Institute of Solid State Physics

University of Latvia

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2015

Riga 2016

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Riga, Institute of Solid State Physics, University of Latvia, 2016, p.132

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INTRODUCTION

The **Institute of Solid State Physics** (ISSP) of the University of Latvia was established in 1978 on the basis of Laboratory of *Semiconductor Research* and Laboratory of *Ferro- and Piezoelectric Research*. Since 1986 the ISSP has the status of an independent organization of the University and now is the main material science institute in Latvia.

Four laboratories from the Institute of Physics of the Latvian Academy of Sciences joined the Institute in 1995. Twenty scientists of the former Nuclear Research Centre joined the ISSP in 1999 and established Laboratory of Radiation Physics. In 2004 scientists from the Institute of Physical Energetics joined ISSP and established Laboratory of Organic Materials (Table 1).

In mid 90-ties the ISSP has intensified its **teaching activities**. A number of researcher have been elected as professors of the University of Latvia. Post-graduate and graduate curricula were offered in solid-state physics, material physics, chemical physics, physics of condensed matter, semiconductor physics, and experimental methods and instruments. In 2002 the Chair of Solid State and Material Physics University of Latvia was established at ISSP.

Research and training in optometry and vision science is taking place in the Laboratory of Visual Perception of the ISSP since 1992. Co-located with the Institute, the Optometry Centre has been established in 1995 with facilities for primary eye care and serving as a technological research basis for students and staff.

In December 2000 the ISSP was awarded the **Centre of Excellence of the European Commission** (Centre of Excellence for Advanced Material Research and Technologies – **CAMART**). This honorary recognition with the accompanying financial support of 0.7 MEUR has increased research activities at ISSP, particularly extending the list of research partners and scientists from the leading European research centres working at the Institute.

Next step of the development of CAMART was in 2015, when ISSP won Horizon2020 Teaming project: "**The Excellence Centre of Advanced Material Research and Technology Transfer – CAMART^2"**. Having 14.5 out of 15 points, CAMART2 is one of 31 proposals of total 169 submitted which were selected for the next phase – preparation of Business Plans for the development of Centre of Excellence. The project is realized in cooperation with Swedish colleagues from the Royal Institute of Technology (KTH) and Acreo Swedish ICT. During 12 months of the Phase 1, a

Business Plan for the future Centre of Excellence CAMART^2 will be elaborated demonstrating the long-term science and innovation development strategy. Business plan will be based on a SWOT analysis of ISSP and it will be fortified with a financial commitment document from government allocating appropriate funding from national, ESIF or any others resources for the development of infrastructure at ISSP.

The research of the ISSP includes:

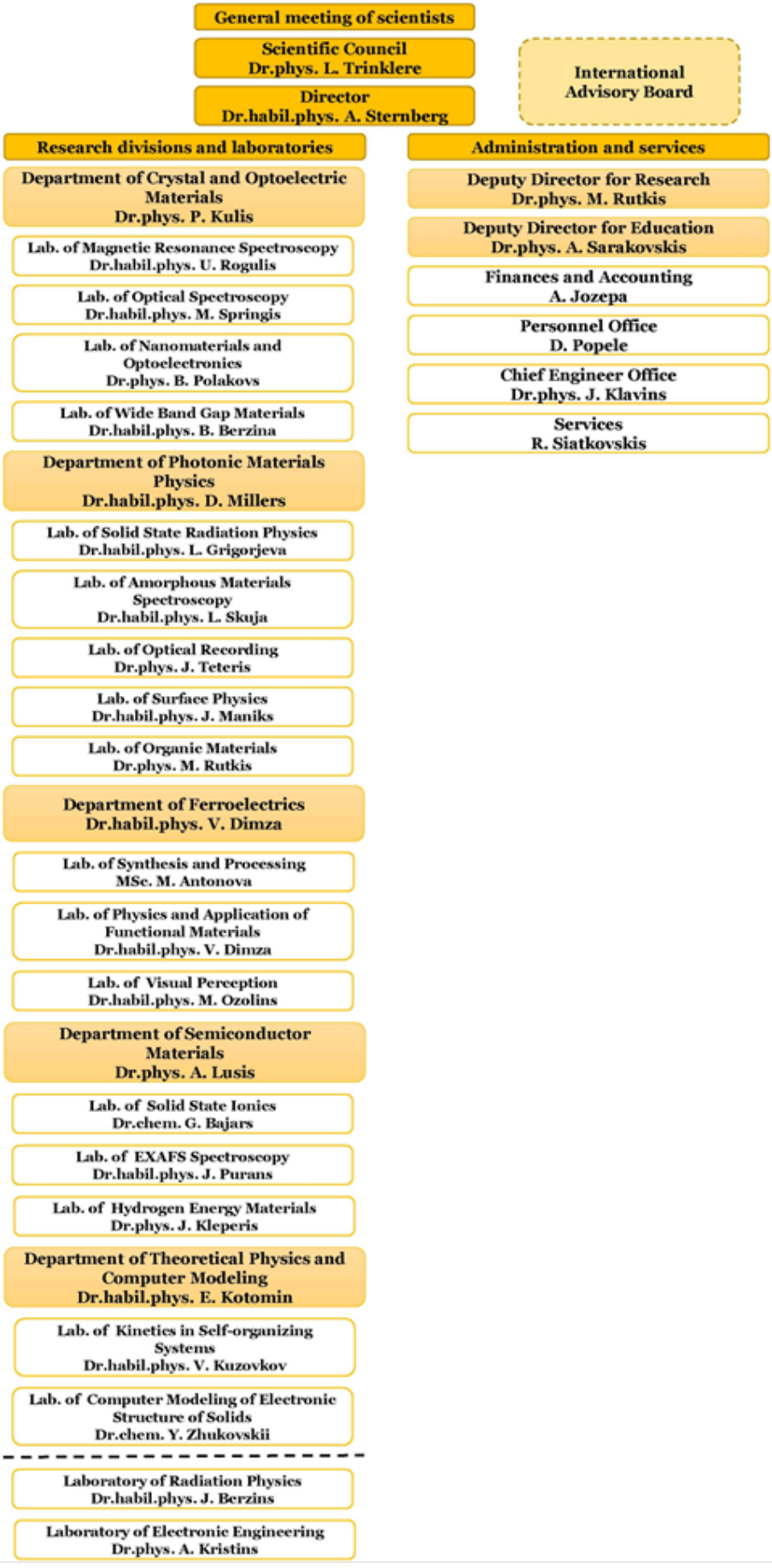
- thin films and coating technologies;
- functional materials for electronics and photonics;
- nanotechnology, nanocomposites and ceramics;
- computational materials science by atomic scale modelling of technologically important materials and devices.

The highest decision-making body of the Institute is the **Scientific Council** of 21 members elected by the employees of the Institute (Table 2). Presently Dr. phys. L.Trinklere is the elected chairperson of the ISSP Council. The Council appoints director and its deputies.

Table 1

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2015

International Supervisory Board	
Council of Institute *Dr.phys*. L.Trinklere	
Director *Dr.habil.phys*. A. Sternberg	
RESEARCH DEPARTMENTS AND LABORATORIES	**ADMINISTRATION AND DOMESTIC SERVICES**


General meeting of scientists
Scientific Council
Dr.phys. L. Trinklere
Director
Dr.habil.phys. A. Sternberg
International Advisory Board
Research divisions and laboratories
Department of Crystal and Optoelectric Materials
Dr.phys. P. Kulis
Lab. of Magnetic Resonance Spectroscopy
Dr.habil.phys. U. Rogulis
Lab. of Optical Spectroscopy
Dr.habil.phys. M. Springis
Lab. of Nanomaterials and Optoelectronics
Dr.phys. B. Polakovs
Lab. of Wide Band Gap Materials
Dr.habil.phys. B. Berzina
Department of Photonic Materials Physics
Dr.habil.phys. D. Millers
Lab. of Solid State Radiation Physics
Dr.habil.phys. L. Grigorjeva
Lab. of Amorphous Materials Spectroscopy
Dr.habil.phys. L. Skuja
Lab. of Optical Recording
Dr.phys. J. Teteris
Lab. of Surface Physics
Dr.habil.phys. J. Maniks
Lab. of Organic Materials
Dr.phys. M. Rutkis
Department of Ferroelectrics
Dr.habil.phys. V. Dimza
Lab. of Synthesis and Processing
MSc. M. Antonova
Lab. of Physics and Application of Functional Materials
Dr.habil.phys. V. Dimza
Lab. of Visual Perception
Dr.habil.phys. M. Ozolins
Department of Semiconductor Materials
Dr.phys. A. Lusis
Lab. of Solid State Ionics
Dr.chem. G. Bajars
Lab. of EXAFS Spectroscopy
Dr.habil.phys. J. Purans
Lab. of Hydrogen Energy Materials
Dr.phys. J. Kleperis
Department of Theoretical Physics and Computer Modeling
Dr.habil.phys. E. Kotomin
Lab. of Kinetics in Self-organizing Systems
Dr.habil.phys. V. Kuzovkov
Lab. of Computer Modeling of Electronic Structure of Solids
Dr.chem. Y. Zhukovskii
Laboratory of Radiation Physics
Dr.habil.phys. J. Berzins
Laboratory of Electronic Engineering
Dr.phys. A. Kristins
Administration and services
Deputy Director for Research
Dr.phys. M. Rutkis
Deputy Director for Education
Dr.phys. A. Sarakovskis
Finances and Accounting
A. Jozepa
Personnel Office
D. Popele
Chief Engineer Office
Dr.phys. J. Klavins
Services
R. Siatkovskis

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff.** At present there are 172 employees working at the Institute, 24 of 116 members of the research staff hold Dr.habil.degrees, 70 hold Dr. or PhD. By the end of 2015, there were 20 PhD students and 48 undergraduate and graduate students in physics, chemistry, materials science and optometry programmes working at the ISSP. By the end of 2015, more than 60 students, master's candidates and doctoral candidates worked in our Institute under the supervision of ISSP scientists.

Table 2

The Scientific Council of the Institute

1. Laima Trinklere, Dr.phys., chairperson of the Council
2. Marcis Auzins, Dr.habil.phys., UL
3. Gunars Bajars, Dr.chem.
4. Larisa Grigorjeva, Dr.habil.phys.
5. Jurģis Grūbe, PhD student
6. Anastasija Jozepa
7. Andris Krumins, Prof., Dr.habil.phys.
8. Peteris Kulis, Dr.phys.
9. Aleksejs Kuzmins, Dr.phys.
10. Raitis Grizibovskis, PhD student
11. Juris Purāns, Dr.phys.
12. Uldis Rogulis, Dr.habil.phys.
13. Mārtins Rutkis, Dr.phys.
14. Andrejs Silins, Prof., Dr.habil.phys.
15. Linards Skuja, Dr.habil.phys.
16. Anatolijs Sharakovskis, Dr.phys.
17. Andris Sternbergs, Dr.habil.phys.
18. Janis Teteris, Dr.phys.
19. Anatolijs Truhins, Dr.habil.phys.
20. Nils Veidemanis, A/S "Sidrabe"
21. Guntars Zvejnieks, Dr.phys.

The annual report summarizes the research activities of the ISSP in 2015. The staff of the Institute has succeed in 5 **national science grants** and in **one national cooperation project** with the total financing 264.4 kEUR

Since 2008 the budgetary increase of science was focused on scientific infrastructure financing and launching of National Research Programmes (NRP). Since then ISSP is a coordinating institution for NRP in Materials Science and ICT as well as collaborator for NRP in Energetics attracting 242.3 kEUR budget in 2015. The base financing for ISSP in 2015 was 1.06 MEUR and it was partly used also for the salaries of the scientific and maintenance staff of the Institute. (Table 3).

In **2015 two international conferences** have been organised:

1. International Young Scientist Conference "Developments in Optics and Communications 2015", April 8 – 10, 2015, Riga, Latvia;
2. Saules kauss 2015, May 16, Riga, Latvia.

Main awards, received at 2015:

No	Author	Award
1.	Dr.habil.phys. Andris Sternbergs	The Great Medal of Latvian Academy of Science
2.	Dr.phys. Martins Rutkis	The Member of Latvian Academy of Science
3.	Dr.phys. Liga Grinberga	The Corresponding Member (physics) of Latvian Academy of Science
4.	Dr.h.c.phys. Janis Jansons	A.Balklavs award for popularisation of science (Latvian Academy of Science)
5.	Dr.phys. Janis Timoshenko	L. and M.Jansons award for young scientists in physics (Latvian Academy of Science)
6.	Dr.habil.phys. Juris Purans Mg.phys. Martins Zubkins	Authors of the best scientific achievement in Latvia (from Latvian Academy of Science)

Table 3

INCOME OF ISSP, THOUSAND EUR, FROM 2008 -2015

Year	Total financing	Grants and programmes from budget	Infrastructure financing	Contracts, market oriented research	Internat. funds	Structural funds from EU
2008	6 063.28	1 457.59	1 385.50	221.83	605.70	2 406.22
2009	2 443.64	898.69	705.40	91.35	348.20	399.97
2010	3 038.68	634.89	664.40	118.53	465.70	1 159.21
2011	3 868.93	637.45	597.30	148.83	308.50	2 176.99
2012	4 925.98	606.57	485.60	170.74	180.00	3 304.05
2013	3 518.90	345.92	599.70	232.21	581.00	1 405.66
2014	3 029.00	562.30	707.20	361.20	362.50	1 035.80
2015	4 246.60	506.70	1 059.90	274.70	953.90	1 392.80

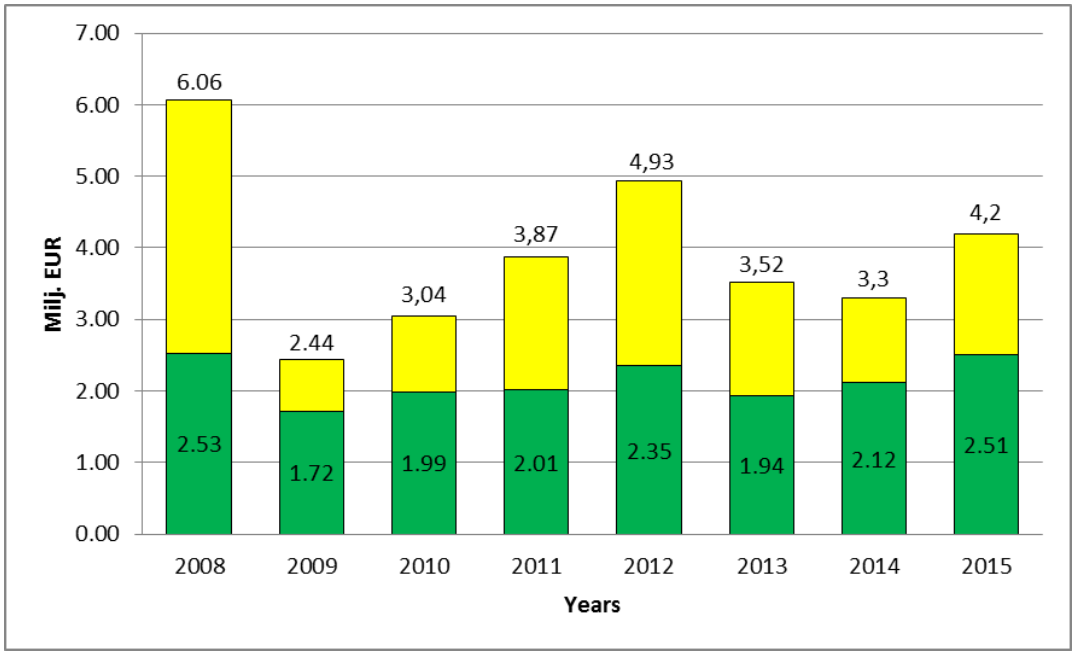


Fig.1. Total financing of the ISSP milj. EUR from 2008 to 2015

- *salaries*

The main source for **international funding** were EC 7th Framework Programme and Horizon 2020 contracts:

- H2020 – WIDESPREAD-2014 project CAMART^2 – 373.1 kEUR;
- 4 EUROFUSSION projects – 273.7 kEUR;
- GREEN-CC project – 77.6 kEUR;
- H2ESOT project – 59.3 thous. EUR.

