

**DEVELOPMENT
OF MATERIALS SCIENCE
IN RESEARCH AND
EDUCATION**

Book of Abstracts of the 24th Joint Seminar
8 – 12 September 2014



Z. Kožíšek
K. Nitsch
Editors



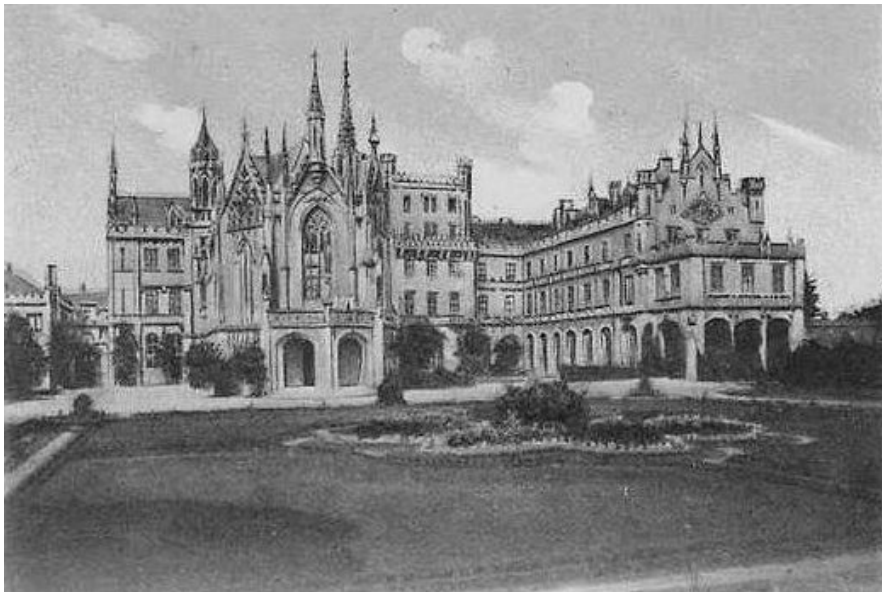
CZECHOSLOVAK ASSOCIATION FOR CRYSTAL GROWTH

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Development of Materials Science in Research and Education

Book of Abstracts of the 24th Joint Seminar

Z. Kožíšek
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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 24th Joint Seminar “Development of Materials Science in Research and Education” (DMSRE24) will be held in Lednice at Lednice spa during 8-12 September 2014. 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 AS CR, 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, nano-crystalline 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 programmes of individual institutions
- Information about equipment for preparation and characterisation of materials
- Results of materials research

The program will include 4 keynote lectures (45 minutes): Pavel Ctibor (Institute of Plasma Physics AS CR, Praha): *Production of ceramics for electrical industry by spark plasma sintering*, Marian Koman (Slovak University of Technology in Bratislava, Bratislava): *100 years of crystallography*, Karel Nitsch (Institute of Physics AS CR, Praha): *Crystal growth techniques*, and Lukáš Válek (ON Semiconductor, Rožnov pod Radhoštěm): *Crystal defects in silicon*. 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 1st September 2014. The authors are responsible for the technical and language quality of the contributions.

The conference will run from Monday afternoon, September 8, till Friday noon, September 12 in Lednice spa.

Dear colleague, we welcome you to the DMSRE24 Joint Seminar and we hope you will enjoy your stay in Lednice spa.

On behalf of the organizers,

Zdeněk Kožíšek, Karel Nitsch, and Marian Koman

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PROGRAM

Monday, 8 September 2014

- 12:30 – 14:15 Registration
Location: Hotel Lounge
- 14:30 – 15:00 Opening
Location: Lecture Hall
- 15:00 – 16:10 **Monday Session I**
Location: Lecture Hall
(chairperson: Zdeněk Kožíšek)
- 15:00 – 15:45: Marian Koman:
100 years of crystallography
- 15:45 – 16:10: Vladimír Jorík:
Application of powder diffraction methods to characterize the products of preparation of cocrystals
- 16:10 – 16:40 Coffee break
Location: Lunchroom
- 16:40 – 17:30 **Monday Session II**
Location: Lecture Hall
(chairperson: Jiří A. Mareš)
- 16:40 – 17:05: Blažena Papánková:
Study of magnetic properties of complexes of Co(II) with N - donors ligands
- 17:05 – 17:30: Ľubor Dlháň:
Magnetic properties of Iron(II) Bithiazole complexes
- 18:00 – 18:30 Dinner

Tuesday, 9 September 2014

08:50 – 10:00 **Tuesday Session I**

Location: Lecture Hall
(chairperson: Vladimír Jorík)

08:50 – 09:35 Lukáš Válek:
Crystal defects in silicon

09:35 – 10:00 Jan Šik:
Optical Interference in SOI wafer

10:00 – 10:30 Coffee break
Location: Lunchroom

10:30 – 11:45 **Tuesday Session II**

Location: Lecture Hall
(chairperson: Karel Nitsch)

10:30 – 10:55 Petr Kalenda:
Lead borophosphate glasses modified by tungsten oxide

10:55 – 11:20 Antonín Račický:
Structure and Properties of Fe_2O_3 - TiO_2 - P_2O_5 Glasses

11:20 – 11:45 Maryna Vorokhta:
Structure and properties of GeO_2 modified lithium phosphate glasses

12:00 – 13:00 Lunch
Location: Lunchroom

14:00 – 15:40 **Tuesday Session III**

Location: Lecture Hall
(chairperson: Lubor Dlháň)

14:00 – 14:25 Zdeněk Potůček:
Photoluminescence of Vanadium Ions in $SrTiO_3$ Crystal

14:25 – 14:50 Tomáš Hlásek:
Infrared luminescence in $Er^{3+}:Yb_3Al_5O_{12}$

- 14:50 – 15:15: Maksym Buryi:
EPR investigation of Ce^{3+} , Er^{3+} , Nd^{3+} impurity centers in $Y_{0.7}Lu_{0.3}AlO_3$ single crystal
- 15:15 – 15:40: Miroslav Menšík:
Anomalous temperature dependence of excitation transfer between quantum dots
- 15:40 – 16:10 Coffee break
Location: Lecture Hall
-
- 16:10 – 17:00 **Tuesday Session IV**
Location: Lecture Hall
(chairperson: Maroš Martinkovič)
- 16:10 – 16:35: Jiří A. Mareš:
Multicomponent $(Lu, Y, Gd)_3(Ga, Al)_5O_{12}$ garnets - new kind of scintillating materials
- 16:35 – 17:00: Apolena Vondrášková:
Nanocrystalline Pr-doped $Lu_3Al_5O_{12}$ phosphor prepared by radiation method
- 18:00 – 18:30 Dinner

Wednesday, 10 September 2014

- 08:50 – 10:00 **Wednesday Session I**
Location: Lecture Hall
(chairperson: Marian Koman)
- 08:50 – 09:35: Karel Nitsch:
Crystal growth from the melt
- 09:35 – 10:00: Petra Zemenová:
Thermal analysis of Er-doped potassium ytterbium lanthanum phosphate glass
- 10:00 – 10:30 Coffee break
Location: LUNCHROOM

-
- 10:30 – 11:45 **Wednesday Session II**
Location: Lecture Hall
(chairperson: Blažena Papánková)
- 10:30 – 10:55: Zdeněk Kožíšek:
Homogeneous nucleation of Ni liquid near critical supercooling
- 10:55 – 11:20: Jan Kulveit:
Application of Ising model to test standard nucleation theory
- 11:20 – 11:45: Michal Havrлік:
Structure of polyvinyl alcohol nanotextiles stabilized by different methods
- 12:00 – 13:00 Lunch
Location: Lunchroom
- 13:00 – 18:00 Joint Meeting
- 18:00 – 22:00 **Conference Dinner and Night Discussion**
Location: Winevault
(chairperson:)
-

Thursday, 11 September 2014

- 08:50 – 10:00 **Thursday Session I**
Location: Lecture Hall
(chairperson: Lukáš Válek)
- 08:50 – 09:35: Pavel Ctibor:
Application of spark plasma sintering technology for ceramic dielectric materials and functionally graded multi-layers
- 09:35 – 10:00: Jaromír Drápala:
Influence of non-ferrous metals and rare-earth elements on structural characteristics of Cr-Mo steels
- 10:00 – 10:30 Coffee break
Location: Lunchroom

