 17:00: Jan Havlíček:
Material optimization study of $GdAlO_3$:Ce for scintillation applications

17:00 – 17:20: Tomáš Thoř:
Transition-metal-doped lithium aluminates for neutron scintillation

17:20 – 17:40: Jan Zich:
Synthesis and study of the thermoelectric properties of $CuFeS_2$ doped with P and Sb

18:10 – 19:00 Dinner

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

Tuesday, 6 September 2022

08:00 – 8:50 Breakfast

09:00 – 10:00 **Tuesday Session I**

Location: Lecture Hall
(chairperson: M. Buryi)

09:00 – 09:20: Tomáš Hostinský:
Sodium borophosphate glasses modified with niobium pentoxide

09:20 – 09:40: Katarína Ridzoňová:
Charge traps in Zn- and Mo-based oxide microstructures. The role of Mo

09:40 – 10:00: Alexandr Stupakov:
Percolating nature of the metal-to-insulator transition in epitaxial films of neodymium nickelate

10:00 – 10:30 Coffee break

10:30 – 12:10 **Tuesday Session II**

Location: Lecture Hall
(chairperson: L'. Dlháň)

10:30 – 10:50: Miroslava Pechočiaková:
Utilization of waste mineral fibers for the production of composite materials

10:50 – 11:10: Blanka Tomková:
Modification of glass/epoxy laminates using micro/nano particles from carbon wastes

11:10 – 11:30: Miroslava Puchoňová:
Opportunities for the further education in chemistry

11:30 – 11:50: Matej Pašák:
Measuring students' learning performance during a pandemic.

11:50 – 12:10: Marian Koman:
The dangerous statistics

12:30 – 13:10 Lunch

14:00 – 16:00 **Tuesday Session III**

Location: Lecture Hall
(chairperson: V. Doležal)

14:00 – 14:20: Zdeněk Kožíšek:
Crystallization of Aluminum droplet at low supercooling: theoretical analysis by homogeneous nucleation model

14:20 – 14:40: Roman Yatskiv:
Tunable visible emission in nanostructured ZnO thin films.

14:40 – 15:00: Maksym Buryi:
Luminescence and scintillation properties of the Si doped InGaN/GaN multiple quantum wells

15:00 – 15:20: Petr Vařák:
The Enhancement of rare-earth ions luminescence in silicate glass

15:20 – 15:40: Zdeněk Potůček:
Study of zero-phonon line splitting in the emission spectrum of vanadium photoluminescence in $SrTiO_3$:V crystal

15:40 – 16:00: Roman Čička:
Computational Thermodynamics - Knowledge, Tools and Applications

16:00 – 16:30 Coffee break

16:30 – 18:10 **Tuesday Session IV**

Location: Lecture Hall
(chairperson: Ľ. Čaplovič)

16:30 – 16:50: Mária Behúlová:
Numerical simulation of laser welding – a review of 3D heat source models

16:50 – 17:10: Valentyn Laguta:
Ultra-broadband EPR spectroscopy in materials research

17:10 – 17:30: Marián Palcut:
Corrosion behavior of Sn-Zn alloys

17:30 – 17:50: Jarmila Oravcová:
The analysis of roughness surface of the samples produced by 3D printing

17:50 – 18:10: Ladislav Rolník:
Influence of geometric parameters and material properties of the reinforcing core on the modal properties of vibrating beam structures.

18:30 – 19:15 Dinner

Wednesday, 7 September 2022

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, 8 September 2022

08:00 – 8:50 Breakfast

09:00 – 10:00 **Thursday Session I**

Location: Lecture Hall
(chairperson: M. Koman)

09:00 – 09:20: Juraj Černák:
Multidentate ligands as a tool in syntheses of complexes with slow magnetic relaxation

09:20 – 09:40: L'ubor Dlháň:
Deposit of the iron oxides in the human spleen

09:40 – 10:00: Vladimír Kuchtanin:
Ni(II) complexes with N,O-benzimidazole ligands

10:00 – 10:30 Coffee break

10:30 – 12:10 **Thursday Session II**

Location: Lecture Hall
(chairperson: J. Černák)

10:30 – 10:50: Rudolf Varga:
New Ni(II) complexes with 2-aminomethylbenzimidazole, preparation and characterization

10:50 – 11:10: Jaroslava Maroszová:
Polychlorinated biphenyls (PCBs) as a significant persistent toxicant in the Slovak environment

11:10 – 11:30: Pavla Ryparová:
Mold growth on pine and spruce wood: The dependence on moisture content, anatomical direction and mold species

11:30 – 11:50: Maroš Eckert:
DMA analysis of 3D prints

11:50 – 12:10: Richard Landl:
Anton-Paar Tritec - Materiálová charakterizácia

12:30 – 13:10 Lunch

14:00 – 15:20 **Thursday Session III (ON-LINE)**

Location: Lecture Hall
(chairperson: R. Čička)

14:00 – 14:20: Iveta Markechová:
Activation function as an inspiration for metamaterial design and gyroid as inspiration for activation function design.

14:20 – 14:40: Lukáš Tóth:
Effect of CO2 concentration on the kinetics of the HYDRALOY C5 alloy

14:40 – 15:00: Irene Villa:
Luminescent materials: from inorganic to hybrid nanoscintillators for medical diagnostic and therapy

15:00 – 15:20: Hüsnügül Yilmaz Atay:
Radar Absorbing Properties of Barium Hexaferrite Accompanying with Cu Powders in Polymer Composite Coatings

15:30 – 16:00 Coffee break

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

Friday, 9 September 2022

08:00 – 8:50 Breakfast

10:00 – 11:00 Departure (individual)

ABSTRACTS

3D FEM thermal transient model for optimization of laser cutting parameters for stainless steel plate.

Eva Babalová and Mária Behúlová

Slovenská technická univerzita v Bratislave, Materiálovotechnologická fakulta so sídlom v Trnave, Ulica Jána Bottu č. 2781/25, 917 24 Trnava, Slovensko

The main area of the research was the proposal of parameters for laser cutting of AISI 304 stainless steel plate based on numerical simulation of laser cutting process using FEM modelling in the ANSYS.

The high-intensity laser beam melts or evaporates the workpiece in the thickness of materials and creates a kerf wall. Molten material is then blown away using an assistant gas. In laser machining, unlike traditional methods, material removal is conducted without applying any force. In laser machining, the final surface quality can be achieved in one step, and no further finishing operations are needed to smooth and clean the surface [1]. Understanding of thermal behaviour resulting from a moving laser beam is essential to control the product quality [1,2].

One of the possibilities for predicting products with the required technological properties and quality is the use of numerical simulation. The 3D FEM model was used for the design of laser cutting parameters. In the numerical simulation of transient thermal behaviour of the laser moving heat source, the conical model with Gaussian laser beam power distribution is widely used [3]. The main data required in the thermal analysis of the moving heat source problem are such as: laser power, spot diameter and intensity distribution of the heat source, the convection of surrounding atmosphere, the thermal properties of the work material, and the moving speed of the heat source [2].

Simulation model for cutting of test samples with the dimensions of $10 \times 35 \times 2$ mm was developed in order to perform numerical experiments applying variable cutting parameters and to design proper combination of these parameters for formation of stainless steel quality cuts. Thermal properties of cutting materials in the dependence on temperature were computed using JMatPro software. The conical model of the heat source was exploited for description of the heat input to the cutting model due to the moving laser beam source. The sample cooling by convection and radiation to the surrounding air and nitrogen process gas was taken into account. Developed simulation model was verified by comparison of obtained results of numerical simulation with the temperatures measured during real experiments of laser cutting by the CO_2 Laser Cutting Machine Bystronic Bysprint 3015.

The research has been supported by the Scientific Grant Agency of the Slovak Republic withinthe Projects VEGA No. 1/0796/20

[1] Mahmoud Moradi, et al. 2021 Optik-International Journal for Light and Electron Optics 225 (2021) 164932.