Main achievments in 2015

1. 146 SCI papers published by the staff of Institute;
2. 12 B.sc. thesis and 21 M.Sc. thesis in physics, optometry, chemistry and materialscience were defended under the supervision of our scientists;
3. Jurgis Grube, Roberts Zabels, Gints Kuchinskis, Ugis Gertners, Kaiva Juraševska, Janis Timošenko, Edgars Nitišs received doctoral degree in physics, Martins Vanags doctoral degree in materials science and Janis Latvelis doctoral degree in environment engineering.

Many thanks to everybody who contributed to this report as well as to the organizations that supported the Institute financially: Science Department of the Latvian Ministry of Education and Science, Latvian Council of Science, University of Latvia, EC 7th Framework and H2020 Programme, Programme of EU Structural funds, COST Programme, and to many foreign Universities and institutions for cooperation.

Prof. Dr. A.Krumins

DEPARTMENT OF CRYSTALS PHYSICS AND OPTOELECTRONIC MATERIALS

Head of Department Dr. phys. P. Kulis

LABORATORY OF MAGNETIC RESONANCE SPECTROSCOPY

Head of Laboratory Prof., Dr. habil. phys. U. Rogulis

RESEARCH TOPICS

Research of defect structure, luminescence centres and mechanisms using magnetic resonance spectroscopy techniques (EPR, ODMR),
Research of intrinsic and activator-related defects in oxyfluoride composites, fluoride micro- and nano-crystals in glass matrixes,
Investigations of luminescence properties of oxyfluoride glass and glass-ceramics, as well as application possibilities of these materials.

LABORATORY EQUIPMENT

ODMR spectrometer: Oxford Instruments Magneto-optical cryostat with magnetic fields up to 7 T at temperatures 1.5-4.2 K, spectral range 200-800 nm and microwave frequencies 36 and 45 GHz.
EPR spectrometer: X-Band (9.3 GHz), magnetic fields up to 0.7 T, temperature range 6-300 K.

SCIENTIFIC STAFF

1. Prof., Dr. habil. phys. U. Rogulis
2. Dr. Phys. A. Fedotovs
3. Dr. Phys. E. Elsts

PhD students
1. A. Antuzevičs
2. M. Ķemere
3. Dz. Bērziņš

Students
1. J. Sperga
2. A. Cvetkovs

SCIENTIFIC VISITS ABROAD

U. Rogulis (2 weeks, Germany)
E. Elsts (1 week in Spain, 1 week in Poland)
M. Ķemere (1 week, Germany, 2 days in Estonia)
A. Antuzēvičs (2 days in Estonia)

COOPERATION

Latvia
1. Department of Physics, Faculty of Physics and Mathematics, LU
2. Laboratory of Semiconductor Physics, Institute of Technical Physics, Riga Technical University (Prof. A. Medvids)

Germany
1. Fachhochschule Südwestfalen, Soest (Prof. Dr. S. Schweizer)
2. University of Paderborn (Prof. Dr. S. Greulich-Weber)

Romania
1. National Institute for Material Physics (INCDFM), Bucharest, Romania (Dr. M. Secu)
2. National Institute for Research and Development for Optoelectronics INOE 2000, Bucharest, Romania (Dr. I. C. Vasiliu)

MAIN RESULTS

STUDIES OF RADIATION DEFECTS IN CERIUM, EUROPIUM AND TERBIUM ACTIVATED OXYFLUORIDE GLASSES AND GLASS CERAMICS

E. Elsts, E. Rogulis, K. Bulindzs, K. Smits, A. Zolotarjovs, L. Trinklere, K. Kundzins

Terbium, cerium and europium activated oxyfluoride glasses and glass ceramics have been studied by thermally stimulated luminescence (TSL) and optical absorption techniques after the X-ray irradiation.
A creation of colour centres in oxyfluoride glass matrix and TSL peaks depending on the activator type were observed. LaF_3 and rare earth activators were analysed by SEM–EDS.

ANGULAR DEPENDENCE OF RECOMBINATION LUMINESCENCE DETECTED EPR IN ZnO CRYSTAL

A. Fedotovs, Dz. Berzins, U. Rogulis, K. Smits, G. Doke, A. Medvids, P. Onufrijevs

Angular dependency of electron paramagnetic resonance, optically detected by UV-excited recombination luminescence (RL-EPR) was measured for nominally pure ZnO single crystals. Observed magnetic resonances belong to the broad “yellow” RL band with slow decay centred at 610 nm, which is characteristic to untreated ZnO crystals. In the sample, irradiated with the 266 nm UV laser, an additional RL band centred at 740 nm appears, which has considerably faster decay time than the “yellow” one. This RL band is characteristic to the luminescence of Fe^{3+} ions in the ZnO crystals. It could be observed only after the UV laser treatment. No RL-EPR signal was detected for this RL band. Our spectral simulations show that the observed angular dependencies of the RL-EPR spectra can be described considering a simultaneous contribution from two types of deep acceptor centres – Li_{Zn} and a zinc vacancy – V_{Zn}.

ELECTRON PARAMAGNETIC RESONANCE AND MAGNETIC CIRCULAR DICHROISM OF Gd^{3+} IONS IN THE OXYFLUORIDE GLASS-CERAMICS CONTAINING CaF_2 NANOCRYSTALS

A. Fedotovs, A. Antuzevics, U. Rogulis, M. Kemere, R. Ignatans

Magnetic resonance investigations of the Gd^{3+} centre structure in the oxyfluoride glass and glass-ceramics (GC) have been carried out. The electron paramagnetic resonance (EPR) measurements showed presence of low symmetry Gd^{3+} centres in the glass

sample. The cubic Gd^{3+} centre appeared in the glass-ceramics after heat treatment of the samples at temperatures above 650 °C. The magnetic circular dichroism (MCD) measurements of both glass and glass-ceramics showed wide absorption band around 310 nm. In the GC samples MCD-EPR of the cubic Gd^{3+} centre has been detected.

EPR STUDY OF Gd^{3+} LOCAL STRUCTURE IN ScF_3 CRYSTAL WITH NEGATIVE THERMAL EXPANSION COEFFICIENT

A. Antuzevics, U. Rogulis, A. Fedotovs, Dz. Berzins, V. N. Voronov and J. Purans

Zero field splitting (ZFS) of Gd^{3+} impurity in ScF_3 is studied by electron paramagnetic resonance at 77 and 295 K. ZFS parameter b4 values obtained from angular dependence simulations show that regardless of negative thermal expansion in ScF_3 temperature dependence of |b4| is similar to other cubic fluoroperovskites. Our analysis of ZFS parameters indicates that the local structure of Gd^{3+} centres expands positively with temperature.

SCIENTIFIC PUBLICATIONS

1. **E. Elsts, E. Rogulis,** K. Bulindzs, K. Smits, A. Zolotarjovs, L. Trinklere, K. Kundzins, Studies of radiation defects in cerium, europium and terbium activated oxyfluoride glasses and glass ceramics, Optical Materials, 2015, vol. 41, pp. 90-93; DOI 10.1016/j.optmat.2014.10.042
2. **A. Fedotovs, Dz. Berzins, U. Rogulis**, K. Smits, G. Doke, A. Medvids, P. Onufrijevs, Angular Dependence of Recombination Luminescence Detected EPR in ZnO Crystal, Physica scripta, 2015, vol. 90, No. 9, 094016. doi:10.1088/0031-8949/90/9/094016
3. **A. Fedotovs**, A. Antuzevics, U. Rogulis, M. Kemere, R. Ignatans, Electron paramagnetic resonance and magnetic circular dichroism of Gd^{3+} ions in the Oxyfluoride Glass-ceramics containing CaF_2 nanocrystals, J. of Non-Crystalline solids, 2015, vol. 429, pp. 118-121. doi:10.1016/j.jnoncrysol.2015.08.036
4. **A Antuzevics, U. Rogulis, A. Fedotovs, Dz. Berzins,** V. N. Voronov and J. Purans, EPR Study of Gd^{3+} local structure in ScF_3 – crystal with negative thermal expansion coefficient, Physica Scripta, 2015, vol. 90, p. 115801.
5. Trukhin, A.N, Smits, K, Jansons, J, **Berzins, D,** Chikvaidze, G, Griscom, D.L, UV and yellow luminescence in phosphorus doped crystalline and glassy silicon dioxide, Journal of Luminescence, 2015, vol. 166, pp. 346-355.

LECTURES ON CONFERENCES

1. A. Antuzevics, U. Rogulis, J. Purans, EPR investigation of Gd^{3+} local structure in ScF_3, Abstracts of the 11th International Young Scientist conference "Developments in Optics and Communications" DOC, 2015, p. 38.
2. O. Kiselova, A. Cvetkovs, U. Rogulis, V. Serga, R. Ignatans, K. Kundzins, Studies of zinc oxide thin films synthesized by extraction – pyrolytic method, Abstracts of the 11th International Young Scientist conference "Developments in Optics and Communications" DOC, 2015, p. 48.
3. J. Sperga, M. Kemere, U. Rogulis, J. Grube, G. Krieke, E. Elsts, Luminescence studies of Europium and coactivator doped oxyfluoride glasses and glass ceramics, Abstracts of the 11th International Young Scientist conference "Developments in Optics and Communications" DOC, 2015, p. 24.
4. U. Rogulis, I. Brice, J. Grube, D. Millers, R. Ignatans, S. Loos, F. Steudel, B. Ahrens, S. Schweizer, Europium luminescence in zinc aluminosilicate glasses containing SrF_2

and CaF_2 nanocrystals, The International Conference EuroNanoForum 2015, Riga, Poster B1-68.

5. A. Antuzevics, A. Fedotovs, U. Rogulis, M. Kemere, Paramagnetic probes for nano-crystalline phase detection in oxyfluoride glass ceramics, The International Conference EuroNanoForum 2015, Riga, Poster B1-89.
6. A. Antuzevics, A. Fedotovs, U. Rogulis, M. Kemere, EPR study of oxyfluoride glass ceramics containing Gd^{3+} ions, Abstracts of the International Conference LUMDETR'2015, Tartu, Estonia, p. We-P-1.
7. M. Kemere, J. Sperga, U. Rogulis, J. Grube, G. Krieke, Photoluminescence properties of double RE doped oxyfluoride glasses and glass-ceramics, Abstracts of the International Conference LUMDETR'2015, Tartu, Estonia, p. Tu-P-36.
8. J. Sperga, M. Ķemere, U. Rogulis, J. Grūbe, G. Krieķe, E. Elsts, Photoluminescence properties of oxyfluoride glasses and glass-ceramics activated with Eu^{3+} and RE ions, Abstracts of the 31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2015, p. 51.
9. A. Antuzevičs, U. Rogulis, J. Purāns, Gd centre and radiation defects in ScF_3, Abstracts of the 31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2015, p. 13.
10. O. Kiseļova, A. Cvetkovs, U. Rogulis, V.Serga, R. Ignatāns, K. Kundziņš, Synthesis of zinc oxide thin films by the extraction-pyrolythic method, Abstracts of the 31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2015, p. 65.
11. A. Fedotovs, U. Rogulis, A. Antuzevičs, M. Ķemere, Dz. Bērziņš, Paramagnetic probes for investigations of the structure of oxyfluoride glass-ceramics zondes, Abstracts of the 31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2015, p. 12.
12. E. Elsts, G. Krieķe, U. Rogulis, K. Šmits, A. Zolotarjovs, J. Jansons, A. Šarakovskis, K. Kundziņš, Investigations of terbium, praseodimium, neodymium and dysprosium activated glasses and glass-ceramics, Abstracts of the 31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, p. 50. lpp.
13. O. Kiseļova, A. Cvetkovs, U. Rogulis, V.Serga, R. Ignatāns, K. Kundziņš, Ar ekstrakcijas – pirolītisko metodi sintezētu cinka oksīdu plāno kārtiņu īpašības, RTU 56. Starptautiskā zinātniskā konference, sekcija: "Daudzfunkcionālie materiāli un kompozīti, fotonika un nanotehnoloģijas", stenda referāts Nr.4.

MASTER THESIS

Meldra Ķemere, „Luminescence studies of oxyfluoride glasses and glass-ceramics co-activated with two rare-earth ions", Master thesis, Riga, LU, 2015

Antons Cvetkovs, „Synthesis and properties of $Zn_xCd_{1-x}O$ policrystalline thin films", Master thesis, Riga, LU, 2015

BACHELOR THESIS

Edvīns Ļetko, „Gadolinium as a paramagnetic probe for nano-crystalline phase detection in oxyfluoride glass ceramics", Bachelor thesis, Riga, LU, 2015

DEPARTMENT OF CRYSTALS PHYSICS AND OPTOELECTRONIC MATERIALS

Head of Department Dr. phys. P. Kulis

LABORATORY OF OPTICAL SPECTROSCOPY

Head of Laboratory Dr.habil.phys. M.Springis

RESEARCH TOPICS

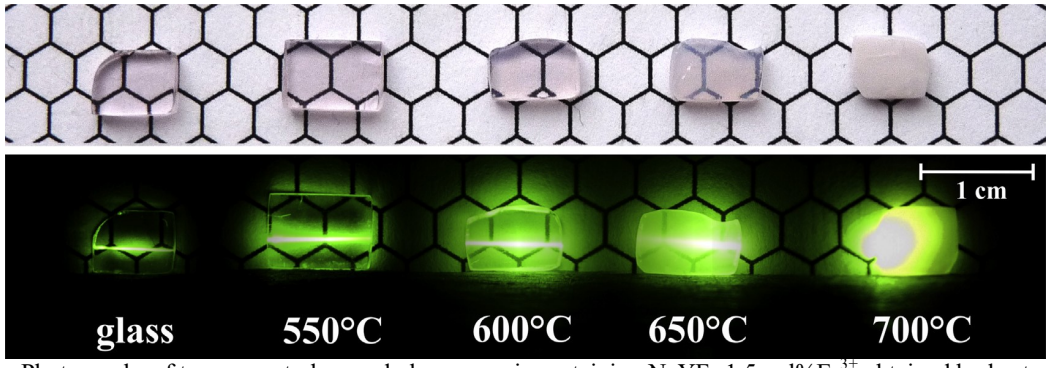
Synthesis of rare-earth doped fluoride and oxyfluoride nanocomposites; studies of radiation energy transfer and relaxation mechanisms in doped nanocomposites by means of optical spectroscopy methods; optical spectroscopy of defects in nanocomposites including studies of up-conversion luminescence.

The impact of defects (including radiation) on spectroscopic properties of several complex fluorides structures (LaF_3, $NaYF_4$, $NaLaF_4$) was studied. Along with the mentioned activities a new research topic related to the luminescence processes in rare-earth (RE) doped oxyfluoride glass and glass ceramics was initiated. The studies are organized in two directions: development of synthesis process of different fluoride nanostructures including oxyfluoride glass and glass ceramics and studies of spectroscopic properties as well as radiation energy relaxation mechanisms in the materials. Special attention is paid to the studies of up-conversion process, i.e. studies of visible or even ultraviolet luminescence excited by several lower-energy photons absorption.

SiO_2 based glasses and nanostructured glass ceramics with RE doped (Er^{3+}, Yb^{3+}, Tm^{3+}) $NaYF_4$ and $NaLaF_4$ nanocrystals were synthesized. Transparent oxyfluoride glass ceramics containing hexagonal $NaYF_4$ nanocrystals, doped with Er^{3+} reveals up-conversion luminescence intensity of which is at least 200 times higher than that of the precursor glass. It was found that in silicate glass ceramics with $NaYF_4$:Er^{3+} the mechanism responsible for Er^{3+} photoluminescence changes significantly with changing Er^{3+} concentration. Oxyfluoride glass and glass ceramics samples with $NaLaF_4$:Pr^{3+} were synthesized and studied. It was found the different Pr^{3+} luminescence mechanisms for precursor glass and glass ceramics.

For the first time transparent glass ceramics containing Er^{3+} activated BaF_2 nanocrystals having efficient up-conversion luminescence was synthesized.

