

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

Book of Abstracts of the 26th Joint Seminar
29 August – 2 September 2016



Z. Kožíšek
R. Král
P. Zemenová
Editors



CZECHOSLOVAK ASSOCIATION FOR CRYSTAL GROWTH

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Development of Materials Science in Research and Education

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

under the auspices of

**the Institute of Physics, Academy of Sciences of the Czech Republic and
the Slovak Society for Industrial Chemistry**

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PREFACE

The 26th Joint Seminar “Development of Materials Science in Research and Education” (DMSRE26) will be held on 29 August - 2 September 2016, in hotel IRIS Pavlov. The first Joint Seminar in these series was held at Gabčíkovo in the Slovak Republic in 1991. Seminar is organized by the Czechoslovak Association for Crystal Growth and the Slovak Expert Group of Solid State Chemistry and Physics under the auspices of the Institute of Physics CAS, Faculty of Chemical and Food Technology SUT Bratislava, and Slovak Society for Industrial Chemistry.

The Seminar is intended to bring together a unique combination of scientists across a multidisciplinary spectrum and provides an ideal forum for the presentations and discussions of recent developments and achievements in all theoretical and experimental aspects of preparation processes, characterization and applications of materials in bulk, thin film, nanocrystalline and glassy states.

The scientific sessions cover the following topics of materials science:

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

The program will include 5 keynote lectures (45 minutes): M. Behúlová (Slovak University of Technology in Bratislava, Trnava, Slovakia): *Numerical simulation of welding processes*, A. Kromka (Institute of Physics CAS, Prague, Czech Republic): *Diamond thin films as a novel platform for life science and biosensors*, J. Pejchal (Institute of Physics CAS, Prague, Czech Republic): *Growth of fluoride and oxide scintillation crystals by micro-pulling-down*, K. Rubešová (Department of Inorganic Chemistry, University of Chemistry and Technology, Prague, Czech Republic): *Perspectives on sol-gel method: crystal growth of functional materials*, and Shih-Jye Sun (Department of Applied Physics, National University of Kaohsiung, Taiwan): *Model simulation and mechanism investigation for ferromagnetic ZnO*. All other contributions will be presented as short lecture talks (25 minutes). The official languages of the seminar are Czech, Slovak, and English.

This booklet contains the abstracts of all contributions, which reached us before 16 August 2016. The authors are responsible for the technical and language quality of the contributions. The conference will run from Monday afternoon, 29 August 2016, till Friday noon, 2 September 2016 in hotel IRIS Pavlov, Czech Republic.

Dear colleague, we welcome you to the DMSRE26 Joint Seminar and we hope you will enjoy your stay in Pavlov.

On behalf of the organizers,

Zdeněk Kožíšek and Marian Koman

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PROGRAM

Monday, 29 August 2016

- 12:50 – 14:20 Registration
Location: Hotel Lounge
- 14:35 – 14:50 Opening
Location: Lecture Hall
-
- 14:50 – 16:00 **Monday Session I**
Location: Lecture Hall
(chairperson: Marian Koman)
- 14:50 – 15:35: Shih-Jye Sun:
Model simulation and mechanism investigation for ferromagnetic ZnO
- 15:35 – 16:00: Hua Shu Hsu:
Magneto-optical properties of Co coated ZnO nanorods
- 16:00 – 16:30 Coffee break
-
- 16:30 – 17:45 **Monday Session II**
Location: Lecture Hall
(chairperson: Zdeněk Remeš)
- 16:30 – 16:55: Z. Kožíšek:
Homogeneous nucleation in small closed systems
- 16:55 – 17:20: Yu-Ying Chang:
Resistive switch mechanism of Au/ZnO/Au crossbar structure
- 17:20 – 17:45: Hsiung Chou:
Heuristic and exploratory education for material science students
- 18:00 – 18:45 Dinner

Tuesday, 30 August 2016

08:50 – 10:00 **Tuesday Session I**

Location: Lecture Hall

(chairperson: Blažena Papánková)

08:50 – 09:35: Alexander Kromka:
Diamond thin films as a novel platform for life science and biosensors

09:35 – 10:00: Anna Artemenko:
In situ XPS depth profiling of polymer films and polymer/diamond interface using Ar⁺ cluster ion beam sputtering

10:00 – 10:30 Coffee break

10:30 – 11:45 **Tuesday Session II**

Location: Lecture Hall

(chairperson: Lubor Dlháň)

10:30 – 10:55: Zdeněk Remeš:
Absorption and photoluminescence spectra of the hydrogenated amorphous silicon with embedded silicon nanoparticles

10:55 – 11:20: Kateřina Dragounová:
Photoluminescence of silicon-vacancy centres in CVD diamond films – characterization and modelling

11:20 – 11:45: Pavla Štenclová:
Atmospheric plasma treatment of detonation nanodiamonds in water

12:00 – 13:00 Lunch

14:00 – 15:40 **Tuesday Session III**

Location: Lecture Hall

(chairperson: Jiří A. Mareš)

14:00 – 14:25: M. Koman:
The influence of the new dipicolinate complexes of Mn (III) and Fe (III) in the process of degradation experiments.

- 14:25 – 14:50: Vladimír Jorík:
Crystalline Polymorphism of 2-((2-(hydroxy)benzylidene)amino)phenolato)(4-methylpiperidine)-nickel(II)
- 14:50 – 15:15: Maroš Martinkovič:
Estimation and utilization of structure anisotropy in forming pieces
- 15:15 – 15:40: Jiří Stuchlík:
Progress of vacuum deposition techniques for Si:H thin films structures
- 15:40 – 16:10 Coffee break
-
- 16:10 – 17:25 **Tuesday Session IV**
Location: Lecture Hall
(chairperson: Zdeněk Kožíšek)
-
- 16:10 – 16:35: Blažena Papánková:
Magnetism and Magnetic Materials
- 16:35 – 17:00: Ľubor Dlháň:
Ferromagnetic ordering in Fe(III) complex mediated by the aromatic rings
- 17:00 – 17:25: Patrik Čermák:
Transport and magnetic properties of $Fe_xBi_2Te_3$ single crystals
- 18:00 – 18:45 Dinner

Wednesday, 31 August 2016

- 08:50 – 10:00 **Wednesday Session I**
Location: Lecture Hall
(chairperson: Robert Král)
- 08:50 – 09:35: Kateřina Rubešová:
Perspectives on sol-gel method: crystal growth of functional materials
- 09:35 – 10:00: Dana Mikolášová:
Use of water-soluble polymers for the $(Er^{3+}/Yb^{3+})\text{:LiNbO}_3$ thin films preparation by sol-gel method
- 10:00 – 10:30 Coffee break
- 10:30 – 11:45 **Wednesday Session II**
Location: Lecture Hall
(chairperson: Jan Pejchal)
- 10:30 – 10:55: Roman Yatskiv:
One-dimensional ZnO nanostructures and their optoelectronic applications.
- 10:55 – 11:20: Miroslav Menšík:
Modelling of charge carrier mobility for transport between elastic polymer nanorods
- 11:20 – 11:45: Kristýna Králová:
Life and research of Niels Steensen
- 12:00 – 13:00 Lunch
- 14:00 – 17:30 **Joint meeting - panel discussions**
- 18:00 – 18:45 Dinner
- 19:45 – 23:00 **Conference Banquet**
Location: Winevault

Thursday, 1 September 2016

- 08:50 – 10:00 **Thursday Session I**
Location: Lecture Hall
(chairperson: Kateřina Rubešová)
- 08:50 – 09:35: Mária Behúlová:
Numerical simulation of welding processes
- 09:35 – 10:00: Michal Horký:
Growth of metastable fcc Fe₇₈Ni₂₂ thin films on Cu/H-Si(100) substrates
- 10:00 – 10:30 Coffee break
- 10:30 – 11:45 **Thursday Session II**
Location: Lecture Hall
(chairperson: Jan Šik)
- 10:30 – 10:55: S. Válková:
New crystal materials prepared by EFG method
- 10:55 – 11:20: Karel Bartoš:
Growth of very large, stress-free YAG crystals with a new method
- 11:20 – 11:45: Karel Kocián:
Humidity condensation during direct wafer bonding for SOI
- 12:00 – 13:00 Lunch
- 14:00 – 16:05 **Thursday Session III**
Location: Lecture Hall
(chairperson: Vladimír Jorík)
- 14:00 – 14:25: Jiří A. Mareš:
Advanced Efficient and Fast LuAG:Ce Optical Ceramic Scintillators
- 14:25 – 14:50: Vít Jakeš:
Preparation of waveguiding Er:YbAG thin films by spin-coating
- 14:50 – 15:15: Pavlína Ruleová:
Optimalization of thermoelectric properties of SnSe
- 15:15 – 15:40: Antonín Račický:
Thermal properties of MgO-Fe₂O₃-B₂O₃-P₂O₅ glasses

