

# DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

Book of Abstracts of the 28th Joint Seminar  
3 – 7 September 2018



*Z. Kožíšek, R. Král, P. Zemenová*

**Editors**





***CZECHOSLOVAK ASSOCIATION FOR CRYSTAL GROWTH***

 **Fyzikální ústav**  
Akademie věd ČR, v. v. i.



# **Development of Materials Science in Research and Education**

*Book of Abstracts of the 28<sup>th</sup> Joint Seminar*

*Z. Kožíšek, R. Král, P. Zemenová*  
Editors



Pavlov  
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*3 – 7 September, 2018*

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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 of the Czech Academy of Sciences and  
the Slovak Society for Industrial Chemistry**

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## Topics

- 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

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# PREFACE

The 28<sup>th</sup> Joint Seminar “Development of Materials Science in Research and Education” (DMSRE28) will be held on 3 – 7 September 2018, 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 of the Czech Academy of Sciences, 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 program will include 5 keynote lectures (35 minutes): Hsiung Chou (Department of Applied Physics, National Pingtung University, Taiwan): *Unconventional Superconductor-Searching for Triplet and Multiband Superconductors*, Hua-Shu Hsu (Department of Applied Physics, National Pingtung University, Taiwan): *Magnetic field controlled absorption effect and its application*, Zdeněk Kožíšek (Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic): *Modelling of polymorphic crystals formation in solution*, Štěpán Potocký (Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic): *Diamond films and nanoparticles for life science*, and Radek Pjatkan (NUVIA a.s., Kralupy nad Vltavou, Czech Republic): *Review of plastic scintillators and development of new materials*.

All other contributions will be presented as short lecture talks (25 minutes). The official languages of the seminar are English, Czech, and Slovak.

This booklet contains the abstracts of all contributions, which reached us before 16 August 2018. The authors are responsible for the technical and language quality of the contributions. The conference will run from Monday afternoon, 3 September 2018, till Friday noon, 7 September 2018 in the hotel IRIS Pavlov, Czech Republic.

Dear colleagues, we welcome you to the DMSRE28 Joint Seminar and we hope you will enjoy your stay in Pavlov.

*Zdeněk Kožíšek, Robert Král, Petra Zemenová (Editors)*



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# PROGRAM

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## Monday, 3 September 2018

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- 13:00 – 14:20 Registration  
*Location: Hotel Lounge*
- 14:30 – 14:40 Conference opening  
*Location: Lecture Hall*
- 
- 14:40 – 15:40 **Monday Session I**  
*Location: Lecture Hall*  
*(chairperson: Zdeněk Kožíšek)*
- 14:40 – 15:15: Hua Shu Hsu:  
*Magnetic field controlled absorption effect and its application*
- 15:15 – 15:40: Maksym Buryi:  
*Charge trapping phenomena in Cs<sub>2</sub>HfCl<sub>6</sub> single crystals: electron paramagnetic resonance and thermally stimulated luminescence study*
- 15:40 – 16:10 Coffee break
- 
- 16:10 – 17:50 **Monday Session II**  
*Location: Lecture Hall*  
*(chairperson: Hua Shu Hsu)*
- 16:10 – 16:35: Zdeněk Remeš:  
*Enhanced UV photoluminescence in hydrogenated ZnO nanocolumns*
- 16:35 – 17:00: Shih-Jye Sun:  
*Theoretical investigation of superconductivity in interface of high T<sub>c</sub> superconductor and ferromagnet*
- 17:00 – 17:25: Zdeněk Potůček:  
*Thawing of ice in the frozen water-saturated quartz sand probed by Raman spectroscopy*

- 17:25 – 17:50: Y. Y. Chang:  
*The electrical and optical properties of nanocrystalline ZnO thin films*
- 18:00 – 19:00 Dinner

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## Tuesday, 4 September 2018

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- 09:00 – 10:00 **Tuesday Session I**  
*Location: Lecture Hall*  
*(chairperson: Zdeněk Remeš)*
- 09:00 – 09:35: Hsiung Chou:  
*Unconventional Superconductor—Searching for Triplet and Multi-band Superconductors*
- 09:35 – 10:00: Miroslav Menšík:  
*Relation between power-law decay of polarons and their transient diffusion coefficient in conducting polymers*
- 10:00 – 10:30 Coffee break
- 10:30 – 11:45 **Tuesday Session II**  
*Location: Lecture Hall*  
*(chairperson: Marian Koman)*
- 10:30 – 10:55: Kateřina Rubešová:  
*Heavily doped Ce:YAG thin films prepared by a non-hydrolytic sol-gel method*
- 10:55 – 11:20: Tomáš Thoř:  
*Lanthanide-doped Lu<sub>2</sub>O<sub>3</sub> phosphors*
- 11:20 – 11:45: Jan Pejchal:  
*Growth of selected single crystals by micro-pulling-down method and their scintillation properties*
- 12:00 – 13:00 Lunch

14:00	–	15:40	<b>Tuesday Session III</b>
			<i>Location: Lecture Hall</i>
			<i>(chairperson: Maroš Martinkovič)</i>
14:00	–	14:25:	Marian Koman: <i>The new heteroligand complexes of Iron(III/II)</i>
14:25	–	14:50:	Juraj Černák: <i>Single crystal X-ray structure analysis as a tool of inorganic chemists</i>
14:50	–	15:15:	Vladimír Jorík: <i>The pitfalls of qualitative phase diffraction analysis of polycrystalline samples</i>
15:15	–	15:40:	Simona Matejová: <i>The quality of the diffraction data and its influence on the crystal structure determination</i>
15:40	–	16:10	Coffee break
			<hr/>
16:10	–	17:50	<b>Tuesday Session IV</b>
			<i>Location: Lecture Hall</i>
			<i>(chairperson: Vladimír Jorík)</i>
16:10	–	16:35:	Jozef Dobrovodský: <i>Development of the Rutherford Backscattering / Channeling (RBS/C) system at the STU Ion Beam Laboratory</i>
16:35	–	17:00:	Karel Král: <i>Charge carrier mobility in polymers. Dependence on charge carrier density and lattice temperature</i>
17:00	–	17:25:	Ľubor Dlháň: <i>Magnetic iron oxides in the human brain</i>
17:25	–	17:50:	Dušan Vaňa: <i>Design of the Time of Flight ERDA system for 6 MV tandem ion accelerator</i>
18:00	–	19:00	Dinner

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## Wednesday, 5 September 2018

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09:00	–	10:00	<b>Wednesday Session I</b>
			<i>Location: Lecture Hall</i> <i>(chairperson: Kateřina Rubešová)</i>
09:00	–	09:35	Zdeněk Kožíšek: <i>Modelling of polymorphic crystals formation in solution</i>
09:35	–	10:00	Ladislav Koudelka: <i>Structure and properties of barium phosphate and borophosphate glasses modified with molybdenum oxide</i>
10:00	–	10:30	Coffee break
10:30	–	11:45	<b>Wednesday Session II</b>
			<i>Location: Lecture Hall</i> <i>(chairperson: Pavlína Ruleová)</i>
10:30	–	10:55	Petr Mošner: <i>Mixed glass former effect in <math>\text{Na}_2\text{O}-\text{P}_2\text{O}_5-\text{TeO}_2</math> glasses</i>
10:55	–	11:20	Viera Zatkalíková: <i>The effect of temperature on the resistance of electropolished <math>\text{Al}_2\text{O}_3</math> stainless steel to pitting</i>
11:20	–	11:45	Lenka Markovičová: <i>Polymer Composites as a Construction Material</i>
12:00	–	13:00	Lunch
14:00	–	17:30	Joint meeting - panel discussions
17:45	–	18:00	Conference Photo
18:00	–	19:00	Dinner
19:45	–	23:00	Conference banquet

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## Thursday, 6 September 2018

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09:00 – 10:00 **Thursday Session I**

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*Location: Lecture Hall  
(chairperson: Jan Pejchal)*

- 09:00 – 09:35: Radek Pjatkan:  
*Review of plastic scintillators and development of new materials*
- 09:35 – 10:00: Robert Král:  
*Cesium hafnium chloride as a new scintillation material, its preparation, growth, and characterization*
- 10:00 – 10:30 Coffee break

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10:30 – 11:45 **Thursday Session II**

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*Location: Lecture Hall  
(chairperson: Petr Mošner)*

- 10:30 – 10:55: Pavlína Ruleová:  
*Examination of effect Ta on transport properties  $Bi_2Se_3$*
- 10:55 – 11:20: Patrik Čermák:  
*Investigation of stability of Tl-doped SnS*
- 11:20 – 11:45: Kateřina Šraitrová:  
*Effect of Tl Doping on Thermoelectric Properties of SnSe Single Crystals*
- 12:00 – 13:00 Lunch

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14:00 – 15:40 **Thursday Session III**

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*Location: Lecture Hall  
(chairperson: Juraj Černák)*

- 14:00 – 14:25: Mária Behúlová:  
*Induction brazing of thin-walled pipes from AISI 304 steel using copper-based solder*
- 14:25 – 14:50: Štefan Vrtiel:  
*Analysis of laser beam welding of the S650MC high strength steel using numerical simulation*

- 14:50 – 15:15: Vladimír Kuchtanin:  
*Preparation and characterization Ni(II) complexes with O,N,O- and O,N,S-Schiff base ligands*
- 15:15 – 15:40: Mate Nagy:  
*Microstructure and mechanical properties of dissimilar Al-Ti joints prepared by GTAW welding-brazing*
- 15:40 – 16:10 Coffee break
- 
- 16:10 – 17:50 **Thursday Session IV**  
*Location: Lecture Hall*  
*(chairperson: Marika Behúlová)*
- 
- 16:10 – 16:35: Martin Necpal:  
*Simulation cold metal forming draw process using different Finite Element Model application software*
- 16:35 – 17:00: Maroš Martinkovič:  
*Comparison of grain boundary orientation to deformation conversion models*
- 17:00 – 17:25: Stanislav Minárik:  
*Influence of Linear Deformation on the Geometry of Grains in Grained Structure*
- 17:25 – 17:50: Miroslava Puchoňová:  
*Structural variability of bis(2-hydroxymethylbenzimidazol) bis(salicylato)copper(II) complexes*
- 18:00 – 19:00 Dinner