The staff of the laboratory is taking part in the preparation and supervision of practical works in solid state physics courses for Master students at the University of Latvia (Dr. hab. phys. M. Springis), supervision of practical works in electricity for Bachelor students and in solid state optical spectroscopy for Master students at the University of Latvia (M. Sc. J. Grube). Dr. phys. A. Sarakovskis is a associate professor at the Faculty of Physics and Mathematics University of Latvia (courses: “Materials in Nature and Technics” and “Spectroscopy of Solid State”).



Photographs of transparent glass and glass ceramics cotaining $NaYF_4$:1.5mol%Er^{3+} obtained by heat treatment of the precursor glass at different temperatures: upper row – as prepared, lower row – excited at 979 nm.

LABORATORY EQUIPMENT

Picosecond wavelength-tunable laser (EKSPLA) excited luminescence measurement equipment with streak-camera (HAMAMATSU). The equipment allows measurement of time-resolved luminescence spectra at different temperatures (10 K – 300 K) in a broad time range (50 ps – 10 ms)
Spectrometer (ANDOR) equipped with CCD camera (ANDOR) for traditional and up-conversion luminescence spectra measurements at different temperatures (10 K – 300 K), excited by Xe lamp or laser diode (808 nm and 980 nm, power up to 1 W).

SCIENTIFIC STAFF

Dr.hab.phys. Maris Springis
Dr.phys. Anatolijs Sarakovskis
Dr.phys. Jurgis Grube

PhD Students
M.Sc. Guna Krieķe
M.Sc. Guna Doķe

Students
A. Ansbergs
G. Zageris
K. Strals

SCIENTIFIC VISITS ABROAD

A.Sarakovskis (4 days Lithuania)

COOPERATION

Latvia
Riga Technical University (Prof. A. Medvid).
RTU Institute of Nonorganical Chemistry (Dr. J. Grabis, Dr. D. Jankovica).
Switzerland
University of Bern, Department of Chemistry, Bern (Prof. K. Kraemer)
Russia
The Joint Institute for Nuclear Research, Dubna (Prof. G. Arzumanyan)
Institute of Spectroscopy, Russian Academy of sciences, Troitsk (Prof. M. Popova)
Finnland
Optoelectronics and Measurement Techniques Laboratory,University of Oulu (PhD, D.Sc.Alexey Popov).

MAIN RESULTS

UPCONVERSION LUMINESCENCE IN ERBIUM DOPED TRANSPARENT OXYFLUORIDEGLASS CERAMICS CONTAINING HEXAGONAL $NaYF_4$ NANOCRYSTALS

A. Sarakovskis, G. Krieke

Transparent erbium doped oxyfluoride glass ceramics containing hexagonal $NaYF_4$ nanocrystals has been prepared by melt-quenching and subsequent heat treatment of the precursor glass. The formation of β - $NaYF_4$ was confirmed by X-ray diffraction measurements. The overall intensity of the upconversion luminescence of the glass ceramics sample is 2 orders of magnitude higher than that of the precursor glass. The observed enhancement of the efficiency is explained by the incorporation of Er^{3+}into low-phonon β - $NaYF_4$crystalline phase.

COMPREHENSIVE STUDY ON DIFFERENT CRYSTAL FIELD ENVIRONMENTS IN HIGHLY EFFICIENT $NaLaF_4:Er^{3+}$ UPCONVERSION PHOSPHOR

A. Sarakovskis, G. Krieke, G. Doke, J, Grube, L. Grinberga,
M. Springis

Complex fluorides, especially rare-earth doped $NaREF_4$ (RE = Y^{3+}, La^{3+} or Gd^{3+}), are promising materials for the upconversion luminescence mostly due to low phonon energy of their matrices and multisite nature of the crystalline lattice. Although multisite formation in hexagonal $NaREF_4$ structures has generally been proved, the actual number of the active sites in different structures varies from two ($NaGdF_4$) to seven ($NaYF_4$). The aim of this work has been to study multisite formation in NaLaF4:Er^{3+}. For this purpose low-temperature site-selective spectroscopy measurements in hexagonal $NaLaF_4:Er^{3+}$ have been performed. Excitation at different wavelengths corresponding to the excitation of 4F7/2 level of Er^{3+} ions has revealed three distinct luminescence spectra in the green spectral region associated with $4S_{3/2} \rightarrow 4I_{15/2}$ electronic transition. The number of the spectra has been sufficient to model experimentally measured luminescence spectra at any excitation wavelength as a linear combination of the distinct spectra. The analysis of the structure of the material and the results of site-selective spectroscopy signify the presence of at least three different crystalline field environments where Er^{3+} ions incorporate. Upon siteselective excitation of Er^{3+} located at a specific site energy transfer to erbium ions located at other sites has been observed in both the upconversion and downconversion luminescence processes. The enhanced energy transfer between the different sites in $NaLaF_4:Er^{3+}$ signifies the importance of the multisite nature of the structure, which is a key factor for an efficient upconversion luminescence.

UP-CONVERSION LUMINESCENCE OF ERBIUM IN BARIUM CONTAINING OXYFLUORIDE GLASS CERAMIC

G. Krieke, A. Sarakovskis

Barium fluoride containing glass ceramics are promising materials because the low phonon energy of the lattice reduces the non-radiative transitions and BaF2 has high solubility of all rare earth ions. In this study glasses with general composition of Na2O-NaF-BaF2-YF3-Al2O3- SiO2:ErF3 containing various amount of BaF2 were prepared. The glass ceramics were obtained after isothermal heat treatment. Introduction of barium

fluoride in aluminosilicate glasses favors the crystallization of Ba2+ containing tetragonally and rhombohedrally distorted fluorite type compounds. These materials exhibit efficient upconversion luminescence. The efficiency of green luminescence is higher than in β-NaYF4 containing glass ceramics. The high efficiency of upconversion luminescence is caused by decreased cross-relaxation rate, increase in the distance between erbium ions and incorporation of erbium ions in cationic positions with low local symmetry. In this study for the first time transparent glass ceramics with rhombohedral and tetragonal Ba2+ containing nanocrystals has been prepared. The upconversion luminescence of these materials has been characterized.

Pr^{3+} LUMINESCENCE IN OXYFLUORIDE GLASS AND OXYFLUORIDE GLASS CERAMIC CONTAINING $NaLaF_4$

Ģ. Zāģeris, J. Grūbe, A. Šarakovskis, G. Krieķe

Rare-earth activated oxyfluoride glass and glass ceramics are interesting luminescent materials which chemical compositions are identical, but luminescence properties are different. The mechanisms that determine how rare-earth ions fit into the crystallographic lattice and, subsequently, how processes of luminescence are different for glass and glass ceramic materials. Oxyfluoride glass samples with various concentrations of praseodymium were obtained – 0.01 mol%, 0.1 mol% and 1 mol%, with each of these samples being created under similar circumstances. Afterwards, the glass samples were heated once more in different temperatures in order to obtain glass ceramic samples containing NaLaF4 crystalline phase. Luminescence spectra both for glass and glass ceramic samples were measured at room temperature as well at low (15 K) temperature. Luminescence kinetics of various luminescence bands were also obtained. The accumulated data allows to conclude that the mechanisms behind luminescence in glass and glass ceramic are indeed different, and they are dependent on the concentration of the rare-earth ion in a given sample. Based on experimental results praseodymium concentration impact on luminescence processes in glass and glass ceramics will be discussed.

NRP IMIS2 2. PROJECT: NANOMATERIALS UN NANOTECHNOLOGY

A. Sarakovskis

The targets of the project are to achieve a world-class knowledge of innovative and advanced materials, smart technologies that contribute to the economic challenges and opportunities to create competitive products. The tasks of the project are: 1. Synthesize and investigate properties of innovative, functional and competitive thin films (nanolayers) including synthesis and application of graphene; 2. Synthesize and investigate properties of innovative, functional and competitive nanomaterials and their application in nanotechnology; 3. Synthesize and investigate properties of innovative, functional and competitive quantum dots and nanowires for efficient electroluminescent light sources; 4. Synthesize and investigate properties of innovative nanocomposite materials for harvesting of waste energy in high performance thermoelectric generators In the presentation the achievements of the scientific groups invovled in the realization of the project will be reported and tasks in the workplan for the 3rd stage will be discussed.

LUMINESCENCES PROCESSES IN $NaLaF_4:Tm^{3+}$

J. Grube

In different kind of materials doped with Tm^{3+} and Yb^{3+} after excitation with infrared light ultraviolet up-conversion luminescence can be observed. Up-conversion excitation appears due to rare-earth interaction as result excitation energy from one ion is transfer to other ion which is excited into higher energy state. In many scientific papers, for example about $NaYF_4:Tm^{3+},Yb^{3+}$, there are proposed energy transfer mechanisms between thulium ions which results in excitation of Tm3+ higher energy state from which ultraviolet luminescence is observed. In this work it will be shown whether in $NaLaF_4$ Tm^{3+} interaction could leads to excitation of Tm^{3+} higher states. In this work $NaLaF_4:Tm^{3+}$ samples with 0.01, 0.1, 0.5, 1 and 2 mol% Tm^{3+} were synthesized. After excitation with various wavelength characteristic Tm^{3+} luminescence bands in the ultraviolet, visible and infrared spectral regions were observed. For the samples with different Tm^{3+} concentration luminescence spectra and luminescence decay kinetics were compared analyzed to thulium ion interaction. Based on the experimental results the impact of Tm^{3+} concentration on the optical properties of $NaLaF_4:Tm^{3+}$ is discussed.

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LECTURES ON CONFERENCES

31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2015, February 24-26.

M.Osis, G.Krieķe, A.Sarakovskis, M.Springis. Up-conversion luminescence of Er doped oxyfluoride glass and glass ceramics. Abstracts, p.7.

K.Strals, G.Krieke, A.Sarakovskis, M.Springis. Up-conversion luminescence in $LaInO_3:Er^{3+}$. Abstracts, p.8.

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A.Sarakovskis. Nanomaterials and nanotechnology.

J. Grube, A. Sarakovskis, G. Doke, G. Krieke, M. Springis. Temperature impact on $NaLaF_4:Er^{3+}$ spectroscopic properties.

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DOCTORAL THESIS

Jurgis Grube. "Luminescence processes in Er^{3+} doped $NaLaF_4$", supervisors Maris Springis and Anatolijs Sarakovskis.

MASTER THESIS

Guna Krieķe. "Luminescence of Erbium ions in oxyfluoride glass and glass ceramics, containing β - $NaYF_4$", supervisors Liga Berzina-Cimdina and Anatolijs Sarakovskis.

BACHELOR THESIS

Kristaps Strals."Up-conversion luminescence ar Er3+ joniem aktivētā $LaInO_3$ ",supervisor Anatolijs Sarakovskis.

DEPARTMENT OF CRYSTALS PHYSICS AND OPTOELECTRONIC MATERIALS

Head of Department Dr. phys. P. Kulis

LABORATORY OF WIDE BAND GAP MATERIALS

Head of Laboratory Dr. hab. phys., Assoc. prof. B. Berzina

RESEARCH AREA AND POSSIBILITIES

The research interests of our laboratory are focused on light-induced processes and defect luminescence in wide band gap materials such as III group nitrides, oxides and others available in form of bulk and nanosize structures. The spectral characterization of materials is realized in order to reveal:

- defect-induced luminescence mechanisms as well as the defect structure and behavior in material;
- processes of energy transfer between defects and host lattice;
- influence of material size on luminescence properties (macrosize and nano-structures in 1D, 2D and 3D forms);
- estimation of practical applications of the materials for the UV light dosimeters, gas sensors, UV and visible light emitters;
- elaboration of new materials for oxygen gas sensing.

The research includes different spectral characterizations of materials in temperature range 8 K – 300 K, such as absorption spectra within the spectral range 190 nm – 1100 nm, photoluminescence spectra (250 nm – 1500 nm), its excitation spectra, luminescence polarization and optically and thermally stimulated luminescence.

SCIENTIFIC STAFF

1. Baiba Berzina, Dr.hab.phys, senior researcher, head of lab.
2. Laima Trinkler, Dr. phys., senior researcher,
3. Valdis Korsaks, Dr. phys., senior researcher.

Students - Technicians:
1. Paula Jankovska, student

COLLABORATIONS

Latvia

Laboratories and departments of ISSP University of Latvia (Drs. J.Maniks, D. Millers, V.Skvortsova, L.Skuja, K.Kundzins, L.Grigorjeva, Y. Zhukovskii, S. Piskunov).
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Institute of Physics of National Academy of Science of Ukraine, Department of Physics of Biological Systems (Prof. Galina Dovbeschko

MAIN INVESTIGATIONS AND RESULTS

SPECTRAL CHARACTERIZATION OF AlN NANOPWDER

L.Trinkler, B.Berzina, V. Korsaks, P.Jankovska

Spectral characterization of AlN nanopowder synthesized in Institute of Inorganic Chemistry, Riga Technical University was done under different environmental conditions, when material is put into a vacuum or surrounded with different gases such as oxygen, nitrogen, argon and air. It was found, that for this material the 420 nm luminescence is sensitive to oxygen gas, which is reducing the luminescence intensity. 420 nm photoluminescence (PL) and its excitation (PLE) spectra of AlN were studied within a temperature range between 8 K and room temperature (RT). It was found that there are two mechanisms responsible for the 420 nm luminescence. One of them is intra-center mechanism, which is realizing, when AlN nanomaterial is excited with 315 nm light. The other one is recombination luminescence mechanism, which is observed when material is excited with light from the spectral region around 260 nm.
Oxygen gas sensing properties of the material such as dependence of the 420 nm luminescence intensity on oxygen gas concentration in mixture of oxygen-nitrogen gases, repeatability of the results etc. were sudied. The results obtained were included in submitted European patent EP 15177885.
These studies were performed within a support of European project ERDF 2014/0047/2DP/2.1.1.1.0/14/APIA/VIAA/007.

SPECTRAL CHARACTERIZATION OF HEXAGONAL BORON NITRIDE

B. Berzina, L.Trinkler, V.Korsaks

Spectral characterization of hBN consisting of macro- or nano-size grains has been performed. Photoluminescence spectra of materials have been studied within a wide temperature range between 8 K and 300 K. It was found that in all materials, which were studied, there are two main phonon-assisted luminescence bands at ~300 nm and ~400 nm. These luminescences are caused by native defects of hBN and appear independently of particle size and material origin. The 400 nm luminescence was specially studied. It was found that the 400 nm luminescence is caused by the F-type defects, which were located at or near the material surface as well as in the bulk. It was also found that the intensity of the 400 nm luminescence is dependent on oxygen content in the ambient atmosphere surrounding the sample. This feature allows to propose hBN as a material suitable for oxygen sensors. The properties, which are characteristic for the gas sensing materials were studied.

These studies were supported by the European projects: ERDF 2014/0047/2DP/2.1.1.1.0/14/APIA/VIAA/007; ESF project "Experimental and theoretical investigation of technologically important materials" and by Latvian National Research Program IMIS2 (2014 – 2017).

LUMINESCENCE PROPERTIES OF LiGaO

L.Trinkler, B. Berzina, V.Korsaks

A special study was performed to investigate the optical properties of the substrate material **$LiGaO_2$ (LGO)** newly produced in Taiwan. LGO is a crystal with orthorhombic distorted wurtzite structure. The samples are cut from the single crystal along [100], [010] and [001] directions. LGO material was studied in more detail by means of absorption, photoluminescence (PL), PL excitation (PLE), polarised luminescence methods. The low-temperature PL spectra of LGO sample contain several bands centered at 4.43 eV, 3.82 eV, 2.38 eV, and 1.77 eV. The corresponding excitation bands are localised at 6.29 eV, 5.85 eV and 4.96 eV. Temperature-dependent PL revealed monotonous decrease of 3.82 eV and 1.77 eV bands, while 4.43 eV band exhibited a maximum at 60 K and then rapidly decreased disappearing at 140 K. 3.82 eV, 2.38 eV, and 1.77 eV bands have polarised luminescence, their polarisation degree and spectral behaviour depend on sample orientation and temperature. The physical origin of the observed PL bands is still under investigation.
These studies were performed within a support of the Latvian-Lithuanian-Taiwan project "Nonpolar ZnO thin films: growth-related structural and optical properties". No. LV-LT-TW/2015/3.