10:30	–	11:45	Thursday Session II
			<i>Location: Lecture Hall</i>
			<i>(chairperson: Jaromír Drápala)</i>
10:30	–	10:55:	Pavλίna Ruleová: <i>Preparation and transport properties of layered semiconductors for thermoelectric applications</i>
10:55	–	11:20:	Veronika Sládková: <i>Cocrystals, their preparation techniques and application</i>
11:20	–	11:45:	Ivana Pilarčíková: <i>Effectiveness of Strategy for Obtaining Quality Applicants to Technical and Life Science Colleges</i>
12:00	–	13:00	Lunch
			<i>Location: Lecture Hall</i>
14:00	–	15:40	Thursday Session III
			<i>Location: Lecture Hall</i>
			<i>(chairperson: Zdeněk Potůček)</i>
14:00	–	14:25:	Mária Domonkos: <i>Nanostructure fabrication using microsphere lithography</i>
14:25	–	14:50:	Blanka Jurková: <i>Testing of nanocrystalline diamond films against bacterial biofilms</i>
14:50	–	15:15:	Jiří Stuchlík: <i>The combined technological methodes for deposition of Si:H thin films and structures with in situ embedded nanoparticles</i>
15:15	–	15:40:	The Ha Stuchlíková: <i>The methodes applied for the characterisation of Si:H thin films with embedded nanoparticles</i>
18:00	–	18:30	Dinner

Friday, 12 September 2014

- 08:50 – 10:05 **Friday Session**
Location: Lecture Hall
(chairperson: Zdeněk Kožíšek)
- 08:50 – 09:15: Maroš Martinkovič:
Analysis of surface local plastic deformation of the workpiece.
- 09:15 – 09:40: Zdeněk Remeš:
Correction method to the surface defective layer in low absorption spectroscopy
- 09:40 – 10:05: Miroslav Menšík:
Dependence of kinetic rates of charge transfer on structural parameters in disordered systems
- 10:05 – 10:30: Alexey Sveshnikov:
Modelling of 3D-structure of nanotextiles
- 10:30 – 10:50 **Closing**
Location: Lecture Hall
(chairperson:)

ABSTRACTS

EPR investigation of Ce³⁺, Er³⁺, Nd³⁺ impurity centers in Y_{0.7}Lu_{0.3}AlO₃ single crystal

Maksym Buryi, Valentyn Laguta, Martin Nikl, and Jan Rosa

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The compositionally disordered compound Y_{0.7}Lu_{0.3}AlO₃:Ce (YLuAP:Ce, 0.19 at.% Ce) belongs to the row of scintillators Y_{1-x}Lu_xAlO₃:Ce (x runs from 0 to 1). Here the critical values of x, 0 and 1, give the cerium doped YAlO₃ and LuAlO₃ scintillators, which find application in the field of medical imaging [1,2]. The Ce³⁺ ions act as the luminiscent centers responsible for scintillation process. Understanding of their distribution and incorporation inside the material is thus essential. During the crystal growth process, uncontrolled impurities could get into the lattice. It is therefore important to clarify the nature of defects occurred in the material and their role in energy transfer.

The EPR spectra measured in the material were consistent with the central strong resonance line referred to as being produced by the main Ce³⁺ center and the satellite lines about 100-1000 times less in intensity similar to those, described in [3]. The satellites originating from the Ce³⁺ ions, were of particular interest. The mirror disposition of the weak cerium satellite lines with regard to the strongest central line allowed us to consider them as being doublets, produced by the coupled Ce³⁺ ions (in contrast with the results, reported in [3]). The g-tensors, exchange constants and orientations of the magnetic axes as well as the relative concentrations of the coupled Ce³⁺ ions have been determined for the first time.

The crystals of YLuAP:Ce contained also noticeable amount of the unexpected defects produced by the Er³⁺ and Nd³⁺ impurity ions. The relative concentration of Er³⁺ was deduced to be about 1.5% of the main Ce³⁺ center concentration. The Er³⁺ and Nd³⁺ impurities create new energy states in the band gap, serving thus as the electron traps. Their spectral parameters were defined as well.

Financial support of Czech TACR TA01011017 project is gratefully acknowledged. This research was also supported by Czech large infrastructure SAFMAT CZ.2.16/3.1.00/22132 project.

- [1] A. Lempicki, M.H. Randles, D. Wisniewski, M. Balcerzyk, C. Brecher, A.J. Wojtowicz, IEEE Trans. Nucl. Sci. 42, 280–284 (1995).
- [2] M. Nikl, Phys. Status. Solidi (a) 178, 595–620 (2000).
- [3] A.G. Asatryan, J. Rosa, J.A. Mareš, Fizika tverdogo tela 45, 8, 1390-1395 (2003).

Application of spark plasma sintering technology for ceramic dielectric materials and functionally graded multi-layers

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²*Faculty of Electrical Engineering, Czech Technical University in Prague, Czech Republic*

The spark-plasma-sintering (SPS) system was developed in 1990-ies. It is a consolidation technique which combines pulsed electric currents and uni-axial compaction. Heating rates, applied pressures and pulsed current patterns are the main factors responsible for the enhancement of densification kinetics and conservation of the submicron-scale structure of the materials. The problems with long sintering times necessary for the sintering of compact fully dense materials by conventional procedures are significantly reduced using SPS. The sintered material is surrounded by graphite elements for application of heating and force to obtain the desirable product form. Therefore just rather simple shapes as tablets, cylinders and small rotation-symmetrical bodies could be manufactured.

- Multi-layers were prepared by SPS using Al_2O_3 and TiO_2 as components. These two materials have markedly different mechanical, optical and electrical properties and in the other hand a high degree of chemical and crystallographic compatibility. When for example one of the components is nanometric and second one not, different character of the boundary and different thickness of interlayers are obtained. Other multi-layers were prepared by spark plasma sintering using Al_2O_3 and MgTiO_3 (or CaTiO_3) as components. These two materials have markedly different mechanical, optical and electrical properties. To promote the compactness at the boundary, TiO_2 could be used as an interlayer. The character of the boundary and thickness of interlayer was studied. Different multi-layers were prepared by SPS using Al_2O_3 . When one side of the sample was composed from a nanometric powder and second one from micrometric powder, different porosities were obtained in proximity of the opposite surfaces. Such material exhibits gradient of microhardness, wear resistance or physical properties.

- Optical FGM was obtained by thermal post-treatment of the SPS-produced YAG:Ce - cerium doped YAG ($\text{Y}_3\text{Al}_5\text{O}_{12}$). The fully crystalline YAG:Ce is useful for cathodoluminescent material production as well as converters of UV radiation to yellow visible light. The as-prepared material by SPS is extremely sensitive to redox conditions. This SPS-prepared material was subjected to a thermal post-treatment at 1000°C in air. The surface, which was in the full contact with a flat ceramic support in the furnace, was reduced and the opposite surface surrounded by air was oxidized. Both parts exhibited after cooling markedly different optical properties, mainly from the emission viewpoint.

- The relative permittivity of SPS-prepared BaTiO_3 was higher and in the same frequency interval also the loss tangent lower for the sintering pressure direction orientation than for the perpendicular orientation. This is probably associated with certain anisotropy of the porosity that should mean more flat pores in the pressure direction and therefore denser structure with easier polarization.

Czech Science Foundation - project P108/12/1872

Magnetic properties of Iron(II) Bithiazole complexes

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A series of Fe(II) complexes has been prepared with bithiazole ligands and NCS coligands. They were characterized by X-ray structure analysis and the magnetic data was taken with the SQUID magnetometer [1].

The SQUID magnetometry has been conducted by taking the temperature dependence of the magnetic susceptibility at small field of $B_0 = 0.1$ T, and field dependence of the magnetization until $B = 7$ T at $T_0 = 2.0$ and 4.6 K, respectively.

Two mononuclear complexes show magnetic behavior typical for the zero-field splitting systems with as a spin Hamiltonian. The fitting procedure gave: $g_z = 2.031$, $g_x = 2.234$, $D/hc = +8.05$ cm⁻¹, $(zj)/hc = -0.159$ cm⁻¹, $c_{TIM} = 0$ for **1**, and $g_z = 2.307$, $g_x = 2.259$, $D/hc = -5.10$ cm⁻¹, $(zj)/hc = -0.108$ cm⁻¹, $c_{TIM} = -5.10 \times 10^{-9}$ m³ mol⁻¹ for **2**. The dinuclear complex exhibits an exchange coupling of the antiferromagnetic nature with $J/hc = -34.2$ cm⁻¹, $g = 2.176$, $x_{PI} = 0.018$, $Q_{PI} = -1.79$ K.