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## Friday, 7 September 2018

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- 09:00 – 10:00 **Friday Session I**  
*Location: Lecture Hall*  
*(chairperson: Zdeněk Potůček)*
- 
- 09:00 – 09:35: Štěpán Potocký:  
*Diamond films and nanoparticles for life science*
- 09:35 – 10:00: Vít Jakeš:  
*Preparation of Er-doped  $\text{Yb}_3(\text{Al,Fe})_5\text{O}_{12}$  garnets*
- 10:00 – 10:30 Coffee break

10:30	–	11:50	<b>Friday Session II</b>
			<i>Location: Lecture Hall</i>
			<i>(chairperson: Robert Král)</i>
10:30	–	10:55:	Václav Doležal: <i>Doped hexagonal aluminates for optical applications</i>
10:55	–	11:20:	Dana Mikolášová: <i>Lithium niobate doped by d- and f-ions</i>
11:20	–	11:35:	Jiří Stuchlík: <i>Technological possibilities and vacuum systems for deposition of Si:H thin films with embedded nanoparticles</i>
11:35	–	11:50:	The Ha Stuchlíková: <i>Characterization of a-Si:H thin films with and without embedded nanoparticles</i>
11:50	–	12:00	Conference Closing <i>Location: Lecture Hall</i>
12:00	–	13:00	Lunch





# **ABSTRACTS**



## **Induction brazing of thin-walled pipes from AISI 304 steel using copper-based solder**

Mária Behúlová, Štefan Vrtiel, and Máté Nagy

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

Pipes made of austenitic stainless steels are widely used in automotive industry. They are connected together or to other components by different joining technologies. The quality of produced joints is often critically important for passenger safety assurance. The joint lifetime is significantly influenced by their corrosion behavior.

The paper deals with induction brazing of thin-walled pipes from austenitic stainless steel using high corrosion-resistant Cu-Ni solder. To design appropriate parameters of induction heating, the effective method of numerical simulation of induction heating using the software ANSYS was applied. Simulation model for evaluation of electro-magnetic and temperature fields in the process of induction brazing of fuel pipes from AISI 304 steel using copper-based solder was developed and verified by experimental temperature measurement during pipe induction heating. Based on performed numerical experiments and results of numerical simulations, appropriate parameters and operating diagram for the induction brazing of thin-walled pipes of the AISI 304 steel using copper-based solder were suggested.

*The research has been supported by the Scientific Grant Agency of the Slovak Republic within the project VEGA No. 1/1010/16, KEGA No. 029STU-4/2018 and project ITMS 26220120048 under the Research & Development Operational Programme funded by the ERDF.*

## Charge trapping phenomena in Cs<sub>2</sub>HfCl<sub>6</sub> single crystals: electron paramagnetic resonance and thermally stimulated luminescence study

Maksym Buryi, Robert Král, Vladimir Babin, Valentyn Laguta, and Martin Nikl

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Cs<sub>2</sub>HfCl<sub>6</sub> (CHC) single crystals (SC) have become attractive for scintillator applications presently due to their good scintillation characteristics. For example, the Cs<sub>2</sub>HfCl<sub>6</sub> powder has been already presented as an efficient X-ray phosphor with a broad blue emission band [1]. In particular, recent experimental studies in the undoped SC samples evidence high intrinsic scintillation efficiency, resulting in the high light yield within 37000-54000 photons/MeV [2,3].

Self-trapping of charge carriers in the CHC single crystals was forecasted theoretically [4]. However, this still needs experimental confirmation as it is commonly known that such a property may have serious impact on the luminescence mechanism. Therefore, the combination of electron paramagnetic resonance (EPR) and thermally stimulated luminescence (TSL) methods is extremely important to study this phenomenon.

EPR experimental data confirm the creation of the so-called V<sub>k</sub> center in the CHC material, a hole localized over two neighboring chlorine anions forming the Cl<sub>2</sub><sup>-</sup> molecular ion. It is stable below the 55-60 K. It does not withstand higher temperatures so after thermal disintegration another charge trapping state at 80 K appears being stable up to about 200 K. This center appeared to be a V<sub>k</sub> center as well, where one of the chlorine anions is regular while the second one creating the new molecular ion is an interstitial Cl<sup>-</sup> by analogy with the H-type center in alkali halides. TSL data show correlation with the EPR, the glow curves contain peaks having maxima at approximately 70 K and 190 K. The hole traps kinetic parameters have been determined.

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## Investigation of stability of Tl-doped SnS

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SnS is an eco-friendly analog of SnSe [1, 2], a very promising thermoelectric material of recent years. However, a stable and effective doping of this compound is still questionable [3]. According to our observation, the main obstacles here are very low solubility of dopants and destabilization of SnS structure due to foreign species (important issue for photovoltaic applications). Regarding a reasonable 60 % doping efficiency of Tl in SnSe [4], we explored Tl-doping of SnS into cation sublattice. Hot-pressed polycrystalline samples were prepared along with single-crystalline samples by various growing technics. Samples were examined for impurity phases by X-ray diffraction, X-ray fluorescence and Energy-dispersive X-ray for chemical analysis. Thermal stability via Differential scanning calorimetry and thermogravimetry was studied. Transport measurements of Seebeck and Hall coefficient, electrical and thermal conductivity were carried out in temperature range 3-775 K, parameter of thermoelectric efficiency ZT was calculated from obtained data. The experiments suggest very low solubility of Tl (i.e. less than 0.1 %). Higher concentrations of Tl or higher temperatures induce decomposition towards Sn<sub>2</sub>S<sub>3</sub> phase.

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## Single crystal X-ray structure analysis as a tool of inorganic chemists

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Since its introduction, the method of single crystal X-ray structure analysis is an important tool in the hands of the inorganic (and not only inorganic) chemists as it is the only direct method yielding information on the spatial arrangement of atoms and molecules in the solid state. Although at early stages of the use of this method the crystal structures were elucidated by lengthy evaluation of photographic data, the results thus obtained helped to clarify the nature of some substances, e.g. [1,2]. The introduction of single crystal diffractometers and computing facilities in the 60s of the 20<sup>th</sup> century contributed to the gradual broad expansion and application of this method. At present, single crystal X-ray structure analysis is considered as a standard method for characterization of crystalline solids; as a consequence, we are witnesses of an explosive increase of number of published crystal structures. For example, currently the Cambridge Structural Database contains more than 900,000 crystal structures, and more than 50,000 entries are added each year [3]. Despite the broad use of this method, its application requires adequate expertise; it should be noted that even cases of abuse of this method have been reported [4]. Within the talk will be given examples of using the method of single crystal X-ray structure analysis in solving problems of inorganic chemistry, the correlation of its results with the results of other methods, and, in addition, some problems associated with its use will be discussed.

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## The electrical and optical properties of nanocrystalline ZnO thin films

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DC reactive magnetron sputtering of Zn metal target in the gas mixture of argon and oxygen plasma has been applied to deposit nominally undoped nanocrystalline ZnO thin films [1-2]. The changes of electrical conductivity, free carrier concentration and localized defect density have been observed in ZnO thin films after hydrogen plasma treatment. To clarify these changes, the mobility and carrier concentration were measured by the temperature dependent electrical resistivity and Hall effect using the van der Pauw method. We show how the plasma treatment is related to the electrical properties and optical absorption, photoluminescence and Raman spectra.

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## Unconventional Superconductor—Searching for Triplet and Multiband Superconductors

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Conventional superconductor consisted of singlet pairs with reverse spins in a single band. When singlet pair is placed in a strong magnetic field or in contact with a strong magnetic material, the single pair amplitude will be suppressed due to de-pairing effect. When the singlet superconductor is made in contact with a strong ferromagnet, the strong magnetic split coupling at the interface may split the energy band of the singlet superconductor and a triplet superconducting pairs could emerge. The triplet pairing state is expected to be enhanced under an external magnetic field and to penetrate deep into ferromagnet conducting as a non-dissipation spin polarized current. This phenomena was realized by Keizer in 2006 in a low- $T_C$ -superconductor/ferromagnet heterostructure system where the triplet pairs was able to transport in the ferromagnet for a long distance of few hundred nanometers. However no further research break through has been discovered since the last experiment in 2010. In the other hand, the multiband superconductor was found in MgB2 system, where two hole bands were opened as superconducting gaps. With two different superconducting gaps, MgB2 exhibits an exotic behavior when it is in the mixing states. Instead of a simple repulsion between magnetic fluxes in a conventional type II superconductor, the magnetic fluxes appears attractive to one another when they are separated far apart and repulsive when they are closed by. Exotic development in these unconventional superconductor will be discuss in this talk.



## Magnetic iron oxides in the human brain

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Samples extracted from the human brain (from the region *Globus Palidus*) have been lyophilized and subjected to investigation by magnetometry [1-4]. A sensitive SQUID apparatus has been exploited for measurements (MPMS-XL7, Quantum Design).

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

The magnetic responses depend from sample to sample and they are essentially unique for each individual. They depend upon the content of magnetocarriers such as magnetic oxides:  $\gamma$ - $\text{Fe}_2\text{O}_3$  (maghemite) and  $\text{Fe}_3\text{O}_4$  (magnetite).

Some samples exhibit magnetic hysteresis not only at low temperature ( $T = 2, 5, 10,$  and  $20$  K) but also at elevated temperature ( $T = 50, 100, 200,$  and  $300$  K).