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2) **V. Korsaks**, Hexagonal boron nitride luminescence dependent on vacuum level and surrounding gases, Material Research Bulletin 70 (2015) 976-979.
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4) V.Skvortsova, N.Mironova-Ulmane, **L.Trinkler**, V.Merkulov, Optical properties of natural and synthetic beryl crystals, IOP Conference Series: Material Science and Engineering 77 (2015) issue 1, article number 012034.

PATENT

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LECTURES ON CONFERENCES

31th Scientific Conference of Institute of solid State Physics, University of Latvia, February 24-26, 2015, Riga, Latvia

1. Paula Jankovska , Valdis Korsaks , Laima Trinkler , Baiba Berzina , Janis Grabis, Luminescence of AlN nanopowder and its dependence on environment, Abstract Book, p. 9.

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2. B.Berzina, L.Trinklere, V.Korsaks, J.Grabis, White light emitters based on AlN nanopowders. http://euronanoforum2015.eu/wp-content/uploads/2015/03/Abstract_Berzina_Baiba.pdf

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3. C.-Y. J. Lu, Y.-T. T. Tu, L. Trinkler, B. Berzina, V. Korsaks, P. Ščajev, S. Tumėnas, R. Nedzinskas, E. Pozingytė, A. Rimkus, S. Paurazaitė, U. Jahn, M.M.C. Chou, L. Chang, Growth and optical properties of rock-salt $Zn_{1-x}Mg_xO$ epilayers on MgO (100) substrate. Abstract Book, p. 82.

4. E. Pozingytė, A. Rimkus, S. Paurazaitė, P. Ščajev, S. Tumėnas, R. Nedzinskas, L. Trinkler, B. Berzina, V. Korsaks, C.L. Chen, L.W. Chang, M.M.C. Chou, Temperature-dependent photoluminescence spectroscopy of nonpolar ZnO/ZnMgO quantum wells, grown on lattice-matched (100) $LiGaO_2$ substrate. Abstract Book, p.122.

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6. B. Berzina, V. Korsaks, L. Trinkler, P. Jankovska, J. Grabis, Surface defect luminescence of AlN powders. Abstract Book, p.124.

DEPARTMENT OF CRYSTALS PHYSICS AND OPTOELECTRONIC MATERIALS

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LABORATORY OF SEMICONDUCTOR OPTOELECTRONICS

Head of Laboratory Dr.phys. B. Polyakov

RESEARCH AREA AND MAIN PROBLEMS

1. Synthesis of inorganic nanocrystals, nanotubes, nanowires for photonics, electronics and biomedicine. Investigation of their structural, optical and other properties.
2. Engineering, synthesis and functional processing of advanced 0D and 1D hybrid nanostructures. Scanning probe and electron microscopy characterization of nanomaterials.
3. Development and implementation of nanomechanical tests for 1D nanostructures and simulations of their mechanical properties; prototyping of nanodevices.
4. Euroatom

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COOPERATION

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Forschungszentrum Juelich GmbH, Julich
Max Plank Institute of Plasma Physics, Garching

Estonia
Institute of Physics, University of Tartu
Estonian Nanotechnology Competence Centre, Tartu

MAIN RESULTS

METAL NANODUMBBELLS FOR NANOMANIPULATIONS AND TRIBOLOGICAL EXPERIMENTS

B. Polyakov, S. Vlassov, J. Butikova, K. Smits, R. Zabels

Manipulation of nanoscale objects provides essential data for development of future nanoscale devices and contributes to fundamental understanding of friction laws. Ag, Au and Cu nanodumbbells were produced by laser induced melting of corresponding nanowires. Formation of NDs by laser-induced partial melting of NWs is a complex dynamic process, which includes melting of the NW ends followed by rapid solidification. Shape and morphology of these structures were studied by SEM and TEM methods. Dependence of the crystalline structure on the size of the end bulb was demonstrated. Small bulbs preserved the original crystalline structure of NW, while for bigger bulbs a twinned structure different from the original one was observed. A grain boundary can be seen at the interface between the melted end and the body of the NW. The medium-sized bulb partially preserved the original structure of the NW. Such association between the structure and size of the bulb may be related to the fact that the temperature gradient between the bulb and the NW is smaller in the case of small bulbs, and the melted part is able to follow the original crystalline structure of the NW. In a bigger bulb, more competing crystallization nuclei forming an independent grain are possible. Nanodumbbells were manipulated by AFM at ambient conditions and inside SEM at high vacuum conditions [fig.1]. Inside SEM manipulations in comparison to AFM manipulation benefit from real-time visual guidance of the manipulation event. The geometry of nanodumbbells makes them promising candidates for applications in MEMS/NEMS and attractive objects for nanotribological studies enabling us to study different regimes of motions (rolling, sliding, rotation).

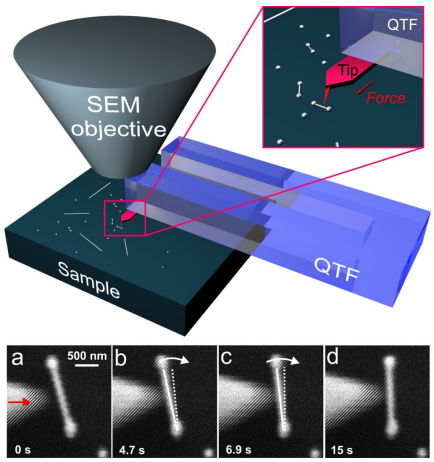

Fig. 1. Schematics of inside SEM manipulation of metal NDs. The metal ND on the silicon wafer is pushed by an AFM tip glued to one prong of the QTF (force sensor). ND manipulation process is monitored in real time by SEM (a-d).

PLASMONIC PHOTOLUMINESCENCE ENHANCEMENT BY SILVER NANOWIRES

B. Polyakov, R. Zabels, A. Sarakovskis, S. Vlassov and A. Kuzmin

The collective excitation of the electron gas in the conduction band of metal nanoparticles (NPs)/nanowires (NWs) can result in strong optical response known as localized surface plasmon resonance (LSPR) and representing considerable interest in the field of nanophotonics and plasmonics. Moreover, metal NWs can be used as a plasmonic waveguide to enhance Raman scattering or photoluminescence (PL) signals very locally for a nanoscale object (single molecule, quantum dot, etc), realizing so called ‘remote surface enhanced Raman spectroscopy’ or PL.
In this study we compare the luminescence enhancement effect on ruthenium-based dye (Ruthenizer 535-bisTBA or

N719) and CdS QDs on the same substrates, that allows direct comparison of obtained results. The analysis of possible geometrical effects and their separation from LSPR-related luminescence enhancement is analysed. PL enhancement for N719 dyes was much more significant in comparison to CdS NCs. The largest enhancement was detected (i) in the case when an NW is placed above the silver film or (ii) at the intersection point of two NWs, where the hot spots are created. The carbon contamination effect at the surface of silver NWs occurs at high laser light intensities and may result in some artifacts; therefore, one should be aware of it during measurements of PL enhanced by LSPR. Silver NW on silver film is proved to be an effective system for LSPR-related PL enhancement.

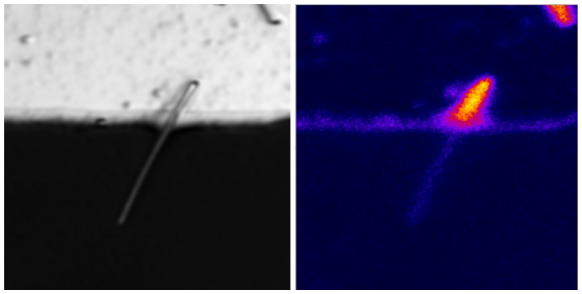

Fig. 2. Confocal and PL spectral images (size 8 × 10 μm) of silver nanowire placed above the silver film on a glass substrate and uniformly covered with ruthenium-based dye (N719). PL spectral image was acquired at 730 nm.

SYNTHESIS AND CHARACTERIZATION OF HETEROSTRUCTURED CUO/CUWO$_4$ CORE/SHELL NANOWIRES

B.Polyakov, A.Kuzmin, K. Smits, S.Vlassov, E.Butanovs, J.Zideluns, J. Butikova

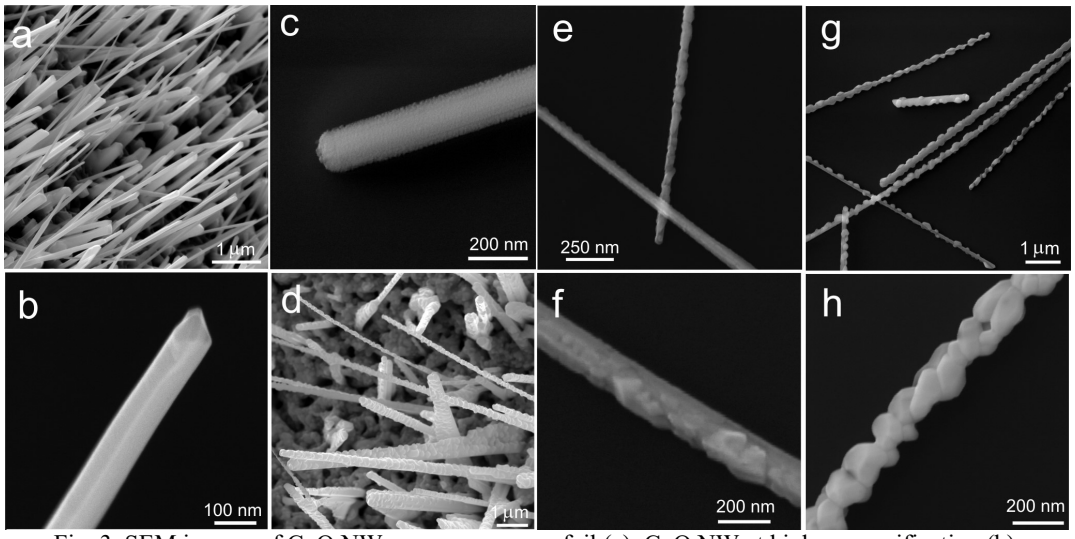

Fig. 3. SEM images of CuO NWs array on copper foil (a), CuO NW at higher magnification (b), WO3-coated CuO NW on silicon substrate (c), core/shell CuO/WO3 NWs array on copper foil annealed at 650ºC (d), core/shell CuO/WO3 NWs on silicon substrate annealed at 450ºC (e, f), core/shell CuO/WO3 NWs on silicon substrate annealed at 650ºC (g, h).

Metal oxide nanowires (NWs) and their heterostructures are promising materials for the next generation of solar power harvesting devices, photocatalyst materials for water splitting, and gas sensing devices. The use of axially heterostructured or core/shell NWs has several important advantages in comparison to thin film technologies: combination of materials with large lattice mismatch and even epitaxial growth of shell material on the core, improved mechanical properties due to a reduction in the number of defects per unit length, superior electroconductive properties of NWs due to their crystallinity and small defect concentration, large surface area and/or large heterojunction area, novel or significantly improved thermal, optical, electronic or field emission properties. Recently CuO/CuWO4 core/shell NW arrays were proposed as well-consisted system with enhanced activity and durability for photoelectrochemical water splitting. In this study

we investigate core/shell CuO/WO3 NWs morphology evolution and CuWO4 formation around CuO core NW upon thermal annealing in air. Degradation of NW core morphology often occurs during solid-state chemical reactions. Therefore, the important question to be addressed in this study is morphology evolution of heterostructured NWs upon reaction between core and shell materials, and a preservation of integrity and crystallinity of the core NW. This is the first study of evolution of the internal microstructure of core-shell CuO/WO3/CuWO4 NWs upon heating.

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2. **B.Polyakov, S.Vlassov**, L.Dorogin, **J.Butikova,** K.Smits, M.Antsov, S.Oras, R.Zabels, R.Lõhmus. Metal nanodumbbells for nanomanipulations and tribological experiments. *Physica Scripta*, 2015, 90, 094007 (7pp).
3. I.Kokina, I.Jahundovila, I.Mickevila, E.Sledevskis, A.Ogurcovs, **B.Polyakov**, M.Jermaonoka, J.Strautiš, V.Gerbreders. The Impact of CdS Nanoparticles on Ploidy and DNA Damage of Rucola (Eruca sativa Mill.) Plants. *Journal of Nanomaterials,* Volume 2015, Article ID 470250, 7 pages.
4. M.Vahtrus, M.Umalas, **B.Polyakov**, L.Dorogin, R.Lõhmus, **S.Vlassov**. Mechanical characterization of annealed Al2O3 nanofibers. *Materials Characterization*. 107, 119–124, 2015.
5. M.Vahtrus, A.Shutka, **S.Vlassov**, A.Shutka, **B.Polyakov**, R.Saar, L.Dorogin, R.Lõhmus. Mechanical characterization of TiO2 nanofibers produced by different electrospinning techniques. *Materials Characterization*, 2015, 100, 98–103.
6. M.Umalas, **S.Vlassov, B.Polyakov,** L.Dorogin, R.Saar, I.Kink, R. Lõhmus, A.Lõhmus, A.Romanov. Electron beam induced growth of silver nanowhiskers. *Journal of Crystal Growth* 410, 2015, 63–68.
7. **B.Polyakov,** L.Dorogin, **S.Vlassov,** I.Kink, R.Lohmus. Tribological Aspects of In Situ Manipulation of Nanostructures Inside Scanning Electron Microscope. *Fundamentals of Friction and Wear on the Nanoscale*, Chapter 18, Springer International Publishing, Switzerland, 2015.
8. A.N. Trukhin, K. Smits, **J. Jansons**, A. Kuzmin. Luminescence of polymorphous SiO2. – *Radiation Measurements*, (2015), 1 – 8 pp

Other Articles

1. **J. Jansons.** LU profesors Jurijs Kuzmins (12.10.1940. – 02.09.2014.). – "Zvaigžņotā Debess" 2015. g. pavasaris (227), 31. – 35. lpp., un nobeigums – "ZvD" 2015. g. vasara (228), 25. – 30. lpp.

LECTURES ON CONFERENCES

Fourth International Conference on Multifunctional, Hybrid and Nanomaterials, 9-13 March 2015, Sitges, Spain:
B. Polyakov, S.Vlassov, L. M. Dorogin, M. Antsov, R. Lohmus. "*Mechanical properties of hybrid Ag-SiO2 core-shell nanowires*".

Euronanoforum 10-12 June 2015, Riga, Latvia:
B. Polyakov,S.Vlassov, L. M. Dorogin, Jelena Butikova, M. Antsov, R. Zabels R. Lohmus. "*Synthesis and Processing of Metal Nanowires*".

J. Butikova, B. Polyakov, S. Vlassov, R. Lohmus. "*Conditioning of Metal Nanowires in Liquids by Laser Processing*".

The International Conference on Understanding and Controlling Nano and Mesoscale Friction, June 22-26 2015, Istanbul, Turkey:
S.Vlassov, B. Polyakov, L. Dorogin, S.Oras, M. Vahtrus, M.Antsov, R.Lohmus. "*Rotational Friction of ZnO nanowires*".
B. Polyakov, S. Vlassov, L.Dorogin, M.Antsov, J. Butikova, R.Zabels, R.Lohmus. "*Metal nanodumbbell as a test object for a nanojoint*"**.**

DEPARTMENT OF PHOTONICS AND MATERIAL PHYSICS

Head of Department Dr.habil.phys. D.Millers

SOLID STATE RADIATION PHYSICS LABORATORY

Head of laboratory Dr.habil.phys.L.Grigorjeva

RESEARCH AREA

The time-resolved luminescence and absorption methods were used for electronic properties studies of single crystals, ceramics, nanopowders and coatings. The basic research includes study of different interactions of electronic excitations, while the applied research is focused on materials for radiation detectors, sensors and luminescent light sources.