15:40 – 16:05: Jaroslav Jíra:
Antibacterial properties of nanomaterials

18:00 – 18:45 Dinner

Friday, 2 September 2016

08:50 – 10:25 **Friday Session I**

Location: Lecture Hall

(chairperson: Pavlína Ruleová)

08:50 – 09:35: Jan Pejchal:
Growth of fluoride and oxide scintillation crystals by micro-pulling-down method

09:35 – 10:00: Petra Zemenová:
Study of the natural ageing in the Er:LiY(PO₃)₄ glassy system by thermal analysis

10:00 – 10:25: R. Král:
Synthesis, purification, and characterization of ternary cesium hafnium chloride

10:25 – 10:50 **Closing**

11:30 – 12:30 Lunch

ABSTRACTS

In situ XPS depth profiling of polymer films and polymer/diamond interface using Ar⁺ cluster ion beam sputtering

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Iurii Melnichuk², Karel Hruška¹, and Alexander Kromka¹

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X-ray photoelectron spectroscopy (XPS) depth profiling is known as useful tool for obtaining information about the chemical composition of thin solid films at different depths. The combination of XPS measurements with monoatomic ion beam sputtering of soft and solid surfaces is commonly used for surface cleaning and concentration depth profiling. However, ion-surface interactions can cause a modification of near-surface layer with the changes in composition and chemical bonding. Recently, a new approach for depth profiling so called cluster ion beam sputtering have attracted a considerable attention as versatile tool with minimal surface damage. Rapid progress has been made in depth profiling of soft films, especially polymers, through the use of cluster ion beams. This technique may be rather useful in XPS analysis where sputter depth profiling of soft/solid structured films could give access to band bending measurements at interfaces.

In this work we present XPS depth profiling of three polymer films (plasma polymerized poly(ethylene oxide); fluorocarbon plasma polymer (PTFE) and amine-containing plasma polymer) via in situ lateral sputtering by Ar⁺ clusters ion beam. These plasma polymers differ in density of functional groups or degree of cross-linking, therefore, they show different adhesive surface properties important for bioapplications. The results of depth profiling by Ar⁺ clusters ion beam and ellipsometry thickness measurements allow calculating the sputtering yield of each polymer. It was estimated that the PTFE films have the lowest sputtering yield (about 1.25 nm/min) in comparison with other polymer films. The XPS analysis of C 1s peaks of the polymers also revealed preservation of the original state of surface chemistry with minimal changes even after 10 min of sputtering.

Next, we investigate polymer/diamond interfaces by in situ XPS depth profiling employing Ar⁺ clusters ion beam sputtering. The amine-containing plasma polymer (27 nm thick) was deposited on the surfaces of H- or O-terminated nano- and microcrystalline diamond (NCD and MCD) films and then sputtered to the polymer/diamond interfaces by Ar⁺ clusters ion beam. After the sputtering of about 90 % of the plasma polymers layer the deconvoluted C 1s XPS spectra showed the dominant signal from sp³ carbon phase which corresponds to the diamond surface. In the case of O-terminated diamond surfaces at this depth still 14 at. % of oxygen were detected by XPS. The possibility of the preservation of O-termination of diamonds under the thin plasma polymer layer will be discussed. In addition, the valence band spectra of polymer/diamond interfaces measured by XPS will be presented.

This work was supported by project GACR 15-01687S. The authors acknowledge the support from the Charles University in Prague through the project SVV-2016-260324.

Growth of very large, stress-free YAG crystals with a new method

Karel Bartoš, Jan Polák, and Jindřich Houžvička

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Yttrium-aluminium garnet (YAG, $Y_3Al_5O_{12}$) is known for more than 40 years and is widely used as a host material mainly for solid-state lasers and scintillators. Czochralski method with automatic diameter control is commonly used for YAG production. The standard furnaces result in crystals with typical diameters below 100 mm. Larger crystals can be prepared by Kyropoulos, Heat Exchange Method, Temperature Gradient Technique or Horizontal Solidification Method, but their quality is typically insufficient, so these crystals did not find broader applications.

The newly developed method aims on production of very large and stress-free crystals. Crystals as large as 125 mm in diameter and 8 kg heavy without core will be presented. 150 mm crystals will be produced in the newly designed furnace this year. And since the system seems to be very robust, even larger crystals can possibly be achieved. The key features of the method are: i) tungsten crucible to cope with temperature gradient along the large area, ii) use of hydrogen protective atmosphere as gas with very high temperature conductivity, and iii) inside process configuration substantially different to the original Czochralski method. Homogeneous temperature distribution results in a very stable and flat growth front.

Technology of growth large garnet crystals can be used with advantage for several applications. Undoped YAG can, for example, replace sapphire as a material for high-power laser systems. Unlike sapphire, YAG is not birefringent. This brings a substantial advantage in any application where subtle differences in index of refraction can be a problem. Size matters also with doped materials. YAG:Ce is a perfect material for large imaging screens with sub-micron resolution using UV, X-ray, electrons or heavier radiation. Newly grown crystals will allow using much bigger “screens” to achieve larger field-of-view than it was ever possible. Yb:YAG is used for laser high-power application. This material is the key material considered to reach thermonuclear fusion within the HiPER reactor. Homogeneity of the grown material is good enough now to manufacture laser Yb/Cr:YAG slabs of the size and parameters necessary for this application. Laser slabs as large as 120x120 mm are now being manufactured. Large Yb:YAG thus now offers attractive option to a large YAG ceramics, which might face problems with a high-power beam depolarization due to different orientation of small YAG grains.

Numerical simulation of welding processes

Mária Behúlová

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Numerical modelling and computer simulation represent a powerful tool for the design, analysis and optimization of welding processes. Numerical simulation of welding processes has been exploited with many advantages to study and explain the physical principles of complex phenomena connected with metallurgical joining processes [1-3]. Results of computer simulations can be applied for the relatively fast and inexpensive evaluation of the influence of welding parameters on the quality of the weld joints and the definition of optimal process parameters for the weld manufacturing.

In most cases, numerical simulation of welding processes requires to solve coupled electromagnetic, thermal-fluid and stress-strain problems involving phase transformations [1, 3]. Using this approach, it is possible to evaluate e. g. the temperature fields developed during conventional fusion welding taken into account the melt convection in the weld pool and also the deformations of welded components. In addition, the stresses arising in the welding process and residual stresses remaining in the material after the weld cooling can be predicted in order to eliminate the possible cracking and failure of the weld joint.

Transient temperature fields developed during welding processes can be described by the Fourier-Kirchhoff's partial differential equation [4]. To solve this equation, it is necessary to specify geometrical, physical, initial and boundary conditions, i. e. geometrical shapes and dimensions of welded structures, material properties, intensity of internal heat sources, temperature distribution at the beginning of the welding process and also the conditions and thermal effects at the interface of welded structures and environment. The heat input in fusion welding can be modeled by different methods including moving point or line heat sources, surface or volumetric heat sources [5-7].

The paper deals with fundamentals of numerical simulation of welding processes providing examples of numerical analysis of arc, laser beam welding and friction stir welding.

The research has been supported by the Scientific Grant Agency of the Slovak Republic (VEGA) within the project No. 1/1010/16.

- [1] F. Boitout et al. Transient simulation of welding processes. ESI Group, SYSWELD, 2004.
- [2] A. P. Mackwood, R. C., Opt Laser Technol 37 (2005) 99-115.
- [3] L.-E. Lindgren, Comput Method App M 195 48-49 (2006) 6710-6736.
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- [6] J. Goldak, A. Chakravarti, M. Bibby, Metall Trans B, 15 (1984) 299-305.
- [7] C. S. Wu, G. Wang, Y. M. Zhang, Weld J 85 (2006) 284-291.

Transport and magnetic properties of $\text{Fe}_x\text{Bi}_2\text{Te}_3$ single crystals

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Recently emerged topological insulators form a new branch of materials with specific surface states, which span ordinary bulk energy gap. The states spanning the energy gap form so called Dirac cone. These conductive surface states are produced due to spin-orbital coupling. Such states are protected by time-reversal symmetry. These materials are interesting both from the point of basic research and the spintronic applications. Crystals Bi_2Se_3 and Bi_2Te_3 receive considerable attention in this field. Doping with transition metals could lead to ferromagnetic arrangement in these materials presumably as a result of RKKY interaction (*Diluted Magnetic Semiconductor*). Thus, doping of these materials by magnetic ions could lead to breaking time-reversal symmetry and opening energy band gap of the surface states.

Aim of this work is to contribute to the discussion of effect of doping on electric and magnetic properties of Bi_2Te_3 . The key point is to elucidate the way of incorporation of doping atoms into host structure (matrix) and further to find a correlation between the way of incorporation of doping atoms and variation of physical parameters. As these materials contain considerable amount of native defects, the interaction of doping atoms with native defects must be included in the scenario.