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Numerical simulation of laser welding – a review of 3D heat source models

Mária Behúlová and Eva Babalová

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In general, numerical modelling and computer simulation represent a powerful tool for the design, analysis, and optimization of fusion welding processes, including laser welding. Depending on the process parameters, laser welding can include the interaction of different physical phenomena (thermal, fluid, metallurgical, chemical, mechanical, diffusion, and others). For this reason, the development of a simulation model for laser welding is quite complicated and requires the accurate setting of a considerable amount of input data [1]. In addition to the geometric characteristics of the components to be welded, initial and nonlinear boundary conditions, it is necessary to define the material properties of the base and possibly also the filler materials in a wide temperature range [2-3].

Probably the most difficult problem in the development of simulation models for fusion welding processes is how to model the energy transfer from the laser beam to the welded material, i.e. how to define the heat input to the weld [2-5]. To solve this task, it is necessary to choose a suitable mathematical model of the heat source and to specify the characteristics of the selected heat source.

This paper presents a review of the most important 3D mathematical models of the heat source for numerical simulation of laser welding. The selected heat source models are applied to the numerical analysis of laser welding of aluminium plates. The results of numerical simulations are compared and discussed.

The research has been supported by the Scientific Grant Agency of the Slovak Republic within the VEGA Project No. 1/0796/20.

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Luminescence and scintillation properties of the Si doped InGaN/GaN multiple quantum wells

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The invention of first blue light emitting diodes led to the wide implementation of the heterostructures based on nitride semiconductors (e.g., the InGaN/GaN multiple quantum wells (MQW) structures [1, 2]) in various branches of human activities. In particular, relatively recently, they appeared in the cross-hair of the researchers engaged in the hot field of ultrafast scintillators due to high exciton binding energy, relatively wide direct bandgap (3.4 eV at room temperature), radiation and chemical stability.

The growth of InGaN/GaN heterostructures is more complicated than the growth of thick GaN layers due to the necessity of the low temperature growth of InGaN. There are few ways how to growth upper interface between InGaN quantum wells and GaN barriers. The growth of InGaN quantum wells with and without QW cap was tested. It has been found that InGaN excitonic luminescence band was increased by about one order of magnitude when the InGaN QW cap had been grown. The defects-related band was complex, composed of at least two contributions at about 2.43 eV (510 nm, cyan) and 2.2 eV (564 nm, yellow). The intensity of the cyan band has also been enhanced by about twice in the sample with the cap.

The samples with the Si or Ge doped GaN barriers were grown with different growth temperature of InGaN QWs to obtain different indium content and excitonic emission wavelength. The best way how to control indium content in InGaN QWs is to control growth temperature. For example, the 15°C temperature difference resulted in the 20 nm blueshift of the maximum of excitonic emission wavelength (maximum emission around 3.02 eV (410 nm)). The excitonic band is suppressed for 325 nm excitation wavelength measurement and there is stronger contribution of the defect cyan band compared to the Si- or Ge-free samples. This increase is probably connected with the stronger incorporation of accidental acceptor defect (zinc) when Si or Ge atoms (donors) are embedded. Comparison of luminescence spectra of the Si- or Ge-free and Ge or Si doped InGaN/GaN MQW samples shows that the defect band is weaker in the Si- or Ge-free samples. In general, it can be concluded that Si or Ge has similar character of influence on luminescent properties of MQW as discussed for the GaN thin films [1].

This work was supported by the Czech Science Foundation project No. 20-05497Y

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[2] T. Hubáček et al., CrystEngComm 21 (2019) 356-362

Multidentate ligands as a tool in syntheses of complexes with slow magnetic relaxation

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We are living in the era of information society so there is a strong demand on storage of information [1]. As perspective materials for molecule-based information storage are considered Single Molecule Magnets (SMM), materials which can exist in two magnetic states [2,3]. Consequently, at present, the magnetic properties including SMM magnetism of various complexes are intensively studied [4,5]. SMMs from chemical point of view (composition, crystal structure) can be very variable and among these the lanthanide complexes with prevailing O-donor ligands are especially popular. One way leading to complexes exhibiting slow magnetic relaxation is the use of multidentate ligands, e.g. based on polycarboxylato ligands as purely O-donor or Schiff base type ligands as O,N-donors. Within the lecture will be given several examples of the use of the above-mentioned ligands for syntheses, characterizations, and crystal structures of (mainly) lanthanide complexes as magnetic materials.

This work was supported by grants VEGA 1/0189/22 and APVV-18-0016.

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Computational Thermodynamics - Knowledge, Tools and Applications

Roman Čička

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Computational thermodynamics is a very important tool in materials science. Although the fundamentals of materials thermodynamics are well known for the long time [1], only with increasing the computational power it became possible to calculate thermodynamic properties and phase equilibria in multi-component materials system [2]. To make the calculations the suitable software and related thermodynamic and mobility databases should be used. For example Thermo-Calc software [3] allows to calculate the state of the materials system to obtain the amounts and compositions of phases, transformation temperatures, solubility limits, driving forces for phase formation, activities and chemical potentials, phase diagrams and potential diagrams. These results can be used for prediction of materials property data, as thermophysical properties, kinetic properties and properties related to equilibrium and non-equilibrium solidification. All results can be exported e.g. to MATLAB software [4] and processed in complex models enabling the more detailed description and simulation of materials processes and properties of materials. This approach is considered as a part of "materials genome" [5] and is used for effective development of new materials and optimization of properties of existing materials.

This work was supported by the Grant Agency KEGA (project 006STU-4/2020).

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Deposit of the iron oxides in the human spleen

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Three samples were extracted from the human spleen of donors suffering dysfunction of the iron metabolism. Fresh material was lyophilized and subjected to investigation by the SQUID magnetometry using MPMS-XL7 apparatus (Quantum Design) [1,2]. Electron microscopy in the SEM/TEM mode confirmed the presence of the iron-oxide minerals of the scale 10 - 1000 nm.

The magnetic susceptibility has been taken at small external field B_{DC}= 0.1 T in the temperature range T = 1.9 - 300 K. The magnetization data was scanned at T = 2.0 and 4.6 K with fields between B = 0 - 7 T. The zero-field cooled magnetization and field-cooled magnetization (ZFCM/FCM) data was acquired at B = 100 mT. The hysteresis loops have been probed between B = +5 to -5 to +5 T.

Slovak grant agencies (APVV 18-0016 and VEGA 1/0191/22) are acknowledged for the financial support.

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Dielectric properties of calcium and europium copper titanate ceramics prepared by a sol-gel method

Václav Doležal[1], Vít Jakeš[1], Jan Petrášek[2], Pavel Ctibor[2], Ondřej Jankovský[1], and Kateřina Rubešová[1]

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Calcium copper titanate is an inorganic compound with a chemical formula $CaCu_3Ti_4O_{12}$. It was first synthesized in 1967 by Alfred Deschanv and his colleagues, but it was not until 2000 that Mas Subramanian and his colleagues at DuPont Central discovered a dielectric permittivity in this material that was greater than 10 000 at room temperature. Since then, it has found a widespread use in various fields related to its dielectric properties [1, 2]. $CaCu_3Ti_4O_{12}$perovskite-type phase possesses promising dielectric properties; however, the giant permittivity phenomenon in this material has not been satisfactorily described yet. One of the positive factors could be the presence of secondary phases or substitution of calcium in a dodecahedral position by europium(II). This rare earth cation shows similar ionic radius and electronegativity but differs in valence shell configuration. Such a substitution has not been studied yet more detailed. We prepared a series with a composition of $CaCu_3Ti_4O_{12}$, $Eu_{0,4}Ca_{0,6}Cu_3Ti_4O_{12}$ and $EuCu_3Ti_4O_{12}$. A sol-gel method was used to synthetize precursors, followed by sintering in a temperature range of 1000 °C-1120 °C. Europium was substituted in full stoichiometry of Ca^{II} with the aim to observe whether i) Eu^{II} is stabilized in the perovskite structure and/or ii) possible secondary phases induced by the excess of Eu^{III}positively affect the dielectric characteristics. Samples were characterized by XPS, XRD and SEM. Influence of the microstructure and phase composition on the dielectric properties of the samples (in relation to the sintering temperature) is discussed. Secondary phases and microstructure played an important role in improving the permittivity values. The obtained values of permittivity measured at room temperature are giant up to higher frequencies but differ significantly for some compositions. We found out that the stoichiometric excess of europium in the fully substituted sample produces secondary phases that could be one of the reasons why dielectric characteristics of this sample were much better than those without europium substitution. The sample $EuCu_3Ti_4O_{12}$ pressed by isostatic pressing and sintered at 1120 °C showed a giant permittivity together with very low losses: ε = 20 874 and $tan\ \delta$ = 0.041 (at 10 kHz). These results confirm the published results describing a positive influence of secondary phases on the dielectric behavior.

