

DEVELOPMENT OF MATERIALS SCIENCE IN RESEARCH AND EDUCATION

Book of Abstracts of the 30th Joint Seminar
7 – 11 September 2020



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

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Pavlov
Czech Republic

7 – 11 September, 2020

Supported by the Czechoslovak Association for Crystal Growth (CSACG)
CZ-162 00 Prague 6, Cukrovarnická 10, Czech Republic

Published by the Institute of Physics of the Czech Academy of Sciences, v. v. i.
CZ-182 21 Prague 8, Na Slovance 1999/2, Czech Republic

Editors: Z. Kožíšek, R. Král, P. Zemenová
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ISBN 978-80-907237-1-9

The 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 and
the Slovak Society for Industrial Chemistry**

Conference Chairman

Dr. Z. Kožíšek

Chairman of the Czechoslovak Association for Crystal Growth
Institute of Physics of the Czech Academy of Sciences
Cukrovarnická 10, 162 00 Prague 6, Czech Republic
Phone (+420) 220 318 574, E-mail: kozisek@fzu.cz

Conference Co-Chairman

Prof. M. Koman

Chairman of the Slovak Expert Group of Solid State Chemistry and Physics
Faculty of Chemical and Food Technology SUT
Radlinského 9, 812 37 Bratislava, Slovak Republic
Phone (+421) 259 325 622, E-mail: marian.koman@stuba.sk

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

Scientific Committee

Mária Behúlová, Faculty of Material Science and Technology SUT, Trnava

Jaromír Drápala, Technical University of Ostrava, Ostrava

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Robert Král, Institute of Physics of the Czech Academy of Sciences, Prague

Zdeňka Poláčková, Institute of Physics of the Czech Academy of Sciences, Prague

Petra Zemenová, Institute of Physics of the Czech Academy of Sciences, Prague

PREFACE

The 30th Joint Seminar “Development of Materials Science in Research and Education” (DMSRE30) will be held on 7 – 11 September 2020, in hotel IRIS Pavlov. The first Joint Seminar in these series was held at Gabčíkovo in Czechoslovakia 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, nanocrystalline and glassy states.

The program will include 5 keynote lectures (35 minutes): Marian Koman (Faculty of Chemical and Food Technology STU, Bratislava, Slovak Republic) *30 years of DMSRE seminars*, Maksym Buryi (Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic): *ZnO nanorods heavily doped with Mo/Er. The effect of post-deposition treatment on defect states and luminescence*, Ladislav Koudelka (University of Pardubice, Pardubice, Czech Republic): *Phosphate glasses modified with transition metals*, Zdeněk Remeš (Institute of Physics of the Czech Academy of Sciences, Prague, Czech Republic): *The optical emission spectroscopy of the inductively coupled plasma used for modification of chemical, optical and electronic properties of nanostructured ZnO*, Kateřina Rubešová (University of Chemistry and Technology, Prague, Czech Republic): *151 years of the periodic table of elements*.

All other contributions will be presented as short lecture talks (20 minutes). The official languages of the seminar are English, Czech, and Slovak.

This booklet contains the abstracts of all contributions, which reached us before 21 August 2020. The authors are responsible for the technical and language quality of the contributions. The conference will run from Monday afternoon, 7 September 2020, until Friday noon, 11 September 2020 in the hotel IRIS Pavlov, Czech Republic.

Dear colleagues, we welcome you to the 30th DMSRE Joint Seminar and we hope you will enjoy your stay in Pavlov.

Zdeněk Kožíšek, Robert Král, Petra Zemenová (Editors)

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PROGRAM

Monday, 7 September 2020

11:45 – 13:00 Lunch

13:00 – 14:40 Registration
Location: Hotel Lounge (near reception)

15:00 – 15:05 Opening

15:05 – 16:00 **Monday Session 1**

*Location: Lecture Hall
(chairperson: Zdeněk Kožíšek)*

15:05 – 15:40: Marian Koman:
Thirty years of seminars “Development of Materials Science in Research and Education”

15:40 – 16:00: Mária Behúlová:
Comparison of microstructures and mechanical properties of Al-Ti weld joints prepared by different welding technologies

16:00 – 16:30 Coffee break

16:30 – 17:30 **Monday Session 2**

*Location: Lecture Hall
(chairperson: Marian Koman)*

16:30 – 16:50: David Rutherford:
Bactericidal effect of zinc oxide nanoparticles on Gram-positive and Gram-negative strains for water decontamination using reverse spin technology

16:50 – 17:10: Jaroslav Jíra:
Effect of ZnO nanoparticles and illumination on growth inhibition of Escherichia coli and Staphylococcus aureus bacteria in cultivation medium.

17:10 – 17:30: Bohuslav Rezek:
Microscopic study of zinc oxide molecular biointerface

18:00 – 19:00 Dinner

Tuesday, 8 September 2020

07:30 – 8:45 Breakfast

09:00 – 9:55 **Tuesday Session 1**

Location: Lecture Hall
(chairperson: Zdeněk Potůček)

09:00 – 09:35: Maksym Buryi:
ZnO nanorods heavily doped with Mo/Er. The effect of post-deposition treatment on defect states and luminescence

09:35 – 09:55: Vladimir Babin:
On the luminescence origin in $Y_2SiO_5:Ce$ and $Lu_2SiO_5:Ce$ single crystals

09:55 – 10:25 Coffee break

10:25 – 11:45 **Tuesday Session 2**

Location: Lecture Hall
(chairperson: Kateřina Rubešová)

10:25 – 10:45: Takahiko Horiai:
Relationship between crystal structure and luminescence properties for Ce^{3+} -doped rare-earth pyrosilicate

10:45 – 11:05: Jan Pejchal:
Growth of perovskite oxide single crystals and their luminescence and scintillation properties

11:05 – 11:25: Robert Král:
Growth and characterization of zirconium-doped cesium hafnium chloride crystals for scintillators

11:25 – 11:45: Zdeněk Kožíšek:
Crystallization of aluminum droplet

11:45 – 12:45 Lunch

14:00 – 15:40 **Tuesday Session 3**

*Location: Lecture Hall
(chairperson: Robert Král)*

- 14:00 – 14:20: Jan Grym:
Zinc oxide nanorods grown from solutions: What is next?
- 14:20 – 14:40: Šárka Kučerová:
High-quality seed layers for patterned growth of ordered ZnO nanorod arrays
- 14:40 – 15:00: Nikola Bašinová:
Growth kinetics of ZnO nanorods prepared by chemical bath deposition
- 15:00 – 15:20: Hana Faitová:
Heterostructures of ZnO on GaN Substrates Modified by Focused Ion Beam
- 15:20 – 15:40: Ondřej Černohorský:
Modeling of the growth of ZnO nanorods in batch and flow reactors
- 15:40 – 16:10 Coffee break

16:10 – 17:50 **Tuesday Session 4**

*Location: Lecture Hall
(chairperson: Mária Behúlová)*

- 16:10 – 16:30: Vladimír Jorík:
Do we really perform physicochemical measurements on polycrystalline substances always with a known crystal structure?
- 16:30 – 16:50: Ľubor Dlháň:
Magnetic response of bovine spleen.
- 16:50 – 17:10: Martin Necpal:
Examination Crystal plasticity in Cool draw tube forming using FEM and Voronoi Tessellation
- 17:10 – 17:30: Rastislav Ďuriš:
A comparison of the optical and tensometric methods of the tensile test evaluation
- 17:30 – 17:50: Štefan Vrtiel:
Influence of laser welding parameters on the microstructure and mechanical properties of butt weld joints of a TRIP steel

18:00 – 19:00 Dinner

Wednesday, 9 September 2020

07:30 – 8:45 Breakfast

09:00 – 9:55 **Wednesday Session 1**

Location: Lecture Hall
(chairperson: Petr Mošner)

09:00 – 09:35: Kateřina Rubešová:

151 years of the periodic table of elements

09:35 – 09:55: Vít Jakeš:

Preparation of mixed strontium-lead hafnate by wet chemical methods

09:55 – 10:25 Coffee break

10:25 – 11:45 **Wednesday Session 2**

Location: Lecture Hall
(chairperson: Jan Pejchal)

10:25 – 10:45: Václav Doležal:

Dielectric properties of (Ca,Eu)Cu₃Ti₄O₁₂ ceramics prepared by a sol-gel method

10:45 – 11:05: Dana Mikolášová:

Impact of solution ageing on the Er³⁺/Yb³⁺:LiNbO₃ thin films properties

11:05 – 11:25: Tomáš Thoř:

Spark plasma sintering of lanthanide doped Lu₂O₃

11:45 – 12:45 Lunch

14:00 – 17:00 **Joint meeting - panel discussion**

18:30 – 22:00 **Conference Banquet**

Location: Hotel Terrace

Thursday, 10 September 2020

07:30 – 8:45 Breakfast

09:00 – 9:55 **Thursday Session 1**

Location: Lecture Hall

(chairperson: Bohuslav Rezek)

09:00 – 09:35 Ladislav Koudelka:

Phosphate glasses modified with transition metals

09:35 – 09:55 Petr Mošner:

Effect of titanium dioxide on thermal behavior and properties of niobate-phosphate glasses

09:55 – 10:25 Coffee break

10:25 – 11:45 **Thursday Session 2**

Location: Lecture Hall

(chairperson: Vít Jakeš)

10:25 – 10:45 Petr Kalenda:

Structure and properties of barium tungstate-phosphate glasses

10:45 – 11:05 Jan Havlíček:

On development of materials and crystal growth in Crytur, spol. s r. o.

11:05 – 11:25 Mária Behúlová:

Current state in the field of life-long learning of employees in the mechanical engineering and automotive industries in the Slovak Republic and the Czech Republic

11:25 – 11:45 Roman Yatskiv:

Luminescence and up-conversion of Er doped TeO₂-PbCl₂-WO₃ glasses

11:45	–	12:45	Lunch
14:00	–	15:40	Thursday Session 3: video conference
			<i>Location: Lecture Hall</i>
			<i>(chairperson: Zdeněk Kožíšek)</i>
14:00	–	14:20:	Serge Nagorny: <i>The Cs₂HfCl₆ crystal scintillators as a perspective detector to search for rare nuclear process</i>
14:20	–	14:40:	Anna Artemenko: <i>XPS as an advanced method for analysis of organic materials</i>
14:40	–	15:00:	Iveta Markechová: <i>Origami-kirigami approach to materials structures modelling</i>
15:00	–	15:20:	Milan Nad': <i>Dynamic analysis of cone waveguide for ultrasonic assisted technological processes</i>
15:20	–	15:40:	Štefan Hajdu: <i>Using optimization in new design of tribometer specimen clamping system</i>
15:40	–	16:00:	Hüsnügül Yilmaz Atay: <i>Welding of S690QL steels with different welding consumables, comparing their microstructure and mechanical properties</i>
16:00	–	16:30	Coffee break
18:00	–	19:00	Dinner

Friday, 11 September 2020

- 07:30 – 8:45 Breakfast
- 09:00 – 9:55 **Friday Session 1**
(chairperson: Ladislav Koudelka)
- 09:00 – 09:35: Zdeněk Remeš:
The optical emission spectroscopy of the inductively coupled plasma used for modification of chemical, optical and electronic properties of nanostructured ZnO
- 09:35 – 09:55: Zdeněk Potůček:
Temperature behavior of the zero-phonon line of vanadium photoluminescence in SrTiO₃:V crystal
- 09:55 – 10:25 Coffee break
- 10:25 – 11:25 **Friday Session 2**
Location: Lecture Hall
(chairperson: Zdeněk Remeš)
- 10:25 – 10:45: Stanislav Tiagulskyi:
Characterization of Graphene/ZnO Schottky Barriers Formed on Zn and O polar faces of ZnO substrates
- 10:45 – 11:05: Pavla Dvořáková:
Moisture expansion of Ca-rich ceramic body
- 11:05 – 11:25: Kateřina Zloužeová:
Dielectric properties, preparation and characterization of lead-free ceramics from piezoelectric powders
- 11:25 – 11:30 Closing
- 11:30 – 12:30 Lunch

ABSTRACTS

XPS as an advanced method for analysis of organic materials

Anna Artemenko¹, Pavla Štenclová¹, Oleg Babčenko¹, Thomas Wågberg², Jonas Segervald², Xueen Jia², Andrey Shchukarev³, Marián Marton⁴, Marián Vojs⁴, and Alexander Kromka¹

¹*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, Prague 6, Czech Republic*

²*Department of Physics, Umeå University, Linnaeus väg 24, Umeå 90187, Sweden*

³*Department of Chemistry, Umeå University, Linnaeus väg 10, Umeå 90736, Sweden*

⁴*Institute of Electronics and Photonics, Slovak University of Technology, Ilkovičova 3, SK-812 19 Bratislava, Slovakia*

X-ray photoelectron spectroscopy (XPS) is known as a surface-sensitive method that allows us to obtain quantitative information about the chemical composition of different organic materials: for simple biomolecules (amino acids (AAs)) to complex organic material (bacteria, cells). However, it is still a challenge to make in situ XPS measurements of organic materials in their solid or liquid form and to provide a correct interpretation of measured data. For non-destructive measurements, the cryogenic XPS approach is often used and capable to reveal novel insights on the chemical structure and composition of organic materials.

Here we present technological challenges in XPS analysis of two different organic materials - AAs and cells (geobacter, Algae), respectively. The first part focuses on an understanding of the actual mechanisms of AAs interaction with carbon-based surfaces, namely with H-/O-terminated nanocrystalline diamond (NCD) and diamond-like carbon (DLC) films using XPS. The depth distribution (<10 nm) of bonding states was calculated from the angular-resolved XPS spectra using the maximum entropy method (MEM), i.e. the in-depth reconstructions of the bonding states at the interface of carbon-based materials. The detailed processing of XPS data revealed the dependence of AAs adhesion on the surface termination of carbon-based materials. The XPS data are corroborated with AFM, SEM and WCA measurements.