The hysteresis loops adopt a complex shape owing to presence of a dominating diamagnetic portion of the organic tissue and a minor response of the ferromagnetic deposits.

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## Development of the Rutherford Backscattering / Channeling (RBS/C) system at the STU Ion Beam Laboratory

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Rutherford backscattering spectrometry under channeling mode (RBS/C) is a powerful tool for characterization of defect densities and structures in the near surface region of monocrystalline thin layers. It has been applied to defect analysis for more than four decades to determine the damage profile and crystalline quality in monocrystalline thin films. RBS is based on the well-known channeling effect [1], when the ion beam is aligned within a crystallographic axis or a planar symmetry direction, a significant fraction of the incident ions have trajectories guided between the atomic rows called the “channels”. Aligning a beam of high energy positively charged ions along a low index crystal axis results in a significant reduction of the backscattered yield which become very sensitive to imperfections of the lattice and in particular to atoms shifted from their lattice positions to interstitial sites blocking the channels, space between the axial rows of atoms in the lattice. However this technique requires high-energy ion accelerators which are available in quite a limited number of the world research centers.

To find the channeling directions in practice means to take over hundred individual RBS measurements at different combinations of angles in tilt and azimuth directions. This process is highly time-consuming since a sample energy spectrum is taken for each point in angle space. Usually “gross” channeling spectrum serves for alignment of the crystal sample after which follows the “fine” channeling spectrum measurement over the selected crystal axis.

To make this process user-friendly and faster, the software in MATLAB including links with the accelerator and process devices were developed to support the automation of RBS/C measurements on 6 MV tandem ion accelerator system [2] and sample angular orientation. Contribution describes the developed code and presents the examples of measured channeling spectra.

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## Doped hexagonal aluminates for optical applications

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Due to their physical properties and high chemical stability up to high temperatures, aluminates are widely used for optical applications. The aluminates can be divided into several groups according to their crystal structure, such as garnets, spinels, perovskites and hexagonal aluminates. This work is focused on the preparation and doping of  $\text{LaMgAl}_{11}\text{O}_{19}$  belonging to the group of hexagonal aluminates.

In the first step, a highly reactive precursor was prepared using polyesterification and chelation sol-gel methods, from which the resulting aluminate was synthesized in the bulk form. The bulk samples were annealed under various conditions which resulted, in some cases, in the formation of a single-phase material. Bulk samples in a given stoichiometry of  $\text{La}_{1-x}\text{Ce}_x\text{MgAl}_{11}\text{O}_{19}$  were prepared using the most appropriate method.

In the second stage, the material was prepared using spin-coating in the form of thin films. Stable solutions were prepared using polymers soluble in water - polyvinylpyrrolidone and auxiliary chelation reagents acetylacetone and acetic acid.

The phase evolution in the stages of precursors and final samples was studied by thermal analysis (TG/DTA) and X-Ray diffraction. The microstructure of prepared precursors and crystalline samples was characterized by scanning and transmission electron microscopy. The surface and microstructure of thin films were observed by optical microscopy. The photoluminescence properties of Ce ions in hexagonal aluminate were studied by photoluminescence spectroscopy in the UV-VIS range.

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## Magnetic field controlled absorption effect and its application

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For the purpose of optoelectronic applications such as photo-detector, the basic principle is to absorb photon energy to delocalize electrons in the materials and this electrons flow can produce an electric current that can be used. According to the present disclosure, it has been discovered that magnetic fields may be used to modify the absorption characteristics of semiconductor materials. This phenomena is known as “magneto-absorption (MA) effect”. However, the MA effect of magnetic material/semiconductor hybrid structures remains less explored. In our previous study, a sizable MA effect was observed in Co/ZnO nanowires (NWs). Our magnetic circular dichroism (MCD) results have showed that this MA behavior is attributed to the the spin-polarized band in the ZnO NWs, which is induced by Co/ZnO interfacial hybridization [1]. The sizeable MA effect is negative and gradually saturated in the UV region. In this study, a transition from negative MA to positive MA have been have been achieved by additional Au coating, via engineering the density and nature of the energy states at the Fermi level. Our delicate design of the hybrid structure sheds new light on effective manipulation of magneoborption between magnetic impurities near the surface on oxide nanostructures for future spintronic applications.

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## Preparation of Er-doped $\text{Yb}_3(\text{Al,Fe})_5\text{O}_{12}$ garnets

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Iron garnets belong to a large family of mixed oxide ceramics with a cubic crystal structure and a general formula of  $\text{A}_3^{+III}\text{Fe}_3^{+II}\text{Fe}_2^{+III}\text{O}_{12}$ , where A = Y, Bi or a rare earth metal. Yttrium-iron garnets ( $\text{Y}_3\text{Fe}_5\text{O}_{12}$  or YIG) were discovered in 1957, since which time iron garnets have been widely studied for their magnetic or electrical properties (ferrimagnetism, high electrical resistivity and thermal conductivity, etc.). The substitution of other metals at the Fe site in the YIG structure leads to a change in the magnetic and electrical properties of the material. While  $\text{Y}_3\text{Fe}_5\text{O}_{12}$  remains the most extensively studied iron garnet, with substitutions being performed at both yttrium and iron sites, other members of this group (e.g.  $\text{Yb}_3\text{Fe}_5\text{O}_{12}$ ,  $\text{Ho}_3\text{Fe}_5\text{O}_{12}$  or  $\text{Tb}_3\text{Fe}_5\text{O}_{12}$ ) were rather neglected and most attention was paid to their magnetic properties.

In order to extend their applicability in photonics, garnets can be doped with optically active cations. Erbium cations show photoluminescence at around 1530 nm which enables their use in the third telecommunication window.

In this work, we focused on mixed YbAG/YbIG garnet, where aluminium and iron occupy the small cation sites (tetrahedral or octahedral) in a progressive substitution Al/Fe. Bulk samples of Er-doped ytterbium-aluminium garnet with a gradual substitution of aluminium with iron ( $\text{Yb}_{2.94}\text{Er}_{0.06}\text{Al}_{5-x}\text{Fe}_x\text{O}_{12}$ ;  $x = 0-5$ ) were prepared by a sol-gel method based on Pechini process with citric acid and ethyleneglycol as polyesterification agents. Subsequent annealing at 1100 °C in oxygen atmosphere was necessary to stabilize  $\text{Fe}^{III}$  in the phase equilibrium. Photoluminescence and magnetic properties of such samples were measured.

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## The pitfalls of qualitative phase diffraction analysis of polycrystalline samples

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A suitable technique for characterizing the crystalline solid phase is X-ray diffraction analysis. The most common method is a qualitative phase diffraction analysis that provides elemental chemical information on the substance. The success of qualitative phase analysis depends largely on the nature of the analyzed sample, the diffractometer experimental arrangement, and carefully selected experimental conditions.

Essential parts of the diffractometer are **X-ray lamp** (source of characteristic x-ray radiation given by the anode material), **incident-beam optics** (condition the X-ray beam before it hits the sample), **the goniometer** (holds and moves the sample, optics, detector, and/or tube), **receiving-side optics** (condition the X-ray beam after it has encountered the sample), **detector** (count the number of X Rays scattered by the sample)

Instrumental aberrations (X-rays have several characteristic wavelengths, "white" radiation and is divergent):

- spectral contamination of the diffraction pattern:  $K \alpha_1$  and  $K \alpha_2$ ,  $K \beta$  or  $W L \alpha_1$  and fluorescence radiation (monochromator, beta filter, energy sensitive detector)
- varying irradiated area of the sample causes a problem if the sample is non-homogeneous
- sample displacement error (the sample surface does not lie on the focusing circle) causes the displacement of the diffraction lines
- sample transparency error (X-rays penetrate deeper below the sample surface) produces peak position errors and peak asymmetry
- flat specimen error (entire surface of specimen cannot lie on the focusing circle) creates asymmetric broadening toward low  $2 \Theta$  angles
- axial divergence (due to divergence of the X-ray beam in plane with the sample) creates asymmetric broadening of the peak toward low  $2 \Theta$  angles and peak shift

Sample preparation (ideal and non-ideal sample):

- ideal powder sample should be prepared with smooth flat surface, densely packed, 'infinitely' thick and homogeneous
- it should have many grains/crystallites in random orientations with size less than  $10 \mu$  - non-ideal sample does not contain sufficient amount of grains/crystallites, poor particle statistics cause random error in the observed diffraction peak intensities
- preferred orientation (grains/crystallites are not randomly oriented) creates a systematic error in the observed diffraction peak intensities

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## The new heteroligand complexes of Iron(III/II)

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This contribution present complexes of Fe(III) with two anionic ligands, anion of pyridine-2,6-dicarboxylic acid (H<sub>2</sub>dipic) and thiocyanate anion (NCS<sup>-</sup>). Anion of pyridine-2,6-dicarboxylic (dipicolinic) acid has attracted interest as potential bidentate, tridentate and/or bridging ligand with variety of coordination modes transition metal centres and abundant structural motifs [1]. The dipicolinate metal complexes are also used in environmentally friendly catalysis and crystal engineering. Anion NCS<sup>-</sup> as ligand may be bonded in complexes of eleven possible manners [2]. The new type of ionic complexes with formula (cat)<sub>2</sub>[Fe<sup>III</sup>(dipic)(NCS)<sub>3</sub>]<sup>-</sup> - **A** and (cat)[Fe<sup>III</sup>(dipic)(H<sub>2</sub>O)(NCS)<sub>2</sub>]<sup>-</sup> - **B** where dipic<sup>2-</sup> = pyridine-2,6-dicarboxylate anion, cat<sup>+</sup> = organic cation (protonated pyridine-like cations as quinolinium, 3-methylisoquinolinium, 2-methylpyridinium or half of 4,4-bipyridinium).