For this purpose, single crystals of overstoichiometric system $\text{Fe}_x\text{Bi}_2\text{Te}_3$ were prepared. Two effects were examined: (1) solubility of Fe in Bi_2Te_3 , where $x = 0, 0.02, 0.04, 0.06, 0.08, 0.1, 0.12, 0.14, 0.16$ and 0.18 after three weeks annealing below melting point of host matrix; (2) equilibrium concentration of Fe (solubility) for $x = 0.06$ without and with annealing for 1 day, 1, 2, 3, 5, 8 and 12 weeks. These materials were characterized by XRD, SEM EDX, ICP OES and LIBS analysis. Temperature dependence of electric conductivity $\sigma_{\perp c}$, Hall coefficient $R_H(\mathbf{B} \parallel c)$, Seebeck coefficient $\alpha_{\Delta T \perp c}$ and magnetic susceptibility $\chi(\mathbf{B} \parallel c, \mathbf{B} \perp c)$ were measured. Results of magnetic susceptibility show merely antiferromagnetic arrangement caused presumably by RKKY interaction. Effective magnetic moments per Fe ion calculated from susceptibility measurements and ICP OES concentrations give effective magnetic moment $\sim 2 \mu_B$. Examined materials are *p*-type semiconductors to 475 K. Based on comparison of electric and magnetic properties we suppose presence of at least two types of Fe ions incorporation in octahedral coordination in both strengths of crystal field. Further research is running.

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Resistive switch mechanism of Au/ZnO/Au crossbar structure

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Resistive random access memory (RRAM) is a new non-volatile memory technology. The advantage is not only non-volatile but also low power, simple structure and fast switching speed. RRAM can keep information when the electrical field was turned off. RRAM is switched the material resistance state and store the information by electron field. But the resistive switching is still controversial.

In this paper, this resistive switch mechanism of the Au/ZnO/Au crossbar structure was investigated. Au has been considered as a good metallic electrode for its low oxygen affinity and high stability. Au/ZnO/Au crossbar was deposited using sputtering. The crossbar area size is $100 \mu\text{m}^2$ with ZnO layer thickness ~ 140 nm and Au electrodes layer ~ 60 nm. The bipolar resistive switching behavior can be observed in our device, which the set voltage (V_{SET}) and the reset voltage (V_{RESET}) is -2.25 V. By further electrical transport analysis, the space-charge-limited-current (SCLC) dominate the carrier transport in the high resistance state (HRS). On the other, low resistance (LRS) is follow the ohmic transport. Our result shows that the oxygen ion migration plays an important role in the resistive switch mechanism.

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Heuristic and exploratory education for material science students

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Learning process of science is a matter of learning by experience. Especially for new generation who was born in the influence of internet, media dominated world, a new approach to bring resonance and permanent engraving to their brain is crucial for the success of learning. In old world, the experience of an idea relies strongly on imagination to create a vivid picture in brain and on occasionally practice in lab's works. These old techniques are still important in present time; but their efficiency have declined as quickly as an exponential decay function. Various new approaches and new unforgettable touches that may regain new generation's attention and carve deep gloves in their mind that may benefit to their entire life must introduce to the modern science education. In this talk, few major examples are presented to show a new way of teaching. The subjects of learning is decomposed into a series of problem hutting, discussion, material reading and finally to solve the problem. In addition to the subjects that teacher wants to deliver, self-exploration and group cooperation are the manner to keep student's high interest to the subject and to develop student's skill to work and contribute in group working. This new way of teaching need a minor to major revolution in today's education system as well as the devotion of teachers' will and time and of course, the support of administration.

Ferromagnetic ordering in Fe(III) complex mediated by the aromatic rings

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The violuric acid, H₃Vi (5-hydroxyimino-1,3-diazinane-2,4,6-trione; 5-isonitroso-barbituric acid) has been combined with Fe(III) salts to yield a hexacoordinate complex of the composition [Fe(H₂Vi)₃] · py · 4H₂O (**1**). This compound has been structurally fully characterized by the single-crystal X-ray diffraction [1]. The violuric anion acts as a bidentate O-N donor ligand.

The magnetic data of (**1**) was studied by the SQUID magnetometer (QuantumDesign MPMS-XL7) in the RSO mode of detection. The susceptibility data was acquired at the applied field $B_{DC} = 0.1$ T and the raw data was transformed to the effective magnetic moment. The magnetization was taken at $T = 2.0$ and 4.6 K, respectively, and presented in the form of the magnetization per formula unit $M_1 = M_{mol}/N_A \mu_B$. The zero-field cooling magnetization and field cooling magnetization experiments (ZFCM/FCM) were conducted at the applied field of $B = 10$ mT between $2 - 100 - 2$ K.

The temperature evolution of the effective magnetic moment for (**1**) at the room temperature possesses a subnormal value of $\mu_{eff} = 1.04 \mu_B$; on cooling it decreases gradually and below 50 K abruptly. This behavior is a fingerprint of the sizable exchange interaction of an antiferromagnetic nature. However, the magnetic susceptibility on cooling is increasing showing no a maximum.

The magnetization per formula unit also adopts a subnormal value of $M_1 = 0.0165$ at $T = 2.0$ and $B = 7$ T. The temperature rising to 4.6 K brings only a minor effect to the magnetization curve. As the data taking was done in the field-decreasing mode, some remnant magnetization remains at the zero field: $M_{1r} = 8.7 \times 10^{-4}$ and 5.3×10^{-4} for $T = 2.0$ and 4.6 K, respectively.

The zero-field cooled magnetization / field cooled magnetization experiments show that the two magnetization curves diverge at the critical temperature $T_C = 50$ K when the paramagnetic phase switches to the ordered one. A test for the magnetic hysteresis was positive at $T = 2.0$ and 5.0 K, respectively. The coercive fields were $B_c = 59$ mT and 69 mT respectively.

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Photoluminescence of silicon-vacancy centres in CVD diamond films – characterization and modelling

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Silicon-vacancy (Si-V) centres in diamond films and nanoparticles attract a great interest due to their perspective applications as solid-state light emitters or fluorescent markers in bio-imaging. Si-V colour centres consist of silicon atom incorporated between two vacant lattice positions in diamond and create so-called split-vacancy configuration [1]. This special geometry results in a weak electron-phonon coupling, which is reflected in emission spectra as dominant narrow zero-phonon line (ZPL) at 738 nm at room temperature and practically invisible phonon sideband. From a technological point of view, large attention is devoted to achieve Si-V photoluminescence (PL) intensity enhancement by means of influence on the deposition conditions as gas composition [2], or substrate temperature [3]. Additionally, temperature dependent photoluminescence, polarisation and EPR measurements [1] were performed to investigate this centre electronic transitions, structure and geometry. Nevertheless, unambiguous interpretation of luminescence process still lacks.

In this contribution, we investigate the temperature behaviour of steady-state photoluminescence of Si-V centre in diamond thin films prepared by the microwave plasma assisted CVD process. Photoluminescence emission spectra were measured in the temperature range of 11-300 K. Accumulated PL spectra were analysed as temperature dependent zero-phonon-line parameters (full width at half maxima, peak position and integral intensity) and compared with theoretical models to discuss possible effects influencing the PL. Our study reveals ZPL narrowing from 123 cm⁻¹ (~6 nm) to 40 cm⁻¹ (~2 nm) for temperature decrease from 300 K to 11 K, respectively. This behavior was well described by the T³ dependence expressing the homogenous broadening determined by vibrations of perturbed host lattice and quadratic electron-phonon interaction. In addition, the blue shift by 29 cm⁻¹ (~1.5 nm) in ZPL position from room temperature to the 11 K was observed. This blue shift was fitted by the T² + T⁴ function reflecting effects of lattice contraction and weakening of strength of electron-phonon coupling. Integral intensity was analyzed in sense of the Boltzmann activation process.

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Growth of metastable fcc Fe₇₈Ni₂₂ thin films on Cu/H-Si(100) substrates

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Ultrathin fcc Fe films on Cu(100) have been studied for their unique capability of magnetic (paramagnetic to ferromagnetic) and structural (fcc to bcc) transformation upon ion beam irradiation. However, pure fcc Fe films undergo a spontaneous transformation when their thickness exceeds 10 ML (~ 2 nm) [1]. We have shown that it is possible to grow thicker transformable fcc Fe₇₈Ni₂₂ films on Cu(100) single crystal where Ni stabilizes the fcc structure. Therefore, 44 ML (8 nm) thick films of transformable Fe₇₈Ni₂₂ have been deposited [2].

Due to the low industrial potential and high production costs of single crystal (Cu substrate), hydrogen terminated Si(100) (H-Si(100)) was chosen as another promising substrate.

In this study an epitaxial Cu(100) interlayer was deposited on H-Si(100) as a suitable substrate for transformable fcc Fe-Ni films [3].

A 44 ML thick Fe₇₈Ni₂₂ was prepared selectively on Cu/H-Si(100) and transformed by irradiation with 30 keV Ga⁺ ion beam. The result of the transformation was observed by Scanning Electron Microscope (SEM) and Magneto-Optical Kerr Effect (MOKE).

The possibility of direct focused ion beam writing of ferromagnetic elements embedded in a paramagnetic thin film makes this system Fe₇₈Ni₂₂/Cu(100)/H-Si(100) as an ideal candidate for the fabrication of magnetic nanostructures and prospective metamaterials [4].