The second part focuses on the investigation of intact interfaces (based on freeze-drying or direct freeze-drying on sample holder) of centrifuged wet pastes of geobacter and Algae followed by standard XPS measurements at liquid nitrogen temperatures. The geobacter with/without yeast in the medium were investigated. The detailed XPS analysis of C 1s, O 1s and N 1s peaks was provided to obtain the information about the chemical composition of geobacter. The XPS study revealed that medium with yeast caused a dramatic increase of peptides and lipids contribution in the C 1s peaks. Moreover, the cryogenic XPS analysis was used to investigate the surface chemical composition of hydrophilic and hydrophobic types of Algae (both grown for 5 and 10 days) to understand as a key factor for the understanding of their hydrophilic/hydrophobic properties. The differences in processed C 1s and S 2p peaks for both types of Algae in dependence on the growth period will be discussed.

This work was supported by project ESIF and MEYS (Project “FZU- researchers, technical and administrative staff mobility” – CZ.02.2.69/0.0/0.0/18_053/0016627), by project VEGA 1/0554/20 and by the Czech Science Foundation (project No. 20-00925Y).

On the luminescence origin in $\text{Y}_2\text{SiO}_5\text{:Ce}$ and $\text{Lu}_2\text{SiO}_5\text{:Ce}$ single crystals

Vladimir Babin¹, Valentin Laguta¹, Martin Nikl¹, Jan Pejchal¹, Akira Yoshikawa², and Svetlana Zazubovich³

¹*Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, 16200 Prague, Czech Republic*

²*Institute of Materials Research, Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Miyagi, 980-8577, Japan*

³*Institute of Physics, University of Tartu, W. Ostwaldi 1, 50411 Tartu, Estonia*

Ce^{3+} -doped rare-earth (RE) oxyorthosilicates RE_2SiO_5 (RE: Y, Lu) have been intensively studied as promising scintillation materials owing to their high density, short luminescence decay time, high light yield, high stopping power, effective atomic number, emission wavelength compatible with common detectors, relatively high radiation hardness, as well as good mechanical properties and chemical stability.

The luminescence characteristics of YSO:Ce and LSO:Ce were intensively studied. In their emission spectra, two main emission bands were observed, the intense violet doublet band and weaker broad blue band. The origin of violet band usually ascribed to the allowed $5d_1 \rightarrow {}^2F_{5/2}, {}^2F_{7/2}$ transitions of the Ce^{3+} ions, while the origin of the blue emission is not clear and still under discussion.

In present work, photoluminescence characteristics of single crystals of Ce^{3+} -doped LSO and YSO with different Ce^{3+} concentrations are studied in wide temperature range by the steady-state and time-resolved spectroscopy methods. The concentrations of single and dimer Ce^{3+} -related centers of different types in the investigated crystals are evaluated from their EPR spectra. On the basis of the obtained results the origin of the Ce^{3+} -related centers responsible for the luminescence of these crystals is clarified and a new interpretation of their luminescence spectra is proposed. The suggestion is made that the dominating violet doublet emission band arises from the Ce^{3+} ions substituting for the host crystal lattice rare-earth ions in two lattice sites and, thus, can be considered as the superposition of the strong Ce1 and weak Ce2 emission bands. The weaker blue broad emission band is ascribed to the dimer Ce^{3+} - Ce^{3+} centers.

The work was supported by the project 20-12885S of the Czech Science Foundation, the ERDF funding in Estonia granted to the Center of Excellence TK141 project No. 2014-2020.4.01.15-0011, the CSA-EAS project ETA-18-01 and the GIMRT Program of the Institute for Materials Research, Tohoku University (Proposal No. 19K0514). Partial support of the project from the Ministry of Education, Youth and Sports of Czech Republic no. CZ.02.1.01/0.0/0.0/16 013/0001406 is also gratefully acknowledged.

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Growth kinetics of ZnO nanorods prepared by chemical bath deposition

Nikola Bašínová, Ondřej Černohorský, and Jan Grym

*Institute of Photonics and Electronics of the Czech Academy of Sciences, Chaberska 57,
Prague, Czech Republic*

Zinc oxide nanorods have been extensively studied in the last two decades for their outstanding properties and prospective applications in photonics and electronics. There is a large number of deposition techniques to prepare arrays of ZnO nanorods. Chemical bath deposition (CBD) on a seeded substrate is a frequently used method, which is easily accessible and non-expensive, with many adjustable parameters. In the growth solution, both homogeneous and heterogeneous nucleation take place, which is followed by precipitation and growth of zinc oxide crystals. To obtain well-ordered nanorods with desired physical properties, it is necessary to control the growth conditions. The growth conditions strongly affect the growth mechanism. A key parameter, which significantly alters the growth rates, is the precursor concentration in the growth solution. It is therefore essential to analyse the time evolution of zinc ion concentration and to evaluate the kinetic parameters.

The precursor solution for CBD consists of zinc nitrate and hexamethylenetetramine (HMTA) equimolar solution. Zinc nitrate acts as a source of zinc ions and HMTA supplies hydroxyl ions, both needed to produce ZnO. The OH^- ions are in excess to Zn^{2+} ions; therefore, it is important to analyse the decrease of the Zn^{2+} concentration with time. The consumption of zinc ions corresponds to the formation of ZnO crystals grown directly on the seeded substrate, as well as in the solution. An effective tool for this purpose is a quantitative chemical analysis - titration. It is an accessible and reliable analytical method that provides information about unknown concentration of an identified substance in an analyte solution. The chelatometric titration was used to determine the zinc concentration in the growth solution. The time and temperature dependence of the zinc concentration was investigated. The obtained data together with the SEM image analysis of the grown nanorods are discussed in terms of reversible first-order reaction model and serve for the calculation of the reaction kinetic parameters, from which the growth mechanism can be identified.

This work was supported by the Czech Science Foundation project 17-00355S.

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Comparison of microstructures and mechanical properties of Al-Ti weld joints prepared by different welding technologies

Máté Nagy, Štefan Vrtiel, and Mária Behúlová

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

The difficulties in joining aluminum to titanium alloys by fusion welding technologies result not only from significant differences in the physical, mechanical and thermal properties of the two materials but mainly from the unavoidable formation of brittle intermetallic compounds [1-4]. Various conventional and unconventional welding technologies were tested to obtain sound weld joints of these materials, and the influence of welding parameters on the quality of produced weld joints was evaluated [5-6].

In this study, the butt welded-brazed joints of two plates with the thickness of 2 mm of EN AW5083-H111 alloy and titanium Grade 2 were prepared applying two different welding technologies: laser beam welding (LBW) and gas tungsten arc welding (GTAW). ER4047 and ER4043 welding wires with the diameter of 1.2 mm were used as filler materials. The microstructure and mechanical properties of experimental weld joints were analyzed and compared. In general, the strength of welded-brazed joints prepared by laser welding was higher than the strength of samples after GTAW. The highest tensile strength at the level of 245 MPa was measured for the welded-brazed joint manufactured by LBW using following welding parameters: the laser power of 1800 W, the welding speed of 30 mm.s⁻¹, the laser beam offset to Al-sheet of 400 μm and the wire feed speed of 2.4 m.min⁻¹.

The research has been supported by the Scientific Grant Agency of the Slovak Republic within the Projects VEGA No. 1/0796/20 and KEGA No. 029STU-4/2018.

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ZnO nanorods heavily doped with Mo/Er. The effect of post-deposition treatment on defect states and luminescence

Maksym Buryi¹, Zdeněk Remeš¹, Vladimír Babin¹, Vojtěch Vaněček¹, Kateřina Dragounová¹, Lucie Landová¹, and Julia Mičová²

¹*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, 162 00 Prague 6, Czech Republic*

²*Institute of Chemistry SAS, Dúbravská cesta 9, 845 38, Bratislava, Slovakia*

Among the most attractive classes of materials one may point out scintillators which transform high energy ionizing radiation into optical photons. This allows detection tools to operate basing on conventional photomultipliers or semiconductor-based devices. Diseases diagnostics is one of the most demanding fields of the scintillators application. It is supplied by the data provided by e.g., computer tomography (CT) and positron emission tomography (PET). The latter is exceedingly sensitive in the time-of-flight (TOF) PET extension. This requires the improved timing coincidence resolution (TCR) of the scintillating system. The TCR reaching 500 ps is now realized in commercial devices, however, the expected limit of the TCR for a scintillating material is 10 ps.

Presently, excellent timing properties have been observed in zinc oxide (ZnO) nanostructures like, e.g., nanopowders, free-standing (hedgehog) or deposited nanorods. Photoluminescence (PL) spectrum measured in these ZnO-based nanomaterials is complex. In most cases (as grown material) it is composed of a very broad defect-related band covering almost the whole visible range. It exhibits slow decay. Post-deposition treatment, conditions of growth, additional doping or all this altogether can result in a narrow UV exciton band appearance whereas the defect-related band can be suppressed [1, 2]. This paves the way for the material properties tuning to make use of each of these bands separately. This in turn requires deep understanding of the energy and charge transfer processes including trapping of charge and defects creation. Therefore, this work is aiming at comparison of undoped and the heavily Er, Mo-doped zinc oxide nanorods to find out the peculiarities of the energy and charge transfer and the possibilities of the nanorods improvement. Paramagnetic Er³⁺, Mo³⁺ and Mo⁵⁺ ions can be detected by means of electron paramagnetic resonance (EPR). Therefore, they can serve as local point probes in the material. Post-growth treatment of the ZnO:Er/Mo by air annealing results in reduction of F⁺ centers. Red emission appears. EPR results were correlated to the RL, PL and thermally stimulated luminescence (TSL) data as well.

This work was supported by the Czech Science Foundation project 20-05497Y and by the Scientific Grant Agency of Ministry of Education, Science, Research and Sport of Slovak Republic and Slovak Academy of Sciences (VEGA 2/0157/20).

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Modeling of the growth of ZnO nanorods in batch and flow reactors

Ondřej Černohorský, Hana Faitová, Nikola Bašínová, Šárka Kučerová, and Jan Grym

*Institute of Photonics and Electronics of the Czech Academy of Sciences, Chaberská 57,
Praha 8 - Kobylisy, 182 51, Czech Republic*

Chemical bath deposition is an attractive method for the preparation of semiconductor nanostructures. This method is cost-efficient, scalable, can be easily implemented, and takes place at temperatures below water boiling point, which allows for the deposition on a large variety of substrates. Various shapes and properties of the nanostructures can be achieved by controlling the interface supersaturation during the growth process. The interface supersaturation is, however, a complex function of many parameters, such as the chemical reactive environment, the transport of growth units to the growth front of nanostructures, and the structure and morphology of the substrate on which the nanostructures grow. As the growth proceeds, these parameters vary, which results in temporal and spatial variation of the interface supersaturation. Determination of the temporal and spatial variation of the interface supersaturation is essential to understand the growth mechanism of semiconductor nanostructures.

In most cases, the growth is carried out in batch reactors without a continual addition of reactants, where the concentration of chemical precursors, and thus also the supersaturation, decreases with time, which can affect the growth mechanism of the grown nanostructures. On the other hand, continuous flow reactors with constant inflow of reactants establish a time-independent supersaturation in a particular position on the sample. To understand the role of substrate, we prepared nanostructures on ZnO seed layers with a non-regular distribution of ZnO seeds and on patterned substrates with precise control over the position of ZnO seeds. To analyse the interface supersaturation, we prepared samples in both types of reactors on both patterned and non-patterned substrates. The growth velocities and the surface area of the growth front were then determined from SEM images. A model of transport phenomena using the measured reaction kinetics was implemented in COMSOL Multiphysics. The solution of the model was used to estimate the interface supersaturation and to compare it with experimentally collected data.

This work was supported by the Czech Science Foundation project 17-00355S and GA UK No 1501318.

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Magnetic response of bovine spleen.

L'ubor Dlháň¹, Roman Boča², and Martin Kopani³

¹*Institute of Inorganic Chemistry (FCHPT), Slovak University of Technology, Radlinskeho 9, SK-812 37 Bratislava, Slovakia*

²*Department of Chemistry, Faculty of Natural Sciences, University of SS. Cyril and Methodius in Trnava, Trnava, SK-917 01, Slovakia*

³*Institute of Medicinal Physics, Faculty of Medicine, Comenius University, Bratislava, SK-81372, Slovakia*

Bovine spleen has been used as a sample for deep magnetochemical investigation. Temperature dependence of the magnetic susceptibility and field dependence of the magnetization reveal a paramagnetic behaviour that violates the Curie law. The zero-field cooled magnetization and field cooled magnetization experiments show the bifurcation point at ca TC = 20 K and the blocking temperature TB = 10 K confirming a dominating portion of ferritin along with the organic tissue. There is a remnant magnetization at temperature below 20 K and the search for the magnetic hysteresis was positive.