In group **A** the central atom in complex [Fe<sup>III</sup>(dipic)(NCS)<sub>3</sub>]<sup>2-</sup> anion is six coordinated by one nitrogen atom of pyridine ring, two oxygen atoms of carboxylate group of dipicolinate anion and three nitrogen atoms of isothiocyanate groups with chromophore FeN<sub>4</sub>O<sub>2</sub>. Compound **B** contain complex [Fe<sup>III</sup>(dipic)(H<sub>2</sub>O)(NCS)<sub>2</sub>]<sup>-</sup> anion. The central Fe(III) atom in complex anion is coordinated by one nitrogen atom of pyridine ring, two oxygen atoms of carboxylate group of dipicolinate anion, two nitrogen atoms if NCS<sup>-</sup> groups and by one oxygen atom of coordinated water molecule with chromophore FeN<sub>3</sub>O<sub>3</sub>. The new Fe(II) complex [Fe(NCS)<sub>2</sub>(CH<sub>3</sub>OH)<sub>2</sub>(bpta)<sub>2</sub>] (bpta = 3,5-bis(3-pyridyl)-1,2,4-thiadiazole) has been prepared by refluxing Fe(NCS)<sub>3</sub> or Fe(NCS)<sub>2</sub> with thionicotinamide in methanol solution. It is supposed that the bpta ligand is generated in situ by oxidative dimerization of thionicotinamide [3].

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## Structure and properties of barium phosphate and borophosphate glasses modified with molybdenum oxide

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Doping phosphate glasses by heavy metal oxides like MoO<sub>3</sub> and WO<sub>3</sub> is interesting due to their semiconducting properties ascribed to the presence of transition metal ions in multivalent states. Borophosphate glasses belong among important classes of glassy materials because they offer better thermal stability and chemical durability than phosphate glasses. In this contribution, phosphate glasses in the ternary system BaO-MoO<sub>3</sub>-P<sub>2</sub>O<sub>5</sub> and the borophosphate glasses of the system BaO-P<sub>2</sub>O<sub>5</sub>-B<sub>2</sub>O<sub>3</sub>-MoO<sub>3</sub> were studied. Phosphate glasses were studied in four different compositional series, while borophosphate glasses were studied in two compositional series. The determined glass-forming region in the ternary system is very large and covers the concentration range from pure P<sub>2</sub>O<sub>5</sub> up to the glass compositions with only 20 mol% P<sub>2</sub>O<sub>5</sub> and 60 mol% MoO<sub>3</sub>. Basic physical properties and thermal behavior of the prepared phosphate and borophosphate glasses were determined. For structural studies <sup>31</sup>P and <sup>11</sup>B MAS NMR spectroscopies were applied as well as Raman spectroscopy. Basic structural units in phosphate and borophosphate glasses were identified in several compositional series. By the deconvolution of NMR spectra, compositional dependences of basic phosphate and borate units present in the glass network were obtained.

<sup>31</sup>P MAS NMR spectra showed on the depolymerization of phosphate chains with increasing MoO<sub>3</sub> content due to the formation of Mo-O-P bonds between octahedral MoO<sub>6</sub> structural units and tetrahedral PO<sub>4</sub> units. <sup>11</sup>B MAS NMR spectroscopy was able to supply information on the boron coordination in the studied borophosphate glasses because these spectra possess an ability to discriminate between tetrahedral BO<sub>4</sub> and trigonal BO<sub>3</sub> coordination.

Crystallization of phosphate glasses was studied as well and crystallized samples were studied by X-ray diffraction analysis and Raman spectroscopy. The only ternary compound identified in the ternary system was Ba(MoO<sub>2</sub>)<sub>2</sub>(PO<sub>4</sub>)<sub>2</sub>. The compound belongs to monoclinic system and its lattice parameters were determined. Raman spectra and <sup>31</sup>P MAS NMR of crystalline and glassy samples were compared and discussed.

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## Modelling of polymorphic crystals formation in solution

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Modelling of the polymorph crystals nucleation and growth in solution is complicated due to the phase transition induced by the supersaturation decrease. In molecular simulations, it is complicated to capture decrease in supersaturation because of too short timescale.

We developed the model of the formation of polymorphic crystals in solution based on the standard kinetic nucleation model. Our model was applied to crystallization of  $\alpha$  and  $\beta$  forms of L-glutamic acid (Lglu) [1]. Numerical solution of kinetic equations at various temperatures showed that small nuclei (< 40 nm) can dissolve with time in consequence of supersaturation decrease. Thus the nucleation rate, in contrast with the classical nucleation theory, can reach negative values (dissolution of small nuclei). In some cases, the total decay of small clusters occurs, which is in agreement with the Ostwald rule of stages. Our model can be generalized for crystallization of several polymorphic phases. However, the numerical solution of kinetic equation is time consuming in this case.

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## Charge carrier mobility in polymers. Dependence on charge carrier density and lattice temperature

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The mobility of charge carriers in certain polymers is studied by theoretical methods upon performing numerical calculations of the behavior of this quantity as it depends on the carrier concentration on the individual localized sites, and also as it depends on the atomic lattice temperature of the sample. For this purpose we utilize the earlier derived formula for the charge carrier mobility, obtained with the help of the quantum kinetic equations based on the nonequilibrium Green's functions. The mobility formula is derived using approximations going beyond the finite order perturbation calculation for including the interaction of the charge carriers with the vibrations of the atomic lattice [1]. The numerical calculations obtained appear to support the idea that the charge carrier motion in the electric conductivity of the polymer can be often expressed by the model of the charge carrier being transferred in an irreversible way between two neighboring sites, with help of the nonadiabatic influence of the lattice vibrations on the charge carrier motion. We show that the effect of the negative differential conductivity in the bulk material consisting of interacting quantum dots might depend considerably on the density of the charge carriers in the corresponding electronic device.

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## Cesium hafnium chloride as a new scintillation material, its preparation, growth, and characterization

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Recently, various new halide materials have been studied for their promising scintillation properties. The lately discovered cesium hafnium chloride ( $\text{Cs}_2\text{HfCl}_6$ ) belongs within these materials due to its high atomic number  $Z = 58$ , high light yield up to 54 000 ph/MeV, energy resolution of 3.3 % at 662 keV, scintillation response of 4.4 ms (95 % of energy) at 662 keV, and moderate density of  $3.86 \text{ g/cm}^3$  [1]. Furthermore, its low hygroscopic nature [2], which is not typical for other halide materials, fulfills the demands on the properties and application of radiation detectors.

The  $\text{Cs}_2\text{HfCl}_6$  is formed by mixing CsCl and  $\text{HfCl}_4$  in the stoichiometric ratio 2:1, congruently melts at ca. 826 °C, and crystallizes in cubic crystallographic structure with lattice parameters  $a = 10.42 \pm 0.01 \text{ \AA}$  [3]. Self-trapping of holes and electrons in the form of temperature dependent  $V_K$  and polarons centers is responsible for scintillation mechanism in the  $\text{Cs}_2\text{HfCl}_6$  matrix as presented in [4].

In this contribution we present results on the preparation and growth of the  $\text{Cs}_2\text{HfCl}_6$  single crystal by the vertical Bridgman method. The element and phase purity was evaluated using X-ray fluorescence (XRF) and X-ray diffraction (XRD) analyses. Further, we report on the characterization of the optical and luminescence properties of the  $\text{Cs}_2\text{HfCl}_6$  measuring the absorption, photoluminescence (PL), and radioluminescence (RL) spectra as well as the PL decay kinetics. Obtained luminescence spectra were analyzed using the Gaussian fitting to identify the contributions of observed transition bands.

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## Preparation and characterization Ni(II) complexes with O,N,O- and O,N,S-Schiff base ligands

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Schiff base ligands have been extensively studied in coordination chemistry mainly due to their facile synthesis, easily tunable steric and electronic properties as well as good solubility in common solvents [1]. Transition metal complexes with Schiff bases, which contain oxygen and nitrogen as donor atoms are of particular interest, because of their ability to possess square-planar or octahedral stereochemistry [2]. These complexes can be Ni-SOD mimetics [3].

In this work we focused on preparation and reactivity Ni(II) coordination compounds with O,N,O and O,N,S-chelating Schiff base ligands (H<sub>2</sub>L). In dependence on conditions and substrates we can prepare square-planar complexes [NiLP] (where P are phosphine ligands), as well as complexes with octahedral stereochemistry of Ni(II) ion [NiL(bipy)(MeOH)] and [NiL(phen)(MeOH)], eventually polynuclear coordination compounds with different composition.

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

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## Polymer Composites as a Construction Material

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Applications of advanced composite materials have demonstrated significant system-level benefits over conventional materials. First and foremost, composites are engineered materials that have been designed to provide significantly higher specific stiffness and specific strength (stiffness or strength divided by material density) - that is, higher structural efficiency - relative to previously available structural materials. In composite materials, strength and stiffness are provided by the high-strength, high-modulus reinforcements. The actual magnitude in composite strength and stiffness can be controlled over a significant range by controlling the volume fraction of reinforcements and by selecting reinforcements with the desired levels of strength and stiffness. In fibre-reinforced composites, the strength and stiffness may be further controlled by specifying the fibre orientation. The highest levels of properties are achieved when all fibres are aligned along the primary loading direction within the composite. However, this simultaneously produces a material with the lowest specific properties for loads perpendicular to the fibre direction. These highly anisotropic properties must be considered in the use of the material.

Polymer composites, their composition, and their properties are the major causes of their application as a construction material. Last century composites with polymer matrix were considered as the most perspective constructional material. Previous researches have only focused on mechanical characteristics of polymer composites but it is also important to observe their mechanical properties before and after UV radiation. The aim of this study is to analyse the change in mechanical properties which are influenced by UV radiation.

It was decided that the optimal method for this investigation was to accelerate ageing in UV box. The test samples were evaluated by the selected mechanical parameters - tensile strength, three-point bend, hardness, Vicat temperature. The same parameters were assessed before and after 500 hours UV radiation. These results extend our knowledge of polymer composites and their behaviour before and after UV radiation. This work shown that UV radiation has significant influence on the change of selective mechanical properties.