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Magneto-optical properties of Co coated ZnO nanorods

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Hybrid transition metal/semiconductor nanostructures embrace two possible applications - as semiconductors and ferromagnetic nanostructures. In addition, the integration of magnetic material and semiconductor has also attracted a considerable research interest due to the potential application for magnetic field control device. ZnO is one of the most explored oxide integrated with magnetic elements for its special properties of optoelectronics application. However, the magneto-absorption effect and related magneto-optical properties of ZnO based hybrid magnetic nanostructure remains less explored.

ZnO NRs array were fabricated by electro-chemical deposition. After electro-chemical deposition, Co layers were coated on the ZnO NRs array also using sputtering. As the Co capping, band tailing becomes evident in the data with the onset of absorption at lower energy. The absorption at low energy in Co capped films may indicate the Co derived states near the band edge 3.4 eV. A sizeable magnetoabsorption change can be observed after the band tail at room temperature under magnetic field ~ 0.8 T. A ferromagnetic interfacial spin-polarized semiconductor band of Co-coated ZnO NRs is also observed by measuring magnetic circular dichroism effect. A phenomenological model related to magnetic field-dependent spin splitting band structures near the Co/ZnO interfaces due to charge transfer between the Co d orbit and the defect-related band has been proposed to describe the observed magneto-optical properties .

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Preparation of waveguiding Er:YbAG thin films by spin-coating

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Garnet structure is a very suitable matrix for doping of optically active cations thanks to its isotropic character. One of the most widely used dopants is Er³⁺ whose emission at around 1530 nm (⁴I_{13/2} → ⁴I_{15/2}) falls within the third communication window. To increase the efficiency of Er³⁺ luminescence, co-doping with Yb³⁺ is usually applied where ytterbium works as a sensitizer. In YbAG (Yb₃Al₅O₁₂), ytterbium is already part of the host matrix, so after doping with Er³⁺, it can be used to produce an active optical material, e.g. a planar waveguiding structure.

Our goal was to prepare the films of Er:YbAG that would be planar waveguides in the IR range. A water-based sol-gel method was used to prepare a solution to be deposited. After optimizing the spin-coater parameters and determining the heat treatment regime, thin films of erbium-doped YbAG were spin-coated on monocrystalline or amorphous SiO₂ substrates and heat-treated at either ambient or low pressure. The influence of the pressure at crystallization, together with the presence of a sintering agent (TEOS), was investigated with respect to surface morphology and waveguiding properties of the films.

The phase composition of prepared films was determined by XRD and their surface morphology by SEM and AFM. All samples were single-phase YbAG with a crystallite size up to 120 nm. When processed in a low pressure atmosphere, the roughness of the samples decreased; this decrease is further enhanced by using a minute amount of TEOS as a sintering agent. However, using a higher amount of TEOS leads to crack formation in the films.

The optical properties of the samples were evaluated using m-line and luminescence spectroscopy. Luminescence measurement showed a typical emission band at around 1530 nm in all samples. Waveguiding properties depend, among other factors, on the thickness of the film. The actual thickness of the prepared films was higher than the theoretically calculated value for one mode guided. The films deposited on amorphous silica substrate guided one mode at higher wavelengths only, contrary to the films deposited on monocrystalline SiO₂ which were one mode waveguides at all measured wavelengths.

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Antibacterial properties of nanomaterials

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Nanodiamonds (NDs) and graphene oxide (GO) are carbon based nanomaterials with promising properties for the microorganism growth ability modification. In this study we used nanodiamonds produced by a detonation process with average diameter of 5 nm. As-received NDs with numerous C-H bonds and positive z-potential are labeled as H-ND. Annealing of H-ND in air at 450 °C for 30 min leads to the surface oxidization and such NDs are labeled as O-ND. GO flakes were prepared according to the Bangal-modified Hummers method. Reduced GO (rGO) flakes were prepared by a two-step procedure, where chemical oxidation was followed by the subsequent thermal reduction of graphite powder oxidized by the Brodie method.

All examined nanomaterials (H-ND, O-ND, GO and rGO) indicate significant influence on the growth of *Escherichia coli*. Growth conditions were modified by the choice of cultivation media: the Mueller-Hinton broth (MH) and the Luria-Bertani broth (LB). The effect of nanomaterials was tested after 5 hour and 24 hour cultivation in the broth. The colony forming ability (CFA) of *E. coli* was compared with the control sample. In case of the MH broth we found that after 5 hours H-ND and GO decreased the CFA of *E. coli* at least by 50 %, after 24 hours only H-ND decreased CFA by 50 % and other nanomaterials had no statistically significant antibacterial effect. Experiment with LB broth gave us different results: all used materials indicated significant decrease of the CFA both for 5 hour and 24 hour measurement while the decrease varied between 20 % and 45 %.

Factors influencing antibacterial activity of used nanomaterials against the *E. coli* in nutrient substances with different ion abundance are discussed.

Crystalline Polymorphism of 2-((2-(hydroxy)benzylidene)amino)phenolato)(4-methylpiperidine)-nickel(II)

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It has been prepared and solved crystal structure of the empirical formula $C_{19}H_{22}N_3NiO$. Square-planar complexes with the electron configuration of the central atom d^8 is expected diamagnetic. A powder sample prepared from the crystals used in the single crystal structure analysis, however, showed a significant paramagnetic properties. The simulated powder diffraction pattern of the solved crystal structure clearly ruled out that it is the same substance. Le Bail analysis allowed separate phase with solved the crystal structure and the remaining diffraction pattern was successfully indexed. This has prompted a number of synthesis in a variety of conditions that manage to prepare and then to solve the crystal structure the second polymorph. The simulated powder diffraction pattern of the solved crystal structure is identical with the diffraction pattern obtained by separation Le Bail analysis. Moreover, it was prepared next, third polymorph of the composition of the substance. While outstanding issue remains whether the crystals used to measure the magnetic properties is a mixture of two already known polymorphs or they are the fourth polymorph.

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Humidity condensation during direct wafer bonding for SOI

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The Silicon-On-Insulator (SOI) wafer consists of three layers: a thin single crystal silicon layer (device layer), a thick silicon layer which provides mechanical support (handle wafer) and a dielectric layer which separates the two silicon layers and is predominantly formed by silicon dioxide (buried oxide, BOX). The electrical insulation of devices from the thick silicon layer enables simpler, smaller and more robust solutions. Devices can achieve higher performance (power, frequency) and robustness (reduced latch-up, higher radiation hardness and voltage isolation) at lower cost (reduced process complexity, higher density).

The key process step in SOI manufacturing is the direct wafer bonding, i.e., joining of the wafers without the use of adhesives or any intermediate layers. Surface of the wafers need to be sufficiently smooth, flat and clean for spontaneous wafer bonding.

There are two types of direct wafer bonding according to chemical structure of the wafer surface: hydrophilic and hydrophobic. Hydrophilic bonding uses wafers prepared by standard cleaning procedures which create hydrophilic wafer surface. On the other hand hydrophobic bonding requires special treatment during wafer cleaning suppressing the native oxide formation.

Because of water adsorption on the hydrophilic wafer surface, the gas at the front of the bonding wave tends to be saturated with water. Cooling caused by gas expansion at the rim of the bonded pair results in supersaturation of the gas with water and its subsequent condensation [1]. On the contrary hydrophilic character of the wafers surfaces greatly reduces the nucleation barrier for the droplet condensation.

The contribution deals with direct wafer bonding, droplet condensation, and its consequences. Techniques leading to suppress this phenomenon are also discussed.

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The influence of the new dipicolinate complexes of Mn (III) and Fe (III) in the process of degradation experiments.