APVV-16-0039, APVV-14-0078, I/0919/17

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Dielectric properties of (Ca,Eu)Cu₃Ti₄O₁₂ ceramics prepared by a sol-gel method

Václav Doležal¹, Jan Petrášek², Kateřina Rubešová¹, Vít Jakeš¹, Ondřej Jankovský¹, and Pavel Ctibor²

¹University of Chemistry and Technology Prague, Technická 5, Prague 6, Czech Republic

²Faculty of Electrical Engineering, Czech Technical University, Technická 2, Prague 6, 166 27, Czech Republic

The ACu₃Ti₄O₁₂ (where A = Ca, Sr, Ba) material belongs to the oxides with perovskite-based structure. The CaCu₃Ti₄O₁₂ was first synthesized in 1967 by Alfred Deschanvres, but no physical properties were measured until 2000, when it was found that this material - in the form of bulk ceramics - exhibits giant dielectric permittivity values as high as 10,000 for frequencies up to 1 MHz. However, the origin of this phenomenon is still not well understood. One suggested explanation is the mixed valence state of copper and/or the presence of secondary phases that are always formed during the synthesis (some authors proposed that the CaCu₃Ti₄O₁₂ is not stoichiometric). In any case, as acknowledged in other perovskite dielectrics, partial or full substitution in the ABO₃ stoichiometry can lead to a significant change in dielectric characteristics. Possible substitution of the alkaline earth metals in a dodecahedral position by europium(II), showing similar ionic radius and electronegativity but differing in valence shell configuration, has not been studied yet.

In this work, we focused on the mixed (Ca,Eu)Cu₃Ti₄O₁₂ perovskite prepared by the Pechini polyesterification sol-gel method. The powder precursors were pressed and sintered in air at different temperatures (1000, 1050, 1100 and 1120 °C) to obtain the desired ceramics. The phase composition of the ceramics was determined by XRD and the thermal behavior was measured by means of thermal analysis. Further, the microstructure and dielectric properties of the material were studied.

This work was financially supported by SGS20/058/OHK3/1T/13 and specific university research (MSMT No 21-SVV/2020).

A comparison of the optical and tensometric methods of the tensile test evaluation

Rastislav Ďuriš and Eva Labašová

Slovak university of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, J. Bottu 25, Trnava, 917 24, Slovak Republic

In the experimental mechanics, various contact and contactless techniques for measurement of surface deformations and strains can be used. Direct measurement techniques are mainly based on strain gauge method. The most popular contactless methods include Moiré interferometry, holography, speckle interferometry and Digital Image Correlation (DIC) [1]. Some of these methods have stringent requirements on the measurement equipment, setup procedure or coherent light source.

In the last years, the more robust and effective computational algorithms were developed for tracking the material points and estimation of whole displacement and strain fields. From this reason, the relatively simple and less expensive Digital Image Correlation optical method has been extensively used for displacement and strain field estimation in various applications like material characterization, structural health monitoring, fatigue crack growth, high temperature testing etc. The adaptability of DIC technique is in the image capturing technology obtained by standard cameras to estimate displacement and strain data from the tracking of the material points [2].

The paper focuses on determination the utility of open source MATLAB based 2D DIC software Ncorr [3] for static tensile test evaluation. The tensile tests on flat rectangular specimens were conducted and corresponding displacement and strain fields were estimated using Ncorr. The results generated by Ncorr were compared with commercially available 2D DIC software Vic 2D from correlated solutions. Results of uniaxial strains obtained by optical method were verified by experimental measurements using an installed strain gauge and extensometer.

The good agreement between results attained by evaluation of experiments using optical and standard tensometric methods was found.

This work has been supported by the Scientific Grant Agency of the Slovak Republic KEGA under the grant No. 029STU-4/2018.

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Moisture expansion of Ca-rich ceramic body

Pavla Dvořáková¹, Alexandra Kloužková¹, Martina Kohoutková², and Mária Kolářová¹

¹*Department of Glass and Ceramics, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague, Czech Republic*

²*Central Laboratories, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague*

The calcareous ceramic body is typical for historical pottery, e.g. maiolica, faience, as well as for contemporary production of ceramic tiles. The amount of the calcium component and the ratio of the other phases together with the firing temperature control the final properties of the ceramic body. The amount of the calcium component has a fundamental effect on relative expansion of the ceramic body after firing and also during long-term usage or eventually during storage. The expansion behaviour is mainly associated with the planarity of the final product which is required in the case of large-format tiles. Expansion of the ceramic body is also related to the long-term stability of historical ceramics especially glazed ceramic objects. In the case of low-fired porous ceramics the moisture expansion of the ceramic body occurs due to a humid environment. It is a process of rehydration/rehydroxylation of unstable non-crystalline residues which remains from clay minerals in the ceramic body after firing. Ceramic body expansion by the action of air or soil moisture is the main indication of the rehydration/rehydroxylation process which can lead to the deterioration of the ceramic body or the glazed surface. It is spontaneous irreversible process that begins immediately after firing and lasts for many years. Body expansion is mainly affected by the composition and porosity of the shard, as well as by the surrounding environment and the way the ceramic product is used. This process can be suppressed with a suitable mineralogical composition of calcareous ceramics. The main aim of this work is to study moisture expansion behaviour of calcareous ceramic bodies with a focus on both historical and contemporary ceramics.

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Heterostructures of ZnO on GaN Substrates Modified by Focused Ion Beam

Hana Faitová^{1,2}, Šárka Kučerová^{1,2}, Nikola Bašínová¹, Ondřej Černohorský¹, Stanislav Tiagulskiy¹, Jan Vaniš¹, Jan Grym¹, and Jozef Veselý²

¹*Institute of Photonics and Electronics, CAS, Chaberská 57, Prague 182 51, Czech Republic*

²*Faculty of Mathematics and Physics, Charles University, Prague, Czech Republic*

Zinc oxide (ZnO) is a wide bandgap semiconductor with a broad range of applications in optoelectronic devices. ZnO nanostructures can be grown by chemical bath deposition (CBD), which benefits from low temperature, large areas, and low cost. The necessary condition for CBD epitaxial growth of ZnO nanostructures is a crystallographically suitable substrate. While the preparation of high-quality ZnO seed layers remains an active topic, it is also possible to use other materials with similar lattice parameters as a substrate. Gallium nitride (GaN) is a great candidate for its mismatch of only 1,9 % to ZnO. GaN epitaxial layers are available on common substrates (Si, sapphire) with both n-type and p-type doping. This is an advantage since the production of reliable ZnO p-type is still restricted by its residual n-type conductivity. Therefore, the heterostructures of ZnO on GaN are promising for the realization of p-n junctions in optoelectronic devices.

We report on the preparation of well-defined heterostructures of ZnO/GaN on the nano-to-micro-scale using focused ion beam (FIB) lithography and solution growth. The FIB lithography enables direct patterning of the substrates by ion milling, where the shapes and the diameters of the structures are limited by the FIB resolution (several tens of nanometres). We show that the single-dot patterns can be used for the growth of highly ordered arrays of ZnO nanorods. Recent studies have demonstrated that the electronic properties of such nanorods are significantly enhanced in comparison with the nanorods grown on plain substrates without FIB patterning [1]. Our aim is to investigate the influence of the FIB treatment of the GaN substrate on the nucleation, growth, and the properties of the ZnO nanostructures.

A FIB-SEM system was used for the preparation and observation of the nanostructures, as well as for the preparation of cross-sections and lamellas for transmission electron microscopy (TEM). The ZnO/GaN interface was investigated by TEM.

The FIB patterning significantly changed the morphology and the crystal quality of the substrate. We investigated the influence of the FIB dose on these changes and thus on the nucleation and growth of the ZnO nanostructures. The results were used for further modelling of the growth processes [2], bringing us closer to the understanding of the growth mechanisms.

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Zinc oxide nanorods grown from solutions: What is next?

Jan Grym, Roman Yatskiv, Stanislav Tiagulskyi, Ondřej Černohorský, Šárka Kučerová,
Hana Faitová, Nikola Bašinová, Jan Vaniš, and Robert Hlaváč

*Institute of Photonics and Electronics of the Czech Academy of Sciences, Chaberska 57,
Prague, Czech Republic*

Synthesis of nanoscale building blocks of controllable dimensions, morphologies, and materials is central to nanoscience and nanotechnology. A great deal of interest has been recently directed towards the design of new devices using one-dimensional (1D) semiconductor nanostructures such as nanowires and nanorods (NRs). The research into 1D nanostructures has been motivated not only by their unique electrical and optical properties but also by the fact that their high aspect ratio allows for a full relaxation of elastic strain without the development of extended defects. This opens the door for the integration of different material platforms onto a given substrate, which is one of the key challenges faced by the semiconductor industry.

The question of how the 1D nanostructures grow has long fascinated scientists. While most of the NRs of classic semiconductors, such as Si, Ge, GaAs, InP, and InAs, is grown catalytically by vapor-liquid-solid (VLS) or vapor-solid-solid mechanisms, the NRs of wide bandgap semiconductors, such as GaN and ZnO, can be grown by catalyst-free methods. The catalyst-driven growth mechanisms, and particularly the vapor-liquid-solid (VLS) mechanism, have received considerable attention. On the contrary, the mechanisms of the nucleation and growth by catalyst-free methods are not deeply understood and the growth technology strongly relies on empirical results.

In this presentation, we take a critical look at the research progress in the growth of ZnO NRs from solutions. We discuss the selection, the surface treatment, and the fabrication of suitable substrates and seed layers for a particular application. We show that in conventional batch reactors the solution supersaturation varies with time. The growth rate of ZnO NRs is thus not constant over time and decreases as the growth proceeds due to the depletion of the solution in reactants. The variation of the supersaturation and of the growth rate results in the variation of incorporation of dopants, impurities, and structural defects along the NRs. Moreover, with a different level of supersaturation, the growth mechanism can be altered. We propose a solution to this issue, the so-called continuous-flow reactors, and discuss their design. We further point out key chemical and physical phenomena taking place during the growth and propose approaches to model them. To deeply understand the nucleation and growth phenomena, we developed lithographic techniques using focused electron and ion beams, which allow us to prepare highly uniform arrays of upright-standing ZnO NRs on different substrates and seed layers. Finally, we demonstrate methods of how individual nanorods and their heterojunctions can be electrically characterized with a nanoprobe installed in the scanning electron microscope.

Using optimization in new design of tribometer specimen clamping system

Štefan Hajdu

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

The article deals with the innovation of the clamping part of the tribometer, where the tested specimens are clamped. The new clamping system was designed in the CAD system CATIA V5. The advantages of the new clamping system are compared with the original clamping system of specimens on the tribometer type A30. The new clamping design is evaluated from technical, technological and marginally also from economic point of view. The new clamping design ensures easy handling and exchange of specimens. Easy handling is ensured by the conical collet, which is released by the fixation nut, and subsequently the specimen can be pulled out and replaced with a new one without disassembly the device.

The content of the article is also the strength analysis of the conical clamping collet and subsequent optimization. In the strength analysis, the conical collet is pushed into the conical cavity of the tribometer rotor by an outer fixation nut. The result is a numerical simulation of the new designed clamping system which will consist of the rotor, the conical collet, fixation nut and the tested specimen. The stress von Misses, deformations and reaction forces acting on the collet will be determined by the numerical analysis. Subsequent optimization consisting of defining the target function, boundary conditions and type of optimization will be found the minimum necessary fixation force which will be obtained from the fixation nut to ensure the transmission of torque to the clamped specimen without slip.

This contribution was written with financial support of VEGA agency within the project 1/0232/18 “Using the methods of multi-objective optimization in production processes control”.

On development of materials and crystal growth in Crytur, spol. s r. o.

Jan Havlíček^{1,2}, Jan Polák¹, and Martin Klejch¹

¹*Crytur, spol. s r.o., Na Lukách 2283, Turnov 51101, Czech Republic*

²*VŠCHT Praha, Technická 5, Praha 6 166 28, Czech Republic*

Crytur is one of the world's leading companies in synthetic crystal manufacturing and processing. Attention is paid to niche applications and client specific projects built on high expertise and close cooperation in research and development. Crytur key products are oxide single crystals grown by Czochralski method and devices containing these materials (e.g. electron microscopy detectors, radiation detectors, X-ray cameras etc.).

This contribution presents Crytur company and introduces current topics in material and technology development of Czochralski grown crystals. Namely, results of developing Czochralski technology for growth of large garnet single crystals and optimized properties of yttrium aluminium perovskite will be discussed.

Relationship between crystal structure and luminescence properties for Ce³⁺-doped rare-earth pyrosilicate

Takahiko Horiai¹, Shunsuke Kurosawa^{2,3}, Jan Pejchal¹, Takashi Hanada², Masao Yoshino², Akihiro Yamaji^{2,3}, Satoshi Toyoda^{2,3}, Hiroki Sato^{2,3}, Yuji Ohashi^{2,3}, Kei Kamada^{2,3}, Yuui Yokota², Akira Yoshikawa^{2,3}, and Martin Nikl¹

¹*Institute of Physics of the Czech Academy of Sciences, 162 00 Prague 6, Czech Republic*

²*Institute for Materials Research, Tohoku University, Sendai 980-8577, Japan*

³*New Industry Creation Hatchery Center, Tohoku University, Sendai 980-8579, Japan*

Ce³⁺-doped rare-earth (RE) pyrosilicate (Ce:RE₂Si₂O₇) have been reported as a scintillator capable of converting energy of ionizing radiation to ultra-violet or visible light [1,2]. The electric configuration of Ce³⁺ ion is defined to be [Xe]4f¹ and Ce³⁺ ion can be excited into [Xe]4f⁰5d¹ electronic configuration [3]. Since the 5d electron of Ce³⁺ ion is existed in the outermost-shell, degenerated 5d levels of Ce³⁺ ion splits due to both of the crystal field strength in Ce³⁺ site and the deviation of the electric charges in the crystal field of Ce³⁺ ion. Here, the crystal structures of Ce:RE₂Si₂O₇ have diverse range of crystal systems and space groups depending on the average RE ionic radii [4]. In this study, we performed a comprehensive study of Ce:RE₂Si₂O₇ to investigate the relationship between the crystal structure and the luminescence properties.