EQUIPMENTS

Excitation sources: a pulsed electron beam accelerator (10 ns, 270 keV, 10^{12} electrons/pulse), YAG:Nd and nitrogen lasers (266 nm and 532 nm, 2 ns; 337 nm, 10ns); for steady state luminescence spectra and radiation defect creation X-ray source and 980 nm laser diode were used. TSL methods were developed.
Steady state and time resolved absorption spectroscopy. VIS-UV absorption spectrometer LABOMED for measurements in 190-1100 nm range. FTIR absorption spectroscopy: EQUINOX 55 (10000-400 cm^{-1} and 22000-7000 cm^{-1} spectral regions) developed also for dispersed materials in wide temperature range.
Luminescence measurements. The luminescence was measured through monochromator MDR-3 with HAMAMATSU H8259 photon counting head and photon counting board FastComTech module P7887 with 500 channels. The minimal time bins is 250 ps. The laser frequency and time bins can be adjusted. The luminescence spectra were recorded using the Andor Shamrock B-303i spectrograph equipped with CCD camera (ANDOR DU-401A-BV). The luminescence measurements will be carried at temperature regions 8-300K and 300K-500K.
The excitation spectra was measured by two Horiba JOBIN YVON monohromators iHR320 and TRIAX320.
TSL and FGT methods. The temperature regimes are easy realized by using special programs. The activation energies were calculated according to Hoogenstraaten and fraction glow methods.

SCIENTIFIC STAFF

Dr.habil.phys. D.Millers
Dr.habil.phys. L.Grigorjeva
Dr.K.Smits

Students
M.Vanks
A.Zolotarjovs
A.Krumina
D.Olšteins

SCIENTIFIC VISITS ABROAD

1. Dr,L.Grigorjeva, Estonia (5 days)
2. Dr.K.Smits. Germany (5 days).
3. Dr.K.Smits, France, PROMES, 2 weeks.
4. A.Zolotarjovs, France, PROMES, 2 weeks.
5. Dr.L.Grigorjeva, France, PROMES, 2 weeks.
6. A.Zolotarjovs, Sant-Peterburg, Russia 7 days.
7. A.Zolotarjovs, Prague, Czech Republic, 10 days.

COOPERATION

Latvia

Riga Technical University, Institute of Inorganic Chemistry (Dr.habil.sc.ing. J.Grabis).

LU Institute of Microbiology (M.Gavare, J.Liepiņš).

Institute of Chemical physics, UL (Dr. G.Kizāne, Dr.E.Pajuste).

Estonia

Institute of Physics, Tartu (Dr.S.Zazubovich, Dr. I.Sildos))

Russia

GIREDMET, Moscow (Pr. I.S Lisitskii)

St.Peterburg, Prof. P.Rodnyi, E.Gorohova, K.Chernenko.

Institute of Electrophysics, Ural Branch, Russian Academy of Sciences, Yekaterinburg, Russia (Prof.S.Sokovnin)

France

CNRS Processes, Material and Solar Energy Laboratory, (PROMES), Odeillo (Dr.C.Monty)

China

Shanghai Institute of Technology (SIT), Dr. Jiayue Xu.

MAIN RESULTS

LUMINESCENCE PROPERTIES OF ZIRCONIA, HAFNIUM AND ZINC OXIDES NANOCRYSTALS AND CERAMICS PREPARED BY SOLAR PHYSICAL VAPOR DEPOSITION.

K.Smits, L.Grigorjeva, D.Millers, A.Zolotarjovs, C.Monty.

In the frame of cooperation with PROMES CNRS (France) the well-separated metal oxide nanocrystals and ceramics were obtained in a Heliotron reactor via the solar physical vapor deposition (SPVD) method. The obtained nanocrystals were used for ceramic sintering. The SEM, TEM, luminescence properties of materials were investigated.

THE EFFECT OF ELECTRON RECOMBINATION PROCESSES ON THE LUMINESCENCE KINETICS OF ZnO CERAMICS

K. A. Chernenko, L. Grigorjeva, E. I. Gorokhova and P. A. Rodnyi

The spectral and kinetic properties of photoluminescence of zinc oxide ceramics with and without addition of gallium have been studied. In the photoluminescence spectrum, we have observed two luminescence bands with maxima at 377–379 (near-band-edge luminescence) and 490 nm (green luminescence). It has been shown that the decay

curves of the green luminescence are complex processes with different decay times and temperature properties, as well as the kinetics of release of
carriers from electron traps. The relations between luminescence decay curves and mechanisms of luminescence excitation, as well as energy transfer processes, have been discussed.

GAS SENSITIVE LUMINESCENCE OF ZnO COATINGS OBTAINED BY PLAZMAELECTROLYTIC OXIDATION

L. Grigorjeva, D. Millers, K. Smits, A. Zolotarjovs

ZnO coatings on Zn substrate were obtained using plasma electrolytic oxidation method. The XRD and SEM methods were used for structural and morphological characterization of obtained coatings. The luminescence of ZnO coatings were studied and compared with luminescence characteristics of ZnO single crystal. It is shown that luminescence intensity in ZnO defect band depends on oxygen concentration in ambient atmosphere. The effect is of interest for oxygen sensing based on ZnO coating luminescence.

STRUCTURE, NANOHARDNESS AND PHOTOLUMINESCENCE OF ZnO CERAMICS BASED ON NANOPOWDERS

Faina Muktepavela, Larisa Grigorjeva, Karlis Kundzins,
Elena Gorokhova and Piotr Rodnyi

ZnO ceramics obtained from grained powders with different grain size by hot pressing and ceramics from tetrapods nanopowders obtained by press-less sintering have been investigated. Ceramics obtained by hot pressing were optically transparent but were composed of large inhomogeneous grains (d=8–35 μm) exhibiting a substructure. Decreased values of elastic modulus within a grain and a wide defect associated 'green' luminescence with a weak excitonic band indicate a high concentration of residual point defects in hot pressed ZnO ceramics. Utilization of more small-grained powders contributes to the formation of more uniform microstructure (d=5–15 μm) and extraction of point defects. This reflects as a substantially decreased defect PL band and increased excitonic band. Ceramics obtained by press-less sintering from tetrapods had fine-grained structure (d=1–4 μm) with no signs of a substructure. PL spectrum has a narrow excitonic band with phonon replicas (1LO_ExD0), whereas the defect 'green' luminescence is negligible. The effects of powders morphologies have been explained in terms of a interaction processes between initial particles on the formation of a microstructure and defect distribution on the grain growth stages during the sintering of ZnO ceramics.

LUMINESCENCE OF Eu ION IN ALUMINA PREPARED BY PLASMA ELECTROLYTIC OXIDATION

Krisjanis Smits, Donats Millers, Aleksejs Zolotarjovs, Reinis Drunka, Martins Vanks.

Eu ion luminescence in aluminium oxide nanocrystals and layers prepared by plasma electrolytic oxidation (PEO) are investigated. The Eu ion in PEO coatings has intense luminescence allowing such material to be used for preparation of various phosphor. In this study, Eu ion doped coatings were prepared with two methods: anodization and pulsed bipolar PEO. Also, for comparative studies, alumina nanocrystals with the same amount of Eu ions were prepared using SolGel and molten salts methods. Obtained Eu-

doped coatings were studied using luminescence methods. Typical Eu ion luminescence bands were observed, however intensity and spectral distribution differs drastically depending on preparation method and parameters used, therefore the Eu ion luminescence could be used as coating quality luminescent probe. Additionally, the possibility to incorporate the Eu ions in trivalent or divalent state exhibiting bright red or blue luminescence by using different oxidation process parameters.

SCIENTIFIC PUBLICATIONS

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2. **K. Smits,** A. Sarakovskis**, L. Grigorjeva, D. Millers** and J. Grabis. The role of Nb in intensity increase of Er ion up-conversion luminescence in zirconia J. Appl. Phys. 2014, 115, 213520 . DOI: 10.1063/1.4882262.
3. V. Bondar, **L. Grigorjeva,** T. Kärner, O. Sidletskiy, **K. Smits,** S. Zazubovich**, A. Zolotarjovs.** Thermally stimulated luminescence of undoped and Ce^{3+}-doped Gd_2SiO_5 and $(Lu,Gd)_2SiO_5$ single crystals. Journal of Luminescence, 2014, v. 159, 229–237. DOI: 10.1016/j.jum.2014.11. 034.
4. A.N. Trukhin, **K. Smits,** G. Chikvaidze, T.I. Dyuzheva, L.M. Lityagina. Luminescence of rutile structured crystalline silicon dioxide (stishovite). Solid State Communications, 2014, v. 189,10–14. DOI: 0.1016/j.ssc.2014.03.010.
5. **K. Smits,** A. Sarakovskis, **L. Grigorjeva, D. Millers** and J. Grabis. The role of Nb in intensity increase of Er ion upconversion luminescence in zirconia K. Smits1,a), A. Sarakovskis, L. Grigorjeva, D. Millers and J. Grabis. J. Appl. Phys.2014, 115, 213520; http://dx.doi.org/10.1063/1.4882262.
6. **Grigorjeva, L., Smits, K., Millers, D.,** Jankovia, Dz. Luminescence of Er/Yb and Tm/Yb doped FAp nanoparticles and ceramics. IOP Conference Series: Materials Science and Engineering 2015,77, 012036; doi:10.1088/1757-899X/77/1/012036.
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8. **Smits, K., Millers, D., Zolotarjovs,** A., Drunka, R., **Vanks, M.** Luminescence of Eu ion in alumina prepared by plasma electrolytic oxidation. Applied Surface Science, 2015, 337, 166-171, DOI:10.1016/j.apsusc. 2015.02.085.
9. Chernenko, K., **Grigorjeva, L.,** Gorohova, E.I., Rodnyi, P.A. The Effect of electron recombination processes on the luminescence kinetics of ZnO ceramics. Optics and Spectroscopy , 2015, 118, pp.425-430. DOI: 10.1134/s0030-400x15030108.
10. Elsts, E., Rogulis, U., Bulindzs, **K., Smits, K., Zolotarjovs, A.,** Trinkler, L., Kundzins, K. Studies of radiation defects in cerium, europium and terbium activated oxyfluoride glasses and glass ceramics. Optical Materials, 2015, 41, pp. 90-93. DOI: 10.1016/j.optmat.2014.10.042.
11. Trukhin, A.N., **Smits, K.,** Jansons, J., Kuzmin, A. Luminescence of polymorphous SiO_2. Rad.Meas. 2015, 1-8. DOI: 10.1016/j.radmea.2015.12.002.

LECTURES ON CONFERENCES

LU CFI 31th Scientific Conference, 2015, 24-26. Febr. Riga, Latvia

1. A.Zolotarjovs, K.Šmits, D.Millers, M.Vanks, L.Grigorjeva, R.Drunka, R.Ignatāns. Alumina coatings obtained by plasma electrolytic oxidation: synthesis and characterization. P.14.
2. M.Vanks, D.Millers, L.Grigorjeva, K.Šmits, V.Dimza. 3. A.Truins, K.Šmits, J.Jansons, A.Kuzmins. Luminescence of cristobolite. P.6.
3. E.Elssts, G.Krieke, U.Rogulis, K.Šmits, A.Zolotarjevs, J.Jansons, A.Sarakovskis, K.Kundzins. Studies of terbium, praseodymium, neodymium, dysprosium activated glass and glass-ceramics. P.50.
4. L.Grigorjeva, D.Millers, K.Šmits, A.Zolotarjovs. Luminescence of Europium doped FAp and HAp ceramics. P.52.
5. M.Vanks, D.Millers, L.Grigorjeva, K.Šmits, V.Dimza. The induced absorption dependence on temperature in PZLT ceramics. P.54
5. D.Millers, K.Šmits, L.Grigorjrva, A.Zolotarjovs. Oxigen exchange in sistem – metal oxide –atmosphere. P.53.

The International Conference EuroNanoForum 10-12 06.2015, Riga

1. K.Šmits, D.Millers, L.Grigorjeva, A.Zolotarjovs. Luminescence properties of metal oxides nanostructures, coatings and ceramics. Poster 2E-164.
2. K.Šmits. Oxygen sensors based on zirconia nanoparticls. Oral.

International Conference LUMDETR'2015, 20-25 Sept., Tartu, Estonia

1. L.Grigorjeva, D.Millers, K.Smits, A.Zolotarjovs. Luminescence of ZnO nanopowders and coatings. Abstracts of the International Conference LUMDETR'2015, Tartu, Estonia, Tu-P-8.

MASTER THESIS

Martiņš Vanks. Electron beam induced optical absorption in PZLT ceramics. LU Fiz.-mat. Fac. Riga, 2015.
Anete Krūmiņa,Eu ion luminescent coatings prepared by plasma electrolytic oxidation. LU Chem.fac. Riga, 2015.

DEPARTMENT OF PHOTONICS AND MATERIAL PHYSICS

Head of Department Dr.habil.phys. D.Millers

OPTICAL RECORDING

Head of Laboratory Dr. J.Teteris

RESEARCH AREA AND MAIN PROBLEMS

Synthesis and research of amorphous chalcogenide semiconductor (As-S, As-Se and As-S-Se) and azobenzene containing organic polymer thin films for optical recording, nanotechnology and holography have been performed. Photoinduced changes of optical properties, holographic recording and hologram self-enhancement effects, and relaxation processes in amorphous films are studied. The main task was RTD of high sensitive photoresists in the visible region for holography and lithography for production of diffractive optical elements. Rainbow hologram production technology based on chalcogenide semiconductor photoresists was developed. The methods for fabrication of subwavelength-gratings and surface-relief features with nanometer scale have been developed.

SCIENTIFIC STAFF

1. Dr. M.Reinfelde
2. Dr. J.Teteris
3. Dr. A.Gerbreders
4. Dr.hab. A.Krūmiņš

PhD Students

1. J.Aleksejeva
2. U.Gertners

Students

1. K. Klismeta

COOPERATION

Latvia
1. Riga Technical University (prof. A.Ozols).
2. Daugavpils Pedagogical University (Dr. Vj.Gerbreders).

USA
3. Boise State University Prof. M. Mitkova).

Czech Republic
4. University of Pardubice (Prof. M.Vlcek).

Bulgaria
5. Institute of Solid State Physics, Bulgarian Academy of Sciences (Prof. Z.Ivanova).

FOREIGN SCIENTIST VISITS IN LABORATORY

1. Assoc. Prof., Dr. Zoya Ivanova, Institute of Solid State Physics, Bulgarian Academy of Sciences, 18.05.2015- 01.06.2015.

MAIN RESULTS

SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

Mara Reinfelde and Janis Teteris

Thin films of amorphous chalcogenide semiconductor As_2S_3, As-Se and As-S-Se systems were used for recording of refractive index and surface-relief modulated gratings. Amorphous chalcogenide semiconductors are high index materials with refractive index in the range 2.2 – 3.5, depending on the film composition and light wavelength. The photoinduced changes of refractive index down to $\Delta n \approx 0.15 – 0.5$ are observed in these systems.

The photo- and electron-beam stimulated changes of wet etching rate in amorphous As-S, As-Se and As-S-Se films have been studied. Amorphous chalcogenide semiconductor (AChS) resists obtained by thermal deposition in vacuum are characterized by very high resolution capability and they possess a number of peculiarities that make them attractive for application in many photo- and electron-beam lithographic (EBL) processes.

The recording of the subwavelength gratings with a period of 0.15 μm – 1 μm was performed by holographic method. The fringe period for two intersecting light beams in a media with high refractive index n can be expressed as $\Lambda = \lambda_0/2\ n \sin\theta$, where λ_0 is the wavelength of laser light in vacuum, n is refractive index of the resist and θ is the half-angle between the laser beams inside the resist. The right angle prisms with n= 1.8 – 2.6 were used to increase the value of θ. The grating period and profile after chemical etching was measured by AFM. The transmission, reflection and polarization properties of the obtained gratings were studied.

OPTICAL RECORDING IN AMORPHOUS CHALCOGENIDE THIN FILMS

Janis Teteris

During the past 10 years, research in the field of optical materials based on amorphous chalcogenide semiconductors has made significant advances. Much of this research is driven by applied interest and this field of research is extremely broad and active. The use of amorphous chalcogenide thin films in holography and lithography has probably only just begun, but already produced some promising results.