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The chemistry of manganese and iron complexes has been investigated recently since these metals are present in a various biological redox systems including peroxidases, catalases, superoxide dismutases, dioxygenases and lipoxidases. Dipicolinic acid is known to be a major component of bacterial spores. The metal dipicolinate complexes are also used in environmentally friendly “green” catalysis. In this study we report the structural characterization of $(\text{H}_5\text{O}_2)[\text{Fe}^{\text{III}}(\text{dipic})_2]$ (**1**) and $(\text{H}_3\text{O})[\text{Mn}^{\text{III}}(\text{dipic})_2]\cdot 3\text{H}_2\text{O}$ (**2**) compounds which were precursors for preparation of new Manganese(III) and Iron(III) dipicolinate complexes with selected cations of pyridinecarboxamides. There are four pairs Fe^{III} and Mn^{III} isostructural compounds: $(\text{H-inia})[\text{Fe}^{\text{III}}(\text{dipic})_2]\cdot 3\text{H}_2\text{O}$ (**3**) and $(\text{H-inia})[\text{Mn}^{\text{III}}(\text{dipic})_2]\cdot 3\text{H}_2\text{O}$ (**7**) (H-inia = isonicotinamidium cation), $(\text{H-pyda})[\text{Fe}^{\text{III}}(\text{dipic})_2]$ (**5**) and $(\text{H-pyda})[\text{Fe}^{\text{III}}(\text{dipic})_2]$ (**8**) (H-pyda = 3,4-dicarbamoylpyridinium cation), $(\text{H-4-pyme})[\text{Fe}^{\text{III}}(\text{dipic})_2]\cdot 2\text{H}_2\text{O}$ (**5**) and $(\text{H-4-pyme})[\text{Mn}^{\text{III}}(\text{dipic})_2]\cdot 2\text{H}_2\text{O}$ (**9**) (H-4-pyme = 4-hydroxymethylpyridinium cation) and $(\text{H-2,2'-bipy})[\text{Fe}^{\text{III}}(\text{dipic})_2]\cdot 3\text{H}_2\text{O}$ (**6**) and $(\text{H-2,2'-bipy})[\text{Mn}^{\text{III}}(\text{dipic})_2]\cdot 3\text{H}_2\text{O}$ (**10**) (H-2,2'-bipy = 2,2'-bipyridinium). Basic compounds $(\text{H}_5\text{O}_2)[\text{Fe}(\text{dipic})_2]$ (**1**) and $(\text{H}_3\text{O})[\text{Mn}(\text{dipic})_2]\cdot 3\text{H}_2\text{O}$ (**2**) were used for testing degradation reaction of waste-water. The degradation experiments were performed with model water which contained a mixture of petroleum hydrocarbon BTEX (benzene, toluene, ethylbenzene, o-xylene, p-xylene). With exception of ethylbenzene, all BTEX substances are on the list of synthetic specific organic pollutants [1]. Benzene is on the list of priority substance [2,3]. Toluene and xylenes are relevant substances for the Slovak Republic [1].

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Homogeneous nucleation in small closed systems

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Phase transition process starts via formation of a new phase clusters in the supersaturated (or supercooled) parent phase due to fluctuation. Subcritical clusters have tendency to diminish and supercritical ones (called nuclei) continue in growth. During such process it is necessary to overcome some energy barrier, so-called nucleation barrier, which depends on the conditions within system. Recent experiments on nucleation kinetics are based on light transmission or differential scanning calorimetry to determine induction times and metastable zone widths [1]. Analysis of these experiments with the mean first-passage time (MFPT) and survival probability (SP) methods [2] enable to determine nucleation rate, i.e., the number of nuclei formed in unit volume per unit time. These methods use the stationary nucleation rate approach to determine basic parameters of nucleation.

In this work we solve the kinetic equations to determine the size distribution of nuclei. As a model system we chose crystal nucleation of Ni droplets due to availability of experimental data [1]. In smaller systems one needs higher supercooling to occur formation of nuclei. At lower supercooling (larger volumes) the number of forming nuclei is relatively low due to higher nucleation barrier and that is why the classical nucleation theory (CNT) works quite well. In a short time some stationary state is reached and approximation of stationary nucleation rate gives a reasonable estimation of nucleation process. In small volumes ($\leq 10^{-18}$ mm³) formation of nuclei requires higher supercooling when depletion of molecules in the parent phase is not negligible [3]. As a consequence the number of nuclei of a certain nucleus size increases after a certain time delay to some maximum value and continues to decrease as the number of molecules in parent phase lowers. In this case using of CNT model is not justified. Computation of the size distribution of nuclei in Ni droplets (using nucleation parameters obtained from experimental data by MFPT and SP methods) shows that no supercritical clusters are formed within considered system. This discrepancy diminishes when the size dependence of the interfacial energy is included.

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Synthesis, purification, and characterization of ternary cesium hafnium chloride

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Recently, a growing interest in a new class of ternary halides based on the general formula A_2MX_6 , where A is alkali metal (Li, Na, K, Rb, Cs), M is metal in 4+ valence state (e.g. Ti, Zr, Hf, Sn, Se, Te), and X is halide (F, Cl, Br, and I), has appeared [1, 2]. The cesium hafnium chloride with formula Cs_2HfCl_6 (CHC) belongs into this group as well. Due to its high atomic number $Z = 58$, high light yield around 54 000 ph/MeV, energy resolution of 3.3 % at 662 keV, moderate density 3.86 g/cm³, and low hygroscopicity, it is a suitable candidate for application in radiation detectors as a scintillator.

The CHC is formed by CsCl (m.p. 645 °C) and HfCl₄ (subl. p. 320 °C) mixed together in stoichiometric ratio 2:1, it melts congruently at 826 °C, and crystallizes in cubic structure with lattice parameters $a = 10.42 \pm 0.01$ Å (space group Fm-3m) [3]. However, the CHC direct synthesis is uneasy due to HfCl₄ sublimation point as well as of its high hygroscopicity. Therefore, the preparation of high quality and purity starting CHC material is a difficult task requiring firstly successful CHC synthesis and secondly the removal of oxidic impurities before crystal growth.

In this contribution, the direct synthesis of undoped CHC from CsCl and HfCl₄ at different experimental arrangements was performed. Two purification methods - introduction of gaseous mixture of halogenation agents into molten CHC and zone refining of prepared CHC ingot, were carried out as well. Prepared and purified CHC material was characterized using X-ray fluorescence analysis, X-ray diffraction analysis, and thermal analysis to determine its purity, phase composition, and thermal properties. Furthermore, preliminary results of the CHC crystal growth by the vertical Bridgman method will be presented as well.

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Life and research of Niels Steensen

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Niels Steensen's contribution to natural sciences is of a great importance as he was one of the first to suggest a modern approach to the research. According to Steensen, science must be based on logic and individual research made with accuracy and precision. In his early work, so called *Chaos - manuscript*, Steensen criticizes the contemporary state of the natural sciences as too conservative, related to the ancient authors and the Bible and closed to scientific progress. His motto was: "Experimental exactitude, reproducible results". Niels Steensen was born in Copenhagen in 1638 and he did not follow steps of his father, a goldsmith, but entered the University of Copenhagen to pursue the medical studies. As a student he began, in accordance with the academic customs of his time, to use Latin name Nicolaus Stenonis. The commonly used name Steno is probably an incorrect derivation from this [1]. Steensen is considered to be one of the last polymaths, i.e. scientists who focused on a wide range of scientific disciplines. His research deals not only with medicine and anatomy, but also with geology and crystallography as well as crystal growth. Steensen's contribution to crystal growth and crystallography was published in his geological studies *De solido intra solidum naturaliter contento dissertationis prodromus* ("Preliminary discourse to a dissertation on a solid body naturally contained within a solid") in 1669. Steensen's observations concerning crystals are impressive, if we realize that he made them in the time, when no analytical methods were used. He observed that crystals do not grow from inside like flowers, but from outside as a result of material deposition on the surface of the existing crystal. Furthermore, Steensen divided crystals into different groups according to parent material and thus disproved the common belief that all crystals were formed from ice [2]. It was also Steensen, who discovered that the interfacial angles of quartz crystals were the same regardless of the size or shape of the crystal [3]. This principle was later named after him and has been known as *Steno's law* or *Steno's law of constant angles*. The last Steensen's conclusion of great importance relates to the reciprocity of crystal growth and its dissolution. It took over 300 years before modern research on the crystal growth confirmed these observations [4]. In 1675 Steensen became a priest and a theologian and did not continue the scientific research.

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Diamond thin films as a novel platform for life science and biosensors

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Diamond is considered as a perspective material for life sciences, especially as a functional artificial substrate for tissue engineering and regenerative medicine [1,2]. In addition to unique mechanical, thermal, chemical, optical and electrical properties, diamond is also biocompatible and its hydrogen terminated surface exhibits p-type induced conductivity which is highly sensitive to changes in surrounding environment due to surface transfer doping mechanism [3]. Thanks to this extraordinary combination of properties optically transparent (bio-) sensors [4] can be realized including also electrically active elements as impedance gas sensors [5], protein and cell field effect transistors [6], or DNA sensors based on change of charge density [7].

Realization of such bio-sensoric devices often requires the deposition of diamond films of tailored properties and therefore, there is still highly demanded a technological progress in growing diamond films on variety substrates and at low temperatures [8,9].

The scope of this presentation is viewing our technological achievements in the diamond synthesis on variety of substrates. Diamond thin films will be highlighted as a novel platform for life science and biosensors.

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Advanced Efficient and Fast LuAG:Ce Optical Ceramic Scintillators

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Scintillating materials (crystals or even ceramic ones) are used in various medical imaging methods (computed CT, PET, etc.), nuclear medicine, homeland security equipments and in high energy physics [1-4]. Majority of application needs scintillators characterized by (i) high light yield (L.Y.), (ii) high Z_{eff} atomic number, (iii) fast scintillating decay, (iv) good optical quality and also good mechanical and chemical stability [3, 4]. One of the heavy, with high L.Y. and fast decay garnet is lutetium aluminum garnet $\text{Lu}_3\text{Al}_5\text{O}_{12}:\text{Ce}$ (LuAG:Ce). Growth (by the Czochralski Cz method [4]) of LuAG:Ce takes place at high temperature, with low growth rate and large energy consumption. Especially, the high temperature of growth resulted in an arising of so called antisite defects (AD Al^{3+} instead Lu^{3+} lattice ion) [4,5]. The above mentioned properties of Cz grown LuAG:Ce crystals are not present if their optical ceramic (OC) analogues are prepared [2,5]. Fabrication of OC ceramics is characterized by (i) lower temperature of growth, (ii) better homogeneity of dopants and also (iii) larger size samples can be produced [5-7].