Since the most RE₂Si₂O₇ have incongruently melting compound and difficult to grow single crystals from the melt, we synthesized the sintered compacts using solid reaction method. As starting materials, commercial oxide powders (SiO₂, Y₂O₃, La₂O₃, CeO₂, Gd₂O₃ and Lu₂O₃) with purities of over 99.99% were used. After weighing according to (Ce_{0.01} RE_{0.99})₂Si₂O₇ (RE= La, Gd, Y and Lu), (Ce_{0.01} RE_{0.50} RE'_{0.49})₂Si₂O₇ ((RE,RE') = (La,Gd), (La,Y), (La,Lu), (Y, Gd), (Gd, Lu) and (Lu, Y)) and (Ce_{0.01} Y_{0.24} Lu_{0.75})₂Si₂O₇, the powders were formed into pellets by a hydraulic press. The pellets were pre-sintered at 1550°C for 12 hours under air atmosphere. After that, main sintering was performed at 1600°C for over 48 hours under air atmosphere.

The powder X-ray diffraction analysis results show that the phases of (Gd,Lu)₂Si₂O₇ and (La,Lu)₂Si₂O₇ are not single phase. On the other hand, the other samples were obtained single phase and classified into three kinds crystalline systems (*C2/m*, *Pna2₁* and *P2₁/c*) according to the average RE ionic radii. The crystal structure information (lattice parameters and atomic coordinates) was identified by the Rietveld refinement technique, and it was found that the average RE-O bond lengths were increased as the average RE ionic radii were increased.

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Preparation of mixed strontium-lead hafnate by wet chemical methods

Vít Jakeš¹, Kateřina Rubešová¹, Herbert Kindl¹, Romana Kučerková², and Martin Nikl²

¹*Dept of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic*

²*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6, Czech Republic*

The search for new oxides applicable as high-energy radiation detectors is connected to parameters such as high effective atomic number Z_{eff} , high light yield and resolution, and, in some applications, fast response. The first quality - Z_{eff} - is closely related to the material density that, at high values, can be also beneficial in enhancing the compactness and may allow for smaller dimensions of constructed detectors. In the case of mixed oxides, the density is generally related to the density of the constituent oxides. Therefore oxides based on heavy cations, e.g. Lu^{3+} , Bi^{3+} , Pb^{2+} , are explored, among them also HfO_2 and hafnates.

The scientific investigation of strontium hafnate, SrHfO_3 , started due to its high dielectric constant and large band gap. Additionally, it has a high effective atomic number ($Z_{eff} = 63.10$) and high density (7.56 g/cm^3) which makes it a promising material for ionizing radiation detection. As activators, Ce^{3+} ions are usually used and $\text{Ce}:\text{SrHfO}_3$ has been thoroughly studied. In search for other dopants, Pb^{2+} was proposed due to its ionic radius in 12-fold coordination being similar to that of Sr^{2+} (1.58 and 1.63 Å, respectively). Supposedly, as the content of lead increases in $(\text{Sr,Pb})\text{HfO}_3$, the density increases up to 10.2 g/cm^3 in PbHfO_3 . Additionally, unlike Ce^{3+} , the equal charge of strontium and lead cations does not induce the necessity to compensate the charge imbalance. Moreover, the Pb^{2+} cations emit at about 340 nm thanks to the partially allowed 6s-6p transition.

Historically, a solid state reaction has been the most widely used way to synthesize mixed oxides. However, apart from high energy and time demands (long sintering times at high temperatures), the major drawback of this method is the impossibility to guarantee homogeneity of the samples, which is crucial when the material is being doped with a minor fraction of a dopant cation. Wet chemical methods, on the other hand, thanks to their ability to transfer the homogeneity of a solution to the solid state, have been increasingly successful in the preparation of a huge range of materials. In this work, two wet routes were used to prepare $(\text{Pb,Sr})\text{HfO}_3$: standard Pechini polyesterification and oxidative precipitation using hydrogen peroxide. A series of hafnate samples, in which the ratio of strontium and lead cations was gradually changing according to the stoichiometry $\text{Sr}_{1-x}\text{Pb}_x\text{HfO}_3$ ($x = 0-1$), were prepared. Their phase composition was determined by XRD and their luminescence properties were measured.

This work was financially supported by MVCR as a project No. VI20192022152.

Effect of ZnO nanoparticles and illumination on growth inhibition of *Escherichia coli* and *Staphylococcus aureus* bacteria in cultivation medium.

Jaroslav Jíra¹, David Rutherford¹, Zdeněk Remeš², and Bohuslav Rezek¹

¹CTU - Faculty of Electrical Engineering, Technická 2, 166 27 Prague 6, Czech Republic

²Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6, Czech Republic

This is a study of antibacterial effects of the ZnO nanoparticles in cultivation medium (Mueller-Hinton broth) on the two basic representatives of gram-negative (*Escherichia coli*) and gram-positive (*Staphylococcus aureus*) bacteria. The broth was chosen to be able to study bacteria and antibacterial effects in bacterial natural environment.

We used three types of the ZnO nanoparticles in our experiments. There was our synthesized ZnO sample and two commercial ZnO samples for comparison - a sample with 50 nm particles and a sample with 20 μm particles. These materials were characterized by the DLS, zeta potential and SEM. The experiments were performed with two different concentrations of the ZnO (1 mg/mL and 0.1 mg/mL). The incubation was performed for 24 hours in the incubator with presence of fluorescent light or in the dark. Samples were taken at given times to be able to obtain the growth curve.

Our results show that the *E. coli* bacteria are more sensitive to the ZnO presence in the cultivation media than the *S. aureus*. We observed the reduction of viable bacteria in time during treatment compared to the reference and after 24 hours there was up to the six order decrease of colony forming units (CFU) number compared to the reference in case of the *E. coli*. The highest sensitivity of the *E. coli* was observed at the sample with our ZnO. In case of the *S. aureus* we observed approximately four order decrease of the CFU number at all samples with higher ZnO concentration. We also tested influence of light to the antibacterial effect. The fluorescent light presence had no significant effect compared to the dark cultivation.

From all possible antibacterial mechanisms of the ZnO particles (reactive oxygen species, releasing of the Zn^{2+} ions, electrostatic interaction and mechanical disruption) we estimate that the most important one is the mechanical factor, which strongly depends on the particle size and shape, which could explain the bacteria inhibition differences between used ZnO samples at the gram-negative *E. coli* with thin outer membrane and small differences at the gram-positive *S. aureus* with thick membrane.

Do we really perform physicochemical measurements on polycrystalline substances always with a known crystal structure?

Vladimír Jorík and Simona Matejová

*Faculty of Chemical and Food Technology, Slovak University of Technology, Radlinského 9,
Bratislava 81237, Slovakia*

Despite great advances in single crystal structural analysis, growing a suitable single crystal for a routine experiment can be a difficult task. Often only a few single crystals can be prepared, or it is necessary to select a single crystal from a polycrystalline mixture - usually more phase. After solving the crystal structure, it is common practice to correlate it with the results of other physicochemical methods such as e.g. infrared and UV / VIS spectroscopy, EPR spectroscopy, magnetic measurements, etc. However, one single crystal is not sufficient for these methods, and repeated preparation of a larger amount of predominantly polycrystalline sample requires control for the purity and "identity" of the crystal structure of the powder sample and single crystal. Powder diffraction analysis is a suitable method, but in its practical application we have observed occasional, commonly overlooked discrepancies. Standard powder diffraction analysis is performed at room temperature ($\sim 298\text{K}$) but single crystal structural analysis at 100K . By comparing the experimental diffractogram of the powder sample with the simulated from the structural data of the solved crystal structure, we can eliminate the influence of the thermal expansion of the sample. In many cases, however, this will not help, and even if the diffractograms on the eye are the same, we will not achieve their "identity". It has been shown and other physicochemical measurements (but also single crystal structural analysis) have confirmed that a change in temperature in the experiments can also lead to phase changes, the formation and interconversion of polymorphs or the formation / extinction of a disorder. These transformations can be irreversible as well as reversible and significant as well as subtle.

This work was supported by the Slovak Research and Development Agency, grant No. APVV-18-0016 and Slovak Grant Agency KEGA (KEGA 018STU-4/2020)

Structure and properties of barium tungstate-phosphate glasses

Petr Kalenda, Ladislav Koudelka, and Petr Mořner

University of Pardubice, Studentská 95, 532 10 Pardubice, Czech Republic

Phosphate glasses of the BaO-P₂O₅-WO₃ system were studied in five compositional series: (A) (50-x/2)BaO-xWO₃-(50-x/2)P₂O₅, (B) 50BaO-yWO₃-(50-y)P₂O₅, (C) 40BaO-zWO₃-(60-z)P₂O₅, (D) (60-u)BaO-uWO₃-40P₂O₅ and (E) vBaO-40WO₃-(60-v)P₂O₅. Thermal behavior of the glasses was studied by differential thermal analysis and dilatometry and the glass structure was studied by Raman and ³¹P MAS NMR spectroscopies. The glass transition temperature, T_g, increases in all compositional series with increasing WO₃ content. In glasses with a low WO₃ content Raman spectra show on the domination of strong vibrational bands of terminal oxygen atoms in WO₆ octahedra at 885 and 945 cm⁻¹ (vibration of W=O and W-O⁻ bonds in tungstate structural units). On the Raman spectra of glasses with a high WO₃ content, a broad band at 820-841 cm⁻¹, ascribed to W-O-W bonds, was assigned to the formation of clusters composed of WO₆ units. ³¹P MAS NMR spectra shows on the shortening of phosphate chains in the glass network.

The authors are grateful for the financial support from the Grant Agency of the Czech Republic (Grant No. 18-01976S).

Thirty years of seminars “Development of Materials Science in Research and Education”

Marian Koman¹ and Zdeněk Kožíšek²

¹*Department of Inorganic Chemistry, Slovak University of Technology, Radlinského 9, 812 37 Bratislava, Slovakia*

²*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6, Czech Republic*

The seminar “Development of Materials Science in Research and Education” started at Gabčíkovo in 1991 by the initiative of the Czech and Slovak Association for Crystal Growth and the Slovak Expert Group of Solid State Chemistry and Physics.

The objective of this meeting is to offer an opportunity to Czech and Slovak teachers and scientists as well as guests from other countries who are working in the field of Materials Science to present their recent results and experience and to exchange new ideas and information.

The scientific session will cover the following topics on materials science:

- Trends in the 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 characterization of materials
- Results of materials research

A total of 1369 participants (some repeatedly) attended the previous 29 seminars, and 1172 lectures were given. The first four seminars also included poster sections. 6 Schools of Crystal growth (total: 38 lectures, 184 participants) were organized in the period 2000-2010. Proceedings of each seminar have been published, since 1994 in English and with an ISBN number. Papers were published on 2132 pages. The proceedings were edited by a total of 15 editors.

The focus of the papers also changed during the seminars. The main areas are listed above, but some areas have received more attention. The composition of the papers also depended on the focus of the seminar participants. In the beginning, more attention was paid to pedagogical issues and programs. Gradually, attention was focused on new technological processes and our own results. An important part of the papers was the study of the properties of materials, mechanical, electrical, optical, magnetic, etc. These have been investigated on various types of materials, single crystals, sintered materials, ceramic and glass materials, polymers as well as concretes, thin films and, more recently, nanomaterials.

During these thirty years, generations of scientists and educators - participants in seminars - have also exchanged, and it is gratifying that the young next generation is also involved in the development of materials science and the study of new materials.

The authors wish to thank the APVV-18-0016 for financial support.

Phosphate glasses modified with transition metals

Ladislav Koudelka, Petr Mošner, and Petr Kalenda

University of Pardubice, Faculty of Chemical Technology, Studentská 95, 532 10 Pardubice, Czech Republic

Phosphate glasses present an important group of glass materials having several commercial applications. The most important applications of these glasses are laser glasses, glasses for the deposition of radioactive wastes, and glass solders. Nd-doped laser glasses are produced and tested for the application in fusion reactors. For the storage of radioactive wastes, Fe₂O₃-P₂O₅ glasses were proposed due to their high chemical durability and the ability to include a high content of radioactive oxides. Glasses of the ternary system SnO-ZnO-P₂O₅ were investigated for the application in solders replacing lead-based glasses. These glasses reveal a sufficient chemical durability, low values of the glass transition temperature and a low coefficient of thermal expansion.

Our studies of ternary phosphate glasses were devoted mainly to three transition metal oxides MoO₃, WO₃ and Nb₂O₅, which are able to form large glass forming regions in various ternary systems. These studies will be demonstrated on two ternary systems BaO-MoO₃-P₂O₅ and BaO-Nb₂O₅-P₂O₅.

Structure of glasses in the BaO-MoO₃-P₂O₅ ternary system was studied by Raman and ³¹P NMR spectroscopies. The glass-forming region in the ternary system was determined, and stable glasses with 0-70 mol% MoO₃ were obtained. From the NMR and Raman spectra of glasses, a structural model was proposed. Structural network contains mostly MoO₆ octahedra and PO₄ tetrahedra. In glasses with a high MoO₃ content, the presence of a broad Raman band 854 cm⁻¹, ascribed to Mo-O-Mo bonds, showed on the formation of clusters composed of MoO₆ units. MoO₆ octahedra prevailed in the glass structure, similarly to crystalline MoO₃ and to the compound Ba(MoO₂)₂(PO₄)₂. Formation of MoO₄ tetrahedra was proposed in the glasses with a low P₂O₅ content.