Current polymer composites are sensitive to UV radiation which minimize their mechanical properties which change due to partial cross-linking of the matrix and crack at the interface of the matrix and reinforcement.

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## Comparison of grain boundary orientation to deformation conversion models

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Mechanical working of polycrystalline materials leads to deformation of grains caused by deformation. Amount of grain surface per unit volume ( $S_V$ ) is a parameter for description of the deformation. Direction of grain boundaries orientation caused by deformation is the same as direction of deformation. If deformation scheme is known, grain boundaries can be decomposed into isotropic, planar and linear oriented components. Saltykov stereology methods with oriented test lines were used in case of grain surface  $S_V$  - common boundary of two grains [1]. On metallographic cuts total specific surface area  $S_V$  of grains and planar and linear oriented part of specific surface area  $(S_V)_{OR}$  of grains were estimated. Degree of grain boundaries orientation  $O$  can be estimated as  $(S_V)_{OR}$  to  $S_V$  ratio. From these results analytical formulas relating structure parameters and strain in each position inside the bulk sample can be developed. One of the methods using idealized tetrakaidecahedron (Kelvin cell) shape of grain (mathematical description of real state shape of grain is quite impossible) is based on analysis of orientation - deformation relation of a grain. Dependence of strain on orientation  $O$  was derived from three basic equations - definition of deformation, definition of degree of orientation and invariability of volume (initial volume is equal volume after plastic deformation). Solution of the system of equations for used idealized grain shapes is independent on the initial dimension of grain - strain depends only on shape of grain and it does not depend on its dimension. In the first case deformation of tetrakaidecahedron in one direction was considered - perpendicular to square on its surface. In undeformed state tetrakaidecahedron consists of six squares and eight hexagons but is not fully isometric. Therefore in the second case deformation of tetrakaidecahedron in all direction was considered - mean value of deformation was estimated. Fully isometric object is sphere. So the same method using idealized spherical shape of grain was considered in third case. Another method was used in the fourth case - Monte Carlo simulation of the grain boundary orientation (the case of "random"grained structure). There are some differences between results of these methods, however results of the first and fourth method most correspond. Mentioned methods enable estimation of local plastic deformation from the microstructure anisotropy in any position of the grained material with arbitrary state of its initial deformation. Which method is the more right, it required experimental verification of them.

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## The quality of the diffraction data and its influence on the crystal structure determination

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Knowledge of the crystal structure of various materials is crucial to understanding their chemical, physical and biological properties. The single crystal structure analysis is preferred X-ray diffraction technique, but powder structure analysis is a useful alternative, when suitable single crystal is not available.

Presented work deals with the impact of the quality of powder diffraction data on the obtained crystal structure or on the process of its solutions. The quality of experimental diffraction data is influenced by many factors, such as sample properties, effect of real structure and the choice of measurement conditions.

Structure analysis from powder diffraction data is a sequential process and at each stage there can be problems that make structure determination impossible to proceed. The most of problems are caused by the collapse of the three-dimensional reciprocal space into one dimension of powder diffraction pattern, which leads to Bragg-peak overlap [1]. Preferred orientation of the sample is another effect that can disable or complicate solving the crystal structure, because it changes the distribution of intensity of diffraction.

In order to assess the impact of the measurement conditions on the crystal structure solution from powder, experiments were carried out on three different transmission diffractometers: Stoe Stadi-P (CuK  $\alpha_1$ , Mylar foil) and measurement of the powder sample in the capillary on the Empyrean PANalytical (Cu K  $\alpha_1\alpha_2$ ) and Rigaku Smartlab (CuK  $\alpha_1$ ). Afterwards, the structural information obtained from both single-crystal and powder X-ray diffraction have been compared using the program COMPSTRU [2]. Also influence of variable count time (VCT) data collection has been studied.

Results showed that the more accurate structure solution were obtained using Rigaku and also VCT led to improved accuracy. In the case of a sample with a significant preferred orientation, it was not possible to obtain the correct solution by using the diffractometer Stoe Stadi-P. This confirms that the best way to reduce the preferred orientation is using of a rotating cylindrical specimen.

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## Relation between power-law decay of polarons and their transient diffusion coefficient in conducting polymers

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Transient absorption spectroscopy provides a powerful tool for analysis of time-resolved kinetics of photoexcited species in organized layers of conducting polymers. Time-resolved kinetics of excitons, polaron pairs and polarons after photoexcitation was experimentally determined recently in 10 nm thick thin films of regioregular poly(3-hexyl-thiophene) (rr-P3HT) in Ref. 1. It was confirmed that after initial formation of singlet excitons (S), inter-chain polaron pairs (PP) are created during ca 200 fs and then, polarons (P) are formed within ca 2-3 ps. Concerning the transient kinetics of the population of S excitons, the experimentally observed power-law decay of the order of  $t^{-0.5}$  was explained by the S-S collision process controlled by a 1-d diffusion kinetics of excitons along polymer chains in crystalline-like domains of P3HT [1]. For the kinetics of PP states two characteristic kinetic regimes were found. For short times (ca below ps), the hot PPs decay undergoes an interplay with P state formation by a coherent up/down conversion process. In this process, one of the bound counter-charges of the inter-chain PP hops coherently to another parallel polymer chain, forming thus a couple of isolated  $P^+$  and  $P^-$  states, which are detected as “free” polarons by the incident probe pulse [2]. For longer times (ca few ps), the PPs thermalize and exhibit a power-law decay of the order of  $t^{-0.4}$ , indicating thus a bi-molecular collision process of the inter-chain PPs controlled by the 1-d diffusion kinetics. On the other hand, decay kinetics of P states showed significantly slower decay of the order of  $t^{-0.25}$  [1], which was slower than predictions by models of diffusion controlled collision processes with time-independent diffusion coefficients. Motivated by this fact we have elaborated a new approach based on the time-dependent diffusion coefficient of excited species and showed a method of the determination of time-dependent diffusion coefficient from decay population kinetics of photoexcited species controlled by the collision processes [3]. Our approach can be used for arbitrary systems where the decay kinetics of photoexcited species is controlled by their diffusion motion and collision events.

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## Lithium niobate doped by d- and f-ions

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Lithium niobate is a ferroelectric material suitable for electrooptic applications. Its versatility is caused by the diverse properties like electro-optical, nonlinear-optical and piezoelectrical. The field of application becomes much wider when LiNbO<sub>3</sub> is doped by various ions. One of the most widely used dopant in NIR region is Er<sup>3+</sup> with photoluminescence at around 1530 nm. Er<sup>3+</sup> ions have problems with the low probability of photon capture and with following excitation. Therefore, different ions are used as sensitizers, Yb<sup>3+</sup>- Er<sup>3+</sup> energy transition being the most known and utilized.

Because LiNbO<sub>3</sub> is transparent in a wide range of wavelength (350 - 5000 nm), it is a suitable matrix for multifunctional or structured materials. Although LiNbO<sub>3</sub> is an important dielectric material, such applications are described very marginally. For the use of LiNbO<sub>3</sub> in optical multifunctional elements or sensors, the study of doped LiNbO<sub>3</sub> in the form of thin films is required.

This work presents the preparation of LiNbO<sub>3</sub> thin films doped by several ions, e.g. Cu<sup>2+</sup>, Ni<sup>2+</sup>, Fe<sup>3+</sup>, Cr<sup>3+</sup>, Ce<sup>3+</sup>, alternatively co-doped with Er<sup>3+</sup>. For the preparation of LiNbO<sub>3</sub> thin films, a sol-gel method using water-soluble polymer polyethylene glycol (PEG) was used. The films were deposited by spin-coating on sapphire substrates. The influence of doped ions on final microstructure, photoluminescence was investigated. With respect to potential use in waveguiding applications, waveguiding properties of thin films were studied as well.

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## Influence of Linear Deformation on the Geometry of Grains in Grained Structure

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The change of geometric orientation of grain-surface in 3D space can be observed during the grain deformation. The change of the grains orientation during the grained structure deformation can be easily quantified experimentally. If the correlation between the degree of grain orientation and its deformation parameters would be known an explicit deformation map of the structure could be designed. Then we could evaluate local strain in any position in the structure on this basis. In our work we present the brief mathematical considerations aimed at the problem of single grain-surface area deformation. Mathematical formulation of single grain-surface area transformation during deformation using standard deformation tensor is found. To treat this problem, a suitable mathematical procedures are proposed and justified in our work. Novel approaches to quantification of local plastic deformation in grained structure appear on the basis of our result. We try to make accessible mathematically rigorous results for a wide range of researchers mainly in the field of materials deformation.

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## Mixed glass former effect in Na<sub>2</sub>O-P<sub>2</sub>O<sub>5</sub>-TeO<sub>2</sub> glasses

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Glasses were studied in the compositional series 40Na<sub>2</sub>O-(60-x)P<sub>2</sub>O<sub>5</sub>-xTeO<sub>2</sub> within the concentration range of x=0-50 mol% TeO<sub>2</sub> and characterized by the measurements of density, molar volume, chemical durability and refractive index. The structure of glasses was investigated by <sup>31</sup>P MAS NMR and Raman spectroscopy, their thermal properties were studied by DSC and thermodilatometry. Raman and NMR spectra showed that the structure of starting 40Na<sub>2</sub>O-60P<sub>2</sub>O<sub>5</sub> glass is formed mainly by metaphosphate (Q<sup>2</sup>) and diphosphate (Q<sup>1</sup>) structural units interconnected by P–O–P bonds. The replacement of P<sub>2</sub>O<sub>5</sub> by TeO<sub>2</sub> leads to the depolymerisation of the phosphate structural network and to the partial transformation of Q<sup>2</sup> units into Q<sup>1</sup> units and finally to the isolated Q<sup>0</sup> orthophosphate units. TeO<sub>2</sub> is incorporated in the structural network in the form of TeO<sub>3</sub>, TeO<sub>3+1</sub> and TeO<sub>4</sub> structural units. The ratio of TeO<sub>4</sub>/TeO<sub>3</sub> increases with increasing TeO<sub>2</sub> content in the glasses. Glasses show the almost linear increase in the refractive index, whereas Abbe number gradually decreases with increasing TeO<sub>2</sub> content. The highest values of glass transition temperature, T<sub>g</sub>, and dilatometric softening temperature, T<sub>d</sub>, were obtained for the glass containing 30 mol% TeO<sub>2</sub>. This glass revealed also the highest chemical durability against water attack.