The main functional principles and practical application of amorphous chalcogenide photoresists for production of the embossed *rainbow* holograms and holographic optical elements are discused. The laser interference lithography is used as a low-cost method for the exposure of large surfaces with regular patterns like subwavelength-gratings and microsieves. The regular features with the sizes of about 50 nm and less can be fabricated by this method. The Bragg reflection gratings were recorded and studied in amorphous As_2S_3 and As-S-Se films. Amorphous chalcogenide thin films are thought to be one of the potential materials for all-optical integrated circuits for the optical communication systems due to their excellent infrared transparency, large nonlinear refractive index, and low phonon energies. The possibility to use the amorphous chalcogenide films as a media for holographic recording, processing and storage of information with high density is discussed.

HOLOGRAPHIC LITHOGRAPHY IN AMORPHOUS CHALCOGENIDE THIN FILMS

J.Teteris, J.Aleksejeva and M.Reinfelde

The recording of the surface-relief and refractive index modulated gratings with a period of 0.15 – 1.0 μm was performed by solid immersion holographic method. The grating period for two intersecting light beams in a coupling prism with refractive index n can be expressed as $\Lambda=\lambda_0/2\ n\ \sin\theta$, where λ_0 is the wavelength of laser light in vacuum, n is refractive index of the prism and θ is the half-angle between the laser beams inside the prism. The right angle prisms with n= 1.5 – 2.6 were used. Amorphous As-S-Se based photoresist with refractive index n_1=3.2 at 0.488 μm was used for the recording of surface-relief gratings. After recording, wet etching of the photoresist was performed to obtain a surface-relief grating. The grating period and profile were measured by AFM. If the recording was performed in air (n=1) and the angle between the beams was equal to 90^o, a grating with a period of 0.345 μm was obtained. If the intersection of the laser beams is performed in a prism with a refractive index of 1.75, a grating period of 0.197 μm was obtained. The application of a prism as an immersion medium decreases the period of the recorded grating *n* times. The transmission, reflection and polarization properties of the subwavelength transmission gratings in As_2S_3 amorphous films were studied. The angular selectivity of holographic recording in amorphous chalcogenide thin films has been improved significantly by a decrease of grating period.

SURFACE RELIEF FORMATION DURING HOLOGRAPHIC RECORDING

U.Gertners and J.Teteris

The key element for the production of surface-relief holographic optical elements is photoresist or light sensitive material. Changes of the chemical properties induced in resist material by light or e-beam exposure enable the surface relief structuring by *wet* or *dry* etching. Therefore this process includes two steps: recording and development by etching. Recently a number of organic and inorganic materials have been studied for direct surface relief formation during the exposure process by a light or e-beam. It is very promising for practical application enabling the possibility to simplify technology of the surface patterning.

In this research the study of direct holographic recording of the surface-relief gratings on amorphous As-S and As-S-Se films has been presented from the side of light polarization. Because of direct surface relief formation, efficiency of the relief formation also depends on softening temperature of the sample what in this case is about 170^0C. Results have shown that the surface relief formation efficiency is many times larger in case of extra softening by additional incoherent light during recording. The mechanism of the direct recording of surface relief on amorphous chalcogenide films based on the photoinduced plasticity has been discussed.

OPTICAL RECORDING IN AZOBENZENE CONTAINING POLYMER FILMS

A. Gerbreders and J. Teteris.

Preparation method and optical properties of spiropyran and polymer composite thin films was studied. Polyvinyl acetate, polymethylmetacrylate and copolymer of poly(vinyl butyral-co-vinyl alcohol-co-vinyl acetate) were used as base for composite.

The transmission spectra of composites were measured before and after illumination by laser beams with different wavelengths. Transmission of composite film of merocianine form was measured by laser beam wavelength 532 nm in dependence on beam intensity. The holographic recording of diffraction gratings was performed by different laser lines (325, 532 nm). During recording the diffraction efficiency was measured in transmission mode. The profiles of the gratings area were analyzed by AFM microscope.

SCIENTIFIC PUBLICATIONS

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2. **A.Gerbreders**, A.Bulanovs, **J.Mikelsone**, K.Traskovskis, **E.Potanina**, A.Vembris, **J. Teteris**, *Photoinduced mass transport in low molecular organic glasses and its practical application in holographyite films based on copper chloride in PMMA matrix,* JNCS, **421** (2015) 48-53.
3. **A.Gerbreders, J.Aleksejeva**, A.Bulanovs, A.Ogurcovs, E.Zarins, A.Tokmakovs, A.Vembris, *Optical properties of the low-molecular amorphous azochromophores and their application in holography,* Journ.Phys.: Conf.Ser., **619** (2015) 012055.
4. **K.Klismeta, J.Teteris**, *The photoinduced birefringence and mass transport in azo compound K-D-2,* Journ.Phys.: Conf.Ser., **619** (2015) 012027.
5. A.Ogurcovs, Vj.Gerbreders, E.Tamanis, **A.Gerbreders**, *Changes in screen-printed ZnO/CuInSe$_2$ p-n junction before and after laser ablation,* Journ.Phys.: Conf.Ser., **619** (2015) 012017.
6. L.Loghina, **J.Teteris**, M.Vlcek, *Holographic recording of surface gratings in $As_{40}S_{60-x}Se_x$ thin films*, Proc.of 3rd International Conference on Photonics, Optics and Laser Technology, Berlin, Germany, 12-14 March, 2015, p.121-124.
7. **U.Gertners, J.Teteris**, *All-Optical Surface Micropatterning by Electric Field Intensity Gradient,* Adv.in OptoElectronics, vol.2015, ID917029, 8 pages.
8. **U.Gertners**, Z.Gertnere, **E.Potanina**, *Optical field-induced surface-relief micropatterning of amorphous chalcogenide thin films,* J.Micro/Nanolith. MEMS MOEMS, 14(4), 044504, 2015

LECTURES ON CONFERENCES

31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Rīga, Latvia, February 24-26, 2015.

1. K.Klismeta, J.Teteris, Fotoinducētā anizotropija azobenzolu saturošā molekulārajā stiklā (Photoinduced anisotropy in azobenzene containing molecular glass), *LU CFI 31. zinātniskā konference*, Rīga, 2015.gada 24.-26.februāris*, 31st Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 24-26, 2015, Book of Abstracts, p.47.

58th Scientific Conference for Students of Physics and Natural Sciences; March 24-27, 2015, Vilnius.

2. U.Gertners, J.Teteris, A.Gerbreders, All-Optical Surface Patterning in Amorphous Chalcogenide and Azopolymer Thin Films, 58th *Scientific Conference for Students of Physics and Natural Sciences*; March 24-27, Vilnius, abstract book p.181.

International Young Scientist Conference "Developments in Optics and Communications 2015", Riga, Latvia, April 8-10, 2015:

3. K.Klismeta, J.Teteris, Azobenzene containing molecular glass as an optical recordind material, , Book of abstracts, p. 17.

SPIE Photonics West Conference, San Francisco, 7-12.02.2015

4. U.Gertners, J.Teteris, Investigation of All-optical laser-based direct-write technique, , 9374-42.

3rd Int. Conf. on Photonics, Optics and Laser Technology-"Photoptics 2015", Berlin, 13-15. March 2015

5. L.Loghina, J.Teteris, M.Vlcek, Holographic Recording of Surface Relief Gratings on $As_{40}S_{60-x}Se_x$ Thin Films.

10th International Symposium on Display Holohraphy, 28.06.-03.07., 2015, Saint Petersburg, Russia.

6. A.Gerbreders, A.Bulanovs, K.Traskovskis, J.Teteris, Direct recording of the surface relief holographic gratings,

7th International Conference on Amorphous and Nanostructured Chalcogenides, July5-10, 2015, Cluj-Napoca, Romania.

7. J.Teteris, Optical field induced mass transport in amorphous materials
8. M. Reinfelde, L. Loghina, J. Teteris, S. Slang, M. Vlcek, Photoinduced birefringence and surface relief grating formation in As40S60-xSex thin films.
9. U. Gertners, A. Gerbreders, J. Teteris, All-optical surface micro-patterning by electric field intensity gradient.

The 5th International school and conference on photonics (Photonica2015), 24-28 August, 2015, Belgrade, Serbia

10. U.Gertners, J.Teteris, All-optical surface micro-patterning by electric field intensity gradient, Book of Abstracts, p. 216.
11. Z.Gertnere, J.Teteris, Adhesion and friction studies of metal nanoparticle arrays for optoelectronic devices, Book of Abstracts, p. 216.

26th International Conference on Amorphous and Nanocrystalline Semiconductors, 13-18 September, 2015, Aachen, Germany

12. J.Teteris, Optical field induced mass transport in amorphous chalcogenide and azobenzene containing polymers, Book of abstracts, ID 141, p. 151.

SPIE Scanning Microscopics Conference, 29.09.-01.10.2015, Monterey, California, USA

13. U.Gertners, Z.Gertnere, J.Teteris, Investigation of all-optical micro- and nanolithography by electric field intensity gradient.

RTU 56. Starptautiskā zinātniskā konference, Rīga, 2015.gada 14.-16.oktobris

14. J.Teteris, M.Reinfelde, Fotoinducētā virsmas reljefa veidošanās amorfos halkogenīdos un organiskos azo-savienojumos, programma 32.lpp.

DEPARTMENT OF PHOTONICS AND MATERIAL PHYSICS

Head of Department Dr.habil.phys. D.Millers

LABORATORY OF AMORPHOUS MATERIALS SPECTROSCOPY

Head of laboratory Dr.habil.phys. L.Skuja

RESEARCH AREA AND MAIN PROBLEMS

The optical and electronic properties of advanced wide-band gap materials for applications in optical elements for high power laser optics, optical fibers, for deep-ultraviolet and vacuum-ultraviolet spectral ranges, for radiation environments and for nanoscience. The research is mainly focused on silicon-dioxide based glasses and related materials.

SCIENTIFIC STAFF

Dr.habil.phys. L. Skuja (Head of laboratory)
Dr.habil.phys. A. Trukhin
Dr.habil.Phys A.Siliņš

EXPERIMENTAL METHODS AND EQUIPMENT

The research is performed mainly by spectroscopic methods, including optical absorption and luminescence spectroscopy, magnetic resonance spectroscopy (electron paramagnetic resonance), infrared absorption and Raman scattering, vacuum-UV spectroscopy, energy-dispersive X-ray microanalysis, thermal desorption mass-spectrometry. In-house-built optical systems are controlled by Labview-based software.
Several of these experimental techniques are available through collaboration with other laboratories of ISSP or with our research partners in other institutions in Latvia or abroad. The equipment, available directly in the laboratory is listed here below.

Optical absorption spectroscopy. Absorption measurements in the NIR-VIS-UV range by double monochromator (AMKO-LTI), single monochromator (MDR2) or CCD-based spectrometers (Andor/Shamrock 303-i) and Hamamatsu TM-UV/VIS C10082CAH portable spectrograph. Configurations for NIR-VIS-UV measurements of attenuation in optical fibers are available (using OceanOptics DH-2000-S-TTL D_2-halogen light source).
Luminescence spectroscopy. Luminescence excitation by the following sources is available: diode-pumped solid state lasers (266 nm, 532 nm, and 473nm), nitrogen laser (337 nm), excimer lasers (248, 193 and 157 nm), semiconductor lasers (650, 765 nm), deuterium and xenon lamps, 50kV X-rays. Luminescence detection is performed using photomultipliers/monochromators and cooled CCD camera coupled with spectrograph. Time-resolved luminescence is detected by digital oscilloscopes, multichannel photon counters or time-correlated single-photon counting.
Vacuum ultraviolet spectroscopy: McPherson 234/302 200 mm monochromator with D_2 lamp with MgF_2-window serving as light source (120-250 nm) is used in configurations for optical absorption and photoluminescence excitation measurements. Capability to investigate optical fibers in deep-UV and vacuum UV range is developed.

Raman spectroscopy: Andor Shamrock303i spectrometer with Newton DU971N electron multiplying cooled CCD, NIR to UV spectral range Raman spectra with excitation at 532nm, 266nm and 632.8nm can be taken in 90° or backscattering geometries.
Energy-dispersive X-ray fluorescence microanalysis (EDAX Eagle III spectrometer, Rhodium X-ray source with micro-capillary focusing lens, detected elements from Na to U, spatial resolution ~50 μm).
Mass spectrometry: Dycor LCD-300 quadrupole mass-spectrometer, 1-300 a.m.u. with oil-free vacuum station.

SCIENTIFIC VISITS ABROAD

1. Anatoly Trukhin, 9th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation (LUMDETR 2015), Tartu, Sept. 20–25,2015, Tartu, Estonia.
2. Linards Skuja, Official referee to PhD work, Diego DiFrancesca "Role of Dopants, Interstitial O_2 and Temperature in the Effects of Irradiation of Silica-based Optical Fibers", Université Jean Monnet Saint-Etienne (France), Feb.4- Feb.6, 2015.

COOPERATION

Latvia
Institute of Atomic Physics and Spectroscopy, University of Latvia (Prof. J.Spigulis, Dr. A.Skudra)
Laser center of University of Latvia (Prof. R. Ferbers, Dr. F. Gahbauer)
Estonia
Institute of Physics, Tartu (Dr. S. Zazubovich)
Russia
GOI, St.Peterburg (Dr.L.Maksimov)
Russian Academy of Sciences, Kotelnikov Institute of Radio-engineering and Electronics Moscow, Russia (Dr. K.Golant).
Vereschagin Institute of High pressure Physics of RAS, Troitsk, Russia (Dr. T. I. Dyzheva).
France
Université Jean Monnet Saint-Etienne (France) (Prof. Y Ouerdane, Prof. A. Boukenter).
Laboratory of Irradiated Solids (LSI), Department of Physics, Ecole Polytechnique, University of Paris-Saclay, prof. N.Ollier.
Italy
University of Palermo (Prof. M. Cannas, S. Agnello, L.Vaccaro)
Japan
Tokyo Institute of Technology (Prof. H. Hosono)
Tokyo Metropolitan University (Prof. K. Kajihara)
USA
Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831-6044(Dr. L. Boatner).

MAIN RESULTS

UV AND YELLOW LUMINESCENCE IN PHOSPHORUS DOPED CRYSTALLINE AND GLASSY SILICON DIOXIDE

A.N.Trukhin, K. Smits, J. Jansons, D. Berzins, G. Chikvaidze, D.L. Griscom

Luminescence of phosphorus doped crystalline α -quartz and phosphosilicate glass with content $3P_2O_5$ $7SiO_2$ was studied. Water and OH groups are found by IR spectra in these materials. The spectrum of luminescence contains many bands in the range 1.5–5.5 eV. The luminescence bands in UV range at 4.5–5 eV are similar in those materials. Decay duration in exponential approximation manifests a time constant about 37 ns. Also a component in ms range was detected. PL band of ms component is shifted to low energy with respect to that of ~37 ns component. This shift is about 0.6 eV. It is explained as singlet–triplet splitting of excited state. Below 14 K increase of luminescence kinetics duration in ms range was observed and it was ascribed to zero magnetic field splitting of triplet excited state of the center.

Yellow–red luminescence was induced by irradiation in phosphorus doped crystalline α –quartz and phosphosilicate glasses. The yellow luminescence contains two bands at 600 and 740 nm. Their decay is similar under 193 nm laser and may be fitted with the first order fractal kinetics or stretched exponent. Thermally stimulated luminescence contains only band at 600 nm. The 248 nm laser excites luminescence at 740 nm according to intra center process with decay time constant about 4ms at 9K.

Both types of luminescence, UV and yellow were ascribed to different defects containing phosphorus.

P-doped α -quartz sample heated at 550 °C become opalescent. IR spectra related to water and OH groups are changed. Photoluminescence intensity of all three bands, UV (250 nm), yellow (600 nm) and red (740 nm) strongly diminished and disappeared after heating to 660 °C. Radiation induced red luminescence of non-bridging oxygen luminescence center (NBO) appeared in crystal after heat treatment. We had observed a crystalline version of this center (Skuja et al., Nuclear Instruments and Methods in Physics Research Section B Beam Interactions with Materials and Atoms. 2012; 286: pp. 159–168). Effect of heat treatment is explained as sedimentation of phosphorus in some state. Keeping of treated sample at 450–500°C leads to partial revival of ability to create yellow luminescence center under irradiation.