Phosphate glasses of the ternary system BaO-Nb₂O₅-P₂O₅ were studied in two compositional series with a constant BaO or Nb₂O₅ content. Chemical durability of the Nb₂O₅-containing glasses is high and the glass transition temperature increases significantly with increasing Nb₂O₅ content as well as the index of refraction. According to the Raman spectra at low Nb₂O₅ content niobium forms isolated octahedra NbO₆ incorporated in the glass network, but when Nb₂O₅ content increases, these octahedra are linked into chains and further into three-dimensional clusters. NbO₆ octahedra clustering is reflected also in the ³¹P MAS NMR spectra.

Study of the glass to crystal transformation was realized for two ternary compounds in the glass-forming region of the BaO-Nb₂O₅-P₂O₅ system: Ba₃Nb₂(PO₄)₄O₂ with 16.66 mol% Nb₂O₅ (glass composition 3BaO.1Nb₂O₅.2P₂O₅) and BaNb₂P₂O₁₁ with 33.33 mol% Nb₂O₅ (glass composition 1BaO.1Nb₂O₅.1P₂O₅).

The authors are grateful for the financial support to the research project No. 18-01976S of the Grant Agency of Czech Republic.

Crystallization of aluminum droplet

Zdeněk Kožíšek, Robert Král, and Petra Zemenová

*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Praha 6,
Czech Republic*

Aluminum (Al) melted droplet of mass $m = 9.9$ mg was undercooled with the cooling rates 2-20 K/min and the crystallization temperature $T_c \approx 642$ °C ($\Delta T \approx 18$ K) was detected by the Differential Scanning Calorimetry (DSC) apparatus under non-isothermal conditions. Experimental data were analysed by the Johnson-Mehl-Avrami (JMA) model under assumption that nucleation and growth occur at T_c . It seems to be a reasonable presumption as the growth rate of Al is high (tens of meters per second). JMA model enables us to determine the kinetic Avrami coefficient $n = d + 1 \leq 2$ from experimental data. However, $n \leq 2$ shows that the JMA model fails as the dimensionality of growth $d < 1$ is unrealistic.

Similarly, we analysed the DSC data recorded at isothermal conditions with crystallization occurring at $\Delta T \approx 6$ K below the melting temperature T_m . Al liquid droplet was cooled down repeatedly to the temperature $T > T_c$ and kept at the isotherm sufficiently long time. Even at this low supercooling, the crystallization of droplet occurred after a time delay τ . The time delay since the beginning of the isotherm T up to crystallization event changed occasionally: $\tau \approx 10 - 50$ minutes. Experimental data confirmed stochastic nature of crystal nucleation similarly to other systems [1].

We have numerically solved the kinetic equation of the crystal nucleation within standard model [2] to determine the time dependent number of nuclei as a function of their size. Small clusters have a tendency to diminish and only supercritical clusters (nuclei) grow independently. At crystallization, it is necessary to form a sufficient number of nuclei to initiate growth. The number of Al atoms in the liquid droplet decreases as the crystal phase is formed and this effect was taken into account. The stochastic data of the time delay τ are often analysed with stochastic method, when Poisson distribution of nuclei is considered. However, as a fit parameter the stationary nucleation rate is used and that is why this analysis fails due to non-stationary process. Standard nucleation model enables us to determine the interfacial energy limit, when the first nuclei are formed within the system. Experimental value of time delay of crystallization event is high in respect to high growth rate. Crystallization probably occurs by two step mechanism [3] when the structure of small sub-critical clusters differs from larger ones and thus kinetics of small clusters is slow.

This work was partially supported by Operational Programme Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760).

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Growth and characterization of zirconium-doped cesium hafnium chloride crystals for scintillators

Robert Král¹, Vojtěch Vaněček^{1,2}, Juraj Páterek^{1,2}, Maksym Buryi¹, Vladimír Babin¹,
Vítězslav Jarý¹, Petra Zemenová^{1,3}, Kateřina Zloužeová^{1,3}, Aleš Bystřický¹,
and Martin Nikl¹

¹*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6,
Czech Republic*

²*Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical
Engineering, Břehová 7, 110 00 Prague 1, Czech Republic*

³*University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6,
Czech Republic*

Currently, cesium hafnium chloride (Cs₂HfCl₆) has been widely studied for its promising scintillation properties. Due to its high light yield up to 54,000 ph/MeV, energy resolution of 2.8 % at 662 keV, scintillation response of 4.4 us (95 % of energy) at 662 keV, density of 3.86 g/cm³ [1], and low hygroscopicity, it is considered for possible application as a new cost effective scintillator for gamma ray spectroscopy. The scintillating mechanism in the undoped Cs₂HfCl₆ is ascribed to intrinsic luminescence originating in a self-trapped excitons represented by a V_k center [3]. Furthermore, an influence of nonstoichiometry on the magnetic properties was reported as well [4]. The Cs₂HfCl₆ is formed by cesium chloride and hafnium chloride mixed together in stoichiometric ratio 2:1 congruently melting at ca. 821°C [5]. The Cs₂HfCl₆ crystallizes in cubic structure with lattice parameters $a = 10.42 \pm 0.01 \text{ \AA}$ (space group Fm-3m).

This work is aimed on the preparation of starting materials (CsCl, HfCl₄), synthesis of Cs₂HfCl₆, doping of Cs₂HfCl₆ by tetravalent elements A⁴⁺ (such as Zr⁴⁺), and growth of Cs₂HfCl₆:Zr⁴⁺ crystals by the vertical Bridgman method. Prepared crystals were cut and polished for subsequent examination concerning their physical, structural, optical, luminescence, and scintillation properties.

The support of Czech Science Foundation by project no. 18-17555Y and partial support by Operational Programme Research, Development and Education financed by European Structural and Investment Funds and the Czech Ministry of Education, Youth and Sports (Project No. SOLID21 CZ.02.1.01/0.0/0.0/16_019/0000760) is gratefully acknowledged. The authors thank to Mr. A. Cihlář for preparation and purification of starting materials.

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High-quality seed layers for patterned growth of ordered ZnO nanorod arrays

Šárka Kučerová^{1,2}, Nikola Bašínová¹, Ondřej Černohorský¹, Jozef Veselý², Roman Yatskiv¹, Stanislav Tiagulskyi¹, Jan Vaniš¹, and Jan Grym¹

¹*Institute of Photonics and Electronics, CAS, Chaberská 57, Prague, 182 51, Czech Republic*

²*Faculty of Mathematics and Physics, Charles University, Ke Karlovu 3, Prague, 121 16, Czech Republic*

Properties of ZnO seed layers (SLs) are fundamental for the growth of ZnO nanorods (NRs). Crystalline structure of the ZnO SL affects the nucleation and growth of ZnO NRs in ways, which significantly differ from the nucleation and growth of ZnO NRs on ZnO bulk substrates or from heteroepitaxially prepared ZnO layers.

The size, the shape, and the preferential orientation along the c-axis as well as the in-plane orientation of the crystallites within the ZnO SL are crucial for the uniform nucleation, vertical alignment, and crystalline quality of the ZnO NRs. We have recently prepared high-quality ZnO SL by the sol-gel process [1].

However, the influence of the ZnO SLs is even more significant and visible during patterned growth, where the NRs do not nucleate randomly - their positions are lithographically defined. Any deviation from the orientation of the crystallites along c-axis causes visible misalignment of the grown nanorods. For good crystallinity, ideally monocrystallinity, of the ZnO NRs grown on patterned ZnO SL, the correlation between the size of an opening in the patterning mask and the size of the crystallites in the SL is crucial. If the size of the opening is equal or smaller than the average size of the crystallites in the SL, the probability of the nucleation and growth of a monocrystalline NR from a single crystallite is significantly increased. Consequently, the requirements for the SL are a high texture with the c-axis oriented perpendicular to the substrate surface, maximum size of the crystallites with a small dispersion of sizes, and a low surface roughness to ensure high quality and reproducibility of lithographic patterning. When all the requirements are fulfilled, highly ordered arrays of identical, monocrystalline, well aligned ZnO NRs can be grown.

We present patterned growth of ordered ZnO NRs on the SLs, where the parameters of the sol-gel process are varied. The SLs were examined with SEM, EBSD, photoluminescence, AFM, AC impedance measurements, TEM, ACOM-ASTAR, and EDX. A significant influence of the concentration of precursors on the average size of the crystallites was observed and the impact of the heat treatment on the shape of the crystallites was investigated. Finally, a patterned growth of ZnO nanorod arrays was performed by chemical bath deposition. The NRs were investigated by SEM, TEM, ACOM-ASTAR, and EDX to describe the relationship between the properties of the patterned ZnO seed layers and the properties of the ZnO nanorods and to shed light on their nucleation and growth.

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Origami-kirigami approach to materials structures modelling

Iveta Markechová and Hana Stúpalová

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

Additive manufacturing and origami/kirigami principles fit together like a coffee cup and saucer. Recently derived translational surface with an elliptic curve (not an ellipse), as the governing one, led to constructing an origami-like object. Set of eight surfaces, each with a square-shaped orthogonal projection, turned out to be enchantingly similar to heaven-and-hell-origami. The Starting Translational Surface (STS), engaged in the presented work, is originally subjected to the selected linear and nonlinear transformations in two ways. The first one is dedicated to spacial placement of STS replicas. Shape STS variations represent the second approach. Square-shape of STS orthogonal projection is preserved during all the mappings. On the other hand, especially in this point, the similarity with origami/kirigami structures is broken; generally, square-shaped sheet of paper changes via folding. In our paper, preserved orthogonal projection offers suitable opportunities to illustrate a structure of the hypothetical material. Explicit and parametric equations of geometrical elements, transformational matrices and MATLAB application MuPAD serve as useful mathematical and computational tools for formal and graphical representation of the modeled structures.

This publication is the outcome of the "UNIVERSITY SCIENTIFIC PARK: CAMPUS MTF STU – CAMBO" project implementation (ITMS: 26220220179) supported by the Research & Development Operational Program funded by the EFRR. This contribution was also funded by the institutional project 1609 04/2018-12/2019 of "Relation elliptic curve - ellipse from the viewpoint of selected differential equations and geometric design of virtual model of robogami". The first author is especially grateful to Marek Rariga for his creative interest in the theme within a bachelor thesis framework.

Current state in the field of life-long learning of employees in the mechanical engineering and automotive industries in the Slovak Republic and the Czech Republic

Mária Behúlová¹, Ivo Říha², Jan Václav³, and Jana Mesárošová¹

¹*Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, Ulica Jána Bottu 2781/25, 917 24 Trnava, Slovakia*

²*National Cluster Association, Studentská 6202/17, 708 00 Ostrava, Czech Republic*

³*Slovak Chamber of Commerce and Industry in Bratislava, Regional Chamber in Trenčín, Jilemnického 2, 911 01 Trenčín, Slovakia*

Since February 2020, a project entitled “Establishment strategic partnerships and preparation of advanced life-long learning courses for companies and clusters with innovative potential in the field of mechanical engineering and automotive industry - EDU-MATech“ has been implemented within the Operational Program 304000 - Interreg VA Slovak Republic - Czech Republic 2014-2020, which is co-funded by the European Regional Development Fund (ERDF). The project partners are the Slovak University of Technology in Bratislava, Faculty of Materials Science and Technology in Trnava, National Cluster Association, Ostrava - Poruba and the Slovak Chamber of Commerce and Industry in Bratislava, Regional Chamber in Trenčín.

The main aim of the project is to establish strategic partnerships and develop a cross-border strategy for life-long learning in selected technically oriented fields for companies in the mechanical engineering and automotive industries, taking into account the application of common European qualifications frameworks for the recognition of acquired qualifications. The project goals are based on the real requirements and needs of employers and the labor market. The key output will be the preparation and pilot implementation of advanced life-long learning programs in the fields of

- materials science and production quality assurance;
- engineering technologies and computer support of production preparation;
- automation and control of technological processes and mechatronic systems

and the development of a common database of training programs as a tool to increase knowledge, skills and competencies of employees, as well as competitiveness and innovation potential of companies.

The paper presents an overview of the current state in the field of life-long learning in the Slovak Republic and the Czech Republic, the main problems, needs and requirements of the labor market and compares their compliance with current trends and strategic documents at the regional, national and European level.

The contribution is supported by the project ITMS2014+ 304011U768 under the Operational Programme 304000 - Interreg VA Slovak Republic - Czech Republic 2014-2020 funded by the ERDF.

Impact of solution ageing on the Er³⁺/Yb³⁺:LiNbO₃ thin films properties

Dana Mikolášová¹, Kateřina Rubešová¹, Vít Jakeš¹, Pavla Nekvindová¹, Marcela Dendisová², and Jiří Oswald³

¹*Dept of Inorganic Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic*

²*Dept of Physical Chemistry, University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic*

³*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6, Czech Republic*

LiNbO₃ is still one of the most applied oxides in optoelectronics, acousto-optics, ferroelectrics etc. The LiNbO₃ thin films are produced by various methods, e.g. liquid phase epitaxy, molecular beam epitaxy, pulsed laser deposition, chemical vapour deposition, physical vapour deposition or sol-gel techniques. Generally, sol-gel methods are cheaper than other deposition methods and can ensure the homogeneous distribution of potentially functionalizing dopants. On the other hand, the quality of thin films is ensured only if the synthesis and deposition of solutions is reproducible and standardized. Therefore, mainly freshly prepared solutions are utilized, which, apart from being time-demanding, requires high purity starting compounds that are not cheap.

To solve this problem, not only freshly prepared solutions could be used, especially in the case of automatized deposition. In such a case, however, the time-dependent physical-chemical behaviour of solutions, which can affect the microstructure and thus physical properties of films, needs to be studied.