Supported by the Grant of Specific University Research - grant No. A1_FCHT_2022_008.

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A comparison of the optical and strain gauge methods for evaluating tensile test

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In the experimental measurement of essential material properties, various contact and contactless techniques can be used to evaluate surface deformations and strains. Direct measurement techniques are mainly based on the strain gauge method. The most popular contactless methods include Moiré interferometry, holography, speckle interferometry, and nowadays the Digital Image Correlation (DIC), too [1]. Some of these methods have stringent requirements on the measurement equipment, setup procedure, or coherent light source, which make these methods more difficult to use and increase the cost of laboratory instrumentation. In recent years, more robust and effective computational correlation algorithms have been developed to track test specimen material points and estimate the whole displacement and strain fields. From this reason, the relatively simple and less expensive optical DIC method has been extensively used for displacement and strain field estimation in material characterization. The adaptability of the DIC technique in image capture technology is obtained by standard cameras to estimate the displacement and strain data from the tracking of the material points [2]. The paper focuses on the determination of deformations using the open source MATLAB based 2D DIC software Ncorr [3] as the static tensile test evaluation. Tensile tests on flat rectangular specimens were stressed, and the corresponding displacement and strain fields were estimated using Ncorr. The influence of selected parameters of the correlation algorithm on the settings of the Ncorr program on the estimation of the deformation was assessed. The results of uniaxial strains obtained by the optical method were verified by experimental measurements using an installed strain gauge and reference extensometer. The good agreement between the results attained by the evaluation of experiments using optical and standard strain gage methods was found.

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DMA analysis of 3D prints

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The main goal of the work is to analyze the viscoelastic properties of parts manufactured by using the fused filament fabrication (FFF) technology. This technology is currently among the most widespread 3D printing technologies in various areas of industry. Experiments were performed for samples from PET-G and PLA materials using a Dynamic mechanical analyzer, which is intended to perform the dynamic mechanical analysis (DMA) and the dynamic response of fused filament fabrication specimens. This specimens are studied while they are subjected to dual cantilever loading under periodic stress. The samples were printed in different filling density and shape from 50 to 100 % and layer thickness of 0.1 and 0.2 mm. DMA is performed with temperature ranging from room temperature to 100 °C at a frequency of 10 Hz. The effect of process parameters of fused filament fabrication on the viscoelastic properties of 3D printed PETG specimens is explored in the form of glass transition temperature, storage modulus and loss modulus.

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Material optimization study of $GdAlO_3$:Ce for scintillation applications

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Scintillation materials are used for the conversion of high energy particles energy to UV/VIS light in detection systems. One of commercially used scintillators is the $YAlO_3:Ce^{3+}$ perovskite (YAP:Ce) produced as a single crystal. YAP:Ce has suitable properties for its application in electron microscopy, gamma spectroscopy, X-ray and gamma counting and X-ray imaging screens. On the base of commercial success of YAP:Ce, other aluminate materials with the perovskite structure were studied with the aim to find a material with better scintillation properties. One of studied materials is cerium-doped gadolinium aluminium perovskite $GdAlO_3$:Ce (GAP:Ce). It exhibits higher density and effective atomic number compared to YAP:Ce. However, its light yield is lower than expected for this material and its scintillation kinetics contains slow components. These unwanted properties come from the energy transfer between gadolinium and cerium.

This work pursues a new approach to improve the scintillation properties of this material. Ceramic pellets of gadolinium aluminium perovskite doped with cerium and admixed with lanthanum ((Gd,La)AlO_3:Ce) were prepared using co-precipitation method. The effect of cerium and lanthanum content was studied using radioluminescence and photoluminescence spectroscopies. An improvement of scintillation properties (emission intensity and decay kinetics), in comparison to $GdAlO_3$:Ce reported so far, was achieved.

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Sodium borophosphate glasses modified with niobium pentoxide

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In this contribution borophosphate glasses of the series (100-x)[0.4Na_2O-0.2Nb_2O_5-0.4P_2O_5]-xB_2O_3 were studied in a composition range of x = 0-48 mol% B_2O_3. Basic physical properties were determined, and thermal properties studied by differential thermal analysis, thermomechanical analysis, and hot-stage microscopy. The glass structure was investigated using Raman spectroscopy and ^{11}B and ^{31}P MAS NMR. The electrical properties of the glasses were obtained by using impedance spectroscopy.

Glass transition temperature increases in range of 0-16 mol% B_2O_3, further additions of B_2O_3 results in a decrease of T_g. All glasses except samples x = 8, 16 crystallize in the temperature range 650-700 ° C. The glass refractive index values follow the trend of T_g. From ^{11}B MAS NMR spectra development is visible that the relative number of BO_4 boron species with tetragonal coordination decreases with increasing B_2O_3 content, while the number of trigonal BO_3 species increases. ^{31}P MAS NMR spectra of studied glasses contain one major resonance which shifts upfield with increasing content of B_2O_3. This shift is due to the increasing connectedness of the glass network, which is based on the decrease in the number of Na^+ cations. Raman spectra are mainly dominated by the vibration of the Nb-O bond in the NbO_6 octahedra. The intensity of this vibration decreases with decreasing Nb_2O_5 content. With the addition of B_2O_3, a decrease in DC conductivity is observed, which is attributed to the decrease in the concentration of Na^+ ions.

The dangerous statistics

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The vector model of chemical structure is based on vector analyses of valence bonds, non-valence interactions and selected interatomic distances in the structure of chemical compounds. The vector structural model is applied to known structures of coordination compounds of the type $Cu_4OCl_6L_4$, L = ligands with N and O donor atoms. In Cambridge Structural Database are 69 crystal structures with such a composition. The $Cu_4OCl_6L_4$ molecule is regarded as a supramolecular model of interactions between ligand L and hypothetical "round-shaped" coordination tetra-receptor Cu_4OCl_6. For vector calculations each $Cu_4OX_6L_4$structure is placed into the three dimensional Cartesian coordinate system with the central oxygen atom O placed in origin 0. Studied ligands are compared and described by molecular structural dynamics and corresponding shifts of electron densities by means of bond lengths (O1-Cu, Cu-L, Cu-Cl) and structural distances (O1···Cl, O1···L). In this paper, we focused on the study of the deformation of the trigonal-bipyramidal coordination polyhedron of copper atoms. The ligands L were divided into four groups depending on the presumed electron density on the donor atoms. The principles of vector methods and calculations have been described[1−3].

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Crystallization of Aluminum droplet at low supercooling: theoretical analysis by homogeneous nucleation model

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Crystallization in an undercooled Aluminum (Al) droplet occurs via the formation of crystalline nuclei by homogeneous or heterogeneous nucleation and successive growth of nuclei. Clusters of a new phase appear in the system due to fluctuations and after reaching of a critical size i^*, nuclei form a new phase. Crystallization event at low undercooling 6.4 ^oC of 9.91 mg of a compact Al sample was detected using isothermal differential scanning calorimetry (DSC) after several tenths of minutes. Standard analysis based on Johnson-Mehl-Avram-Kolmogorov (JMAK) model is not appropriate in this case [1] as Avrami parameter n, which is closely connected to the dimensionality of the system, is too low to fit the crystallization data via JMAK model. Al growth rate is extremely high [2] and that is why we presume that the time delay of crystallization, detected by DSC, is slightly higher then nucleation time delay. Homogeneous nucleation model is applied to determine the basic characteristics of nucleation: the size distribution of nuclei, nucleation rate, total number of nuclei and crystallization fraction at the nucleation process. Interfacial energy σ was selected to get only several supercritical nuclei within the Al droplet and the kinetic barrier of nucleation, E, was chosen to get a reasonable value in the time delay of nucleation due to high Al growth rate. The number of atoms in a liquid Aluminum droplet decreases with time as a formation of a new crystalline phase occurs. In consequence, the decrease in stationary nucleation occurs. It is shown that the decrease in the number of atoms in a liquid Al droplet is predominantly caused by a formation of subcritical clusters.