The DSC curves showed that all glasses crystallize on heating. The lowest tendency towards crystallization was found for the glass with the ratio of P<sub>2</sub>O<sub>5</sub>/TeO<sub>2</sub> = 1. The contribution of the internal crystallization mechanism increases with increasing TeO<sub>2</sub> content. Study of nucleation rate shows that with increasing TeO<sub>2</sub> content the temperature of maximum nucleation rate is gradually shifted towards the value close to the glass transition temperature.

The observed changes in the refractive index reflects increasing electron density by adding TeO<sub>2</sub>. The reason for increase in T<sub>g</sub> values and chemical durability of glasses, within the compositional range of 0-30 mol% TeO<sub>2</sub>, is the reticulation of the glass network with the formation of P-O-Te linkages, where Te species to cross-link the phosphate chains, resulting in a higher packing density. In addition, the electronegativity difference between P (2.19) and Te (2) implies a polar character of P-O-Te linkages, making them stronger than homoatomic P-O-P or Te-O-Te linkages. A further decrease of T<sub>g</sub> and chemical durability with increasing TeO<sub>2</sub> content (>30 mol%) can therefore be associated with the formation of Te-O-Te bonds and a decrease in the number of P-O-Te connections.

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## Microstructure and mechanical properties of dissimilar Al-Ti joints prepared by GTAW welding-brazing

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Dissimilar joining of light metals and alloys including Al-Ti is of great interest of researchers and producers particularly from automotive and aerospace industries. It results from increasing demands on production of lightweight but on the other hand high-strength constructions [1-3]. Joining titanium and aluminium as well as their alloys using fusion welding technologies is difficult due to very different material properties of these materials and mainly due to development of different metastable phases and formation of brittle intermetallic compounds in interphase layers [4-5]. To produce high-quality weld joints of Al-Ti alloys, the thickness of the brittle intermetallic layer shall be minimized.

In this paper, conventional GTAW welding-brazing method was applied to join the plates of wrought AA5083-H111 aluminium alloy with titanium Grade 2 using ER4043 filler metal. Butt and double butt welded-brazed joints of two plates with the thickness of 2 mm were produced using various welding currents. Mechanical properties of prepared welded-brazed joints were evaluated by tensile tests and microhardness measurements. Microstructural analyses were carried out using light microscopy. The weld zones and Al-Ti interfaces were observed by scanning electron microscope. EDX microanalysis was used to identify variations in chemical composition across the welded-brazed joints. Finally, the analysis of the influence of welding parameters on the mechanical properties and dimensions of the fusion and the heat affected zones were accomplished.

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## **Simulation cold metal forming draw process using different Finite Element Model application software**

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To improve the metal forming processes reducing lead times and try out and improving product free of defects is essential for manufacturing productions. Finite Element Method (FEM) is one of the most satisfactory approaches make forming process superior and forming products of better quality. The IT companies develop the unique FEM applications that are intended to use of forming operations. One of the most commercially used apps of forming simulation is DEFORM, developed by Scientific Forming Technologies Corporations. On the other hand, it is possible to use universal FEM software. COMSOL Multiphysics is a general-purpose platform software for modeling engineering applications. This work discusses the possibilities of using DEFORM and COMSOL software to simulate the cold drawing process. In both cases, the Lagrange FEM method is used, the boundary conditions and the process conditions are set equally. The resulting stress-strain forming conditions of the draw process are compared with the other possibilities of the used software.

## Growth of selected single crystals by micro-pulling-down method and their scintillation properties

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Inorganic scintillation single crystals have been utilized in many fields of technology and research, such as high-energy physics, environmental monitoring, geological survey, oil well logging, astronomy or medical imaging and security scanning. To accelerate the scintillation single-crystal development, fast material composition screening is desirable. 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 to its present form in the 90's for oxide crystals [1, 2]. Aluminum perovskites represent an important group of promising scintillation materials [3], but due to a difficult crystal growth, not much attention has been paid to them so far. The crystal growth of perovskite crystals for gamma-ray detection and by the micro-pulling-down method will be presented and discussed together with brief overview of their structure and luminescence characteristics. 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 [4] or VUV-sensitive photomultipliers (PMT) with CsI-coated photocathodes. Using the micro-pulling-down method modified for fluorides, it was found that further modifications of the carbon hot-zone, 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 BaLu<sub>2</sub>F<sub>8</sub>, ErF<sub>3</sub> and LuF<sub>3</sub> will be presented and discussed together with their luminescence and scintillation properties as well.

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## Review of plastic scintillators and development of new materials

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NUVIA a.s. is an engineering and supply company providing comprehensive supplies and services to customers both in the Czech Republic and abroad.

The Detectors Technology Division is one of the seven divisions of the company, specializing in the unique manufacture and assembling of scintillation detectors, namely the production of inorganic sodium iodide doped with thallium crystals - NaI (Tl) and organic plastic scintillators based on polystyrene. The origin of this production in the Czech Republic (Czechoslovakia) dates back to the 1950s (VÚPJT Tesla Přemyšlení and subsequently SM&D Chemicals and Technology). In 2008, when being taken over by NUVIA a.s. the gradual modernization of production technologies and processes began, and the production was moved to Kralupy nad Vltavou. The Detectors Technology Division supplies scintillation detectors to major manufacturers of radiation monitoring technology and industrial measurement systems mainly in Europe and Eastern markets. Part of the production is also used for the production of the Division of Radiometric Systems within the company NUVIA a.s.

After the relocation of production to new premises in 2010, the division's activities expanded in the field of research and development both within the framework of projects supported from national and international funds, as well as in the framework of contractual cooperation with research entities.

The major research works are targeted in the field plastics materials based on polystyrene.

The basic production technology (cast molding) is gradually expanded with further progressive types of plastics processing (extrusion, injection molding, 3D printing, pressing). In the field of material research, the main development is focused on improving current material by using new luminophores and nanocomposite materials. Part of the activity is also focused on finding new scintillation plastics or new variant standard plastic (microspheres, nonwoven fabrics, microtubes, doped plastics).

In the field of designing new detectors the research is focused on area multilayer and segmental detectors with using fibers for collecting signals and SiPM as replacements of classical PMTs.

## Diamond films and nanoparticles for life science

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Diamond represents a class of material suitable for life science. Boron doped diamond (BDD) films can be used as electrode material for water purification and as an electrochemical electrode in the detection of water contaminants. Nanodiamond particles (NDs) possessing medically significant properties and having a tailorable and easily accessible surface have great potential for use in sensing/imaging and as a component of cell growth scaffolds. In both cases its main advantages are stable and wear resistant surface, extremely high chemical stability, a wide potential window in aqueous media with a low background current and stable surface state without the tendency to fouling.

In case of thin BDD films we show the applicability of BDD electrodes for a water purification demonstrated by the decomposition of organic material, for a disinfection of water contaminated by *Escherichia coli* bacteria and for electrochemical detection of heavy metal ions. In case of nanodiamond particles in vitro interactions of human osteoblast-like SAOS-2 cells with four different groups of NDs.

We have found that during water purification experiments, the diclofenac decomposes to the detection limit of the electrochemical method. During water disinfection, the *E. Coli* bacteria are dead after 10 min treatments. SEM images and optical density measurements indicate the *E. Coli* decomposition and well correlate with impedance spectroscopy and Raman measurements. In electrochemical detection experiments, the RIE etching of BDD resulted in different morphologies, such as dense tiny nanograss or irregular microstructure with increased sp<sup>2</sup> phase. It was found that the optimal BDD morphology is related to the analyte composition.

The comparison of the viability of the cells indicates that the toxicity of NDs is probably dependent on the surface functional groups and the zeta potential, rather than on the diameter of the particles. In our study, oxygen termination emerges as the best surface modification for ND particles from the point of view of their biocompatibility supported also by live cell imaging. A concentration-dependent toxic effect was assigned to mechanical obstruction by NDs preventing cell adhesion, migration and division.

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## Thawing of ice in the frozen water-saturated quartz sand probed by Raman spectroscopy

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The effects associated with the soil thawing and freezing have been investigated for various reasons related in the past particularly to exploitation of cold climate regions. Recently the global warming has enhanced interest in these effects because the bubbles of greenhouse gases trapped in ice in the frozen soils can release in big amounts into the atmosphere upon the thawing, such as the methane from the thawing permafrost in Siberia, and accelerate the global climate change. Even when the soil temperature decreases below the freezing point, a certain part of water in pores among soil particles remains unfrozen due to intermolecular surface forces of soil particles, the pores with sufficiently small dimensions, and water impurities. Thus, thin films of unfrozen liquid water on the surface of mineral particles are simultaneously present with ice within the porous network of frozen fine-grained soils even at temperatures lower than 10 °C below the freezing point. The unfrozen water content that is in dynamic equilibrium with ice in freezing soil decreases with the temperature lowering and under the given external conditions depends on the unsaturated soil properties including soil specific surface area related to the pore-size distribution and geometry, mineral composition of soil particles, water content, and composition and concentration of water solutes.