This work is supported by Slovak grant agencies (VEGA 1/0522/14, VEGA 1/0233/12, APVV-0014-11)

- [1] A. Abedi, V. Amani, R. Boča, L. Dlháň, H. R. Khavasi, N. Safari, *Inorg. Chim. Acta* 395 (2013) 58–66.

Nanostructure fabrication using microsphere lithography

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In this study microsphere lithography (MSL) is demonstrated to be a versatile, simple, inexpensive (in terms of equipment and operation) and materials-independent fabrication process for creating periodic arrays of nanostructures using self-assembled polymer microspheres as templates. Self-assembly is the most feasible way to create monolayers of polymer nano/microspheres with hexagonal-close-packed ordering on a large scale. After mask preparation MSL consists of different post-treatment steps - plasma etching and deposition processes- to create the desired geometrical patterns. The resulting patterned micro- and nanostructures have a wide range of applications, such as substrates for SERS, optical devices, plasmonic biosensors and chemosensors. This study focuses on the modification of microspheres using plasma etching and an overview of applications of 2D colloidal crystals. Specifically, this contribution also deals with structuring of micro- and nanocrystalline diamond thin films.

This work was supported by the Project No. P108/12/G108.

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Influence of non-ferrous metals and rare-earth elements on structural characteristics of Cr-Mo steels

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Theoretical and experimental study on influence of addition of selected non-ferrous metals and mischmetal on microstructural characteristics in special Cr-Mo steel grades were performed. A clear relationship between distribution coefficients of admixtures in iron and their proton numbers was revealed.

Samples of two specific Cr-Mo steels with Ce addition were prepared using a plasma furnace. Microstructure characterization were carried out using light optical microscope, SEM and SEM-EDS. Cerium addition resulted in the formation of micrometer size oxy-sulfide inclusions which can be utilized for controlling the grain size structure of steel castings. The majority of the particles have settled down at the bottom part of the sample, indicating that the convection flow during solidification was very weak. The rare-earth metals (REM) addition slightly diminished hardness of the steel. Segregation behaviour which brought about non-uniform distribution of dissolved cerium over the entire volume of the studied steel samples during relatively fast crystallization process was observed.

The paper presents the first results obtained from laboratory-scale experiments with addition of rare-earth metals, especially of cerium, to two specific steel grades provided by the industrial partner, for achieving finer grain structure of the steel castings. Based on the obtained results and observations it is concluded that addition of REM to the liquid steels brought about formation of REM oxy-sulfide inclusions prior to steel solidification. The inclusions have acted as active heterogeneous nucleation sites for grain nucleation during solidification processes and the grain structure in final as-cast microstructure was remarkably refined. The performed REM addition, thus, produced positive effect on grain structure of the as-cast steel samples. Such improved as-cast microstructure, of course, is greatly desirable in heavy-weight steel castings produced by steel-making industry as it can help to eliminate internal defects occurred in the castings as a consequence of macrosegregation of microalloying and trace elements during solidification (cracking, large-size inclusions and other types of defects).

The study was carried out within the frame of the project TA CR No. TA03010161: Experimental development of non-ferrous metals utilization for microstructure refinement in the production of steel ingots for forgings in the specific work, with the technical support of the Project No. LO1203: Regional Materials Science and Technology Centre - Feasibility Program and Project No. CZ.1.07/2.3.00/30.0016: Opportunity for Young Researchers.

Structure of polyvinyl alcohol nanotextiles stabilized by different methods

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Nanotextile is a promising type of material with possible areas of application ranging from tissue engineering in medicine and air filtration in aircrafts to protective layers of construction materials in civil engineering. High level of interest to nanotextiles is explained by recent progress in technology of production of nanotextiles, allowing fabrication of this material in large scale at relatively low cost. Nanospider technology is a modification of electrospinning method of production of unwoven nanotextiles. In our paper we study structure of polyvinyl alcohol (PVA) nanotextiles produced by Nanospider technology at the Center for Nanotechnology in Civil Engineering on Faculty of Civil Engineering of CTU in Prague.

PVA nanotextiles can be easily produced by Nanospider, but due to extremely high solubility of PVA in water cannot be directly used in civil engineering. There exist different methods of stabilization of PVA [1, 2]. We have tried thermal stabilization, methanol and aldehyde treatment. The first two methods are applied to already existing nanotextile, while addition of aldehyde to polymer solution allows a direct production of stabilized nanotextile.

Before nanotextiles can be successfully used as protective layers of construction materials their other properties must be studied: mechanical strength, diffusion and antibacterial properties to name just a few. These properties depend on the structure of the nanotextile, which makes the determination of its exact microscopic structure a very important task.

Our paper represents an initial attempt to study the structure of PVA nanotextiles stabilized by different methods by means of SEM photography. There is a room for improvement here, both on experimental and theoretical level. For example, electrical conductivity of PVA nanotextile is very low, which complicates the study of fine structure due to constantly increasing electrical charge. Further analysis is required in order to reconstruct the 3D-structure of the material. However, it is shown that even the results of our preliminary study are important for future applications of nanotextiles.

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Infrared luminescence in $\text{Er}^{3+}:\text{Yb}_3\text{Al}_5\text{O}_{12}$

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The emissions of rare-earth (RE) ions doped materials have attracted much attention because of the potential applications, such as optoelectronics, scintillators, full-colour displays, lasers or planar waveguides. Among RE ions, Er^{3+} is the most attractive activator because it can simultaneously offer the possibility of blue, green, and red upconversion emissions for visible light applications, as well as IR emission for optical amplification in telecommunication.

In this work, the luminescent properties of Er^{3+} doped ytterbium aluminium garnet (YbAG) bulk ceramics and thin films was investigated by excitation at 980 nm. Various sol-gel methods were used to prepare thin films on silicon substrates. Thin films were also deposited by the liquid phase epitaxy (LPE). All samples prepared by the sol-gel methods exhibit the very high resolution of ${}^4\text{I}_{13/2} \rightarrow {}^4\text{I}_{15/2}$ transition fine splitting. However; the thin films prepared using LPE are the only which exhibit waveguiding properties.

According to this work, the erbium doped YbAG seems to be a promising material for planar waveguides. The bulk samples prepared in this work are suitable as standards for the measurement of photoluminescence spectra of the $\text{Er}^{3+}:\text{YbAG}$ thin films.

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Application of powder diffraction methods to characterize the products of preparation of cocrystals

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Herein presented work uses qualitative powder diffraction to characterize the products of preparation of cocrystals. The product can contain unreacted starting components, a new phase (cocrystal) or mixture of both. To identify the individual components of the product, a newly formed user database of reference powder diffraction pattern of the starting materials and their cocrystals was used. The diffraction patterns of cocrystals were obtained experimentally. The real samples of starting materials often contain mixture of polymorphs. Therefore diffractograms of the starting materials and their polymorphs and pseudopolymorphs were calculated on a base of Cambridge CSD [1]. There was characterized a 46 cocrystallization products, 22 samples have been characterized as a pure cocrystal. Some typical cases are shown in a demonstrative examples. Despite the user database making the qualitative analysis more accurate, significantly simpler and quicker, not all products could be clearly characterized by phase analysis (due to overlap of the diffraction lines). The result was verified by other methods.

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Testing of nanocrystalline diamond films against bacterial biofilms

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Nanocrystalline diamond (NCD) films appear to be a promising material for many different applications due to their high physical and chemical stability, great range of possible surface modifications and easy production. NCD films were shown to be well biocompatible with tissue cells; however their possible antibacterial properties have been much less investigated.

For our studies, we grew NCD films by chemical vapour deposition method on glass substrates and treated them by hydrogen, oxygen and CF₄ plasma to achieve different wetting angles (70°, 5°, 100°, respectively). Apart from wetting angle measurements, the surface properties of NCD films were further examined by scanning electron microscopy, Fourier transform infrared spectroscopy, Raman spectroscopy and X-ray photoelectron spectroscopy.

We present two methods of bacterial biofilm cultivation suitable for studying the bacterial growth on solid surfaces, which we will use for testing of possible antibacterial properties of NCD films. The first method comprises modified batch cultivation. The second method employs the commercially available CDC Bioreactor for continuous cultivation of bacteria. For both methods *Escherichia coli*, a gram-negative bacterium, was used as the model organism.