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Ni(II) complexes with N,O-benzimidazole ligands

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Recently, the preparation of coordination compounds of transition metals with biologically active ligands has become one of the popular options for the development of new more effective drugs. Benzimidazole derivatives are one of the substances potentially usable as biologically active ligands, which are also used as drugs in clinical practice and exhibit anti-inflammatory, potentially anticarcinogenic, antiproliferative and antiparasitic properties; they are also used as proton pump inhibitors (Omeprazole), anthelmintics (Albendazole, Mebendazole) or antipsychotics (Pimozide) [1,2]. Therefore presented study demonstrates preparation, characterization of Ni(II) coordination compounds with 2-substitued N,O-benzimidazole ligand.

All newly prepared complex compounds were characterized by X-ray structural analysis and by spectral techniques such as infrared spectroscopy and UV-VIS spectroscopy.

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Comparison of reliability functions of simple mixed four-element systems

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The reliability of the systems depends on the reliability of all the subsystems that create them. In the reliability theory, the term simple systems represents systems that can be decomposed into a sequence of serially and / or parallel subsystems [1].

One of the most important reliability indicators is the hazard rate $\lambda(t)$. We need to know the probability density function $f\ (t)$ and the reliability function $R\ (t)$ to determine the hazard rate of the system. The reliability function expresses the probability of survival of time t and is an additional function to the cumulative distribution function $F\ (t)$ [2].

In the classic reliability theory, systems are classified according to the hazard rate function, which is an increasing, constant or decreasing function of time (operating time, number of rode kilometers, number of monitored events, etc.). The bathtub curve of hazard also represents the dependence of hazard rate function on time. Constant hazard rate is a typical feature of systems with exponential distribution of probability time to failure. A constant value of hazard rate function is also an expected feature of well-designed systems in the period of normal usage, if its value is sufficiently low.

The structure of a simple system is usually serial, parallel and serial-parallel. The paper focuses on the calculation and comparison of reliability indicators such as: reliability function, mean time to failure and hazard rate function. Reliability indicators for a combination of systems with four subsystems are compared. The calculations were realized by using the program MATLAB.

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Ultra-broadband EPR spectroscopy in materials research

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Electron paramagnetic resonance (EPR) spectroscopy is a very powerful tool for investigation of a variety of materials that contain unpaired electrons. It is thus important in branches of physics, chemistry and biology or medicine. It is sensitive to the static electronic properties of paramagnetic system as well as to ionic or molecular dynamics. EPR spectroscopy is also widely used in study of lattice defects created by light and ionizing irradiation. Commercial EPR spectrometers are typically operated at fixed microwave (MW) frequencies of 10 and 34 GHz and a magnetic field of 0 - 1.4 T. However, higher MW frequencies and fields (HFEPR) lead to drastic increases of the absolute sensitivity as a result of the larger MW quantum energy. Furthermore, the advantages of HFEPR also lie in the delivery of much higher spectral resolution, which allows precise determination of the electronic and geometric structures of lattice defects and local properties of materials. Today, HFEPR spectrometers become widespread in scientific research due to commercial availability of MW sources up to THz region and cryomagnets with fields up to 25 T, allowing quite simple construction of laboratory setups.

In this our report, we review our results recently obtained in investigation of optically active impurity ions in wide bandgap oxide materials used as a scintillators in detection of ionizing irradiation by applying the HFEPR technique at frequencies 100-1000 GHz. The advantages of HFEPR will also be shortly demonstrated in studies of other functional materials with magnetic and ferroelectric properties.

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Anton-Paar Tritec - Materiálová charakterizácia

Richard Landl

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Zariadenia z oblasti materiálovej charakterizácie sú produktom dlhoročnej švajčiarskej tradície kvality spoločnosti CSM Instruments, ktorá sa stala súčasťou spoločnosti Anton-Paar v roku 2013. Vývoj a výroba všetkých zariadení materiálovej charakterizácie naďalej prebieha neďaleko hlavného mesta Švajčiarska v mestečku Corcelles-Cormondrèche.

Spoločnosť Anton-Paar v roku 2022 oslávila 100. výročie vzniku a tým zavŕšila jedno storočie úspešnej spolupráce s poprednými predstaviteľmi akademickej obce, ale aj výrobnej sféry. Na akademickej pôde sa spoločnosť najčastejšie sústredí na oblasti stanovenia veľkosti častíc, reometriu, tribometriu, adsorpčné analyzátory a mnoho iných pokročilých metód. V oblasti výroby a kontroly kvality ide o časovo menej náročné merania s prístrojmi ako sú hustomery, viskozimetre, analyzátory bodu vzplanutia, penetrometre a mnoho iných.

V produktovom porfóliu materiálovej charakterizácie sa aktuálne nachádzajú štyri kategórie prístrojov a to inštrumentálne indentory, analyzátory hrúbky vrstiev, skúšky vrypom a tribometre. Spoločnosť Anton-Paar vyvinula jednotlivé zariadenia pre jednoúčelovú charakterizáciu, ale tiež aj kombinované platformy, ktoré umožňujú komplexnú charakterizáciu materiálov v rámci jedného zariadenia.

Activation function as an inspiration for metamaterial design and gyroid as inspiration for activation function design.

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Oscillations accompany us throughout our lives. From the rocking in the cradle, through commuting between living space to working one, and, finally, dived to time flowing - from morning to evening and again to (following) morning, which, maybe, is perceived more sensitively in time period of higher age or lower physical-psychical condition. Life is interwoven with interactions with an infinite variety of materials. The state-of-the-art materials and technologies offer plenty of possibilities and challenges to improve human life. This paper presents an illustration of specifically one oscillation: a) from the design of planar sections of the gyroid structure to the activation function (AF), and vice versa b) from the AF to the design of a specific metamaterial structures. In recent years AF as an necessity element in artificial intelligence algorithms of deep neural nets is also exploated in specific material properties identifications. Here we contribute next AF mission. Mainly based on linear transformations we engage AF sigmoid as the generator of metamaterials structures. Consequently, the candidate for AF was introduced from the features of intersection curves in gyroid. Testing these properties is an opportunity for further research and expanding new knowledge in the field of artificial intelligence.

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Polychlorinated biphenyls (PCBs) as a significant persistent toxicant in the Slovak environment

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Polychlorinated biphenyls (PCBs) are stable organic substances with serious negative impacts on health. Due to their optimal physicochemical properties, they have been mass produced worldwide in the past. In the Czechoslovakia, the Chemko Stražské plant was a major producer of these substances. After the discovery of serious toxic effects on health and the environment, the production of PCB substances was gradually phased out worldwide (Czechoslovakia was one of the last countries to do so). After years of inaction, the Ministry of the Interior (MISR), in cooperation with the municipality and the Slovak University of technology in Bratislava (STU), decided to finally address the issue of PCB disposal in residual solid waste and the environment after more than 30 years. It is estimated that more than 500 tons of toxic waste is involved. STU, as a partner of the MVSR, has been tasked with assisting in the design of appropriate decontamination techniques in relation to the solid waste improperly stored on the former plant site. It is also tasked with addressing the issue of PCB contamination of water and soil and finding appropriate solutions for environmental decontamination**.**

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Modification of the stiffness properties of beam structures filled with aluminum foam.