In our work, the thin films were deposited using an aqueous solution of polyvinylpyrrolidone (PVP) that chelates and stabilizes the present cations (Er^{III}:Yb^{III}:Li^I:Nb^V). The solutions were left to age for up to 10 months. These solutions were characterized by MIR and TG/DTA analysis. Thin films were then deposited from the aged solutions by spin-coating and various thermal treatment regimens were tested. The waveguiding, luminescent and microstructural properties of the final films were examined.

Financial support from specific university research (MSMT No 21-SVV/2020).

Effect of titanium dioxide on thermal behavior and properties of niobate-phosphate glasses

Petr Mošner, Ladislav Koudelka, and Petr Kalenda

Faculty of Chemical Technology, University of Pardubice, Studentská 95, Pardubice 532 10, Czech Republic

Niobium is one of the elements used to modify the structure and properties of phosphate glasses. It was found that niobium containing phosphate glasses show good chemical durability, good VIS to near IR transparency, high transition temperature and high refractive index. These properties contribute to their prospective applicability for various optical devices or as potential candidates for the nuclear waste immobilization. Moreover, niobate-phosphate glasses show also promising biological response with stimulation of alkaline phosphatase activity of osteoblast-like cells. The previous results indicated that the incorporation of larger amounts of Nb₂O₅ into phosphate glasses requires the addition of stronger bases like alkali or alkaline earth oxides. TiO₂ is used as a nucleating agent in silicate glasses, nevertheless recent studies indicate that the TiO₂ addition can markedly improve properties of the phosphate glasses and glass-ceramics, e.g. chemical durability, thermal, mechanical and optical properties.

TiO₂ containing phosphate-niobate glasses were prepared in the compositional series 40Na₂O-40P₂O₅-20Nb₂O₅+xTiO₂ within the range of x=0-36, using conventional melt quenching technique, when the melt (1200-1400 °C) was poured into a tempered graphite mould. Glasses were characterized by the measurements of density, molar volume and chemical durability. The structure of glasses was investigated by Raman spectroscopy, their thermal properties were studied by DSC, thermodilatometry and hot stage microscopy. Crystalline phases were identified by X-ray powder diffraction analysis.

Raman spectra showed that the structure of starting 40Na₂O-40P₂O₅-20Nb₂O₅ glass is formed mainly by metaphosphate (Q²) and diphosphate (Q¹) structural units interconnected by P–O–P bonds. Nb₂O₅ is incorporated in the structural network in the form of NbO₆ octahedral units. Introducing and gradually increasing of TiO₂ content causes a slow depolymerization of the phosphate structural network and the development of probably TiO₆ octahedral units in the local structure of the glass matrix. Glasses show the almost linear increase in the density, whereas molar volume steeply decreases with increasing TiO₂ content. The highest values of glass transition temperature, dilatometric softening temperature, crystallization temperature and flow temperature were obtained for the glass containing 28 mol% TiO₂. This glass revealed also the highest chemical durability against water attract and on the contrary the lowest thermal expansion. The DSC curves indicated that all glasses crystallize on heating.

The authors are grateful for the financial support to the research project No. 18-01976S of the Grant Agency of Czech Republic.

Dynamic analysis of cone waveguide for ultrasonic assisted technological processes

Milan Nad', Štefan Šimon, and Peter Bucha

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

The new modern materials (ceramics, composites and others) developed for specific applications are generally characterized by improved mechanical properties. As a result, it is clear that this situation leads to relatively large problems in their technological processing. For this reason, the hybrid technology processes are used to process these materials, in which the combination of conventional technological processes with ultrasonic vibrations is used. The transmission of vibrations into the technological process [2] is performed by means of the so-called ultrasonic horn, which has to vibrate only in resonant mode. Design and analysis of cone ultrasonic horn with adaptive change of modal properties is solved in this paper. Modification of modal properties [1], [3] is carried out using an embedded core. By the change of dimensions, position and material properties of core, the distribution of the spatial properties of horn structure are modified. The dependence of modal properties (mode shapes and natural frequencies) on the dimension parameters and material properties of core using the numerical simulations by finite element method are investigated in this paper.

The work was supported by the Scientific Grant Agency of the Slovak Republic within the project VEGA No. 1/0796/20.

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The Cs₂HfCl₆ crystal scintillators as a perspective detector to search for rare nuclear process

Serge Nagorny¹, Vincenzo Caracciolo^{2,3}, Pierluigi Belli^{2,3}, Rita Bernabei^{2,3}, Fabio Cappella^{4,5}, Riccardo Cerulli^{2,3}, Antonella Incicchitti^{4,5}, Matthias Laubenstein⁶, Stefano Nisi⁶, and Peng Wang¹

¹Queen's University, 99 University Ave, Kingston, K7L 3N6, Canada

²INFN sezione Roma "Tor Vergata", Rome, Italy

³Dipartimento di Fisica, Università di Roma "Tor Vergata", Rome, Italy

⁴INFN - Sezione di Roma I, Roma, Italy

⁵Dipartimento di Fisica, Università di Roma "La Sapienza", Rome, Italy

⁶INFN - Laboratori Nazionali del Gran Sasso, Assergi, Italy

Nowadays there is significant interest in Cs₂HfCl₆ scintillating crystals because of their outstanding scintillating properties demonstrated in recent measurements - a high light yield (up to 60000 photons/MeV), perfect linearity of the energy response, excellent energy resolution (< 3.5% at 662 keV in the best configuration), a quenching factor for alpha particles around QF = 0.3-0.5, and excellent statistical pulse shape discrimination ability.

The internal background of Cs₂HfCl₆ crystals was also investigated, using an ultra-low background high purity germanium detector. The CHC crystal showed a very low content of U and Th natural decay chains, only limits at the level of few mBq kg⁻¹ could be set after 500 hours of measurement. Nevertheless, it contained man-made and cosmogenic radionuclides as ¹³⁷Cs (about 0.8 Bq/kg), and ^{132,134}Cs and ¹⁸¹Hf with activities at the level of few tens mBq kg⁻¹.

Moreover, one should mention that the Cs₂HfCl₆ crystal is the first scintillating material containing a high fraction of Hf in mass (about 26%). Thus, combination of all above listed scintillating properties and the rather promising radiopurity, together with the high mass fraction of Hf opens up new opportunities to search for rare nuclear processes occurring in Hf isotopes applying of the "source = detector" experimental approach with advanced sensitivity.

As a great example of this crystal use, preliminary results on the first long terms (over about 2800 hours) ultra-low background measurements with a 7 g CHC crystal as scintillating detector performed at the Gran Sasso Underground Laboratory are reported. Rare alpha decay of ¹⁷⁴Hf isotope was clearly detected, and the preliminary value of the measured half-life value is in great agreement with various theoretical models and discards previously measured value 2.0(4) × 10¹⁵ y. Moreover, we are presenting a detailed analysis of the internal background components that will be useful for further applications on such crystal. We have characterized this material by combination of mass-spectrometry, low-background gamma spectrometry, time-amplitude analysis and analysis of scintillating signals pulse shape methods. The current progress in the development and production of radiopure and large volume Cs₂HfCl₆ crystals is reported as well.

The future perspective of the use of Cs₂HfCl₆-like family of scintillating crystals as highly sensitive detectors to search for rare nuclear processes in Os, Zr, Sn and V is also discussed.

Examination Crystal plasticity in Cool draw tube forming using FEM and Voronoi Tessellation

Martin Necpal and Maroš Martinkovič

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

The analyses of the tube drawing process can be divided into two basic parts of investigations. Macro-scale and Micro-scale. Macro-scale analyses involve investigation of dimensional accuracy of the formed specimen, drawing forces, strain, stress, etc. The analyses of the tube drawing process in the macro-scale have been studied experimentally or theoretically using numerical methods for many years. For the final product of drawing process is also important to know the surface quality for example. For this purpose, it is important to know micro-scale material properties (spatial distribution of grain neighborhood orientation etc.), and examine the context of micro forming material.

There has been a trend in the last decade to make a link between macro-scale forming and micro-scale material properties and name it Multi-scale modeling. This research illustrates the possibility to use Voronoi Tessellation grain microstructure model in Deform FEM software to predict grain plasticity. The result obtained from numerical simulation is compared with direct reconstruction, derivation of basic stereology equation, and measurement using the line coincidence method of the oriented line using real specimen grain deformed in the cold forming process drawing the tube through a die.

This work was supported by the Slovak Research and Development Agency under contract No. APVV-15-0319 Grant Agency of the Slovak Republic Ministry of Education.

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Growth of perovskite oxide single crystals and their luminescence and scintillation properties

Jan Pejchal¹, Vladimir Babin¹, Maksym Buryi¹, Lenka Procházková^{1,2}, Christo Gugushev³, Michael Schulze⁴, František Hájek¹, Alena Beitlerová¹, Romana Kučerková¹, Kateřina Rubešová⁵, Vít Jakeš⁵, Jan Bárta¹, Petra Zemenová¹, and Robert Král¹

¹*Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, Prague 16200, Czech Republic*

²*Faculty of Nuclear Sciences and Physical Engineering, Czech Technical University, Břehová 7, Prague 1, Czech Republic*

³*Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany*

⁴*Scientific Instruments Dresden (SciDre) GmbH, Gutzkowstrasse 30, Dresden, Germany*

⁵*Department of Inorganic Chemistry, University of Chemistry and Technology, Technická 5, Prague, Czech Republic*

Inorganic scintillation single crystals have been utilized in many fields of technology and research, such as high-energy physics, environmental monitoring, geological survey and oil well logging or astronomy. The Medical imaging and especially security scanning are nowadays the applications mostly stimulating the development of new scintillation materials due to increasing demands on their performance.

Aluminum perovskites represent an important group of promising scintillation materials [1], 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 [2] will be presented and discussed together with brief overview of their structure and luminescence and scintillation characteristics.

The SrHfO₃(SHO) - based perovskite scintillators have been studied since 1990's [3]. High efficiency and quite fast decay time were reported for Sr-deficient undoped SHO powders [4]. Similar scintillation properties were found for the Sr-deficient lighter, the strontium zirconate SrZrO₃ (SZO). Due to very high melting points (2730 °C for SHO, 2646 °C for SZO), all the research was conducted on powders or ceramics. Therefore, we prepared single crystalline samples of undoped Sr-deficient SHO and SZO using the optical floating zone method to perform a study on their luminescence and scintillation properties. The overall scintillation efficiency of SHO was comparable to the Bi₄Ge₃O₁₂ reference scintillating material, while that of SZO was considerably lower. The luminescence mechanism and scintillation properties of the SHO and SZO crystals will be presented and discussed together with the crystal growth and morphology.

This work was supported by the Czech Science Foundation (GA ČR) project no. 18-14789S.

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Temperature behavior of the zero-phonon line of vanadium photoluminescence in SrTiO₃:V crystal

Zdeněk Potůček¹, Kateřina Aubrechtová¹, Zdeněk Bryknar¹, and Vladimir Trepakov²

¹*Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Trojanova 13, 120 00 Prague, Czech Republic*

²*Ioffe Physical-Technical Institute of the RAS, Polytekhnicheskaya 26, 194021 St.-Petersburg, Russia*

Strontium titanate (SrTiO₃) is a model ABO₃ perovskite-type oxide with highly polarizable structure and soft TO phonon modes. However, SrTiO₃ crystals remain in paraelectric phase down to the lowest temperatures because transition to ferroelectric phase is suppressed by quantum effects. Very unusual and large temperature shift of the zero-phonon R-line was observed in the emission spectra of photoluminescence of Cr³⁺ and Mn⁴⁺ impurity ions (3d³ electron configuration) substituted for octahedral coordinated Ti⁴⁺ ions in SrTiO₃:Cr and SrTiO₃:Mn crystals, respectively [1, 2]. Besides, this temperature shift was found to be proportional to the reciprocal permittivity of SrTiO₃ crystals and to the square of temperature-dependent TO₁ soft phonon mode frequency below the temperature of structural phase transition from the cubic to tetragonal phase in the vicinity of 105 K. At the same time, the R-line temperature shift occurs in the case of Cr³⁺ and Mn⁴⁺ ions in the opposite direction. Better understanding of these effects that are very unusual in the spectroscopy of transition metal impurity ions in ionic crystals requires an analysis of temperature behavior of zero-phonon emission lines for other impurity ions with different 3dⁿ electron configuration in SrTiO₃ crystals.

Recently we have found structured photoluminescence in the near infrared spectral region in the slightly vanadium doped SrTiO₃ single crystals that at low temperatures consisted of a pronounced zero-phonon line near 1157 nm accompanied by well developed vibrational sidebands. We suppose that this photoluminescence originates from V³⁺ ions (3d² electron configuration) substituted for Ti⁴⁺ ions in SrTiO₃:V crystal. Present detailed analysis of emission spectra at temperatures between 4.2 and 300 K showed an unusually large temperature shift of the zero-phonon line for studied photoluminescence of SrTiO₃:V crystal as well. The origin of the observed line shift to lower energy side with increasing temperature will be discussed taking into consideration structure of vanadium impurity center in SrTiO₃:V crystal and the specificity of impurity-lattice interaction in ABO₃ perovskite-type oxides with soft TO phonon modes.

This work was supported by the project "Center of Advanced Applied Sciences", Reg. No. CZ.02.1.01/0.0/0.0/16-019/0000778, of the Operational Program Research, Development and Education co-financed by the European Structural and Investment Funds and the state budget of the Czech Republic.