LUMINESCENCE OF COESITE

A. N.Trukhin, K.Smits, J.Jansons, G. Chikvaidze, T. I. Dyuzheva, L. M.Lityagina

Coesite is a polymorph modification of crystalline silicon dioxide with a tetrahedral structure. The luminescence of a single crystal of synthetic coesite was studied under excitation using X-rays, an electron beam, and excimer lasers KrF (248 nm), ArF (193 nm) and F 2 (157 nm). Luminescence bands in the regions of 2.5 eV and 4.4 eV appear. The blue band is dependent on temperature and has composite decay kinetics. Three main decay times are revealed, exhibiting luminescence contributions of a different nature in the same spectral range. One is in the ns range of time with a time constant of about 2 ns. The two other decay times are in the regions of 5 μs and 700 μs. The 5 μs component is also seen under KrF excitation, whereas both the 5μs and 700μs components are seen under ArF excitation. The time resolved spectra are mutually similar and they correspond to those under X-ray and e-beam excitation. The UV band is fast with a time constant of less than 1 ns, independent of temperature. Only the 2 ns and 5 μs components are revealed for the blue band under the KrF laser excitation. Blue luminescence thermal quenching takes place for temperatures above 50 K, with good correspondence between the intensities of the thermal dependences under different

excitation and that of the decay time constant. The quenching parameters used are 0.05 eV of energy and a frequency factor of $6 \cdot 10^5$ s^{-1}. The UV band is practically independent of temperature in the range 10–290 K.
The nature of luminescence is ascribed to the coexistence of a host defect and a self-trapped exciton. The defect is similar to the known oxygen-deficient luminescence center in pure silica glass. The blue luminescence at 700μs is ascribed to the self-trapped exciton being characteristic of silicon dioxide with a tetrahedral structure.

LUMINESCENCE OF POLYMORPHOUS SiO_2

A. N. Trukhin, K. Smits, J. Jansons, A. Kuzmin

The luminescence of self-trapped exciton (STE) was found and systematically studied in tetrahedron-structured silica crystals (α-quartz, coesite, cristobalite) and SiO_2 glass. In octahedron structured stishovite only host material defect luminescence was observed. It strongly resembles luminescence of oxygen deficient silica glass and γ- or neutron-irradiated α-quartz. The energetic yield of STE luminescence for α -quartz and coesite is about 20% of absorbed energy and about 5(7)% for cristobalite. Two types of STE were found in α -quartz. Two overlapping bands of STEs are located at 2.5 - 2.7 eV. The model of STE is proposed as Si-O bond rupture, relaxation of the created non-bridging oxygen (NBO) with foundation of a bond with bridging oxygen on the opposite side of c or x,y channel. The strength of this bond is responsible for the thermal stability of STE. Similar model of STE was ascribed for coesite and cristobalite with difference related to different structure. STE of silica glass is strongly affected by disordered structure.

SCIENTIFIC PUBLICATIONS

1. **A.N.Trukhin**, K. Smits, J. Jansons, D. Berzins, G. Chikvaidze, D.L. Griscom, UV and yellow luminescence in phosphorus doped crystalline and glassy silicon dioxide, Journal of Luminescence 166 (2015) 346–355 (doi: 10.1016/j.jlumin.2015.05.045).
2. **A.N.Trukhin**, K.Smits, J.Jansons, G.Chikvaidze, T.I.Dyuzheva, L.M.Lityagina, Luminescence of coesite, Phys. Scr. 90 (2015) 094009 doi:10.1088/0031-8949/90/9/094009
3. **A.N.Trukhin**, K.Smits, J.Jansons, A.Kuzmin Luminescence of polymorphous SiO_2. Radiation Measurements, (2015 online), doi: 10.1016/j.radmeas.2015.12.002

LECTURES ON CONFERENCES

9th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation (LUMDETR 2015), Tartu, Sept. 20–25,2015, Tartu, Estonia.

A.N. Trukhin, K. Smits, J. Jansons, A. Kuzmin, Luminescence of polymorphous SiO_2 (talk Mo-O-4), Abstract book, p.42).

Energy, Materials, and Nanotechnology (EMN) Ceramics Meeting 2015, Jan.26 – Jan.29 Orlando, Florida:

K.Kajihara, L.Skuja, H.Hosono "Diffusion and reactions of interstitial excess oxygen species in amorphous SiO_2" (invited), Talk D30, Abstract book p.111-112.

31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, Latvia, February 24-25, 2015:

1) L. Skuja, K. Kajihara, J.Gube, A. Siliņš, H. Hosono New luminescence bands of non-bridginhg oxygen center in crystalline SiO_2. Abstracts, p.11.

2) A. Trukhin, K. Smits, J. Jansons, A. Kuzmin Luminescence of cristobalite, Abstracts, p.6

DEPARTMENT OF PHOTONICS AND MATERIAL PHYSICS

Head of Department Dr.habil.phys. D.Millers

LABORATORY OF SURFACE PHYSICS

Head of Laboratory Dr.habil. phys. J. Maniks

RESEARCH AREA AND MAIN PROBLEMS

The main areas of interest concern structural and micro-mechanical investigation of simple and complex functional materials. Another research direction is investigation of modification processes of structure and micro-mechanical properties in wide-gap ion crystals and carbon-based materials induced by high dose irradiation, including irradiation with swift ions and laser treatment. Another topic deals with structural and mechanical characterization of complex nano-composite coatings for tribological and protective applications.
An important area of interest is processes at grain boundaries in homogeneous as well as heterogeneous materials (nanopowders, oxides, superplastic alloys, ceramics, nuclear materials etc.). These include investigation of interaction processes and mass transfer at interphase boundaries, such as adhesion, wetting and corrosion.

The main research topics in 2015 were:

- Structural, micro- and nano-mechanical characterization of swift ion irradiated wide gap ion crystals (MgO, LiF).
- Structural and mechanical investigation of carbon-based nanocomposite coatings for tribological applications.
- Investigation of structure and nano-mechanical response of thin protective ALD oxide-based nanolaminate coatings.
- Structural and optical investigation of translucent ZnO-based ceramic materials
- Micro- and nano-mechanical characterization of grain boundaries and interaction processes (adhesion, wetting and corrosion) on contact surfaces

SCIENTIFIC STAFF

1. Dr.habil.phys., emeritus J.Maniks
2. Dr.phys. F.Muktepavela
3. Dr.phys. I.Manika
4. Dr.phys. R.Zabels

Students
B.sc. R.Grants

VISITORS FROM ABROAD

Prof.K.Schwartz, GSI, Darmstadt, Germany (6 days).

COOPERATION

Latvia
Daugavpils University, Innovative Microscopy Centre (Dr.E.Tamanis);
Institute of Physics, University of Latvia (Dr.A.Shisko, Dr.E.Platacis);
NACO Technologies (Dr.V.Mitin, Dr.V.Kovalenko)

Estonia
Institute of Physics, University of Tartu (Dr. K. Kukli, T. Jogiaas)
Germany
GSI, Darmstadt, (Prof. K.Schwartz).
Spain
V Dr. Teresa Hernández- National Laboratory for Magnetic Fusion. Materials CIEMAT Avda. Madrid.
Kazakhstan
L. Gumilyov Eurasian National University (Dr.A.Dauletbekova)
Russia
Institute of Solid State Physics RAN, Chernogolovka (Dr.V.Sursajeva)
National University of Science and Technology "MISIS, Moscow, (Prof. B. Straumal)
Research and Technological Institute of Optical Materials, Scientific Center "S.I. Vavilov State Optical Institute" St. Petersburg, Russia (Dr E. Gorokhova).

MAIN RESULTS

DEPTH PROFILES OF INDENTATION HARDNESS AND DISLOCATION MOBILITY IN MgO SINGLE CRYSTALS IRRADIATED WITH SWIFT ^{84}Kr AND ^{14}N IONS

R. Zabels, I. Manika, K. Schwartz, J. Maniks, R. Grants, M. Sorokin, M. Zdorovets

MgO single crystals exhibit a high resistance to radiation damage and withstand high temperatures, therefore having a potential in nuclear applications, such as a host of inert matrix fuels, a component material for fusion devices and others. An actual topic is the reliability of MgO under conditions of severe irradiation with high-energy particles, particularly with swift heavy ions (SHI), energy loss of which is of the same order as for nuclear fission fragments. The depth dependence of damage and modification of micromechanical properties in MgO single crystals irradiated with 150 MeV ^{84}Kr and 24.5 MeV ^{14}N ions (specific energy 1.75 MeV/u) at fluences up to 10^{15} ions/cm^2 has been studied. The effects of ion-induced increase in hardness and reduction in dislocation mobility, magnitude of which varies along the ion range, were observed. These effects are related to ion-induced dislocations which were revealed by chemical etching. The results confirm a joint contribution of electronic excitations and atomic displacements by elastic collisions in the structural damage of MgO. The excitation mechanism in hardening dominates in the incoming part of ion range (up to the Bragg's maximum), while the role of impact mechanism becomes dominant only at the end of ion range.

MECHANICAL PROPERTIES OF ALUMINUM, ZIRCONIUM, HAFNIUM AND TANTALUM OXIDES AND THEIR NANOLAMINATES GROWN BY ATOMIC LAYER DEPOSITION

T. Jõgiaas, R.Zabels, A.Tamm, M. Merisalu, I. Hussainova, M. Heikkilä, H. Mändar, K. Kukli, M. Ritala, M. Leskelä

The microstructural design has attracted a certain interest in the development of hard coatings consisting of a variety of materials ranging from single metal oxides to composites or nanolaminates of chemically distinctive compounds. Metal oxide laminates have been studied as protective coatings on surfaces of demanding metal alloys, e.g. Al_2O_3–TiO_2 or Al_2O_3–Ta_2O_5 laminates on steel. In nanolaminates, different useful physical properties of constituent material layers can be tailored e.g. crystallinity and higher local density of one component with amorphous and laterally homogeneous,

uniformly disordered structure of another component material, accompanied by the repeatedly formed interfaces between constituent layers. Among other potential applications, wear-resistant oxide–metal multilayers deposited on glass have been of interest as hard and stable optical coatings.
The mechanical properties of two different metal oxide nanolaminates comprised of Ta_2O_5 and Al_2O_3, HfO_2 or ZrO_2, grown on soda–lime glass substrate by atomic layer deposition, were investigated. Ta_2O_5 and Al_2O_3 layers were amorphous, whereas ZrO_2 and HfO_2 possessed crystalline structure. Thickness of single oxide layers was varied between 2.5 and 15 nm. The total thickness of the laminate stacks was in the range of 160–170 nm. The indentation results implied a correlation between mechanical properties and the relative content of constituent single oxides.

THE ROLE OF NANOPOWDER MORPHOLOGY ON PROPERTIES OF ZnO TRANSPARENT CERAMICS

F. Muktepavela, R.Zabels

ZnO ceramics obtained from grained powders with varying grain sizes by hot pressing and ceramic from tetrapod-shaped nanopowders obtained by press-less sintering have been investigated at identical conditions. Ceramics obtained by hot pressing were optically transparent but were composed of large inhomogeneous grains exhibiting a substructure. Decreased values of elastic modulus (E) within a grain and a wide defect-associated (”green”) photoluminescence (PL) band at 2.2-2.8 eV in conjunction with a weak excitonic band indicate on a high concentration of residual point defects in hot pressed ZnO ceramics. Ceramics obtained by press-less sintering from tetrapods which don’t have a tendency for agglomeration had fine-grained structure (d=1-4μm) with no signs of a substructure. PL spectrum has a narrow excitonic band with phonon replicas ($1LO\_ExD^0$) whereas the defect-associated “green” luminescence is negligible. The effects of powders morphologies have been explained in terms of a hereditary influence of interaction processes between initial particles on the formation of a microstructure and kinetics of defect distribution during the sintering of ZnO ceramics.

STRAIN-INDUCED WETTING OF NON-EQUILIBRIUM GRAIN BOUNDARIES IN Sn-Pb SYSTEM

F.Muktepavela, B.Straumal

The grain boundary (GB) wetting by the melt and second solid phase has been studied in the Sn–Pb system both in equilibrium conditions and during continuous strain. The percentage of Sn/Sn GBs completely wetted by the melt increases from 80% at eutectic temperature T_e =183 °C and to 100% at 220 °C. The percentage of Pb/Pb GBs completely wetted by the melt increases from 0% at T_e to 100% at 270 °C. Below T_e only incomplete wetting of Pb/Pb GBs by solid Sn and Sn/Sn GBs by solid Pb has been observed after long annealing. However, during straining the lattice dislocations are continuously absorbed by GBs increasing the GB energy. As a result, the complete wetting of such non-equilibrium Sn/Sn GBs by the second solid phase Pb appears. Therefore, the difference in energies between equilibrium and non-equilibrium grain boundaries has been experimentally demonstrated for the first time.

MAGNETIC FIELD EFFECT ON THE CORROSION PROCESSES AT THE EUROFER / Pb-17Li FLOW INTERFACE

F.Muktepavela, T. Hernández, E.Platacis, A.Shishko

Structure and elemental analysis of the interface between *EUROFER 97* steel and flowing Pb-17Li eutectic alloy (velocity 5 cm/s at 5500 ^{o}C, 1000h) under an action of strong magnetic field (B=1.7 T) were examined using optical microscopy, SEM, confocal microscopy, precision micro-hardness methods, SIMS and EDX point and line-scan measuring approaches. Magnetic field causes a faster crushing of martensite phases, deep dissolution of grain boundaries, an increased mass transfer of Fe and Cr and a fast detachment of corrosion layers due MHD effects.

SCIENTIFIC PUBLICATIONS

1. **R. Zabels, I. Manika**, K. Schwartz, **J. Maniks, R. Grants**, M. Sorokin, M. Zdorovets, Depth profiles of indentation hardness and dislocation mobility in MgO single crystals irradiated with swift ^{84}Kr and ^{14}N ions, *Applied Physics A: Materials Science and Processing*, 120 (2015) 167.
2. **J. Maniks**, V. Mitin, U. Kanders, V. Kovalenko, P. Nazarovs, M. Baitimirova, R. Meija, **R. Zabels**, K. Kundzins, D. Erts, Deformation behavior and interfacial sliding in carbon/copper nanocomposite films deposited by high power DC magnetron sputtering, *Surface & Coatings Technology*, 276 (2015) 279.
3. T. Jogiass, **R. Zabels**, A. Tamm, M. Merisalu, I. Hussainova, M. Heikkila, H. Mandar, K. Kukli, M. Ritala, M. Leskela, Mechanical properties of aluminum, zirconium, hafnium and tantalum oxides and their nanolaminates grown by atomic layer deposition, *Surface & Coatings Technology*, 282 (2015) 36.
4. B.B. Straumal, O.A. Kogtenkova, **F. Muktepavela**, K.I. Kolesnikova, M.F. Bulatov, P.B. Straumal, B. Baretzky. Direct observation of strain-induced non-equilibrium grain boundaries. *Materials Letters* 159 (2015) 432.
5. M.C. Gázque, T.Hernández, **F.Muktepavela**, E. Platacis, A. Shishko. Magnetic field effect on the corrosion processes at the Eurofer-Pb-17Li flow interface. *Journal of Nuclear Materials* 465 (49162) (2015) 633.
6. **F. Muktepavela**, L. Grigorjeva, K. Kundzins, E. Gorokhova, P. Rodnyi. Structure, nanohardness and photoluminescence of ZnO ceramics based on nanopowders, *Physica Scripta* 90 (2015) 094018.
7. K Schwartz**, J Maniks, I Manika**. A review of colour center and nanostructure creation in LiF under heavy ion irradiation. *Physica Scripta* 90 (2015) 094011.
8. U. Kanders, K. Kanders, **J.Maniks,** V.Mitins, V. Kovalenko, P. Nazarovs, D. Erts. Nanoindentation response analysis of Cu-rich carbon–copper composite films deposited by PVD technique. *Surface & Coatings Technology* 280 (2015) 308.
9. B.Polyakov, S.Vlassov, L.Dorogin, J.Butikova, K.Smits, M.Antsov, S.Oras, **R.Zabels**, Metal nanodumbbells for nanomanipulations and tribilogical experiments, *Physica Scripta* 90 (2015) 094007.
10. B. Polyakov, **R.Zabels**, A.Sarakovskis, S.Vlassov, A.Kuzmin, Plasmonic photoluminescence enhancement by silver nanowires, *Physica Scripta* 90 (2015) 094008.