Roughly after year 2005 an extensive development of LuAG:Ce ceramics has started [5,6]. Our first studies of LuAG:Ce OC ceramics in 2007 (M. Nikl, et. al. in [5]) have shown L.Y. of ~ 5000 ph/MeV and this is very low value compared with that of LuAG:Ce crystal (~ 26000 ph/MeV in 2010 see C. Dujardin et al. in [8]). But during last 10 years a significant progress in the technology of OC materials [6,7] resulted in substantial improvement of scintillating properties of LuAG:Ce and similar ones OC materials. The most used technology to produce LuAG:Ce OC is solid state reaction method [6,7]. Now, LuAG:Ce,Mg OC's exhibit L.Y. ~ 25000 ph/MeV and ER $\sim 5\%$ at 662 keV with short 1 μs shaping time [1] which is very close to L.Y. of LuAG:Ce crystal mentioned above [8].

The main goal of this report is to present the newest data of scintillating properties of LuAG:Ce OC including (i) an influence of Mg^{2+} co-doping and (ii) effects of deviations from stoichiometry (an excess or deficiency of Lu^{3+} lattice ions).

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Estimation and utilization of structure anisotropy in forming pieces

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Anisotropy of microstructure in case of forming of metal or plastics depends on technology parameters of processes. In case of deformation of metals grain boundaries orientation can be observed, in case of short fibre reinforced plastics orientation of fibres. In the polycrystalline material (metal, alloy) the main microstructural parameter is grain boundary - surface interface between individual grains. In case of isotropic non deformed structure the grains have isometric dimension mean grain size or specific surface area of grain boundaries can be measured. In case of anisotropic plastically deformed structure the grains have anisometric dimension, it is necessary to describe their anisotropy [1]. The anisotropic microstructure is decomposed into isotropic, planar and/or linear oriented components - specific surface area of grain boundaries and these parameters are measured using stereology. Degree of grain boundary orientation is estimated as ratio of oriented specific surface area to total specific surface area. These results can be used for estimation of local plastic deformation in arbitrary places in volume of forming pieces. Real state of grain shape is quit impossible to describe, therefore model of conversion of degree of grain boundary orientation to deformation based on an idealized shape (tetrakaidecahedron) of grains has been proposed. Our conversion model is independent on an initial grain size (as it is in another model [2]) - strain depends only on the shape of the grain and does not depend on its dimension, what allows experimental estimation of local plastic deformation in various areas of plastically deformed parts. Fibre orientation in short fibre reinforced thermoplastics depends on injection moulding parameters. Stereological metallography was used for estimation of experimental orientation of fibres, and degree of orientation is estimated as oriented specific length of fibres (specific length of linear oriented components) to total specific length of fibres (specific length of all components). These results can be directly compared with numerical modeled ones - orientation tensor, what leads to experimental verification of numerical simulation model, which can be optimized to obtain coincidence with experiments. The measurement is very simple in comparison with a current method [3], which is based on measurement of dimensions (major and minor axes) and orientation of major axes of a lot of fibre intersections in analysed plane. These method can be applied for all types of materials as metals, plastics or ceramics.

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Modelling of charge carrier mobility for transport between elastic polymer nanorods

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Organic semiconductors keep going on attracting our attentions due to their some extremely good intrinsic properties for the device applications as well as for the benefits of low cost fabrications for industry concerns [1]. Among others, the idea of organic field effect transistors (OFET) [2] utilizes the fact the charge current increases by the increase of the charge carriers densities induced by the attracting field of the applied gate voltage in the direction perpendicularly to the plane of conducting thin layers. Next, for the increased charge concentration the mobility increases due to the filling of less mobile trap states [3], which additionally increases the effect of the gate voltage on the charge current in the conducting layer. However, at the surface interface between the conducting layer and the insulating dielectrics (separating the gate contact and the conducting layer), an environmental coupling of the conducting layer can change the charge densities due to the hybridization effects (partial charge transfer to trap states).

It is the scope of this work to study the mobility dependences on the charge carrier concentration and the hybridization coupling for the charge transport between closely stacked polymer lamellas. For the hopping transport between lamellas the model assumes the Marcus theory, while for the respective lamellas, the density of states are calculated taking into account the electron-phonon coupling of the elastic string model (dimerization effects) as well as the hybridization effects.

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Use of water-soluble polymers for the (Er³⁺/Yb³⁺):LiNbO₃ thin films preparation by sol-gel method

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Nowadays, with the development of economy and the growth of electricity consumption in telecommunications it is necessary to seek ways increase the effectivity of optical signal guiding. Lithium niobate doped with erbium ions, which are capable to emit in the near infrared region (1530 nm), seems to be a promising material to solve problem. The LiNbO₃ thin films are produced by various methods e.g. ion implantation, liquid phase epitaxy, molecular beam epitaxy, pulsed laser deposition, chemical vapour deposition, physical vapour deposition or sol-gel techniques. The preparation of homogeneous layers with sufficient thickness for their possible application to guide an optical signal is not an easy task when using sol-gel methods. This problem can be solved by the use of starting solutions containing additional gelling and/or stress-relaxing agents such as polyvinylpyrrolidone (PVP), polyethylene glycol (PEG), polyvinyl alcohol (PVA) or polyacrylic acid (PAA).

Our work presents the preparation of LiNbO₃ thin films doped with 0.5 at % of Er³⁺ and 0.5 at % of Yb³⁺ using PVP, PEG, PVA and PAA polymers. The influence of polymers on final microstructure, the Er³⁺/Yb³⁺:LiNbO₃ luminescence and waveguiding properties were investigated. After overcoming the problems with strongly hydrolysing Nb(V) ion, the PVP and PEG seems as promising for LiNbO₃ films preparation by a non-hydrolytic sol-gel method.

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Magnetism and Magnetic Materials

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The history of molecular magnetism began in 1951 with the study of a dinuclear complex, copper(II) acetate [1], however it was not until the 1990s that it received a strong impetus with the discovery of the first molecular-based solids that exhibited spontaneous magnetization [2] and [3]. Many important discoveries have been made since then by European teams in particular [ESF Scientific Programme Molecular Magnets (MM), October 2, 1999]: the synthesis of the first bimetallic molecular magnets and organic magnets with the highest Curie temperature known so far; the synthesis of room-temperature molecular-based magnets; the discovery of spin cross-overs that occur with large hysteresis at room temperature; new photomagnetic processes, including light-induced excited spin state trapping; the synthesis of the first molecular-based magnetic superconductor; the first characterization of the magnetic tunneling effect [4].

Molecular materials are systems that may be considered as built of discrete molecules, the so-called “building blocks”. This structural feature creates great opportunities for the modeling of electrical, magnetic and optical properties of materials through the selection of appropriate constituent molecules. The department of Inorganic chemistry of Faculty of Chemical and Food Technology is not only the main slovak center on coordination chemistry but also the place where investigation of molecular magnetism in Slovakia has started. It took place in the 1994s - R. Boča and his research group was one of the researchers who moved magnetochemistry into “Molecular Magnetism”. They revitalized areas like spin crossover, and developed a new language that was a mix of chemistry and physics, largely using theoretical models. Among their everlasting contributions to the field are: Spin crossover, Magnetic anisotropy, Polynuclear complexes, Non-isotropic exchange. Magnetostructural D-correlation for zero-field splitting in nickel(II) and Co(II) complexes.

The following topics have been developed under research activities: magnetic behavior of manganese(II), manganese(III), iron(II), iron(III), cobalt(II), nickel(II), and copper(II) complexes (magnetic anisotropy, spin crossover, molecular magnetism, nanomagnetism).

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Growth of fluoride and oxide scintillation crystals by micro-pulling-down method

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Inorganic scintillation single crystals have been employed in the detection of ionizing radiation including high energy photons, charged particles or neutrons. They are utilized in high-energy physics, environmental monitoring, geological survey and oil well logging or astronomy. Medical imaging and especially security scanning are the applications mostly stimulating the development of new scintillation materials due to increasing demands on their performance. To accelerate the material development, fast material composition screening is often required. The micro-pulling-down method is one of the most suitable for such a task due to its low material consumption and high growth rate which allows growing a crystal within several hours. It has been developed in the 90's for oxide crystals and consists in pulling the melt down from a crucible through a microcapillary in the crucible bottom [1, 2]. The melt spreads over a die and is further delivered to the solid/liquid interface which is formed below due to a temperature gradient. The crystal growth of heavy garnets for gamma-ray detection and Li-containing crystals for neutron detection by the micro-pulling-down method will be presented and discussed together with brief overview of their luminescence and scintillation characteristics, their modification with co-dopants and the influence of stoichiometry.