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The optical emission spectroscopy of the inductively coupled plasma used for modification of chemical, optical and electronic properties of nanostructured ZnO

Zdeněk Remeš¹, Júlia Mičová², Bohuslav Rezek³, and Hua-Shu Hsu⁴

¹*Institute of Physics of the Czech Academy of Sciences, Na Slovance 1999/2, Praha 8, Czech Republic*

²*Institute of Chemistry SAS, Dubravska cesta 9, 84538 Bratislava, Slovakia*

³*CTU Faculty of Electrical Engineering, Technická 2, 166 27 Praha 6, Czech Republic*

⁴*National Pingtung University, Minsheng Rd. 4-18, 900 Pingtung City, Taiwan*

Plasma treatment of the nanostructured surface of thin films has increasingly attracted the attention of scientists and technologists due to the high surface-to-volume ratio and related size effects. The surface and size effects impose challenges for energy conversion or sensing applications, i.e., in solar cells, optoelectronic devices, gas sensors, or electrochemical energy storage. The plasma modification of surfaces by plasma processing provides further adjustment of properties for application. The plasma treatment is done in a novel inductively coupled plasma (ICP) reactor and monitored in-situ by optical emission spectroscopy (OES) in the spectral range 350-1050 nm. The reactor operates at 13.56 MHz, 10-200 W discharge power, pressure 1-100 Pa and gas flow 1-100 sccm using hydrogen (purity 99.999%), oxygen (purity 99.995%), argon (purity 99.998%) and nitrogen (purity 99.999%). After the plasma treatment of single crystal as well as nanostructured ZnO [1] we observe changes in the chemical, optical and electronic properties such as optical absorption spectra, photoluminescence spectra, Raman spectra, surface conductivity, surface energy as measured by contact angle.

This work was supported by the Operational Programme Research, Development and Education project SOLID21 - CZ.02.1.01/0.0/0.0/16_019/0000760, the Czech Science Foundation project 19-02858J, and by the Scientific Grant Agency (VEGA, Slovak Academy of Sciences, Grant No 2/0157/20) and by the Ministry of Science and Technology of Taiwan under Grant Nos. M-153-001-MY3, 107-2119-M-153 -001.

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Microscopic study of zinc oxide molecular biointerface

Bohuslav Rezek¹, Jaroslav Jíra¹, David Rutherford¹, Hadi Hematian¹, Egor Ukraintsev²,
and Zdeněk Remes²

¹*Faculty of Electrical Engineering, Czech Technical University in Prague, Technická 2,
16627 Prague 6, Czech Republic*

²*Institute of Physics of the Czech Academy of Sciences, Cukrovarnicka 10, 16200 Prague 6,
Czech Republic*

Zinc oxide is a semiconductor material well known as transparent conductive electrode as well for its photocatalytic and bactericidal properties. It has been prepared in various forms and sizes and it also available commercially. Properties and functions of various ZnO nanoparticles and nanomaterials are thus intensively investigated also in biological systems for diagnostics, therapy, health risks assessment as well as decontamination purposes. Yet understanding actual processes behind the observed effect is still debated. One of the reason is complexity in terms of ZnO fabrication properties, resulting structural, chemical and electronic properties as well as the effect of biological environment, where the nanomaterials can significantly change the size, shape and zeta potential (even reverse it). The mutual interaction of ZnO nanomaterials and biological environment can manifest itself in various ways and can be very specific for particular nanomaterial and its surface modification.

In this work, we focus on the actual interface between ZnO and biological environment. At first, by using atomic force microscopy (AFM) we have studied adsorption of fetal bovine serum and bovine serum albumin (typical supplement in cell culture medium) on ZnO plates. Droplets of biomolecular solution (20 uL, 30 mg/mL) were deposited on clean ZnO substrates for 10 minutes, rinsed with demi water, dried with nitrogen. We employed CF₄ treated AFM tips to minimize tip contamination by biomolecules during morphology analysis. The RMS surface roughness was below 1 nm in all cases. Globular features were resolved for both FBS and BSA. We also employed so-called nanoshaving method to determine thickness of the biomolecules adsorbed on ZnO. Thickness of FBS 1.9 ± 0.2 nm, BSA was 2.0 ± 0.3 nm, thus very comparable. However, BSA layer was more strongly attached to ZnO compared to FBS layer. Force of 10 ± 5 nN was sufficient to remove FBS layer from ZnO, however, 25 ± 5 nN were needed to remove BSA layer. Compared to our reference, oxidized diamond surfaces, the morphology of molecular layer is similar, however, the binding forces are much stronger on ZnO. We performed atomic scale computing of the ZnO biointerface by force field method to support understanding the above effects and differences. We discuss implications for protein corona on ZnO nanostructures.

The work has been supported by the project GACR 19-02858J.

151 years of the periodic table of elements

Kateřina Rubeřov

*University of Chemistry and Technology, Department of Inorganic Chemistry, Technick 5,
16628 Prague 6, Czech Republic*

The periodic table, as an icon of chemistry, surrounds us in both academic and research areas. The periodic assemble of elements reflecting physical and chemical behavior of elements and their compounds was firstly proposed by Dmitriy Ivanovich Mendeleev in 1869. To honor this event, United Nations General Assembly and UNESCO proclaimed 2019 “The International Year of the Periodic Table of Chemical Elements (IYPT2019)”.

In this presentation, we will look back to the history of human knowledge about elements, paying a special attention to Mendeleev’s periodic law proposal. Today’s periodic table situation and future prospects will be also summarized. The IUPAC criteria for the validation of an element discovery and for naming of a new element will be outlined and, the last but not least, the collection of elements and their stable natural compounds, that was installed at the Department of Inorganic Chemistry in UCT, will be presented as a new tool in the education of general and inorganic chemistry in bachelor study courses.

Bactericidal effect of zinc oxide nanoparticles on Gram-positive and Gram-negative strains for water decontamination using reverse spin technology

David Rutherford¹, Jaroslav Jíra¹, Kateřina Kolářová², Zdeněk Remeš²,
and Bohuslav Rezek¹

¹*Czech Technical University, Faculty of Electrical Engineering, Technická 2,
166 27 Prague 6, Czech Republic*

²*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10, 162 00 Prague 6,
Czech Republic*

We present an experimental study investigating the efficacy of zinc oxide nanoparticle use for water decontamination. A range of concentrations of commercially available spherical 50 nm zinc oxide particles were added to deionised water spiked with bacteria in a final volume of 40 mL contained inside a reverse spin bioreactor. The bioreactor rotated the bacteria-nanoparticle suspension at a defined speed (200 rpm) and duration (5 seconds) in one direction, then in the other direction to ensure constant mixing and enhanced interaction capability. The number of viable bacteria reduced with treatment time, and the rate of inactivation was concentration dependent. Gram-positive *S. aureus* bacteria were more resistant to zinc oxide nanoparticles compared to Gram-negative *E. coli*, however both strains were completely eradicated after 4 hours using a concentration of 10 µg/mL. Nanoparticles did not inhibit growth of bacteria when added to an agar surface, neither in solution before bacteria inoculation nor when loaded onto filter paper disks after bacteria inoculation. Optical properties of zinc oxide nanoparticles were probed using UV-vis spectroscopy and exhibited a strong absorption peak at 363 nm which corresponds to a calculated energy band gap of 3.4 eV. However, the bacteria-nanoparticle interaction inside the reverse spin bioreactor was shielded from ambient light which eliminated any possible photon-induced excitation of the nanoparticle surface. Electron micrographs revealed particle agglomeration on the surface of bacteria, which suggests an important role of physical interaction with the cell wall in the inactivation of bacteria and structural differences in the outer cell wall of Gram-positive and Gram-negative bacteria affected treatment efficacy.

This work was supported by the GAČR (19-02858J), MOST (M-153-001-MY3, 107-2119-M-153-001) and by the Ministry of Education, Youth and Sport (CZ.02.1.01/0.0/0.0/16-019/0000778, CZ.02.2.69/0.0/0.0/16_027/0008465).

Influence of laser welding parameters on the microstructure and mechanical properties of butt weld joints of a TRIP steel

Štefan Vrtiel, Štefan Šimon, and Mária Behúlová

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

Advanced High Strength Steels (AHSS) including TRIP steels are usually produced by unconventional methods of heat and thermo-mechanical treatment. Multiphase TRIP steels generally contain ferrite, carbide-free bainite and retained austenite. During plastic deformation, the retained austenite is transformed into martensite, thus obtaining an exceptional combination of mechanical properties (strength, ductility and ductility) of TRIP steels [1-2]. Joining the TRIP steels by fusion welding processes leads to the destruction of developed microstructure in the fusion and heat-affected zones, which also results in the degradation of mechanical properties [3].

The paper deals with the assessment of the influence of welding parameters on the microstructure and mechanical properties of weld joints of newly developed TRIP steel prepared by laser beam welding. The butt weld joints of sheets with the thickness of 2 mm were produced by the TruDisk 4002 disc laser using different values of laser power, welding speed and beam focustion. Mechanical properties of experimental weld joints were evaluated by tensile tests and microhardness measurements. Microstructural analyses were carried out using NEOPHOT 32 light microscope and the JEOL 7600 scanning electron microscope equipped with EDX analyzer.

The research has been supported by the Scientific Grant Agency of the Slovak Republic within the Projects VEGA No. 1/0796/20 and KEGA No. 029STU-4/2018.

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Spark plasma sintering of lanthanide doped Lu₂O₃

Tomáš Thoř¹, Kateřina Rubešová¹, Vít Jakeš¹, Dana Mikolášová¹, Jakub Cajzl¹, Jan Havlíček¹, Ladislav Nádherný¹, Filip Průša², Romana Kučerková³, and Martin Nikl³

¹*Department of Inorganic Chemistry, University of Chemistry and Technology, Technická 5, Prague 6, 166 28, Czech Republic*

²*Department of Metals and Corrosion Engineering, University of Chemistry and Technology, Technická 5, 166 28 Prague 6, Czech Republic*

³*Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, Prague 6, 162 00, Czech Republic*

Lutetium oxide (Lu₂O₃) is a host material with favourable properties for the detection of high-energy ionizing radiation (X-ray, γ -ray). It features one of the highest densities among inorganic host materials (9.4 g/cm³) along with high effective atomic number ($Z_{eff} = 67$), both of which attribute to a short attenuation length of a high energy photon followed by its scintillation conversion into lower energy UV-Vis light. Due to its high thermal conductivity and low coefficient of thermal expansion, it has also attracted attention for development of high power lasers. Despite its favourable properties for optical applications, its fabrication in the form of single crystals is seriously hindered by the very high melting point of 2490 °C. Because of this, extensive research has been carried out in recent years to prepare this material in the form of a transparent ceramics.

In this work, the fabrication of dense ceramics of Ln:Lu₂O₃ (Ln = Pr, Eu, Tb, Dy) by spark plasma sintering is presented. Nanocrystalline powders of Ln:Lu₂O₃ were prepared using co-precipitation followed by a pre-annealing treatment at a high temperature of 1000 °C or 1250 °C. These powders were SPS-processed into dense ceramics using a two-step sintering program. The pre-annealing affected the microstructure and transmittance of sintered ceramics. Transparency was achieved for samples pre-annealed at the higher temperature of 1250 °C. Post-annealing of sintered ceramics increased its transmittance in the visible region and removed the dark colouring of SPS-processed ceramics. However, if the post-annealing temperature is too high, the transmittance can decrease instead, to a point where the transparency is lost. The dense ceramics exhibited luminescence corresponding to the element doped into the Lu₂O₃ host. Both radioluminescence and photoluminescence emission of the Ln:Lu₂O₃ dense ceramics is fully determined by radiative transitions of the Ln³⁺ luminescent centres. The luminescence integral light yield increased with post-annealing of the sintered ceramics.

This work was financially supported by specific university research (MSMT No 21-SVV/2020), the TA CR project No. TJ01000411 and the grant agency of MVCR project No. VI20192022152.

Characterization of Graphene/ZnO Schottky Barriers Formed on Zn and O polar faces of ZnO substrates

Stanislav Tiagulskyi, Roman Yatskiv, Hana Faitová, Ondřej Černohorský, Jan Vaniš,
and Jan Grym

*Institute of Photonics and Electronics of the Czech Academy of Sciences, Chaberska 57,
182 51 Prague 8, Czech Republic*

Graphene/semiconductor junctions have been in the forefront of intense research in recent few years. Such interest originates from relatively easy fabrication of the junctions and their unique properties enabling the study of new physical phenomena. Zinc oxide is a direct wide band gap semiconductor with a broad range of unique and technologically useful properties. However, a number of factors (crystallographic surface orientation, crystal defects, residual impurities, etc.) influence the formation of the Schottky contact on ZnO. Fabrication of graphene contact on ZnO and systematic analysis of such junctions is essential for deeper understanding of the physical phenomena occurring at the interface between 2D and 3D materials as well as for their potential optoelectronic applications.

In our previous work, we investigated the polar depended properties of graphite Schottky contacts on ZnO. We showed that the interaction between O- and Zn-polar face of ZnO and graphite contact strongly affects transport properties [1].

In this study, commercially available graphene monolayers (by Graphenea) prepared by CVD on a polymer support film were transferred onto bulk ZnO substrates (by CrysTec). To limit the area of the Schottky junctions to $10\mu\text{m}$ circles, trenches were milled into graphene by Ga^+ focused ion beam (FIB).

The morphology of the graphene deposited onto ZnO was studied by atomic force microscopy (AFM, Nano Wizard 4, JPK Instruments) and scanning electron microscopy (SEM, Lyra 3 GM FIB/SEM, Tescan). The I-V characteristics of the graphene/ZnO structures were measured in the chamber of the SEM. The tip of tungsten needle handled by the nanomanipulator (Omniprobe 400, Oxford Instrument) served as the top electrode to the graphene layer while a drop of InGa alloy rubbed into ZnO substrate served as the second ohmic electrode.