We show the preliminary results of experiments that aimed to the careful optimization of the experimental setup and procedures required for monitoring *E. coli* biofilm formation on glass and NCD films. Untreated glass will serve as negative control material in further studies that will thoroughly explore the potential ability of NCD film to reduce the bacterial growth.

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Lead borophosphate glasses modified by tungsten oxide

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Borophosphate glasses of the $\text{PbO-B}_2\text{O}_3\text{-P}_2\text{O}_5\text{-WO}_3$ system were studied in two compositional series $(1-x)[50\text{PbO-}10\text{B}_2\text{O}_3\text{-}40\text{P}_2\text{O}_5]\text{-}x\text{WO}_3$ with 0-60 mol% WO_3 and $(1-x)[50\text{PbO-}20\text{B}_2\text{O}_3\text{-}30\text{P}_2\text{O}_5]\text{-}x\text{WO}_3$ with 0-40 mol% WO_3 . Moreover, glasses with the ratio $\text{B}_2\text{O}_3/\text{P}_2\text{O}_5 = 5/45$ and $15/35$ were studied as well. Thermal behavior of the glasses was studied by differential thermal analysis, thermodilatometry and hot stage microscopy. Glass structure was studied by Raman spectroscopy and also by ^{31}P and ^{11}B MAS NMR spectroscopy. The glass transition temperature increases with increasing WO_3 content in both compositional series and almost all prepared glasses crystallize within the range of 500-750 °C. ^{31}P MAS NMR spectra of both compositional series revealed the formation of P-O-W bonds with an increasing WO_3 content resulting in the shortening of phosphate-chains. ^{11}B MAS NMR spectra reveal the formation of B-O-W bonds in tetrahedral BO_4 units resulting in the formation of mixed tetrahedral units BO_4 containing B-O-P, B-O-B and B-O-W bonds. Trigonal BO_3 units are formed in the glasses with a higher WO_3 content. Raman spectra of the studied glasses also revealed the incorporation of octahedral WO_6 units into the glass network and formation of W-O-W bonds in glasses with a high WO_3 content.

100 years of crystallography

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Crystallography is the science that examines the arrangement of atoms in solids. The word "crystallography" derives from the Greek words "crystallon" cold drop, frozen drop, in the broad sense covers all solids with some degree of transparency, and "grapho" I write. In July 2012, the United Nations recognised the importance of the science of crystallography by proclaiming that 2014 would be the International Year of Crystallography. X-ray crystallography is used to determine crystal structure of small molecules as well as of large biomolecules such as proteins.

Before the development of X-ray diffraction crystallography, the study of crystals was based on their geometry. This involves a measuring of angles between the faces of crystal relative to theoretical reference axes (crystallographic axes), and establishing the symmetry of the crystal in question.

Crystallographic methods now depend on analysis of the diffraction patterns of a sample targeted by a beam of some type. X-rays are most commonly used; other used beams include electrons or neutrons. Every of these three types of radiation interacts with a solid in different way. X-rays interact with the spatial distribution of the electrons, while electrons are charged particles and therefore feel the total charge distribution of both the atomic nuclei and its electrons. Neutrons are scattered by the atomic nuclei through the strong nuclear forces, but in addition, a magnetic moment of neutrons is non-zero. Therefore they are also scattered by magnetic fields. Due to these different forms of interaction, every of these three types of radiation is suitable for different crystallographic studies.

Homogeneous nucleation of Ni liquid near critical supercooling

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Crystal nucleation from supercooled liquid occurs due to fluctuation at the appropriate conditions. At the critical supercooling $\Delta\mu_C$, where $\Delta\mu$ denotes the difference in chemical potentials of both phases, a detectable small amount of thermodynamically stable phase is formed and a certain maximum size of nuclei i_{max} is reached. Metastable zone width, i. e. the temperature difference between the melting temperature and the temperature at which the crystals are detected upon applying a constant cooling rate, characterizes nucleation process and depends also on sample volume and on a cooling rate. Critical supercooling increases with melt volume decrease and provides important information about nucleation process.

We have numerically solved the kinetic equations within standard nucleation model to determine the size distribution of nuclei F for homogeneous crystal nucleation of Ni melt [1] near the critical supersaturation. The maximum size i_{max} of nuclei is determined from the condition $F_{i_{max}}=1$. It is shown that although the supercritical nucleus is formed, the growth does not occur if the number of supercritical nuclei is low. The size distribution of nuclei reaches the stationary value after some time delay and decreases with nucleus size. The maximum size of nuclei i_{max} rapidly increases with supercooling and decreases with melt volume. The growth rate, determined from i_{max} , reaches some maximum and consequently decreases to zero as the maximum size of nuclei is reached. The classical nucleation theory underestimates the maximum size of nuclei in dependence of supercooling.

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Anomalous temperature dependence of excitation transfer between quantum dots

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The photoluminescence of quantum dots or of systems of low-dimensional nanostructures has been given attention experimentally and theoretically recently. In the present work the temperature dependence of the photoluminescence of the systems with quantum dots is studied theoretically as a response of the quantum dot system to the excitation of the system by a laser pulse. This kinetic process is built on the electron-phonon or on the exciton-phonon interaction of the electronic subsystem with the vibrations of the atomic lattice. The nonequilibrium Green's functions are used to include the electron-phonon interaction in an approximation going beyond the limits of the finite degree of the perturbation theory. The theoretical approach is illustrated by numerical calculations in individual quantum dots and in a system of two interacting quantum dots. The results obtained are discussed in relation to the available experiments.

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Application of Ising model to test standard nucleation theory

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First - order phase transitions begins on scales of individual particles (atoms, molecules, ions) to form portions of a new phase via localized domains within initially metastable phase. Before the recent advances in nanoscience this a quite complex process has been usually studied within context of classical nucleation theory (CNT). Implementation of certain theoretical approaches (in particular, Ising model) succesfully applied in other physical fields (in this case, magnetism) allow to describe phase changes in nanoscaled world.

It has to be pointed out, however, that the essential problem to verify the validity of CNT is closely connected with the fact that predictions for a relatively small space of experimental data (e.g. dependence of basic nucleation characteristics on single parameter like temperature) are based on generous space of model parameters, resp. assumptions (chemical potentials, surface energies obtained via capillary approximation, etc.). In this case it seems to be very useful to use computer simulations allowing a precise control over the big parameters space to test individual aspects of CNT.

Following earlier studies of CNT and purely numerical modelling (e.g. [1]-[3]), we propose application of Ising model to test standard nucleation theory varying not only the external driving force (as already investigated) but also the temperature, surface energy (exhibiting its heterogeneity due to surface roughness or curvature). Other promising modification is more correct definition of newly-forming clusters (e.g. [4]) possibly forming a more consistent model across broad scale of temperatures and cluster sizes.

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Multicomponent (Lu,Y,Gd)₃(Ga,Al)₅O₁₂ garnets - new kind of scintillating materials

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An intense research of heavy lutetium based Ce³⁺-doped aluminum garnet scintillating crystals as Lu₃Al₅O₁₂ (LuAG) started around year 2000 [1,2]. Besides Ce³⁺ dopant also Pr³⁺ one started to be studied in LuAG from year 2004 [2,3]. Ce³⁺ and Pr³⁺-doped LuAG crystals were prepared by a Czochralski method but from year 2008 also single crystalline layers were grown by a liquid phase epitaxy method [4].

A few years ago (from 2010 year) in Japan a technique called "bandgap engineering" was developed [5]. This technique allows to prepare so called multicomponent garnets of composition (Lu,Y,Gd)₃(Ga,Al)₅O₁₂ mainly Ce³⁺-doped. Both single crystals and single crystalline films were prepared [4,5]. These multicomponent garnet crystals are characterized by high Light Yield and the highest one reached ~50000 ph/MeV on Ce³⁺-doped Gd₃Ga₃Al₂O₁₂:Ce (GGAG:Ce) Czochralski grown crystal [5]. This crystal is also characterized by a good energy resolution of 5.5 % at 662 keV energy of ¹³⁷Cs radioisotope. Besides Ce³⁺-doped GGAG multicomponent crystal also well characterized GGAG single crystalline layers were prepared [4]. Emission spectra of multicomponent garnet single crystals and layers are lying roughly in the same wavelength range as those of classical LuAG:Ce and YAG:Ce single crystals - broad emission bands peaking around 520 nm.

In this talk we will present the newest results of scintillating properties of both Ce³⁺-doped multicomponent garnets and by liquid phase epitaxy prepared single crystalline layers [4,5]. Scintillating properties (Light Yield, Energy Resolution and Non-proportionality) were measured using a HPMT multiplier under different radioisotopes excitation [6].