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The beam constructions can be classified as the most important constructions in the field of mechanical engineering and civil engineering industry. In many cases, current modern trends in these areas of industry lead to the design and creation of beam constructions that meet the required economic savings, are light-weight and especially material-saving. A necessary condition imposed on new approaches in the creation of such constructions is the achievement of the required stiffness parameters and strength properties. One of the design approaches which could meets the mentioned requirements is the use of the material with specific structure, which fills the inner space of the closed cross-section beam element. So-called aluminum foam appears to be one of the suitable filling materials [1], [2] that meets the given requirements. In this application, the technological process of creating aluminum foam is extremely important. The structure of aluminum foam and its material properties depend on the conditions and parameters of the technological process. It is obvious that the distribution, dimensional size and shape of cavities is clearly a stochastic phenomenon. Then, the computer simulation for determining stiffness properties is very complicated when all the mentioned facts are to be taken into account.

The bending stiffness properties of the beam structure filled with aluminum foam are investigated in this paper. The stiffness properties of the beam structure filled with aluminum foam are investigated in the paper. The deterministic structure of the cavities the aluminum foam in the entire interior space of the beam filling is considered. The effect of dimensional size of the cavities with a precisely specified position in the filling on the beam structure stiffness properties is investigated and analyzed.

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A Statistical Approach in the FEM Simulation Analysis of Geometrical Product Specification during the Cold Tube Drawing Process

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Cold tube drawing provides higher accuracy compared to hot approaches. The process can be used to reduce the dimensions of tubes, and depending on the reduction size, the wall thickness of these may be subject to changes. In the process, any form of variability provoked by external factors is highly sensitive, given that the resulting tubes are often the final step in tube production. This paper focused on the evaluation of the influence of pre-tube factors on key variables after the FEM simulation of drawing process, i.e., the outer diameter, and wall thickness of the tubes. For these purposes, a factorial design with fixed factors was implemented. It was also a goal to investigate if the single-pass type of drawing would guarantee good statistical results potentially leading to significant time and financial reductions. The FEM simulation were executed using DEFORM software of Scientific Forming Technologies Corporation with Design of Experiment application module of this software. The results prove that most factors, and their interactions, significantly impacted the response variables.

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The analysis of roughness surface of the samples produced by 3D printing

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The current period in industrial production is characterized by increasing requirements for accuracy and reproducibility of production. Each technology leaves on the surface of the components certain characteristics signs. Macro-roughness and micro-roughness occur on the surface of the components. Appropriate surface quality of components is one of the prerequisites for the correct function of the equipment and significantly affects the service life of components [1].

Surface roughness is the sum of surface irregularities with relatively small distances between protrusions and depressions, which leaves a trace during cutting as a cutting tool, abrasive and the like. One of the parameters that is recommended to be used in the technical documentation for marking the surface roughness is the mean arithmetical deviation of the profile Ra. Ra is defined as the arithmetic mean of the absolute value of the ordinate Z (x) in the range of the fundamental length l [2]. Roughness parameters were detected using a surface roughness tester TR200.

The printer Creality Ender 3 Pro with a control board version 4.2.7 was used for 3D printing of samples. Samples with dimensions 20x20x20 mm were made from material of Gembird white and Verbatim, PLA, white. The following parameters of variables have been set for printing samples: print speed 30 - 50 - 70 mm s^{-1}, layer height of print 0.1 - 0.15 - 0.2 mm, infill 25%, material temperature 200 °C, board temperature 50°C, nozzle MK8, brass, diameter of nozzle 0.4 mm. The roughness of the samples was measured only after they had cooled down to room temperature.

A factor experiment was used to analyze the measured roughness values of material [3]. The aim was to analyze the value of roughness of the samples by two factors (print speed, print layer height) at three levels. It was found that for samples made of Verbatim material, the height of layer of the print has the greatest influence on the value of the parameter of roughness Ra. The print speed has the greatest effect on the surface roughness for samples made of Gembird material. Based on the results of the experiment, the printing parameters can be set according to the desired value of the surface roughness parameter Ra.

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Corrosion behavior of Sn-Zn alloys

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In the present work, the microstructure, phase constitution and corrosion behavior of binary Sn - xZn alloys (x = 5, 8.9 and 15 wt.%) have been investigated. The alloys were prepared by melting Sn and Zn lumps in an induction vacuum furnace under a protective argon atmosphere. The phase constitution of the alloys was studied by room temperature X-ray diffraction. The microstructure of the as-cast alloys was examined using a JEOL JSM 7600F scanning electron microscope. The chemical composition of each constituent was determined by quantitative EDX analysis using a Si(Li) detector X-Max 50 mm^2. The Sn-8.9Zn alloy had a eutectic microstructure. The Sn-5Zn and Sn-15Zn alloys were found to be composed of dendritic Zn(ss) or Sn(ss) and the Sn+Zn eutectic. The corrosion testing of the materials was carried out by means of an electrochemical potentiodynamic corrosion test in a standard three-electrode cell with working, reference, and counter electrodes. The corrosion behavior was studied in aqueous HCl (1 wt. %) and NaCl (3.5 wt. %) at room temperature. Corrosion potentials and corrosion current densities for each alloy were obtained by Tafel extrapolation of the polarization curves. Subsequently, the corrosion rates were calculated using Faraday's laws of electrolysis. It was found that the corrosion rate of the alloys increases with increasing zinc concentration. Furthermore, the corrosion rate of the alloys increases with decreasing pH of the electrolyte. The results have been compared with those of metallic Zn and Sn. A corrosion mechanism is suggested, and implications for practical applications of the Sn-Zn alloys are provided.

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Measuring students' learning performance during a pandemic.

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The educational system has been suddenly collapsed during the lockdown period of the COVID-19 pandemic (coronavirus disease 2019) across all the world. During pandemic lockdown the distance learning process or self learning activities has become more prevalent. Students reported negative experiences of difficulty distance learning and positive experiences such as time and location flexibility. Usually, the performance and success of students is evaluated using grades. However, during online teaching or self-teaching, students need much more time and effort to understand and complete the course materials. The topic of this article is summarize not only the grades but also the time needed to complete this self learning homework. Were used data of online send-in of completed homework before the lockdown period and during the lockdown period. Even though the students had less present teaching, but more time for work the results indicating that performance stay markedly unchanged.

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Utilization of waste mineral fibers for the production of composite materials

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In the construction industry, mineral fibers in the form of a reinforced layer of different thickness are often used for the purpose of thermal and acoustic insulation. At the construction site, these prepared layers are then modified into the desired shape, creating waste that must be landfilled. This waste material can be used as a basic raw material for the production of composite materials.

Customer demands for physical, chemical and heat-resistant technical materials are constantly increasing, so it is necessary to pay attention to this area as well. A large part of this area can be satisfied by mineral fibers. Basalt fibers due to their physical, chemical and thermal stability. Basalt fibers surpass glass and asbestos fibers in their properties, which they are beginning to successfully replace. Glass fibers, mainly because of their more affordable price, and asbestos fibers mainly because of their safety, because asbestos fibers are carcinogenic. This study is focused on mineral fibers, i.e. a mixture of basalt and glass fibers.

Samples of composite materials were created, in which the mechanical properties were measured and the internal structure of the composite was monitored (using SEM). The following tests were chosen for testing the mechanical properties: dynamic 3PB using dynamic-mechanical analysis (DMA DX04T), impact strength (Charpy test CHK 50J) and static 3PB (Tiratest 2400).

The actual composite was made up of a matrix (Lukosil M130) and waste mineral fibers from commonly used mineral insulations. The experiment was designed in such a way that the short fiber basalt waste was mixed together with Lukosil M130 as a matrix to form a consistent mixture. 2 types of composite samples were produced. The first type of composite was stuffing the mold with the mixture and curing it in an oven. The second type of composite was stuffing the mold with mixtures and then pressing and at the same time curing on the press.

The measured data were evaluated and the influence of the production technology on the resulting properties of the composite was assessed. The use of the newly obtained composite material is offered especially in the field of insulating materials. Another possible use is, due to their good dynamic-mechanical properties and low specific weight, in the field of construction for the creation of structures, etc.