We show that the FIB milling technique is a proper approach for prototyping of graphene-based electronic devices. We further demonstrate that the electrical properties of graphene/ZnO Schottky junctions strongly depend on the crystallographic orientation of the ZnO substrate, and we discuss in detail charge transport mechanisms in the graphene/ZnO junctions.

The work was supported by the Czech Science Foundation, Project No. 20-24366S.

[1] R. Yatskiv, S. Tiagulskyi, and J. Grym, Phys. Status Solidi A 216 (2019) 2.

Luminescence and up-conversion of Er doped TeO₂-PbCl₂-WO₃ glasses

Roman Yatskiv¹, Peter Kostka², Jiri Zavadil^{1,2}, and Jan Grym¹

¹*Institute of Photonics and Electronics of the Czech Academy of Sciences, Chaberska 57, 182 51 Prague 8, Czech Republic*

²*Institute of Rock Structure and Mechanics of the Czech Academy of Sciences*

Tellurite glasses are attracting attention for their excellent properties for optoelectronic applications. The glass network consisting exclusively of tellurium oxide is highly unstable and results in rapid devitrification of the glass melt. However, the addition of a wide variety of modifiers leads to stabilization of the tellurite glass network and to the formation of glasses with very different properties. Tungsten oxide is a relatively heavy glass network modifier that effectively stabilizes the TeO₄ network reducing the network's phonon energies and contributing to a high refractive index due to high polarization ability of tungsten valence orbitals. Lead compounds also have a significant stabilizing effect on the tellurium network. Lead chloride has the advantage that it introduces chlorine in addition to heavy lead atoms, which, by its presence, further disrupts the symmetry of structural units present when substituting the oxygen atoms, thus reducing the devitrification tendency of the glass melt and stabilizing its amorphous structure.

In this work, we focus on photoluminescence (PL) properties of erbium-doped TeO₂-PbCl₂-WO₃ (TBW:Er) glasses, IR to VIS/NIR up-conversion, and the temperature dependence of selected PL bands. We have demonstrated that the investigated glasses show promising spectroscopic properties. The visible PL under 514.5 nm excitation is dominated by two green bands centred at 528 and 550 nm; the highest luminescence intensity in near infrared region was observed for the transition at 1530 nm. The FWHM the band centred at 1530 nm exhibits broadening from 54 to 71 nm, when Er³⁺ ions concentration increased from 0.25 to 1 mol%. This result indicates that TBW:Er glass is a good candidate for application as a broadband optical amplifier. We obtained green, red, and NIR up-conversion emissions under 980 nm excitation. The square dependence of the emission on excitation power indicates that two photon absorption dominates to the up-conversion mechanism. The strong green emission was obtained under both VIS (514.5 nm) and NIR (980 nm) excitation. Based on the LIR technique we evaluated the optical temperature sensing abilities of the TBW:Er glass and we conclude that these glasses are suitable for temperature sensing at low temperatures

The work was supported by the Czech Science Foundation, Project No. 19-07456S.

Welding of S690QL steels with different welding consumables, comparing their microstructure and mechanical properties

Hüsnügül Yılmaz Atay, Umut Altıok, and Berkin Esim

İzmir Katip Çelebi University, İzmir Katip Çelebi Üniversitesi Mühendislik Fakültesi, İzmir, Türkiye

In this study, fine-grained, high-strength S690QL steel was welded by gas, submerged and electric arc methods. These welds were made by using three different welding wires (ER110S-G / G 69 4 M21 Mn3Ni1CrMo, ER307 / G 18 8 Mn and ER312 / G 29 9) and equivalent welding consumables in other welding methods of this wire. No preheating was done in the welding processes, the processes took place at room temperature. After the welding processes were completed, tensile, bending, impact tests and SEM were applied for determining the mechanical properties, microstructure and phase changes of the material, respectively. Depending on the test results, compatibility of the main material with different welding method and consumables was observed.

Dielectric properties, preparation and characterization of lead-free ceramics from piezoelectric powders

Kateřina Zloužeová, Soňa Hříbalová, Vojtěch Nečina, and Willi Pabst

University of Chemistry and Technology Prague, Technická 5, 166 28 Prague 6, Czech Republic

Piezoelectric materials are widely used in electrotechnical devices as sensors, energy harvesters, actuators, transducers or as hydrophones. Usually, in the preparation of these materials, an effort is made to achieve the highest possible density, since, for example, the elastic, dielectric and piezoelectric properties decrease with increasing porosity. The decrease in relative permittivity with increasing pore volume fraction is then interesting, as it is related to the increase in the values of some figures of merit, which describe the response rate of the transducer. Porous ceramics then show a significant improvement in properties, for example for the application of hydrophones, even if, for example, piezoelectric, dielectric and elastic properties are worse than for their dense counterparts. This work deals with the preparation of lead-free piezoelectric ceramics - potassium sodium niobate (KNN) and barium titanate (BT) - from commercially available piezoelectric powders by conventional firing and spark plasma sintering (SPS) in order to prepare partially sintered (porous) ceramics. The relative permittivity is then measured by the impedance spectroscopy method in the range from 10 Hz to 1MHz. The aim of this work is to compare the properties of ceramic samples prepared by the SPS method and conventional firing and to discuss the effect of porosity on relative permittivity (or rather its real part).

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LIST OF PARTICIPANTS

Dr. Anna Artemenko
Institute of Physics, Czech Academy of Sciences
Cukrovarnická 10
Prague 6
Czech Republic
artemenko@fzu.cz

Dr. Ľubor Dlháň
Institute of Inorganic Chemistry (FCHPT)
Slovak University of Technology
Radlinskeho 9
SK-812 37 Bratislava
Slovakia
lubor.dlhan@stuba.sk

Dr. Vladimír Babin
Institute of Physics of the Czech Academy of Sciences
Cukrovarnická 10
Prague 16200
Czech Republic
babinv@fzu.cz

Ing. Václav Doležal
University of Chemistry and Technology Prague
Technická 5
Prague 6
Czech Republic
dolezalv@vscht.cz

Ing. Nikola Bašínová
Institute of Photonics and Electronics of the Czech Academy of Sciences
Chaberská 57
182 51 Praha 8
Czech republic
basinova@ufe.cz

Ing. Rastislav Ďuriš
Slovak university of Technology in Bratislava
Faculty of Materials Science and Technology in Trnava
J. Bottu 25
Trnava, 917 24
Slovakia
rastislav.duris@stuba.sk

Doc Mária Behúlová
Slovak University of Technology in Bratislava
Faculty of Materials Science and Technology in Trnava
Ulica Jána Bottu č. 2781/25
917 24 Trnava
Slovakia
maria.behulova@stuba.sk

Ing. Pavla Dvořáková
UCT Prague
Technická
Praha 6
Czech republic
pavla.dvorakova@vscht.cz

Dr. Maksym Buryi
Institute of Physics of the Czech Academy of Sciences
Cukrovarnická 10
162 00 Prague 6
Czech Republic
buryi@fzu.cz

Mgr. Hana Faitová
Institute of Photonics and Electronics
Czech Academy of Sciences
Chaberská 57
182 51 Praha 8
Czech republic
faitova@ufe.cz

Dr. Ondřej Černohorský
Institute of Photonics and Electronics
Czech Academy of Sciences
Chaberská 57
182 51 Praha 8
Czech Republic
cernohorsky@ufe.cz

Dr. Jan Grym
Institute of Photonics and Electronics
of the Czech Academy of Sciences
Chaberska 57
182 51 Praha 8
Czech Republic
grym@ufe.cz

Ing. Štefan Hajdu
Slovak University of Technology in Bratislava
Faculty of Materials Science and Technology in Trnava
Ulica Jána Bottu č. 2781/25
917 24 Trnava
Slovakia
stefan.hajdu@stuba.sk

Dr. Petr Kalenda
University of Pardubice
532 10 Pardubice
Czech Republic
petr.kalenda2@upce.cz

Ing. Jan Havlíček
Crytur, spol. s r.o./ VŠCHT Praha
Na Lukách 2283
Turnov 51101
Czech Republic
jan.havlicek@crytur.cz

Prof. Marian Koman
Fakulta chemickej a potravinárskej technológie STU
Oddelenie anorganickej chémie ÚAČHTM
Radlinského 9
812 37 Bratislava
Slovakia
marian.koman@stuba.sk

Dr. Takahiko Horiai
Institute of Physics of the Czech Academy of Sciences
Cukrovarnická 10
162 00 Prague 6
Czech Republic
horiai@imr.tohoku.ac.jp

Prof. Ladislav Koudelka
University of Pardubice
Faculty of Chemical Technology
Studentská 95
532 10 Pardubice
Czech Republic
ladislav.koudelka@upce.cz

Dr. Vít Jakeš
University of Chemistry and Technology Prague
Department of Inorganic Chemistry
Technická 5
166 28 Prague 6
Czech Republic
vit.jakes@vscht.cz

Dr. Zdeněk Kožíšek
Institute of Physics of the Czech Academy of Sciences
Cukrovarnická 10
162 00 Prague 6
Czech Republic
kozisek@fzu.cz

Ing. Jaroslav Jíra
CTU - Faculty of Electrical Engineering
Technická 2
Prague 6
16627
jira@fel.cvut.cz

Dr. Robert Král
Institute of Physics, Czech Academy of Sciences
Cukrovarnická 10
162 00 Prague 6
Czech Republic
kralr@fzu.cz

Dr. Vladimír Jorík
Faculty of Chemical and Food Technology
Slovak University of Technology
Radlinského 9
Bratislava 81237
Slovakia
vladimir.jorik@stuba.sk

Šárka Kučerová
Institute of Photonics and Electronics
Czech Academy of Sciences
Chaberská 57
182 51 Praha 8
Czech Republic
kucerova@ufe.cz

Dr. Iveta Markechová
Slovak Uni Technol, Fac Mater Sci & Technol, Dept
Math
Jána Bottu 2781/25
917 24 Trnava
Slovakia
iveta.markechova@stuba.sk

Ing. Martin Necpal
Slovak University of Technology in Bratislava,
Faculty of Materials Science and Technology in Trnava
Jána Bottu č. 2781/25
917 24 Trnava
Slovakia
martin.necpal@stuba.sk

Dr. Jana Mesárošová
Slovak University of Technology in Bratislava
Faculty of Materials Science and Technology in Trnava
Ulica Jána Bottu 2781/25
917 24 Trnava
Slovakia
jana.mesarosova@stuba.sk

Dr. Jan Pejchal
Institute of Physics
Academy of Sciences of the Czech Republic
Cukrovarnicka 10
Prague 16200
Czech Republic
pejchal@fzu.cz

Ing. Dana Mikolášová
University of Chemistry and Technology
Department of Inorganic Chemistry
Technická 5
16628 Prague 6
Czech Republic
mikolasd@vscht.cz

Dr. Zdeněk Potůček
Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering
Trojanova 13
120 00 Prague
Czech Republic
potucek@fzu.cz

Prof. Petr Mošner
Faculty of Chemical Technology
University of Pardubice
Studentská 95
Pardubice 532 10
Czech Republic
petr.mosner@upce.cz

Dr. Zdeněk Remeš
Institute of Physics CAS
Na Slovance 1999/2
Prague 8
Czech Republic
remes@fzu.cz

Milan Nad' ¹
Slovak University of Technology in Bratislava
Faculty of Materials Science and Technology
Ulica Jána Bottu 2781/25
Trnava
Slovak Republic
milan.nad@stuba.sk

Prof. Bohuslav Rezek
Faculty of Electrical Engineering
Czech Technical University in Prague
Technická 2
16627 Prague 6
Czech Republic
rezeboh@fel.cvut.cz

Dr. Serge Nagorny
Queen's University
99 Universilty Ave
Kingston, K7L 3N6
Canada
sn65@queensu.ca

Dr. Kateřina Rubešová
University of Chemistry and Technology
Department of Inorganic Chemistry
Technická 5
16628 Prague 6
Czech Republic
rubesovk@vscht.cz

Dr. David Rutherford
Czech Technical University
Faculty of Electrical Engineering
Technická 2
166 27 Praha 6
Czech Republic
david.rutherford@fel.cvut.cz

Ing. Kateřina Zloužeová
University of Chemistry and Technology
Department of Inorganic Chemistry
Technická 5
16628 Prague 6
Czech Republic
k.zlouzeova@gmail.com

Ing. Štefan Šimon
Slovak University of Technology in Bratislava
Faculty of Materials Science and Technology in Trnava
Ulica Jána Bottu 2781/25
Trnava
Slovensko
stefan.simon@stuba.sk

Ing. Tomáš Thoř
University of Chemistry and Technology
Department of Inorganic Chemistry
Technická 5
16628 Prague 6
Czech Republic
tomas.thor@centrum.cz

Dr. Stanislav Tiagulskyi
Institute of Photonics and Electronics
Czech Academy of Sciences
Chaberská 57
182 51 Praha 8
Czech Republic
tiagulskyi@ufe.cz

Dr. Roman Yatskiv
Institute of Photonics and Electronics
Czech Academy of Sciences
Chaberská 57
182 51 Praha 8
Czech Republic
yatskiv@ufe.cz

Dr. Hüsnügül Yılmaz Atay
İzmir Katip Çelebi University
İzmir Katip Çelebi Üniversitesi Mühendislik Fakültesi
Malzem
İzmir
Türkiye
hgulyilmaz@hotmail.com