Special group of fluoride-based very fast scintillation materials are the vacuum ultraviolet (VUV) scintillators, whose development has been started some 2 decades ago. These scintillators can be coupled with advanced VUV photodetectors such as position-sensitive gas electron multipliers (GEM), micro-pixel chambers [3] or VUV-sensitive photomultipliers (PMT) with CsI-coated photocathodes [4]. Using various modifications of the carbon hot-zone [5], introducing the flux-growth or self-cladding phenomenon can enable growth of fluoride compounds that are difficult to grow with conventional crystal growth techniques. Crystal growth of fluorides for VUV scintillators based on BaLu₂F₈, ErF₃ and LuF₃ will be presented and discussed together with their luminescence and scintillation properties.

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Thermal properties of MgO-Fe₂O₃-B₂O₃-P₂O₅ glasses

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Doping of borophosphate glasses by environmentally friendly iron oxide is generally known to improve their chemical resistance against water and therefore these glasses are of interest in the field of nuclear or toxic waste disposal by their vitrification. Magnesium borophosphate glasses doped with Fe₂O₃ were prepared and studied in the compositional series A: (40-x)MgO-xFe₂O₃-10B₂O₃-50P₂O₅ and B: 20MgO-20Fe₂O₃-yB₂O₃-(60-y)P₂O₅ within the concentration range of x (y) = 0-20 mol % Fe₂O₃ (B₂O₃). The structure of the glasses was studied by Raman spectroscopy, Mössbauer spectroscopy was used to monitor the changes in Fe²⁺/Fe³⁺ ratio. Differential thermal analysis, thermodilatometry and heating microscopy have been used to study thermal behaviour and stability of the glasses.

The obtained Raman showed that the structure of starting glasses (x, y = 0) is formed mainly by Q³ and Q² tetrahedral PO₄ structural units. With increasing Fe₂O₃ (A series) or B₂O₃ (B series) content the dominant band in the high-frequency region (1050-1250 cm⁻¹) becomes weaker and shifts down to longer wavelengths, which is due to gradual depolymerisation of phosphate network up to terminal diphosphate (Q¹) structural units. The isomer shift and quadruple splitting for the absorptions in the Mössbauer spectra showed that each glass with Fe₂O₃ contained both Fe²⁺ and Fe³⁺ ions with octahedral and deformed octahedral coordination respectively.

DSC studies showed that most of glasses (their super-cooled liquids) crystallize on heating within the temperature region of 560-760 °C. Major compounds formed by crystallization were Mg(PO₃)₂, Mg₂P₂O₇, Fe₃(P₂O₇)₂, BPO₄ and Fe₂B(PO₄)₃. Glass transition temperature, T_g, and crystallization temperature, T_c, decreases with increasing Fe₂O₃ content in the series A, whereas in B series exhibits a maximum for glass containing 10 mol % B₂O₃ (T_g) and 5 mol % B₂O₃ (T_c).

The highest thermal stability and therefore the lowest tendency towards crystallization were found for the glasses where x = 0 mol % Fe₂O₃ and y = 5 mol % B₂O₃. Most of glasses exhibit good chemical durability against water corrosion.

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Absorption and photoluminescence spectra of the hydrogenated amorphous silicon with embedded silicon nanoparticles

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We investigate the low cost a-Si:H PIN junction with embedded nanoparticles (NPs) for applications such as large area light emitting diodes (LED). In our previous research we applied in-situ techniques to create the heterogeneous NPs embedded in the Si:H thin films using the reactive deposition epitaxy (RDE) [1], laser ablation [2] and the magnetron sputtering followed by plasma treatment [3]. The formation of Mg₂Si NPs by RDE and laser ablation has been confirmed in-situ by the Auger electron spectroscopy (AES) and electron energy loss spectroscopies (EELS) and ex-situ by optical absorbance and Raman spectroscopies. The homogeneous coverage of a-Si:H surface by vacuum evaporated and hydrogen plasma treated Mg₂Si NPs with diameter below 10 nm has been confirmed.

For efficient electroluminescence a good injection of carriers into nanoparticles embedded in p/n junction must be achieved. Therefore we focus in our recent research on silicon nanoparticles (NPs) embedded in the hydrogenated amorphous silicon (a-Si:H). The intrinsic a-Si:H layers were grown on glass substrates at 250° C by the radio frequency silane-hydrogen plasma enhanced chemical vapor deposition (CVD). The optical absorption was measured by the photothermal deflection spectroscopy (PDS). The room temperature photo-luminescence of amorphous layers deposited at high silane concentration is rather low but increases significantly with hydrogen dilution reaching maximum at 5-6 % silane concentration and diminishes abruptly below 5 %. The high resolution transmission electron microscopy (HRTEM) shows in the highly photo-luminescent a-Si:H the presence of silicon nanocrystallites embedded in amorphous matrix.

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Perspectives on sol-gel method: crystal growth of functional materials

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With enormous materials engineering expansion in the last decades, the new technologies of materials preparation have been developed in a wide spectrum of forms, properties and following applications. New technologies enable to control properties at atomic level and to use such functional materials from biomedical applications through optics, electronics, and catalysis to energy storage and conversion. Nevertheless, even at this time, such a simple preparation process - the sol-gel method - finds a broad application.

Sol-gel methods comprise a very wide group of chemical principles that enables to prepare a great variety of functional materials. However, in all sol-gel methods, there is one great advantage important for the preparation of multicomponent functional materials - the homogeneity of precursors at an atomic level. This enables to synthesize multi-cation oxides that are prepared by a solid-state reaction only with a serious difficulty. In addition, there are many other benefits, the most valuable being the lowering of crystallization temperature by hundreds of degrees because of a highly reactive amorphous intermediate. Also variability in material texture and design for a particular application are the advantage of the liquid-solid process. Besides dense ceramics and thin films, the sol-gel methods allow the synthesis of self-assembly structures, nanocomposites, fibres, mesoporous materials, hybrid organic-inorganic structures etc.

The first real sol-gel preparation was described in 60's of the 19th century - tetraethyl orthosilicate (TEOS) formed glassy-like solid after longer stay on air. This finding started a new era of SiO₂ application. The true development of the sol-gel method occurred in 80's of the 20th century. Firstly, materials based on primary oxides (SiO₂, TiO₂, ZrO₂ or Al₂O₃) were synthesized using the alkoxide sol-gel process. Then also multi-cation systems - e.g. PbTiO₃, YBa₂Cu₃O_x - were prepared employing further new methods based not only on the hydrolysis of alkoxides.

In any case, the transformation from a sol to a stable gel determines the nature of -M-O-M- bonding in an arising amorphous/glassy intermediate (linear or network polymer). Naturally, crystallization energetics and mechanism is also determined in the stage of the sol-gel conversion. The difference from the solid state crystallization mechanisms can lead to the above described advantage (the crystallization temperatures are lowered by hundreds of degrees). On the other hand, some parameters - e.g. the solid-state solubility of cation dopants - are governed rather by kinetic aspects than by the thermodynamic stability of the solid state.

The talk will present an overview of the sol-gel methods with respect to differences in a solution composition that is crucial in the sol-gel transformation and in the following structural arrangement in the prepared solid state. Also the survey of functional materials with various structure designs will be presented.

Optimization of thermoelectric properties of SnSe

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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 materials to recover waste heat. Research on thermoelectric (TE) materials is thus a very active field of research. The performance of a TE material is expressed in terms of dimensionless figure of merit, ZT , where $ZT = \alpha^2 \sigma T / \kappa$. In this formula, α , σ , T and κ are the Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity, respectively.

The primary objective of this study was to investigate the behavior of arsenic and yttrium as dopants in SnSe, and to try to increase the value of the parameter ZT . Polycrystalline samples of composition $\text{SnAs}_x\text{Se}_{1-x}$ and $\text{Y}_x\text{Sn}_{1-x}\text{Se}$ (for $x = 0; 0.0025; 0.005; 0.0075; 0.01; 0.02$ and 0.04) were synthesized from elements of 5N purity using a solid-state reaction. The phase purity of the products was verified by X-ray diffraction. Samples for measurement of the transport properties were prepared using hot-pressing. The samples were then characterized by the measurement of electrical conductivity, the Seebeck coefficient, and the thermal conductivity over a temperature range of 300 - 725 K.

All of the samples demonstrate p-type conductivity. From the data, the value of dimensionless figure of merit ZT was calculated. The transport measurements suggest that the incorporation of As atoms in the crystal structure SnSe actually leads to an increase in figure of merit ZT in temperature region 450-550 K.

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Atmospheric plasma treatment of detonation nanodiamonds in water

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Nanodiamonds attract increasing attention due to their special properties such as low toxicity, biocompatibility, fluorescence, and widely adjustable surface properties and chemistry. Detonation nanodiamonds (DNDs), the mostly available and inexpensive type of nanodiamonds, are well known to contain non-diamond carbon phase and complex mixture of surface functional groups. Controlled and reliable surface cleaning and modification is still a challenge. This limits their utilization in otherwise promising biological and electronic applications.