The Raman spectrum of water is dominated by the broad composite band in the spectral region 2900 - 3900 cm<sup>-1</sup> arising from symmetric and asymmetric stretching vibrations of O-H bonds in hydrogen-bonded H<sub>2</sub>O molecules. The intramolecular O-H bonds are influenced by neighboring intermolecular hydrogen couplings, which are sensitive to the temperature. Consequently, the O-H stretching band shows subtle but significant changes with water temperature both in liquid and solid phase. Moreover, the band shape differs considerably for ice and liquid water due to significant change of molecular vibrations at the water phase transition. Therefore, in the case of optically transparent porous materials the Raman spectroscopy allows characterize the state of water in pores and identification at the pore-scale the phase transformation of water accompanying freezing or thawing of both saturated and unsaturated porous material.

We have studied by Raman spectroscopy the distilled water saturated quartz sand with grain diameter between 100 and 630 μm to determine temperature behavior of ice in porous material with broad distribution of pore sizes. The sample was contained in a cylindrical cavity with a volume of about 0.7 cm<sup>3</sup> covered with quartz window that was made in a copper block fixed to a holder of optical cryostat. The unpolarized Raman spectra within the spectral region 2800 - 4000 cm<sup>-1</sup> were recorded at temperatures from -20 to 10 °C with a temperature-raising step of 0.5 °C. Measured temperature dependence of the O-H stretching band was analyzed and obtained results are discussed.

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## Structural variability of bis(2-hydroxymethylbenzimidazol)bis(salicylato)copper(II) complexes

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Copper(II) complexes containing N-donor ligands are traditionally studied from different points of view. For instance, the carboxylatocopper(II) complexes with benzimidazole form various structural motifs [1,2]. The study of preparation and properties of copper(II) complexes with derivatives of salicylic acid in presence of 2-hydroxymethylbenzimidazole have resulted in few methyl- and methoxysalicylatocopper(II) complexes. All compounds can be divided to two groups according to the stoichiometric formulae. First type of complexes are monomeric units of formulae  $[\text{Cu}(\text{Rsal})_2(\text{OHmebz})_2]$  (where Rsal is 3-methylsalicylate or 4-methylsalicylate, OHmebz is 2-(hydroxymethyl)benzimidazole). Complexes of summary formula  $[\text{Cu}(\text{Rsal})_2(\text{OHmebz})_2] \cdot 2\text{Solv}$  belong to second group (where Rsal is 3-methylsalicylate or 5-methylsalicylate or 3-methoxysalicylate anion and Solv is water molecule; Rsal is 4-methylsalicylate anion and Solv is acetonitrile molecule; Rsal is 5-methoxysalicylate and Solv is methanol molecule). The solid state complexes were characterized by spectral methods (infrared, electronic and EPR spectra) and by X-ray analyses. The coordination environment was similar in all systems, however, different hydrogen bond motifs led to creation of various supramolecular structures. First group of compounds is built up by 1D and 2D supramolecular structures. On other hand, the second type is built up by 3D supramolecular structures.

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## Enhanced UV photoluminescence in hydrogenated ZnO nanocolumns

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Zinc oxide (ZnO) nanocolumns are nowadays a subject of a large attention due to their interesting physical properties such as the direct band gap, large exciton binding energy, the optical transparency in the visible spectra range, the high thermal conductivity and the tunable electrical conductivity. We have recently developed the technology of the nominally undoped ZnO nano-crystalline thin films deposited by DC reactive magnetron sputtering of Zn target in the gas mixture of argon and oxygen plasma [1] serving as a seeding layer for hydrothermal growth of the ZnO nanocolumns [2]. We have shown that lack of the seeding layer leads to the random growth of low quality nanocrystals [3]. Our recent results showed a significant increase in the length of the ZnO nanocolumns grown under UV irradiation, as well as the improvement in their uniformity. An enhancement of the optical and opto-electrical quality of the UV irradiated samples was also reported. Here we present the latest results on the enhancement of the photoluminescence in ZnO nano-columns after plasma hydrogenation. The photoluminescence in near UV region (peak at 380 nm) has been enhanced by several orders of magnitude whereas the deep defect related yellow photoluminescence (broad band 550-600 nm) has been significantly decreased. We explain the observed phenomena by passivation of defects at grain boundaries that not only decrease the defect related photoluminescence but it also significantly prolongs the lifetime of excitons and thus increasing the UV photoluminescence. The defects were also detected by the optical absorption spectroscopy and the electron paramagnetic resonance.

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## Heavily doped Ce:YAG thin films prepared by a non-hydrolytic sol-gel method

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Yttrium aluminium garnet doped with Ce<sup>3+</sup> ions (Ce:YAG) belongs to the most widely studied and applied optical materials, especially in fluorescent or cathode-ray tubes, white-light LEDs, and scintillation technology. The allowed *5d-4f* radiative energy transition of Ce<sup>3+</sup> ions with a short lifetime is utilized in all mentioned applications. In spite of the fact that Ce:YAG is so widely used material, there is no thermodynamic study of the Ce<sup>3+</sup> solubility in the YAG crystal structure. The reason may be the strong influence of preparation process (and thus of kinetics) on the solubility of Ce<sup>3+</sup> ions in the YAG crystal structure. The situation described in most details is probably the case of single crystal growth - Czochralski method or liquid phase epitaxial growth. When Ce:YAG is prepared in polycrystalline form (ceramics, nanoparticles, thin films) the scene changes completely. The polycrystalline microstructure is probably able to tolerate higher internal crystal stress compared with a single crystal, namely at nanoscale level. On the other hand, the internal crystal stress can further distort the cubic symmetry, change the *5d* energy levels, and/or vary the position of the valence and conducting band edges - both influencing luminescence properties.

According to our best knowledge, Ce<sup>3+</sup> solubility has not yet been determined in YAG films prepared by a sol-gel method. In this contribution, we present Y<sub>3-x</sub>Ce<sub>x</sub>Al<sub>5</sub>O<sub>12</sub> thin films deposited by spin-coating on sapphire substrates with a concentration range of  $x = 0-0.75$  (i.e. 0-25 mol. % of Ce of the Y stoichiometry). The solutions were prepared by a non-hydrolytic method utilizing a water-soluble polymer polyvinylpyrrolidone (PVP). We achieved a high Ce<sup>3+</sup> concentration in YAG never previously published - 18 mol. % - without any detectable secondary phase. The thin films were characterized by X-ray diffraction, scanning and transmission microscopy, photoluminescence and radioluminescence spectroscopy, and UV-Vis transmission spectroscopy.

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## Examination of effect Ta on transport properties Bi<sub>2</sub>Se<sub>3</sub>

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This study is focused on preparation and characterization of single-crystalline Bi<sub>2</sub>Se<sub>3</sub> doped with tantalum. Single crystals of Bi<sub>2-x</sub>Ta<sub>x</sub>Se<sub>3</sub>, where x = 0; 0,005; 0,01; 0,02; 0,03; 0,04; 0,06 and 0,08 were grown from high purity elements using self-flux method. The samples were characterized by X-ray diffraction. Transport properties, such as electrical conductivity  $\sigma$ , Hall coefficient  $R_H$  and Seebeck coefficient  $\alpha$  were measured over a temperature range of 100 - 470 K.

From the measured results, it is obvious that the  $R_H$  values for all the studied samples are negative and therefore show the n-type of electrical conductivity. With increasing tantalum content the  $R_H$  decreases. This result leads to the conclusion that the Ta-atoms in the Bi<sub>2</sub>Se<sub>3</sub> crystal structure increase the concentration of free electrons and act as a donor in the structure. This is confirmed by the results of both the electrical conductivity and the Seebeck coefficient. With the increasing content of Ta atoms in the Bi<sub>2</sub>Se<sub>3</sub> crystal structure, the mobility of free carriers is reduced and the scattering mechanism does not significantly affect it. The electrical conductivity increased to twice the value of the pristine sample, however the Seebeck coefficient significantly decreased with tantalum, and adversely affected the value of the Power Factor  $PF = \sigma\alpha^2$ . The incorporation of Ta atoms into the Bi<sub>2</sub>Se<sub>3</sub> crystal structure results in a reduction in PF, and therefore it is difficult to assume that the Ta additive improves the thermoelectric properties of Bi<sub>2</sub>Se<sub>3</sub>.

Doping tantalum atoms into the structure of Bi<sub>2</sub>Se<sub>3</sub> led to an increase in the concentration of free carriers - free electrons. This effect was explained by two possible models of point defects in the Bi<sub>2-x</sub>Ta<sub>x</sub>Se<sub>3</sub> crystal structure.

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## Effect of Tl Doping on Thermoelectric Properties of SnSe Single Crystals

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SnSe is a very promising material that can be used in many applications - in photovoltaic cells, batteries, supercapacitors, and especially as thermoelectric (TE) material. Based on the excellent TE properties presented in the article of *Zhao et al* [1], we study this material from thermoelectric point of view. *Zhao et al* [1] presented exceptional thermoelectric properties of this material,  $ZT = 2.6$  at 923 K and extremely low thermal conductivity in single crystals ( $ZT = \alpha^2 \sigma T / \kappa$ , where  $\alpha$ ,  $\sigma$ ,  $T$  and  $\kappa$  are Seebeck coefficient, electrical conductivity, absolute temperature and thermal conductivity). In our previous paper on polycrystals [2] we discussed Tl as a suitable p-type dopant for SnSe. We decided to further study its effect in single crystals.

For this purpose a series of single crystalline samples  $\text{Sn}_{1-x}\text{Tl}_x\text{Se}$ , where  $x = 0.001, 0.0025, 0.005, 0.0075$  and  $0.01$  was prepared. Phase purity was verified by powder X-ray diffraction. Samples were characterized by measurements of electrical conductivity, Hall coefficient and Seebeck coefficient in the temperature range 93 - 473 K. Tl doping increases the concentration of holes in SnSe markedly - from  $4.9^{17}$  to  $6.7^{19} \text{ cm}^{-3}$  at room temperature for  $x = 0.005$ . Thanks to high values of electrical conductivity Tl significantly improves values of *power factor* ( $PF = \alpha^2 \delta$ ) - almost by an order of magnitude at all temperatures.