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Analysis of surface local plastic deformation of the workpiece.

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Final properties of plastic deformed parts of workpieces are affected by production technological processes. Therefore it is needful to know detail structure changes of plastic deformed material caused by machining - milling, turning, drilling etc. Metal cutting, viewed as a plastic deformation process, is quite unique. It is localised, asymmetric deformation which operates at very large strains and exceptionally high strain rates [1]. Cutting zone has three areas of intensive local plastic deformation: the primary area of plastic deformation in shear plane, the secondary area of plastic deformation caused by friction of chip to tool face and the tertiary area of plastic deformation caused by friction of tool to work surface. The primary and secondary areas of plastic deformation has great influence to technological process, the tertiary area of plastic deformation has great influence to quality of work surface and local mechanical properties of surface layer of workpiece. Therefore it is necessary to evaluate degree of local plastic deformation of workpiece.

Local strain in structure can be estimated by measurement of deformation of grains on metallographic cut. In general, the effect of grains boundaries self-orientation caused by grains deformation can be observed. Stereological evaluation of the grain boundary orientation is relatively simple in case if axes of orientation are defined [2]. But the orientation is not the same as deformation and so it is necessary to use a correlation between the grain deformation and grain orientation [3].

Local plastic deformation in deformation zone around the surface of drilled holes, local plastic deformation in deformation zone near the surface of milled workpiece and local plastic deformation in cutting zone of turned material was investigated. Standard cutting parameters were used. The working piece was bulk from carbon steel Ck45 (1.0503). Due to plastic deformation (if it is present) structure anisotropy is increased - grain boundaries orientation in deformed places of piece is observed. Estimation of grain boundary orientation degree leads to determination of local plastic deformation in arbitrary place of workpiece. It allows very simple and effective experimental estimation of local plastic deformation degree by measure of grain boundary orientation in various places of formed parts, at the surface layer deformation at machining. It can leads to consequential technological processes optimization and knowing quantitative dependences technological parameters - microstructure - properties.

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Dependence of kinetic rates of charge transfer on structural parameters in disordered systems

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Charge transfer process in conjugated polymers is widely studied as far as those materials seem to be promising in optoelectronic devices for their low cost and easy processing. The semiconducting properties of those polymers can be utilized in applications as field-effect transistors, various kinds of sensors and switches, and light-emitting diodes, etc.. The concrete application is very sensitive on specific transport phenomena that are controlled by the structural parameters. In our presentation we will study the dependence of charge carrier mobility in disordered chains of conjugated polymers.

For our model assumption we assume that the polymers forming quasi linear chains are parallelly oriented. Simultaneously, we assume that additives carrying dipole moments are randomly dispersed between them. Next, we assume that the major contribution to the 3-dimensional mobility of the charge carriers is given by the hopping of charges between neighbouring chains. For the kinetic modelling we assume that first the charges are delocalized and thermalized in 1-dimensional segments. In the second step, the charges hop to the neighbouring chain. In our approach we calculate the eigenenergies of those thermalized states that are controlled by the transfer integrals between repeating units within polymer chains and by the local energies of charge carriers on units influenced by distributed additives. For the calculation of the hopping rates of charges between segments we use either Marcus or Miller-Abrahams theory. The overall kinetics is governed by the Pauli-like equations that are numerically solved for randomly set structural parameters of the materials (additives and torsion of repeating units). The obtained values of the charge carrier mobility are averaged over Monte-Carlo simulations.

Mobility of charge carriers provides interesting dependences on temperature, measure of static disorder and charge concentration and they will be discussed in our presentation.

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Crystal growth from the melt

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Methods of single crystals growth from the melt are the most important and simultaneously the most frequently used methods of growing crystals of metals and congruently melting compounds. These growth methods have been used for more than 100 years and the reason for their expansive utilization has been the fact that crystals grow from the melt faster and in higher quality than crystals prepared by other methods, for instance from low and high temperature solutions. Currently, huge amounts of crystals of silicon, about 10 000 tons, GaAs nearly 1000 tons, ruby about 500 tons, garnets about 100 tons, zirconium dioxide more than 1000 tons, have been produced in recent years.

As the start of modern era of systematic preparation of synthetic single crystals and crystal growth methods the year 1902 is considered. In this year French professor A.V.L. Verneuil (1856-1913) demonstrated the flame fusion growth apparatus and method for growth of ruby crystals from the melt. In this method a finely powdered starting compound is melted in the oxy-hydrogen flame and originating droplets are deposited on the cooling down surface of the growing crystal. The Verneuil process remains in wide use to this day and in 2000 above 250 tons of crystalline gemstones were grown by this method. This method is just like other growth methods from the melt based on cooling of the melt below its freezing temperature, but their experimental arrangements are quite different. These techniques of growth from the melt can be divided into three groups according to their experimental arrangement:

1. *Directional crystallization, normal or gradient freezing.* In this method the starting material is at the beginning melted in a container and a crystal grows in the temperature gradient from the coldest point of this container. The crystal grows if a container or furnace is moved through the temperature gradient providing by a furnace. The simplest arrangement of this method is very often designed as Bridgman or Bridgman-Stockbarger one, while more sophisticated methods are known as gradient freezing configurations.

2. *Czochralski method (Cz)* is the most employed method for crystal growth of many electronic and optical materials. Crystal grows on a seed mounted on a moveable pulling rod. The growth starts by dipping the seed in the melt and by formation of a meniscus. The furnace temperature must be adjusted so that the melt crystallizes at the crystal/melt interface.

3. *Zone melting (ZM) and floating zone technique (FZ).* In these methods a narrow molten zone of the rod of the material under treating is moved through this rod from its start to its end. While in the *ZM* the treated material is in a long boat, in the *FZ* a vertically standing free rod of polycrystalline metal is treated. At the molten zone pass the starting material melts on its front part and crystallizes on the back one. The *ZM* as well *FZ* can be used as both growth and purification methods. The main advantage of the *FZ* is the fact that any contamination from a crucible material is avoided.

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Study of magnetic properties of complexes of Co(II) with N - donors ligands

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Single molecule magnets (SMM)s have attracted considerable interest as they are a confluence of multiple fields as well as the realization of a large body of theoretical predictions [1-2]. Early work focused on increasing the S value of clusters, the strength of coupling, and highlighted the importance of spin orbit coupling in 3d metals for increasing the overall magnetic moment. More recently researchers have attempted to understand and predict physical structure and its influence on the uniaxial anisotropy term, D . This term is an indicator for SMM phenomena and synthetic control of it would provide a rational synthetic [3]. Meanwhile the magnetic anisotropy quantified by the D parameter (which depends on the spin-orbit contribution) is in principle a difficult property to predict and/or control. The study of the magnetic properties of highly anisotropic paramagnetic molecules is an area of intense current research interest. The various cobalt(II) complexes were synthesized and characterized by common instrumental techniques. The present compounds of cobalt(II) with imidazole, benzimidazole and its derivatives are neutral, mononuclear, octahedral complexes $[\text{Co}(\text{ac})_2(\text{im})_2]$ (ac=acetate, im = imidazole) and $[\text{Co}(\text{ac})_2(\text{L})_4]$ (ac=acetate, L = benzimidazole, methylbenzimidazole, ethylbenzimidazole) were obtained and characterized as a distorted octahedron environment that is responsible for the moderately strong positive anisotropy of high spin Co(II). In the present complexes the imidazole/or benzimidazole is a ligand where an azomethine nitrogen atom of the imidazole/or benzimidazole ring and an oxygen atom of the carboxyl group are donor atoms. The bond of the carboxyl group with the metal ion is marked in the IR spectra by two separate bands assigned to asymmetric and symmetric stretching vibrations (ν_{as} and ν_s , respectively). For the present cobalt(II) complexes the bands are placed in range at $\nu_{as} = 1601\text{-}1563\text{ cm}^{-1}$ and $\nu_{as} = 1398\text{-}1457\text{ cm}^{-1}$. The frequency difference of the vibrations ($\Delta = \nu_{as} - \nu_s = 171\text{-}156\text{ cm}^{-1}$) is not characteristic of either the monodentate group COO^- or the bidentate one [4]. The UV absorption band observed for the present cobalt(II) complexes is broad and irregular. Within the visible range the maximum of absorption corresponding to the d-d bands for the present cobalt(II) complexes appear at 589, 553, 551, 547 nm, respectively. Magnetic moment of 4.25 B.M was measured at room temperature, for $[\text{Co}(\text{ac})_2(\text{im})_2]$ indicating the high-spin nature of this complex.