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Study of zero-phonon line splitting in the emission spectrum of vanadium photoluminescence in $SrTiO_3$:V crystal

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Strontium titanate ($SrTiO_3$) is a model ABO_3 perovskite-type oxide with highly polarizable structure and soft TO phonon modes. However, $SrTiO_3$ crystals remain in paraelectric phase down to the lowest temperatures and only structural phase transition from the cubic to tetragonal phase occurs near 105 K. Recently we have found structured photoluminescence in the near infrared spectral region in vanadium doped $SrTiO_3$ crystals that at low temperatures consisted of a pronounced zero-phonon line near 1157 nm accompanied by well developed vibrational sidebands. We suppose that it originates from V^{3+} ions ($3d^2$ configuration) substituted for octahedral coordinated Ti^{4+} ions. The zero-phonon line shows a surprisingly large shift to lower energy side with increasing temperature. This very unusual effect in the spectroscopy of transition metal impurity ions in ionic crystals seems to be inherent to luminescence centers in $SrTiO_3$ with specific properties of energy levels involved in emission transition because very similar temperature shift of the zero-phonon R-line has been observed earlier in the emission spectra of photoluminescence of Cr^{3+} and Mn^{4+} impurity ions ($3d^3$ configuration) substituted for Ti^{4+} ions in $SrTiO_3$:Cr and $SrTiO_3$:Mn crystals, respectively [1, 2]. However, while the R-line of Cr^{3+} and Mn^{4+} emission shifts with increasing temperature monotonically to higher and lover energy side, respectively, a temperature behavior of position of the zero-phonon line near 1157 nm observed below 30 K is rather complex.

Present study of emission spectra of V^{3+} photoluminescence in $SrTiO_3$:V crystal at high spectral resolution and temperatures between 4.2 and 140 K proved splitting of the zero-phonon line near 1157 nm into four components at low temperatures resulting from the splitting of both ground $^3T_{1g}$ and excited $^1T_{2g}$ states of V^{3+} ions. Consequently, complex temperature behavior of the zero-phonon line position originally observed below 30 K under unresolved line structure is related to the changes of relative intensities of the line components owing to the alteration of thermal population of the higher energy sublevel of the $^1T_{2g}$ excited state. An origin of the ground $^3T_{1g}$ and excited $^1T_{2g}$ state splitting in V^{3+} impurity center in $SrTiO_3$:V crystal will be discussed taking into consideration structural phase transition in $SrTiO_3$ crystal, spin-orbit coupling, and possible action of the Jahn-Teller effect.

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Opportunities for the further education in chemistry

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Why is chemistry important for us? It is well known that chemistry represents an integral part of our life and is interwoven into our every day. In order to understand what is going on, it is necessary to constantly educate oneself as new information appears on a daily basis. There are many ways to learn something new, for example by self-study or by attending various courses. Many institutions provide educational activities for different age groups.

Faculty of Chemical and Food Technology FCHPT STU participates in the development of continuing education courses. We are involved in these activities by organizing seminars for secondary school teachers of science subjects, which has been held since 1987. We therefore try to bring in topics each year that are topical from across the spectrum of chemistry extending into other disciplines. The papers reflect not only current events in science but also emerging trends. The aim of the paper is to promote the educational activities of FCHPT STU and to outline further possibilities for progress in education.

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Charge traps in Zn- and Mo-based oxide microstructures. The role of Mo

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ZnO-based nanostructures are highly promising materials for application in photo-catalysis, supercapacitors, light emitting diodes, energy harvesting and storage systems. Doping the ZnO with different ions may improve fast exciton emission and suppress the defect-related emission bands, which further opens applications in ultrafast scintillation detectors. Here, we specifically focus on the role of Mo doping. We combine X-ray powder diffraction (XRPD), X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM) and electron paramagnetic resonance (EPR) to study the ZnO:Mo(10, 30%) and MoO_3 microstructures synthesized in the powder by the hydrothermal growth method. The ZnO:Mo(10%) has been shown to contain complex molybdenum-based oxides existing in the form of platelet flakes beside the Wurtzite ZnO. The ZnO:Mo(30%) consists mostly of complex zinc molybdates and of only a negligible amount of ZnO phase, which is beyond the detection limits of XRD. According to XPS measurements molybdenum exists as Mo^{6+} on the surface of ZnO:Mo samples. The MoO_3 sample is composed of two phases in the form of microneedles: hydrated and anhydrous MoO_3 phases. We further address an important topic of ZnO:Mo aging under X-ray irradiation, which cannot be avoided during scintillator operation. We observe X-ray induced formation of point defects, which we assign to the oxygen-based electron and hole trapping centers (O^- or $O_2{}^-$) and Mo^{5+}-based electron trapping centers. Part of them is expected to exist in the pure ZnO and MoO_3 phases whereas the rest must appear in the complex zinc molybdates.

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Influence of geometric parameters and material properties of the reinforcing core on the modal properties of vibrating beam structures.

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The occurrence of unwanted phenomena, which arise in various mechanical structures, cause in them unwanted vibrations, in many cases have fatal consequences for their functionality and, in extreme cases, for their structural integrity. Very dangerous states occur when these structures are exposed to an inappropriate dynamic load, which in unfavorable cases causes a resonance state of the structures. There is necessary to eliminate these undesirable states arising during operation, and one of the ways is to create conditions and possibilities for modifying the modal properties [1], [2] of the relevant structural elements of the mechanical system.

The beam structures are considered as fundamental structural elements that are widely used in mechanical and building structures. One of the important tasks in the structural design of beam structures should be the ability to prevent or reduce the level of unwanted vibrations. It is obvious that the dynamic properties of beam structures depend on their shape structure, i.e. from their geometric parameters and material properties. Usually, the beam structures have constant cross-section and made of homogeneous material. However, these structures in many cases do not have the required dynamic properties. The design and analysis of the beam structures that will allow its spatial properties (mass and stiffness) to be redistributed using the sliding core inserted into the beam structure is investigated in this paper.

The change of modal properties of beam structures [3], which are closely related to their resonance behavior, depending on the redistribution of spatial properties (material properties, dimensions and position of the reinforcement core) is investigated. By changing the above-mentioned spatial parameters of beam structures, it is possible to achieve a suitable modification of the natural frequencies and mode shapes of the beam structure. The presented design modifications in the beam structure provide possibilities for redistribution of spatial properties, which can be used to "tune"the modal properties of the beam structures to the desired values and thus eliminate the emergence of resonance states.

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Mold growth on pine and spruce wood: The dependence on moisture content, anatomical direction and mold species

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Mold growth on pine and spruce wood: The dependence on moisture content, anatomical direction and mold species

Wood materials are used in wooden or natural houses as well as in conventional construction. Wood is also a natural substrate for mold growth. The occurrence of mold in homes may pose a threat to human health. Better knowledge about the conditions for mold growth on wood could improve the mold growth prediction models, prevent health risks, and increase the durability of wood without any additional biocidal treatment.

Mold growth depends on the surrounding condition and the available nutrients. The main requirements for mold growth are suitable relative humidity, temperature, wood specie, and availability of nutrients. The most effective measure to prevent the mold growth in wood-based houses is to keep the indoor relative humidity sufficiently low.

We studied the dependence of mold growth on the ambient relative humidity (75 - 95% RH) at 23 ° C with respect to the anatomical direction of wood and mold species. The mold mixture studied was *Penicillum sp., Aspergillus sp*., and *Alternaria sp.* The samples were prepared from pine and spruce sapwood. The monitored parameters were the time of germination and the degree of coverage of the samples.

It was found that these parameters are more dependent on the relative humidity than on the direction of the wood fibers. Mold growth began at a relative humidity above 75 %. The humidity of around 87 % was more suitable for the germination of Penicillium sp., the humidity of around 95 % for the germination of Aspergillus sp. The liquid water stopped mold germination. The time of germination was between 7 and 24 days in the absence of liquid water in the samples. The time to achieve the maximum coverage of the samples was more dependent on the direction of the wood fibers and was between 24 - 69 days for the conditions without liquid water. The extent of maximum coverage depended on the amount of nutrients available and the direction of the wood fibers.