In this contribution, we report on a novel method for modifying DNDs suspended in water by DC atmospheric plasma sustained above the water suspension. DNDs were used either in as-received form (labeled as H-DND) or after air-annealing at 450 °C for 45 minutes (labeled as O-DND). The influence of applied plasma current (100 and 300 μA) and treatment duration (1, 5 and 10 minutes) on the surface chemistry of DNDs was evaluated by Fourier-transform Infrared spectroscopy (FTIR). Plasma treated H-DND particles reveal *i*) decreasing ratio of CH_3 to CH_2 surface groups; *ii*) disappearance of double bonds (1589 cm^{-1}) present in the graphitic shell of the particles and *iii*) re-arrangement of residual oxygen-containing moieties on the particle surface, i.e. the spectral range from 1400 to 950 cm^{-1} . In contrast to H-DNDs, the chemical state of O-DND surface was not affected by plasma treatment. In this case, newly formed doublet at 1580 and 1604 cm^{-1} was detected whose origin is not clear yet. Furthermore, for both DND types the observed changes were more pronounced for longer treatment times. Complementary XPS and Raman measurements did not reflect any changes of DNDs after the plasma treatment.

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Progress of vacuum deposition techniques for Si:H thin films structures

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A widely used technique for the deposition of thin films with very different qualities is the Plasma Enhanced Chemical Vapor Deposition (PECVD). For the development of effective solar cells the long-time efforts were focused on the group 4 of the periodic table of elements, i.e. C, Si, Ge and their eventual alloys. However the first industrial processes for production of solar panels were based on mixed-phase of hydrogenated silicon in the case of the single solar cells, and on fully amorphous and microcrystalline structures in the case of tandem structures. The photoluminescence of thin films and electroluminescence of diode structures based on hydrogenated silicon have been studied only sporadically due to the very low quantum efficiency of energy transfer.

While the amorphous structure is characterized by higher absorption coefficient of light and thin films can be thinner, the microcrystalline structure has the character of crystalline silicon, i.e. the band gap is non-direct, the absorption coefficient is lower, and the final structure of solar cells has to be thicker. Light emission is similar - the photo- and electro- luminescence of amorphous structure of silicon is very low, and the microcrystalline structure does not exhibit these effects practically at all. One solution how to increase the absorption coefficient or radiative recombination is to integrate another kind of nanocrystals with direct or near direct band gap to this structure. Our work is focused on the forming of silicide nanocrystals as Mg₂Si by application of plasma treatment.

For evaluation of new quality Si:H thin films we already used the samples deposited by two technological procedures, which allows the integration of convenient nanoparticles of different semiconductors into the Si:H structures. The first one is a combination of PECVD and Reactive Deposition Epitaxy (RDE) [1] and second one the PECVD and Reactive Laser Ablation (RLA). In both cases the current technology does not allow to deposit the whole diode structure without interruption of vacuum process. Up to now only in the case of PECVD and Vacuum Evaporation together with Plasma Treatment (VE+PT) the all *in situ* deposition processes were realized in special vacuum chamber. The actual results, namely the influence of integrated Mg₂Si NPs on the electroluminescence and reached basic parameters - V_{oc}, FF and I_{sc} of diode structures measured under illumination will be introduced.

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Model simulation and mechanism investigation for ferromagnetic ZnO

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Undoped ZnO [1] as well as magnetic ions doped ZnO [2] exhibit ferromagnetism which attracts our attention to investigate the ferromagnetic mechanism. From many experimental evidences, for instances, the vacuum annealing drives the appearance of ferromagnetism, which imply the vacancies of oxygen as well as zinc are both key factors for the appearance of ferromagnetism. However, also some evidences do not support that the ferromagnetism is induced from the oxygen vacancy. Besides, UV irradiations can enhance the ferromagnetism of ZnO [3] which imply the ferromagnetism will be enhanced from conduction carrier density.

Above evidences help us to construct the proper ferromagnetic model for ZnO. The Hamiltonian of our model is set up from ZnO unit cell with Zinc (Zn) and Oxygen (O) vacancies, respectively. The ferromagnetism of ZnO is induced from O vacancies and singlet spin bonds are formed from Zn vacancies via magnetic coupling J . Besides, the Hamiltonian include two hybridization interactions between ZnO conduction band and both O and Zn vacancy states.

Our calculation results reveal the facts that the controversy in oxygen vacancy inducing the ferromagnetism is due to the magnetic coupling between Zn vacancy states is too weak. The ferromagnetism increases with the carrier density is consistent with the experimental results.

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New crystal materials prepared by EFG method

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The EFG (Edge-defined Film-fed Growth) method introduced by La Belle [1] is based on capillary elevation of the melt through capillaries of the shaping element. Profiled crystal is grown from a thin layer of melt on top of the shaping element which defines the cross-section of the crystal [2]. Possibility to grow the crystal directly in a shape that is desired for the final applications is a large benefit of this method since it is both economically and technologically advantageous. A method analogous to EFG is μ PD (Micro Pulling Down) that is commonly used for today's crystal development [2].

Although EFG method is primarily applied in sapphire production, it can also be used for a wide range of crystal materials such as YAG (yttrium aluminium garnet) or LuAG (lutecium aluminium garnet) based scintillators. YAP (yttrium aluminium perovskite) is also probably one of the most complex materials for the preparation.

EFG method makes it possible to prepare crystal materials not only as rods but also in form of tubes or thin fibers with 0.5 mm diameter. Several types of materials based on Al_2O_3 , YAG, LuAG and YAP crystal matrix were prepared to achieve dimensions required for the applications.

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One-dimensional ZnO nanostructures and their optoelectronic applications.

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One-dimensional (1D) ZnO nanostructures, and more specifically nanorods (NRs), have attracted an increasing interest in recent years due to their potential in optoelectronic applications. To fully exploit this potential, several problems, such as understanding and controlling Schottky contact on nanostructured ZnO or difficulty in obtaining reliable and controllable p-type ZnO, must be overcome. Preparation of high quality rectifying Schottky contacts on ZnO is a complex task; crystal defects, residual impurities, surface asperities, and chemical reactions forming oxides and eutectics all have a large impact on the formation of a Schottky contact.

We have recently developed a new method for the fabrication of highly rectifying Schottky contacts on different semiconductor materials [1-3]. We showed that the deposition of colloidal graphite allows for the fabrication of highly rectifying junctions with the ideality factor close to one on bulk ZnO. The current transport was dominated by thermionic emission between 300 and 420 K and the extracted barrier height followed the Schottky-Mott relation [4]. The analyses of the current-voltage and the capacitance-voltage characteristics of the graphite/ZnO nanorod heterojunctions provide evidence of the predominance of the tunnel-recombination current transport mechanism via interface state [5].

These nanostructured heterojunctions showed potential in different applications, such as highly sensitive UV photodetectors [6], or hydrogen sensors operated at room temperature [7].

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Study of the natural ageing in the Er:LiY(PO₃)₄ glassy system by thermal analysis

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Phosphate glasses doped with rare earth (RE) elements are promising materials for application as radiation detectors (scintillators) e.g. in medical imaging (PET, CT), homeland security, and high energy physics [1]. Any prepared glass, kept far below glass transition temperature (T_g), loses with time its excess configurational entropy, enthalpy or free volume towards the equilibrium state of supercooled liquid if its matrix permits the corresponding relaxation processes [2]. These processes are characterized by the movement of structural components toward their equilibrium state and depend both on the glass thermal history and the ageing time [2, 3].

These phenomena are studied using different thermal methods such as differential thermal analysis (DTA) and differential scanning calorimetry (DSC), which are widely used to determine thermal properties of glasses. Further they are suitable to describe the relaxation losses of glasses as a function of their thermal history, ageing, composition, and heating and cooling rates [2].

This contribution deals with preparation of the meta-phosphate glass Er:LiY(PO₃)₄ with nominal composition of 0.5Er₂O₃-25.0Li₂O-24.5Y₂O₃-50.0P₂O₅ (in mol %) synthesized directly from the Li₂CO₃, YPO₄, ErPO₄, and P₂O₅ and its characterization using thermal analysis. For further characterization the powder samples were prepared by grinding a part of the glassy ingot in an iron mill and sieving it through sieves with a nominal aperture size ranging from 90 to 106 μ m. These prepared and tested powder samples were aged under defined conditions in a desiccator at room temperature, where they were kept and continuously taken after 1 to 71 days for non-isothermal DSC measurement. The DSC analysis was carried out in an alumina crucible at heating rates of 8, 10, and 25 K/min from room temperature to 1000 °C under inert nitrogen atmosphere using Setaram Setsys Evolution 16. The aim of this work is to study the influence of structural changes occurring during natural ageing of glassy samples. The effects of ageing time and heating rate on the glass transition, crystallization, and thermal stability parameters will be discussed as well.

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