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Effectiveness of Strategy for Obtaining Quality Applicants to Technical and Life Science Colleges

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This study summarizes information about obtaining applicants to study at colleges with focus on technical and life science studies. The theoretical part of the thesis concentrates on studying available literature for quality assurance in the college education system and marketing opportunities in education. It includes an analysis of characteristics for graduates from individual secondary school-leaving examination majors and their transition to tertiary education and the form of marketing communication necessary for education institutes.

Based on studying available literature and the analysis of theoretical and practical information, we managed to come up with a strategy, the goal of which is to obtain quality applicants to technical and life science colleges. The strategy was derived from said analysis within the scope of theoretical analysis, experience and information gained over previous periods, analysis of secondary school student preferences when choosing a college and SWOT analysis.

Issues that came up during research work and hypotheses are defined in the empirical part:

H1: The quality level of students in the winter semester for the 1st year of college is higher for students in the experimental group than for students in the control group.

H2: The extra-economic effectiveness of the created strategy is higher than the traditional procedures for obtaining college applicants.

The following research methods were applied to verify our hypotheses: experiment, general knowledge tests, questionnaire and interview. Also included are the results of implementing the experiment, by which we verified the effectiveness of the created strategy for obtaining quality college applicants. It regarded determining the number of students, which came across the promotion, determining the efficiency of each promotion tool and defining the quality level of students in the control and experimental group.

The experiment was carried out at the Faculty of Electrical Engineering, Czech Technical University in Prague and at secondary schools. The results imply the proposed strategy is more effective than the traditional procedures for obtaining college applicants.

Photoluminescence of Vanadium Ions in SrTiO₃ Crystal

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Crystals of strontium titanate (SrTiO₃) with the highly polarizable perovskite-type structure and soft phonon modes remain in paraelectric phase down to the lowest temperatures because transition to ferroelectric phase is suppressed by quantum effects. Nevertheless their properties result in a whole range of interesting impurity related phenomena that have been observed in this incipient ferroelectric. Thus a very unusual and large temperature shift of the zero-phonon R-line was found in emission spectra of photoluminescence of Cr³⁺ and Mn⁴⁺ ions substituted for octahedral coordinated Ti⁴⁺ ions in SrTiO₃:Cr and SrTiO₃:Mn crystals [1, 2]. Besides, this temperature shift was shown to be proportional to the reciprocal permittivity of SrTiO₃ crystals and to the square of temperature-dependent TO₁ soft phonon mode frequency below the temperature of structural phase transition from the cubic to tetragonal phase in the vicinity of 105 K. At the same time, the R-line temperature shift occurs in the case of emission of Cr³⁺ and Mn⁴⁺ ions in the opposite direction. In this context a study of photoluminescence of other impurity ions with 3d³ electron configuration such as V²⁺ or Fe⁵⁺ substituted in SrTiO₃ crystal for Ti⁴⁺ ions could be very contributing to prove suggested explanation of this difference in the R-line position temperature behavior because the R-line corresponding to ²E → ⁴A₂ transition may also appear in their photoluminescence emission spectra. Therefore, we performed a study of photoluminescence spectra of vanadium doped SrTiO₃:V (300 ppm) crystal grown by the Verneuil technique in order to detect centers formed by vanadium ions and to determine their optical properties. Photoluminescence emission and excitation spectra were examined at temperatures between 12 and 300 K within the 350 - 1600 nm and 250 - 1000 nm spectral range, respectively.

The only emission band related to vanadium doping was revealed in the emission spectra of photoluminescence of the studied SrTiO₃:V crystal in the near infrared spectral region. The emission band consisted at low temperatures of the pronounced zero-phonon line peaking at 1157.1 nm at 77 K accompanied by well developed vibrational sidebands extending up to 1450 nm. Two excitation bands peaking near 500 and 620 nm at 77 K were found below the absorption edge of the SrTiO₃ crystal in the excitation spectra taken for this emission. Spectral features of the obtained emission and excitation spectra are typical for photoluminescence of ions with 3d² electron configuration in octahedral coordination of oxygen ions. Therefore, we suppose that the emission band with zero-phonon line at 1157.1 nm at 77 K corresponds to the ¹T_{2g} → ³T_{1g} transition in V³⁺ ions substituted in Ti⁴⁺ sites.

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Structure and Properties of Fe₂O₃-TiO₂-P₂O₅ Glasses

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Iron phosphate glasses are of interest in the field of nuclear waste disposal by vitrification due to their exceptionally good chemical durability and low processing temperatures.

Iron phosphate glasses doped with TiO₂ were prepared and studied in the compositional series (100-x)(40Fe₂O₃-60P₂O₅)-xTiO₂ within the concentration range of x=0-12 mol% TiO₂. Glasses were characterized by the measurements of density, molar volume, chemical durability and refractive index. The structure of the glasses was studied by Raman spectroscopy. Differential thermal analysis, thermodilatometry and hot stage microscopy have been used to study thermal behaviour of the glasses.

According to the Raman spectra, the glass structure consist mainly of tetrahedral PO₄ diphosphate (Q¹) units and partially of metaphosphate (Q²) and orthophosphate (Q⁰) units. Vibrational bands of TiO_x structural units were not observed in the Raman spectra.

The modification of starting 40Fe₂O₃-60P₂O₅ glass by TiO₂ additions revealed changes in the properties of the glasses. Replacement of both Fe₂O₃ and P₂O₅ by TiO₂ results in an increase of glass density, refractive index and Abbe number, whereas molar volume decreases within the range of 48.6 - 45 cm⁻³ mol⁻¹. All studied glasses reveal high dispersion in the visible spectral region and high durability against water corrosion.

DSC studies showed that all of glasses crystallize on heating within the temperature region of 590-605°C and the surface nucleation mechanism prevails over the internal one. Crystallization temperature and glass transition temperature increase with increasing TiO₂ content, whereas the thermal stability of glasses decreases. The values of thermal expansion coefficient, obtained from dilatometric curves, change from 8,4 to 9,6 ppm °C⁻¹, without compositional dependence on TiO₂ content. Compounds formed by crystallization were Fe₂P₄O₁₂, Fe₃(P₂O₇)₂ and FePO₄.

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Correction method to the surface defective layer in low absorption spectroscopy

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We derive the so-called thin-film limit by a novel approach and present formulae for transmittance (T), reflectance (R) and absorptance (A) in highly versatile and accurate form. We draw attention to two remarkable consequences of the thin-film limit: (i) The optical properties A, R and T do not depend on the absorption coefficient (a), thickness (d) and refraction index (n) individually, but only on their product adn . (ii) The absorptance strongly depends on the index of refraction of the surrounding media. Next, we perform experimental verification on graphene [1]. We also discuss consequences for the optimization and optical simulations of thin-film solar cells. Finally, a new method is presented that allows direct evaluation of ultrathin surface defective layer absorptance. This presents a direct and elegant way avoiding complex evaluation of surface defective layer [2].

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Preparation and transport properties of layered semiconductors for thermoelectric applications

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Bi_2Se_3 , which adopts the tetradymite structure, is a component of n-type legs of thermoelectric (TE) couples used in solid state coolers or generators having the dimensionless figure of merit ZT less than or equal to 1 ($ZT = \sigma S^2 T / \kappa$, where σ is electrical conductivity, S is the Seebeck coefficient, κ is thermal conductivity, and T is thermodynamic temperature) in the range around room temperature. In last decade, number of papers has been published showing that some TE materials of tetradymite structure (p-type) form diluted magnetic semiconductors (DMS) if they are doped with some transition metals. Recently, it has been shown that these materials are bulk topological insulators (TI). Bi_2Se_3 is degenerate semiconductor due to a high concentration of native defects that produce large concentration of free carriers. Selenium vacancies are the dominant defects, and they produce a doping on the order 10^{19} cm^{-3} . Such a high concentration of free carriers affects the exploration and potential usage of this material as topological insulator. Further, n-type conductivity prevents potential carrier induced ferromagnetism in Bi_2Se_3 based DMS. In recent studies, the use of calcium was successfully demonstrated for tuning the free carrier concentration in Bi_2Se_3 . Doping with an electropositive element is rather uncommon within semiconductor chemistry; therefore, this topic is very interesting. We assumed that other alkali earths could induce similar effects in Bi_2Se_3 . With the aim to provide evidence of this assumption and to perform a detailed study on the doping of Bi_2Se_3 with alkaline earths, we examined the next element in the periodic table, strontium [1].