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Percolating nature of the metal-to-insulator transition in epitaxial films of neodymium nickelate

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Perovskite rare-earth nickelates $ReNiO_3$, where Re = La, Pr, Nd, Sm, etc, exhibit a rich scale of structural and physical properties including strong electron-lattice coupling, low-temperature magnetic ordering and opposite signs of the Hall and the Seebeck coefficients. However, a principal functional feature of these materials is a sharp metal-to-insulator transition (MIT), which is governed by a tiny tilting of the Ni-O-Ni bond angle under cooling/pressure. Because of extreme synthesis conditions, there is still a lack of bulky single crystals of the nickelates. Therefore, uniform epitaxial films of tens-nm thickness present the best nowadays approach to study the intriguing physics of these materials and its application potential for innovative electronics devices [1].

Neodymium nickelate with a chemical composition $NdNiO_3$ (NNO) is the best studied representative of the $ReNiO_3$ family. High-quality epitaxial films of NNO can be routinely prepared by modern deposition techniques. The films subjected to a tensile in-plane strain (positive substrate-film misfit) demonstrate a pronounced MIT at T_{MI} = 170 K, below which the electrical resistivity abruptly increases by several orders of magnitude [1]. Therefore, controlling the MIT by external stimuli with an aim to increase T_{MI} up to the room temperature holds potential for novel micro-electronics applications including resistive switching.

In this presentation, I consider effects of percolating nature of the MIT in the thin NNO films, which have been overlooked or assigned to a concomitant antiferromagnetic transition. Recently, a hypothesis of two-phase coexistence in a hysteresis region of the MIT at T = 20-170 K has been proved experimentally. Effective-medium analysis of the resistivity dependencies on temperature in both phases, the insulator phase below 20 K and the metallic phase above 200 K, gives a phase volume ratio in the transitional region T = 20-200 K (Bruggeman-Landauer equations estimating transport properties of inhomogeneous materials). Knowing the phase ratio, non-monotonic dependencies of Seebeck/Hall coefficients in the transitional MIT region is fitted by a proportional combination of the thermal/magnetic voltages induced in the separate phases. Following a universality principle of critical exponents, percolation threshold in these films occurs at T_p = 120 K. At this critical point, a long-range connectivity between fractions of a growing phase (a large component of the order of system size) is formed. Our study reveals a significant drop of thermal conductivity and a small burst of negative magnetoresistance at the percolation threshold.

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Transition-metal-doped lithium aluminates for neutron scintillation

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Neutron radiation and neutron detection systems have become of great importance recently, as the number of their applications in research, medical, security and other advanced fields have been gradually growing. Scintillators for thermal neutrons utilize a nuclear reaction of isotopes with a high cross section for neutron capture, such as ^{6}Li or ^{10}B. The resulting nuclear reaction creates high-energy charged particles that produce scintillating light along their ionization tracks. Important requirements for neutron scintillators are low density and effective atomic number, which are necessary to minimize their sensitivity to high-energy photons (γ-ray background). Promising host materials with high lithium content, low density and atomic number are oxides within the binary Li_2O-Al_2O_3 system. Depending on the Li_2O content, these can be distinguished as the lithium-rich Li_5AlO_4, the intermediate $LiAlO_2$ and the aluminum-rich $LiAl_5O_8$.

In this work, a complementary study of the lithium aluminates $LiAlO_2$, $LiAl_5O_8$ and Li_5AlO_4 doped with transition metal ions Cu^{+} and Ti^{3+} is presented. Bulk ceramic samples of tetragonal γ-$LiAlO_2$ and cubic α-$LiAl_5O_8$ with varying doping concentrations were prepared using the Pechini sol-gel method. Luminescence characterization of the samples was performed using X-ray-excited radioluminescence, photoluminescence excitation and emission spectra, and luminescence decay measurements. Samples of undoped and Cu-doped Li_5AlO_4 were prepared by solid state synthesis based on thermal decomposition of metal nitrates. These samples exhibited strong hygroscopic properties, which makes Li_5AlO_4 an unsuitable host material outside a controlled atmosphere environment.

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Modification of glass/epoxy laminates using micro/nano particles from carbon wastes

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Fibre reinforced plastics (FRP), especially those made from inorganic multifilaments and polymer matrices, belong to the most popular materials for structural application, because they perfectly combine lowest possible weight and high load capacity. While their technical advantages are undisputed, in recent years much attention has been paid to environmental problem they cause, when disposed in landfills at the end of their lifetime. This problem is particularly acute with thermoset matrix composites. Although there are numerous attempts to their recycling, suitable technologies are still lagging behind the growing amount of composite waste [1]. Therefore, the development of new "environmentally friendly"FRP is one of the fastest growing R&D area in composite research.

Promissing solution is offered by various binder modifications. Many recent studies present possibilities of improvement for "green"resins or "bio-based"thermo-plastics, often based on using different combinations of micro/nanofillers, mainly those made from recycled sources. Especially carbon/graphite particles of various shapes and sizes seem like very promising material [2]. Usual filler volume in structural plastics ranges between 15-40wt% depending on the production technology, and requirements on utility properties of final composite product. However, such filler amount is unusable in the resins that serve as the binder for FRP due to striking increase of the resin viscosity. We observed this increase already at a concentration around 3wt% [3].

Our study is therefore focused on influence of selected carbon particles on composite properties in perspective of appropriate balance between the matrix modification and processing requirements in FRP production. We build on our previous research in the development of fibrous assemblies and structural composites from recycled sources [3]. For this study we modified green epoxy resin with 2.5wt% of carbon based fillers. The resin was subsequently applied to glass multifilaments, and vacuum cured to obtain glass fiber/epoxy laminates.

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Effect of CO2 concentration on the kinetics of the HYDRALOY C5 alloy

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The paper discusses the action and effect of a high concentration of carbon dioxide on the kinetics of the hydrogen absorption and desorption process from the metal hydride alloy Hydralloy C5. The alloy is the subject of research into the possibility of hydrogen separation from a mixture of synthetically generated gas with a majority representation of H_2, CO_2, CO and CH_4, such as syngas. The main attention is paid to the effect of CO2 concentration in the process of hydrogen storage into the alloy. Carbon dioxide, as an important oxidant and catalytic poison, greatly affects the kinetics of H_2 storage in a metal hydride alloy, while the rate of degradation of the alloy's properties increases with the increasing percentage of CO_2 in the mixture with hydrogen. The process of contamination of the alloy with carbon dioxide is accompanied by the chemical splitting of carbon dioxide into carbon monoxide and oxygen, which leads to the oxidation of the alloy grains, thereby limiting or significantly reducing the ability of the catalytic splitting of hydrogen and its storage in the intermetallic structure of Hydralloy C5.

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The Enhancement of rare-earth ions luminescence in silicate glass

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Lasers and amplifiers based on glass waveguides doped with rare-earth (RE) ions have a vast potential in various applications, such as material processing, medicine, sensors or defence. The key components of glass-based photonic devices are the optically active ion and host matrix. RE ions such as Er^{3+}or Ho^{3+} are especially perspective due to strong emission around 1.5 μm and 2 μm, since the area beyond approx. 1.4 μm is considered "eye-safer". The co-doping with Yb^{3+} allows effective sensitization by pumping around 980 nm. In the question of host matrix, silica glass remains a perspective option as thanks to its favorable material properties, such as thermal, mechanical and chemical durability, and feasible drawability into optical fiber. However, the photoluminescence of RE ions in pure silica glass is severely limited by the high phonon energy of the silica network and the low solubility of RE ions. To remediate these drawbacks, the silica glass needs to be modified with suitable additives, resulting in the creation of multicomponent silicate glass. Three oxides have emerged as perspective options for enhancing the luminescence of RE ions - germanium oxide (GeO_2) [1], aluminium oxide (Al_2O_3) [2] and zinc oxide (ZnO) [3], which may influence the matrix structure and photoluminescence in various ways, depending on the glass composition and dopant concentrations.