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## Technological possibilities and vacuum systems for deposition of Si:H thin films with embedded nanoparticles

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In the Department of Thin Films and Nanostructures at the Institute of Physics ASCR, we developed the radio frequency plasma enhanced chemical vapour deposition (RF PE CVD) of hydrogenated silicon thin film. Solar cells resp. photovoltaic diode structures based on hydrogenated amorphous (a-Si:H) and hydrogenated micro-crystalline ( $\mu$ c-Si:H) silicon thin films have been developed in the last 35 years with the aim to increase energy conversion efficiency. This technological process of cheap solar cells production was many years perspective to substitute the standard production based on sliced crystalline silicon ingots. We consider (may be as last) a possibility how to improve the cells efficiency is to prepare silicon thin films with embedded nanoparticles to enhance the light absorption in the near infrared region. For this aim we combine different deposition processes and test different semi-conductive nanoparticles to Si:H thin films. 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) 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. 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. Here in our contribution we focus on Ge and Sn nanoparticles in the a-Si:H structures and compare the results with previous results which we get on application of Mg silicide NPs. Structural changes will be observed by SEM and TEM microscopes.

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## Characterization of a-Si:H thin films with and without embedded nanoparticles

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A widely used technique for the deposition of thin films with very different qualities and structures is the Plasma Enhanced Chemical Vapour Deposition (PECVD). For the surface morphology of deposited thin films we use SEM (Scanning Electron Microscope). PDS (Photo-thermal Deflection Spectroscopy) is applied to measure low optical absorptance. Recombination centres in disordered hydrogenated structures are detected by the Photoluminescence spectroscopy excited by laser illumination. For those optical characterizations of individual - homogeneous thin film the films are deposited on convenient substrates, usually Corning glasses or silica fused substrates. For measurement of electrical and optical 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 there are measured the temperature dependences 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 changes at energies near conductive gap (tail) correspond with defects in the disordered structure. The CPM is used together with transmittance and reflectance measurements to get absolute values of the optical absorptance. The basic measurement on diode structures gives as important results the I-V (current-voltage) characteristics, which are measured under or without illumination. As well as the control of the Electroluminescence is important. This configuration is called "sandwich". For this opto-electrical measurements there is necessary to use one from electrodes transparent and conductive (TCO - oxides of metals as ITO or ZnO). All those mentioned methods are applied for characterisation of thin films and structures modified by embedded nanoparticles.

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## **Theoretical investigation of superconductivity in interface of high T<sub>c</sub> superconductor and ferromagnet**

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The superconductivity in the interface of high temperature superconductor and colossal magnet (YBCO/LCMO) was investigated. In the interface, a magnetic frustration is built between the antiferromagnetic Cu-O layer and the ferromagnetic Mn-O layers from YBCO and LCMO, respectively. The d-wave superconducting pairs from YBCO will be affected by the ferromagnetism from LCMO as well as the magnetic frustration in the interface. Owing to the ferromagnetism will be suppressed by the magnetic frustration and the d-wave superconducting pairs also be suppressed by the ferromagnetism as well. Under both competing interactions the triplet superconducting pairs possibly exist in the interface of YBCO. A model for dealing with the transformation of superconducting pairs from singlet to triplet pairs under the magnetic frustrations were proposed.

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## Lanthanide-doped Lu<sub>2</sub>O<sub>3</sub> phosphors

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Cubic lutetium sesquioxide (Lu<sub>2</sub>O<sub>3</sub>) presents a suitable host material because of its favourable properties including chemical and phase stability. Lu<sub>2</sub>O<sub>3</sub> has a wide band gap (> 5.5 eV) and its doping with lanthanide ions, which behave as activators, gives rise to some unique optical properties. Lanthanide-doped lutetium oxide (Ln:Lu<sub>2</sub>O<sub>3</sub>) thus finds use in wide field of lightning-related applications such as fluorescent lamps, plasma display panels, cathode ray tubes etc. Also, due to a high effective atomic number ( $Z_{eff} = 63$ ) and high density (9.4 g/cm<sup>3</sup>) of Lu<sub>2</sub>O<sub>3</sub> host, that prompts high stopping power for ionizing radiation, it has also attracted attention as a scintillator material. Since optical properties are affected by both crystal structure and morphology, which depend strongly on the synthesis method and conditions employed, many different methods have been studied for its synthesis. In our work, we used the sol-gel route to prepare a series of Ln:Lu<sub>2</sub>O<sub>3</sub> (Ln = Eu, Tb, Pr, Dy) phosphors. Luminescence properties with respect to various dopants and dopant concentrations were investigated.

**Keywords:** lutetium oxide; europium; dysprosium; terbium; praseodymium; sol-gel; XRD; luminescence

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## Design of the Time of Flight ERDA system for 6 MV tandem ion accelerator

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Currently the Ion Beam Laboratory of the MTF STU in Trnava [1] utilise the basic IBA (Ion Beam Analysis) methods, namely RBS (Rutherford Backscattering Spectrometry), PIXE (Particle Induced X-ray Emission), in limited extend NRA (Nuclear Reaction Analysis) and ERD (Elastic Recoil Detection) with He beam. The development of the HI ERDA (Heavy Ion Elastic Recoil Detection Analysis) system [2] for our laboratory has started, which utilizes ions from O to Au with energies  $\sim 1$  MeV/amu (tens of MeV) as the analyzing projectiles.

HI ERDA is ideal for measurement of concentration depth profiles of all elements lighter (including hydrogen) than the mass of the primary ion beam, present in thin layers as well as in multilayer sandwich systems.

During the HI ERDA experiment, the high energy heavy ions impinge on the sample at an acute angle, atoms of the sample are elastically recoiled, and it is necessary to determine their energy and mass. We have chosen the energy measurement by Si charge particle detectors and the Time of Flight (ToF) [3] method to distinguish the mass of the elements. Two time gates will be used to acquire the two time stamps. The fast acquisition electronics has to collect the coincidence energy/ToF/yield multiparametric spectra. The ToF system can be realized through the classical fast analog nuclear electronics or using the digital nuclear electronics. The systems used so far have been compared and a new solution based on a fast digital multiparametric collection system has been proposed. The first draft of the ToF HI ERDA for Trnava IBA laboratory is presented.

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## **Analysis of laser beam welding of the S650MC high strength steel using numerical simulation**

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Laser beam welding (LBW) is used in a wide range of industries, e. g. in the mechanical engineering, R&D, electronics, medical, aerospace or automotive industries. LBW technology is very popular not only for the well-known advantages comparing to another processes of fusion welding but also due to the fact that it can be easily integrated into the automated production lines. Modelling and numerical simulation of LBW processes provides a possibility to explore in detail technological principles and complex phenomena associated with this technology.

The contribution is focused on the application of numerical simulation for the analysis and design of parameters for laser welding of S650MC high-strength steel sheets. For this purpose, simulation model of LBW process was developed and applied for numerical simulation of temperature fields in the program code ANSYS. A verification experiment was carried out using TruDisk 4002 disk laser. During the laser welding experiment, temperatures were measured using thermocouples of the K-type. The macrostructure of the produced weld joints was assessed by light microscopy. Measured temperatures and dimensions of welded joints were compared with results obtained by numerical simulation. Finally, using the verified simulation model, suitable parameters for laser welding of sheets from S650MC high-strength steel with the thickness of 4 mm were suggested.

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## The effect of temperature on the resistance of electropolished AISI<sub>304</sub> stainless steel to pitting

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AISI 304 is the most widely used Cr-Ni austenitic stainless steel. It is recommended for a wide variety of applications that require high corrosion resistance, good formability and weldability. Due to the passive surface film the stainless steels are resistant to the uniform corrosion in oxidation environments. However, aggressive substances in environment (most commonly chlorides) can evoke local breakdown of protective film and consequently destructive and dangerous local corrosion, namely pitting.

There are numerous factors that influence the resistance of stainless steels to pitting. In addition to internal factors (chemical composition, surface treatment) important role is played by the environmental conditions (temperature, pH, a concentration of aggressive ions). Temperature is a factor that strongly affects both thermodynamics and kinetics of pitting corrosion. Numerous studies on the effect of temperature on pitting have been carried out (usually for temperature range 20 - 100 °C). An influence of temperature on the pitting corrosion is commonly expressed by the change of electrochemical characteristics - decrease of the pitting potential  $E_p$  and repassivation potential  $E_r$  with temperature.

Many authors have documented an effect of surface characteristics on the pitting corrosion resistance of austenitic stainless steels. Traditional mechanical polishing usually causes deformed layer and residual stresses on the treated surface. Electropolishing is a surface finishing process of electrochemical anodic dissolution which enhances high surface brightness without residual surface tensions. Improved corrosion resistance and reduced bacterial attachment are other benefits of electropolished surfaces important for various industrial and medical applications of these materials.

This paper is focused on the temperature dependence of pitting corrosion resistance of AISI 304 steel in acidified 1 M chloride solution. Resistance of three surface types (“as received”, electropolished and ground + electropolished) is studied and compared at two temperatures (22 ± 3 °C, 50 °C). Evaluation of the corrosion resistance is based on the results of electrochemical cyclic potentiodynamic polarization tests (determination and comparison of pitting potentials  $E_p$ ) and on the microscopic observation of specimen surfaces attacked by pitting during performed testing procedure.

According to obtained results at both temperatures the ground + electropolished reflected the highest thermodynamic stability. However, it should be noted, that elevated temperature (50 °C) caused a strong decrease of corrosion resistance of this type of surface (the pitting potential was almost 5 times lower than at 22 ± 3 °C).

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