System $\text{Bi}_{2-x}\text{Sr}_x\text{Se}_3$ in single crystalline form was prepared using a controlled solidification and characterized with focus on examination of doping efficiency of strontium in Bi_2Se_3 . The doping efficiency of strontium was explained within a model of point defects. The prepared single crystals were characterized by the measurement of IR reflectivity in plasma resonance region and the results were compared with the results derived from transport measurements. Analysis of the transport and optical properties reveal strontium to be an acceptor in Bi_2Se_3 . A strong interaction of strontium with native defects in the host structure is demonstrated on varying the doping efficiency. Strontium is a notable doping element for tuning the electron concentration in Bi_2Se_3 , in all research areas given; it matches the structure and increases the mobility of free carriers in Bi_2Se_3 .

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Optical Interference in SOI wafer

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Silicon-on-insulator (SOI) refers to a semiconductor substrate technology in which traditional bulk silicon starting wafer is replaced by a substrate consisting of three layers: a thin, top layer of single crystalline silicon, middle layer of insulating silicon dioxide (called buried oxide or BOX), and a bulk silicon, which provides the mechanical support. SOI essentially adds a layer of insulation to the substrate under the top silicon in which the transistors are built. The basic SOI technology is provided by “direct wafer bonding”, mechanical back-grinding and polishing. SOI starting wafer offers a number of benefits for electronic devices. The main advantages include higher radiation tolerance, reduced latchup and cross-talk, lower leakage currents, and reduced complexity of isolation processes. Higher complexity of the layered SOI structure brings also new group of phenomena which have to be taken into account.

One of these challenges are the optical interference effects between the top silicon layer and the buried oxide. The total intensity of the reflected light is a sum of all waves reflected from both interfaces, i.e., from the top and bottom of the buried oxide, including multiple reflections back and forth in the top layer and the BOX. The spectral dependence of the normal reflectivity forms a typical Fabry-Perot interference pattern with nodes at specific wavelengths. We discuss the density of interferences and position of these nodes as a function of the device layer thickness and the BOX thickness. Understanding of the physical phenomena can be used for many applications; we will demonstrate three examples.

In the region where the interferences in the device layer are pronounced, i.e., between two neighboring nodes, we can estimate the device layer thickness from the position of the two neighboring minima. Methods of correction will be explained. We have demonstrated this measurement method on the tool built in CEITEC, Masaryk University.

In case the magnitude of the interference pattern needs to be reduced, optimization of the BOX thickness is proposed. Near the nodal positions, the interference in the device layer is significantly suppressed. Such behavior can be successfully utilized for optimization of laser marking, for example.

Lastly, the SOI structure can be used for precise determination of optical constants of silicon. Their knowledge is essential for many applications, but the available spectra of extinction coefficients suffer from a large uncertainty in the spectral region below about 3 eV. For a homogenous device layer the interference phenomena provide very high sensitivity to the optical constants of the device layer material. Optical functions can be extracted from measurements on special SOI structures with a very thin BOX. We report here on the preliminary results; optical constants in the NIR-VIS region will be published elsewhere.

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Cocrystals, their preparation techniques and application

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Cocrystals have been lately established as novel multicomponent solid forms with defined stoichiometry. By narrow definition, two or more neutral input components should be solid at ambient pressure and temperature, which distinguishes cocrystals from clathrates and solvates. Also, they can be distinguished from salts, as no proton transfer occurs between the host and guest compounds. Cocrystal's physicochemical properties differ from other types of solid forms, thus, they can offer a variety of advantageous solid-state properties. The most important domains where cocrystals are applied are improved energetic materials, nonlinear optics and pharmaceuticals.

Cocrystals are widely screened forms of explosives, cocrystalline materials can improve detonation velocity, explosive power, thermal stability or physical sensitivity.

In nonlinear optics (NLO), where materials specifically respond to certain radiation, compounds with otherwise favorable NLO properties can overcome problems such as non-desired centrosymmetric packing by cocrystallization.

For pharmaceutical compounds, especially active pharmaceutical ingredients (API), cocrystals are an attractive option in drug development, as they offer better dissolution profiles, higher stability or are less hygroscopic than pure API.

In the solid form screening strategy, the preparation techniques contribute to the successful discovery of the new form. There are many cocrystallization methods described, which can be divided in two basic groups: solvent-based (crystallization from solution, liquid-assisted grinding, slurring) and solvent-free techniques (co-melting, neat grinding). The most commonly used cocrystallization techniques are presented and compared on the example of trospium chloride's cocrystal screening.

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The combined technological methods for deposition of Si:H thin films and structures with in situ embedded nanoparticles

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The PECVD (Plasma Enhanced Chemical Vapour Deposition) is based on possibility to transport needed elements at a form of gases or vapours of convenient liquids into deposition chamber. But it is not so easy to transport some elements at room temperature by any form like that. For those elements it is necessary to use a common transport method from solid state to solid state - we can use quite standard techniques as it is Vacuum Evaporation /VE/ or Sputtering or Reactive Sputtering. We can deposit thin film multi-structures changing periodically both processes. When we apply a convenient temperature annealing, we can stimulate reaction between elements of thin films. For it we usually need high temperatures which in many cases change a quality of the thin films. It is a case of amorphous or microcrystalline form of hydrogenated silicon. There are reasons why we study processes as Plasma Treatment for formation of compounds, their structures and size of NPs on the surface of Si:H thin films.

Another possibility how to deposit NPs on the surface of Si:H thin films when the PECVD is interrupted is the Laser Ablation /LA/ or Reactive Laser Ablation technique /RLA/. A convenient condition for evaporation of targets /energy in pulse and focusing/ by laser, the selection of material of the target and reactive atmosphere in the case of RLA for the deposition of nanoparticles gives many possibilities how to influence the size and quality deposited nanoparticles.

For deposition of materials convenient for thermoelectric application the Reactive Deposition Epitaxy /RDE/ is applied in UHV chambers. Those structures are studied in non-hydrogenated form up to now. Our developed deposition methods allow the study of their quality in hydrogenated form.

By all the methods mentioned above it is possible to modify the quality of Si:H thin films and that is why we have developed combined deposition chambers for in situ deposition of all diode structures. We expect the embedded nanoparticles can increase PL and EL of Si:H thin films as well as make them convenient for photovoltaic or thermoelectric application.

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The methods applied for the characterisation of Si:H thin films with embedded nanoparticles

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For the characterisation of hydrogenated silicon thin films deposited by CVD (Chemical Vapour Deposition), PECVD (Plasma Enhanced CVD), HW (Hot Wires) and so on with different qualities there are already used standard methods. For measurement of electrical quality the most used configuration is co-planar with gap between two linear well conductive electrodes which there are used as ohmic contacts. On those samples prepared by this way there is measured the temperature dependence of electrical conductivity and evaluated the activation energy. Next important measurement on this sample there is measurement of absorption coefficient as dependence of photon energy by CPM (Constant Photocurrent Method). The level of absorption in the tail of conductive band is important for evaluation of level of defects in disordered structures. The CPM is used together with transmittance and reflectance measurements to get absolute values of the optical absorptance. PDS (Photo-thermal Deflection Spectroscopy) is also applied to measure low optical absorptance (down to 0.01%).

For the surface morphology we use SEM (Scanning Electron Microscope), especially for observation of nanoparticles, their size and surface configuration. Raman spectroscopy was applied to evaluate structural relation between amorphous and microcrystalline silicon as well as nanoparticles. Recombination centres are detected by the Photoluminescence spectroscopy excited by laser illumination.

The I-V (current-voltage) characteristics are as basic measurement on diode structures in sandwich configuration. We observe changes in I-V curves of diodes based on Si:H thin films with embedded different NPs deposited by different deposition techniques. Here the most important is to control their Electroluminescence via the applied Voltage and the Electrical Current through diode. First examples of realised infrared LED are presented.

Our work is performed with financial support by LH12236 (MSMT KONTAKT II, Czech Republic)

Modelling of 3D-structure of nanotextiles

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During the last decade many potential applications of unwoven nanotextiles have been proposed. These applications include but are not limited to protective layers of different kinds on the surface of other materials. Such layers can protect the underlying material from aggressive influence of the environment: humidity, dust, bacteria, molds, etc. Thus, it is very important to know the corresponding properties of the nanotextiles and how to control them. These properties can be studied both experimentally and theoretically. Each approach has its own advantages and disadvantages.