In this work, we aim to investigate the relationship between the matrix structure and photoluminescence properties of RE ions in multicomponent silicate glass. Germano-, alumino- and zinc-silicate glass doped with Er^{3+} or Ho^{3+} ions and co-doped with Yb^{3+} ions were prepared by the melt-quenching method. The structural properties of the glass were analyzed using Raman and NMR (^{27}Al, ^{29}Si, ^{23}Na, ^{67}Zn). The RE ion incorporation was studied by comparing the amount and shape of the NMR signal present in the RE- and La-doped samples. The absorption spectra were analyzed using the Judd-Ofelt analysis. The steady-state and time-resolved luminescence was measured, and the relationship between the matrix structure and the luminescence was analyzed.

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New Ni(II) complexes with 2-aminomethylbenzimidazole, preparation and characterization

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The benzimidazole moiety is involved in a variety of biological processes. For example, N-ribosyl-dimethylbenzimidazole is part of the chemical structure of vitamin B_{12} [1]. Benzimidazole derivatives are of intensive researches due to their coordination ability besides their biological importance [2]. Furthermore, the tendency of bivalent nickel to form tetragonally distorted octahedral complexes is well known. In many series of this type, changes of magnetic behaviour occur when small changes are made in the anion or the neutral ligand, and in some cases dia- and para-magnetic isomers are known [3].

New Ni(II) complexes of general formula NiL_xY_z have been synthesized, where L is 2-aminomethylbenzimidazole and Y are inorganic anions such as Cl^-, Br^-, ClO_3^-, ClO_4^-, NO_2^-, N_3^-, SCN^-, SO_4^{2-} as well as organic anion CH_3COO^-. All newly prepared complex compounds (1-14) were characterized by X-ray structural analysis and by spectral techniques such as infrared spectroscopy and UV-VIS spectroscopy. Magnetic measurements were also performed for compounds (1-6).

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Luminescent materials: from inorganic to hybrid nanoscintillators for medical diagnostic and therapy

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The great advantage of nanomaterials is the tunability of their physico-chemical properties and of their emission features through the control of their structure, morphology, and doping. In biomedical applications exploiting ionizing radiations, such as in radiotherapy (RT) as well as in total body medical imaging techniques, the scintillation performance (intensity and fast timing features), should be optimized towards the improvement of the therapeutic and diagnostic results. The nanoscintillators (NS) are mostly inorganic nanomaterials featuring high atomic number and density that enable the efficient interaction with the ionizing radiation. Recently, a new class of hybrid NS has been coming into the spotlight. Hybrid NS are composed of an inorganic dense scintillating nanoparticle coupled to an organic fast emitter or a cancer killing agent (photosensitizers). Hybrid NS can also be embedded in a polymeric host for the creation of scintillating composite.[1] The exploitation of hybrid NS as co-adjuvant in the established RT protocols would allow to reduce side effects and cancer recurrence. The use of NS, coupled with highly emissive and fast dyes, would result in the upgrading of the final image resolution in medical diagnostic (down to the millimetric range) for early-stage cancer diagnosis. We present the investigation on Hf oxide nanoscintillators (HfO_2) doped with Europium ions (Eu) for biological applications. In the in vitro imaging field, we demonstrate that Eu:HfO_2 can be used as non-toxic, highly stable probes for cell optical imaging and, potentially, as radiosensitive materials for clinical treatments.[2] We present a successful case of biocompatible chrysotile NS functionalized by photosensitizers for RT. The optimized design of the NS surface, of the composition, as well as of the spatial arrangement of dyes allow to boost the performance of NS.[3] Lastly, we propose the preliminary results obtained on HfO_2-based hybrid composite NS for fast timing medical techniques. The high density of Hf enhances the interactions of the X-rays. The investigation on the luminescence/scintillation performance is performed in relation to the surface functionalization and optimization of the polymeric matrix loading to maximize the energy sharing mechanism and boost the luminescence and timing qualities of this hybrid composite.

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Tunable visible emission in nanostructured ZnO thin films.

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ZnO is a promising wide bandgap semiconductor with a wide range of potential applications in different areas[1-4]. It is well known, that the PL spectrum of ZnO is characterized by two features, the near band-edge excitonic emission (NBE) in the UV region and the defect-related emission (DLE) in the visible region [5]. For the majority of optoelectronic applications, the presence of DLE emission is undesirable and a variety of approaches have been developed to suppress the DLE emission by different methods such as hydrogen plasma treatment, thermal treatment, or other surface passivation methods including the deposition of Al_2O_3 or polymer layers. Nevertheless, the broad DLE emission band in ZnO, which covers almost the whole VIS region, can be exploited in the fabrication of white light-emitting diodes, display devices, or biological labeling. Of particular importance is the need to develop new highly efficient materials for white light-emitting diodes (LEDs) and replace conventional lighting sources, which combine a white-light-emitting phosphor with a UV LED chip. While commercial rare-earth phosphors and traditional semiconductor QDs show a narrow bandwidth emission, the characteristic broad emission band makes ZnO an ideal candidate for white LEDs.

In this work, we show that the visible emission from a thin ZnO film can be manipulated by simply varying the annealing atmosphere and temperature, and consequently, the DLE emission can be tailored towards a particular application [6]. We demonstrated a strong correlation of the blue luminescence band with surface-related defects. This band has been rarely observed in ZnO thin films and was mostly associated with zinc-related intrinsic defects. We also confirmed the formation of willemite after annealing at temperatures above 700°C, which can affect the optical properties; however, in previous reports, its presence was not considered.

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Radar Absorbing Properties of Barium Hexaferrite Accompanying with Cu Powders in Polymer Composite Coatings

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Radar, which is an electronic and electromagnetic system that works with the use of radio waves to detect and locate objects, has led to the need for radar absorber materials for some military applications, especially for defense and security. In this study, barium hexaferrite and copper powders were used to produce radar absorbing composite material. Barium hexaferrite powders were synthesized by Sol-Gel method with hexagonal molecular structure in nano size. Barium hexaferrite and copper powders were added to a polyurethane resin to interpolate the radar absorption at different loading levels to see the concentration dependence. Later, metal surfaces were covered with these polymeric composites. Characterization tests such as particle size analysis, X-Ray Diffraction, Scanning Electron Microscopy (SEM) and scratch test were performed. It was done with a Network Analyzer to determine the electromagnetic properties of copper and barium hexaferrite reinforced composites. It was concluded that the increased amount of copper and barium hexaferrite powder in the composites increased the radar absorption performance. Besides, it was concluded that very good synergistic effects were obtained that Cu powders was significantly influential with barium hexaferrite powders.

Synthesis and study of the thermoelectric properties of $CuFeS_2$ doped with P and Sb

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Chalcopyrite is a promising thermoelectric material(TE) due to its low thermal conductivity, non-toxicity, abundance and price. In its native form, low electrical conductivity limits its use as a TE material. We aim to increase its properties with another element substitution. Whereas substitution in cation lattice was widely studied to improve thermoelectric properties, anionic lattice remained unexplored. To study the effects of phosphorus and antimony substitution for sulfur, we prepared polycrystalline samples of P and Sb-doped chalcopyrite with compositions $CuFeS_{2-x}P_x$ and $CuFeS_{2-x}Sb_x$. Synthesis was performed in a resistance furnace from powders (5N purity) with a gradual temperature increase from 300 to 900K. The resulting ingots were grounded in the air. For transport properties measurements, round samples were prepared by hot pressing from synthesized powders. Temperature dependencies of the transport properties were measured and calculated, namely the electrical conductivity, the Hall coefficient, the Seebeck coefficient and the thermal conductivity. In conclusion, we evaluated the effect of substitution in the anionic subgrid on the increase of the ZT parameter. Both phosphorus and antimony led to an increase in the ZT parameter. Newly formed secondary phases are interesting materials for further research.

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