In order to model processes inside the nanotextile one has to know its structure. The combined geometrical shape of all nanofibers forms a scenery for subsequent numerical modelling of physical, chemical and biological phenomena taking place in the nanotextile. Consequently, the creation of 3D model of the nanotextile is the basis of any successful attempt of theoretical analysis of these processes.

In our work we discuss a method to reconstruct the structure of a nanotextile based on SEM photographs of its surface. Due to the lack of information about the distance of nanofibers from the observer we utilize the following approach. We construct a 3D model of the top layer of the nanotextile and then replicate it several times in order to obtain a 3D structure of the whole nanotextile. Such model can be possibly successfully used to model the diffusion in the direction perpendicular to the plane of the textile. However, phenomena which include extensive diffusion parallel to the surface (e.g. growth of molds) will probably require more advanced model, where different layers will intertwine.

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Crystal defects in silicon

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Single crystal silicon has played the fundamental role in electronic industry since the second half of the 20th century and still remains the most widely used material. Electronic devices and integrated circuits are fabricated on single-crystal silicon wafers which are produced from silicon crystals grown primarily by the Czochralski (CZ) technique. Various defects are formed in the growing crystal as well as in the wafers during their processing.

The lecture deals with the topic of crystal defects in the technology of manufacturing silicon single crystals and silicon wafers for the electronic industry. A basic overview of crystal defects found in semiconductor-grade silicon is provided and mechanisms of their formation are introduced. The impact of crystal defects on the manufacturing and performance of electronic devices is outlined and some of the methods of defect analyses are described. Finally, the most important methods for control of defect formation are summarized.

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Nanocrystalline Pr-doped Lu₃Al₅O₁₂ phosphor prepared by radiation method

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Lu₃Al₅O₁₂ (LuAG) based bulk single crystal scintillators have been intensively investigated during the last decade. Ce and Pr-doped ones became extensively tested in various applications due to their high density, fast response and high light yield. At the same time, these materials were also prepared in powder form by various methods.

Recently, the radiation method has been also used to prepare a nanocrystalline precursor for Ce-doped LuAG phosphor [1]. This method provides nanopowder that after proper calcination (>950 °C) consists of well separated grains with diameter of a few tens of nanometers, narrow size distribution and perfect garnet structure containing minimum defects and traps. Such characteristics then ensure high scintillation efficiency. Due to the presence of the Lu³⁺ site, LuAG can be doped by the whole variety of rare earth ions. Therefore, its emission properties can be tuned in a large accessible range determined by the emission transitions of dopants.

In this work, prepared LuAG nanopowders were doped with various Pr concentrations from 0.1 to 10 at.%. Samples were prepared by radiation method and UV light (medium-pressure mercury discharge, polychromatic radiation 180 - 580 nm) was used as radiation source. One additional sample was prepared using different source of UV light (low-pressure mercury discharge, 254 nm) to compare the solid phase composition and scintillation properties of the product formed under different conditions.

All samples were characterised by X-ray powder diffraction (XRPD) method to compare phase purity of the nanocrystalline powder. Real concentration of dopant in all samples was determined by X-ray fluorescence (XRF) measurements of all samples. To determine the effect of concentration quenching the concentration dependence of Pr³⁺ emission spectra and decay course 5d and 4f levels in the UV - visible part of the spectra was studied. Especially the decay kinetics data are essential to identify the concentration quenching. Photoluminescence measurements were complemented with radioluminescence spectra to investigate the scintillation efficiency of all samples. The results were compared with the earlier published characteristics of bulk Pr-doped LuAG single crystals prepared by other methods [2]. Furthermore, based on obtained results we determined the optimum concentration of Pr³⁺ dopant for application of the prepared material as X-ray phosphor.

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Structure and properties of GeO₂ modified lithium phosphate glasses

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GeO₂ containing glasses are promising materials for IR technologies, nonlinear optics and design of laser devices. Furthermore, the high ionic conductivity of GeO₂, makes them interesting candidates for solid electrolyte applications.

Lithium phosphate glasses doped by GeO₂ were prepared in two compositional series: 50Li₂O-(50-x)P₂O₅-xGeO₂ with x=0; 5; 10; 15 mol% GeO₂ (A series of glasses) and 40Li₂O-(60-y)P₂O₅-yGeO₂ in a concentration range of y=0-30 mol% GeO₂ (B series of glasses). Glasses were characterized by the measurements of density, molar volume, chemical durability and refractive index. The structure of glasses was investigated by ³¹P MAS NMR and Raman spectroscopy. Their thermal properties were studied by differential thermal analysis (DTA) and thermodilatometry (TD).

Structural studies of starting 50Li₂O-50P₂O₅ metaphosphate glass (A series) showed the presence of metaphosphate Q² units in the glass structure, whereas the structure of parent 40Li₂O-60P₂O₅ glass (B series) is formed both metaphosphate (Q²) and polyphosphate (Q³) tetrahedral units. The incorporation of germanate structural units was reflected by the presence of vibrational modes associated with P-O-Ge and Ge-O-Ge bonds in the middle-frequency part of the Raman spectra between 400 and 800 cm⁻¹. The replacement of tetrahedral PO₄ structural units by GeO_n units was associated with the depolymerisation of phosphate chains and gradual transformation from Q³ to Q¹ units.

The modification of Li₂O-P₂O₅ by the replacement of P₂O₅ by GeO₂ revealed also changes in the properties of the glasses. The gradual incorporation of germanate structural units into the structural network with increasing GeO₂ content results in a decrease of their molar volume and thermal coefficient, whereas their density, glass transition temperature, dilatometric softening temperature increase. The refractive index has been measured at room temperature at wavelengths 452.9, 532 and 637.3 nm. With the replacement of P₂O₅ by GeO₂, the values of refractive index increase. All glasses reveal low dispersion in the visible spectral region.

DTA and XRD studies showed that most of glasses crystallized on heating within the range 410-570°C. The highest thermal stability was observed for the glasses containing 0 and 5 mol% GeO₂ in the compositional series B. Compounds formed by crystallization were LiPO₃ and GeP₂O₇.

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Thermal analysis of Er-doped potassium ytterbium lanthanum phosphate glass

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Recently, there has been growing interest in search and preparation of new glass materials with prospective properties for applications as scintillators and solid state lasers. This requirement was fulfilled by alkali rare earth phosphate glasses e.g. $\text{Ce}^{3+}:\text{NaGd}(\text{PO}_3)_4$, which is due to their low cost and high intensity of radioluminescence potential materials for detection of γ -rays in medical and technical applications [1].

This contribution deals with the study of preparation and thermal properties of Er-doped potassium ytterbium lanthanum phosphate glass. The aim of this work is to analyze the influence of P_2O_5 excess in the starting charge on the glass transition temperature T_G and crystallization effects occurring in the studied glass samples when thermally treated.

Alkali rare earth phosphate glasses were prepared by rapid quenching of molten mixture of starting K_2CO_3 , YbPO_4 , LaPO_4 , ErPO_4 , and P_2O_5 heated at 1240 °C. Five glass ingots with different ratio of meta- and ortho- phases, depending on the excess of P_2O_5 in the starting charge, were prepared. However, the molar fraction of cations $x(\text{K}^+) = 0.7$, $x(\text{Yb}^{3+}) = 0.135$, $x(\text{La}^{3+}) = 0.16$, and $x(\text{Er}^{3+}) = 0.005$ remained constant. Prepared samples were analyzed by non-isothermal DSC (Setaram Setsys Evolution 16) at heating rates of 2, 5, 10, 20, and 30 K/min from room temperature to 900 °C on powder samples of 60 ± 1 mg in alumina crucible under nitrogen atmosphere flow.

The values of glass transition temperature T_G and crystallization effects were obtained from DSC curves [2]. The activation energy of glass transition E_t was calculated by Moynihan and Kissinger relations [3] and the activation energy of crystallization E_a by Kissinger, Augis-Bennett, and Matusita-Sakka relations [4]. Stereomicroscope Olympus SZX 12 with program Quick Photo Industrial was used to study samples after the thermal treatment.

Obtained values of glass transition temperature T_G and the effect of crystallization depended on the ratio of meta- and ortho- phase and were shifted to higher temperature with the increasing excess of P_2O_5 . Whereas the activation energy of glass transition (E_t) and the activation energy of crystallization (E_a) decreased with the increasing excess of P_2O_5 .

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