PhD. THESIS

R.Zabels, "Swift-ion-induced modifications of structure and micromechanical properties in wide-gap ionic crystals", Institute of Solid State Physics, University of Latvia, Riga, 2015

LECTURES ON CONFERENCES

9th International Symposium on Swift Heavy Ions in Matter (SHIM-2015), May 18-21, 2015, Darmstadt, Germany

1. R. Zabels, I. Manika, K. Schwartz, J. Maniks, R. Grants, E. Tamanis, Formation of dislocations along tracks of swift heavy ions in LiF crystals, Mo-PA25, Abstracts, p. 79.

18th International Conference on Radiation Effects in Insulators (REI-18), 26th to 31st October, 2015, Jaipur, Rajasthan, India

2. I.Manika, J.Maniks, A.Dauletbekova, R.Zabels, R.Grants, M.Baizhumanov. Formation of color centers and extended defects in LiF irradiated with swift ^{131}Xe ions: contribution of electronic excitation and inpact mechanisms. Abstracts, P- 83. p,138.

EuroNanoForum 10-12 June 2015, Riga, Latvia

3. J. Maniks, V. Mitin, U. Kanders, V. Kovalenko, P. Nazarov, D. Erts. Mechanical characterization of a-C/Cu nanocomposite films obtained by high-power DC magnetron sputtering. Abstracts, 2E-149.

International conference "Boundaries, Segregation and Diffusion – BS&D„ October 1–3, 2015, National University of Science and Technology (MISiS), Moscow. Russia

4. F. Muktepavela, E. Gorokhova, L. Grigorjeva, K. Kundzins, R. Zabels. "Hereditary" effects of nanopowders morphology on the ZnO ceramics structure and properties. Abstracts p.43,

Riga Technical University 56th International Scientific Conference, 14–16 October 2015, Riga, Latvia

5. Nanostrukturēšanās un dislokāciju veidošanās procesi ar MeV enerģijas joniem apstarotos LiF un MgO kristālos R. Zabels, I. Manika, R. Grants.Program, p.33.

The 31st Annual scientific conference of Institute of Solid State Physics, University of Latvia, February 24-26, 2015, Riga, Latvia

6. R. Zabels, I. Manika, R. Grants dislocations in Bi tracks in LiF irradiated at various beam incidence angles, Abstracts, p.15.
7. R. Grants, R. Zabels, M. Baizhumanov. Effect of ion energy on structure of LiF crystals irradiated with swift Xe ions. Abstracts, p.56.

DEPARTMENT OF PHOTONICS AND MATERIAL PHYSICS

Head of Department Dr.habil.phys. D.Millers

LABORATORY OF ORGANIC MATERIALS

Head of laboratory Dr. phys. M.Rutkis

SCIENTIFIC STAFF:

Mārtiņš Rutkis	Dr.phys.	**PhD students:**	
Oskars Vilītis	Dr.phys.	Elīna Laizāne	MSc.
Aivars Vembris	Dr.phys.	Kaspars Pudžs	MSc
Edgars Nitišs	Dr.phys.	Raitis Gržibovskis	MSc
Jānis Latvels	Dr.Eng.	Igors Mihailovs	MSc.
Andrejs Tokmakovs	MSc.	Jūlija Perveņecka	MSc
Jānis Busenbergs	MSc.		
Andrejs Jurģis			

Students:
Arturs Bundulis BSc
Elza Lina Linina

RESEARCH AIM:

The fundamental and applied research of organic molecules, materials and their structures are conducted by the laboratory. In most cases the objects of investigations are original organic compounds synthesized by Latvian chemists. The main research goal of laboratory is to develop knowledge about the structure - properties relationship of organic materials for next generation electronics and photonics. Based on concepts derived from these studies, new materials with improved properties are designed in close cooperation with the Latvian chemists. Assessment and demonstration of possible applications of the novel developed materials is an important task of the laboratory. Trained human resources, generated knowledge and technology within the laboratory are a base for development of organic electronics and photonics in Latvia.

RESEARCH TOPICS:

- Quantum chemical investigation of structure and properties of chromophores;
- Design of thin films;
- Energy structure of thin films;
- Electrical and photoelectrical properties;
- Nonlinear optical phenomena;
- Stimulated emission;
- Electroluminescence in thin films;
- Optically induced switching;

RESEARCH METHODOLOGY WITHIN A LABORATORY:

- Quantum chemical modelling by Gaussian 09, GaussView 5.0 and HyperChem 8.0 software packages;
- Deposition of organic thin films by thermal evaporation in vacuum, spin coating, blade casting, Langmuir– Blodgett technology, self-assembled monolayers;
- Space charge limited current, time of flight and carrier extraction by linearly increasing voltage methods are used for acquiring electrical properties of thin films;
- Investigation of energetic structure is done by temperature modulated space charge limited current method, Kelvin probe and photoconductivity measurements;
- Determination of linear optical parameters by absorption and reflection spectroscopy and M-line method;
- Investigation of light emission properties by luminescence, stimulated emission and electroluminescence spectral methods;
- Characterisation of nonlinear optical properties by hyper Rayleigh scattering, optical second harmonic generation, Maker fringe, Kurtz powder, Teng-Man ellipsometric, attenuated total reflection and Mach – Zehnder interferometric methods.

PROJECTS:

National Research Program in MultIfunctional Materials and composItes, photonicS and nanotechnology (IMIS2) (2014-2017):

Project No.1 "Photonics and materials for photonics"
Project No.6 "Nanomaterials and nanotechnology"

ESF project of the activity 1.1.1.2 "Attraction of Human Resources to Science":

No.2013/0045/1DP/1.1.1.2.0/10/APIA/VIAA/018 "Design and investigation of low molecular weight glass forming organic compounds with use in photonics"

INTERNATIONAL PROJECTS:

1. EC 7F project: ***„Waste heat to electrical energy via sustainable organic thermoelectric devices - H2ESOT"***
2. Latvian – Lithuanian – Taiwan partnership program project: ***„Synthesis and studies of organic electroactive materials for effective and reliable optoelectronic devices*"**

COLLABORATION:

Latvia:

- Riga Technical University;
- Institute of Organic Synthesis;
- Institute of Physical Energetics;
- Daugavpils University.

Lithuania:

- Vilnius University (Prof. S. Jursenas);
- Kauņas universitāte (Prof. J. V. Grazulevicius);

- Center for Physical Sciences and Technology (Prof. L. Valkunas un Prof. V. Gulbinas).

Taiwan: National Sun Yat-sen Universty (Dr. Li-Yin Chen).
France: Institut des Nanosciences de Paris (Prof. N. Witkowski).
England: Nottingham University (Prof. S. Woodward).
Germany: Julius-Maximilians Universitaet Wuerzburg (Prof. J. Pflaum).
Bulgaria: Institute of Organic Chemistry, Bulgarian Academy of Sciences (Prof. V. Dimitrov).
Moldova: Universitatea Tehnica a Moldovei (Prof. A. Casian).

MAIN RESULTS

SOLID STATE SOLVATION EFFECT AND REDUCED AMPLIFIED SPONTANEOUS EMISSION THRESHOLD VALUE OF GLASS FORMING DCM DERIVATIVE IN PMMA FILMS

AivarsVembris, ElmarsZarins, ValdisKokars

Molecule crystallization is one of the limitations for obtaining high-gain organic laser systems. One of the examples is well known red laser dye 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran (DCM). The lowest threshold value of amplified spontaneous emission was achieved by doping 2wt% of DCM molecule in tris-(8-hydroxy quinoline) aluminum (Alq3) matrix. Further increase of the DCM dye concentration makes the system less efficient as its threshold value increases. It is due to large intermolecular interaction, which induces photoluminescence quenching. Compounds with reduced intermolecular interaction could be prospective in organic laser systems due to higher possible doping.

In the work photoluminescence and amplified spontaneous emission properties of modified DCM molecule in poly(methyl methacrylate) (PMMA) matrix were investigated. Bulky trityloxyethyl groups were attached to the donor part of DCM. These groups increase intermolecular distance wherewith reduce photoluminescence quenching. More than one order of magnitude lower excitation threshold energy of the amplified spontaneous emission was achieved in doped polymer films with investigated compound in comparison to doped polymer with DCM. It means that the investigated compound is more perspective as a laser material compared to the previously studied. Additionally amplified spontaneous emission maximum could be tuned within 15 nm by changing concentration from 0.1wt% to 10 wt% DWK-1 in PMMA matrix due to solid state solvation effect.

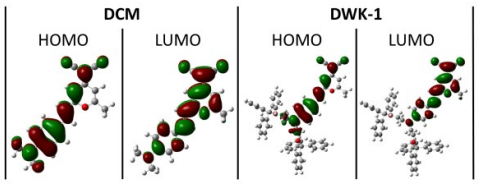


Fig. 1. Highest occupied and lowest unoccupied molecular orbitals of DCM and DWK-1.

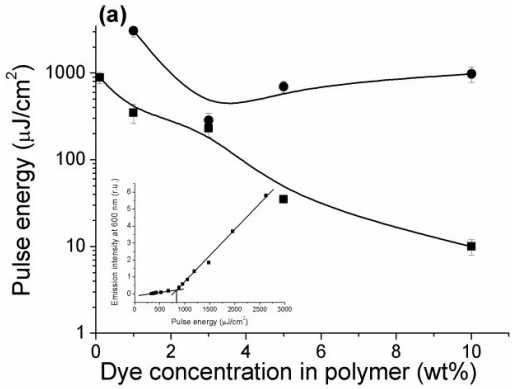


Fig. 3. Dependence of the threshold values of amplified spontaneous emission on active molecule concentration in PMMA matrix(inset—determination of amplified spontaneous emission excitation threshold value). Lines are guideline for eyes.

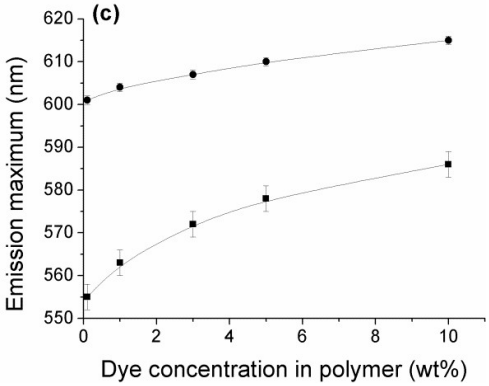


Fig. 2. Dependence of amplified spontaneous emission (circles) and photoluminescence (squares) maximum wavelength on DWK-1 concentration in polymer matrix. Lines are guideline for eyes.

Bulky trityloxyethyl groups attached to the electron donor side of the DCM molecule prevents its aggregation in the polymer matrix which results in higher photoluminescence quantum yield. Photoluminescence and amplified spontaneous emission spectra of DWK-1 films exhibit a red shift with increasing active molecule concentration in polymer. It is explained by solid state solvation effect where the dielectric constant in the system is increasing with the active molecule concentration. Amplified spontaneous emission maximum could be tuned within 15 nm by changing concentration from 0.1wt% to 10 wt% DWK-1 in PMMA matrix. Excitation threshold energy of amplified spontaneous emission is decreasing by the increase of DWK-1TB molecule concentration in PMMA matrix. It is due to negligible photoluminescence quantum yield changes on dye concentration. Moreover, we are able to reduce more than one order of magnitude threshold value in the system DWK-1:PMMA compared to the system DCM:PMMA. It means that DWK-1 compound is prospective for practical use in light amplification systems.

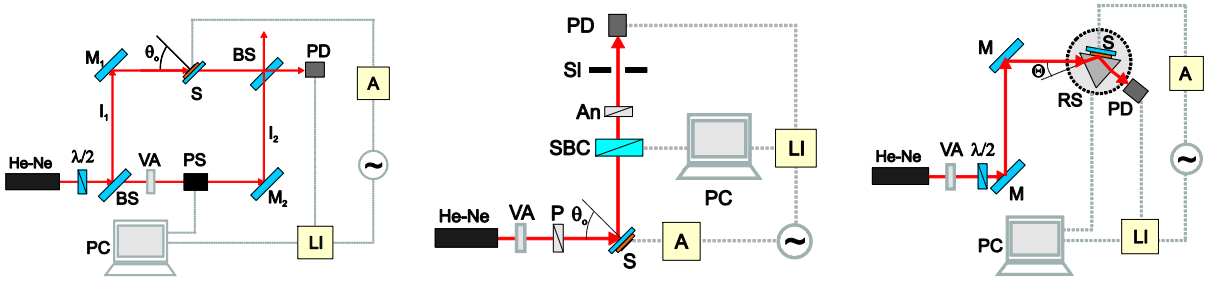
REVIEW AND COMPARISON OF EXPERIMENTAL TECHNIQUES USED FOR DETERMINATION OF THIN FILM ELECTRO-OPTIC COEFFICIENTS

Edgars Nitiss, Arturs Bundulis, Andrey Tokmakov, Janis Busenbergs, Elza Linina, Martins Rutkis

In the last decades nonlinear optical (NLO) materials have been developed, extensively studied and applied in the industry more and more often. New low-cost materials with enhanced second order properties could be used in various electro-optic (EO) devices such as switches, modulators, tunable filters.

The nonlinearity of the organic material can be characterized by means of EO coefficients. Multiple measurement techniques have been developed and applied for the measurement of EO coefficients, however, the most widely used are the Fabry-Perot, the transmission polarimetric, the Mach-Zehnder interferometric (MZI), the Teng-Man

(TM) and the attenuated total reflectance (ATR) technique. All these methods are typically realized by detection of low amplitude EO modulations of the material subjected to a varying electric (AC) field at a frequency of several kHz. The fact that no single technique has been established as the standard for the determination of thin film EO coefficients clearly indicates that not all of the measurements, nor the respective data interpretation are straightforward. In this contribution we review and demonstrate the experimentally retrieved EO coefficients in the low absorbing region of thin films obtained by the three of the mentioned techniques: MZI, TM and ATR. The setups for the measurements are illustrated in Fig. 1.



a. b. c.

Fig. 1. The setups used for EO coefficient measurements by a) MZI, b) TM and c) ATR techniques, where He-Ne – Helium Neon laser 632.8 nm, λ/2 – half-wave plate, BS – beam splitter, M – mirrors, VA – variable attenuator, PS – phase shifter, S – sample, PD – a large area Si photodiode, LI – Lock-in amplifier, A – amplifier, PC – computer, Θ_o – incidence angle, SBC – Soliel-Babinet compensator, P – polarizer, An – analizer, RS – rotating stage.

Each of these techniques has shown to have multiple advantages and drawbacks. The MZI and TM optical setups are very simple. However, a correct interpretation of the experimental data obtained by the mentioned techniques requires full understanding about the effects taking place in the sample. The signal obtained by the MZI and TM techniques is strongly influenced by the multiple internal reflection and piezo- and electrostrictive TC effects, which, in our opinion, have not been sufficiently addressed in the literature. An analytic description containing both of the mentioned effects would be fairly complicated. We have shown that a numerical solution based on the Abelès matrix formalism can be used for the retrieval of the EO coefficient values from the experimental data obtained by MZI and TM methods. The approach requires recording modulated signal measurements at multiple light incidence angles on the sample, which makes the methods quite time-consuming. Moreover, the thickness change of the sample should be known with a high precision. The ATR has shown to be the most precise and the simple technique for the determination of EO coefficients. The entire procedure, which involves measurements of modulated signals with TM and MZI setups and data processing, is quite cumbersome. Moreover, MZI and TM does not guarantee high precision EO coefficients despite the independent determination of the entire set of material constants such as refractive indices, thin film thicknesses and the actual thickness variations due to piezo- and electrostriction effects.

SOLUTION PROCESSABLE 2-(TRITYLOXY)ETHYL AND TERT-BUTYL GROUP CONTAINING AMORPHOUS MOLECULAR GLASSES OF PYRANYLIDENE DERIVATIVES WITH LIGHT EMITTING AND AMPLIFIED SPONTANEOUS EMISSION PROPERTIES

Elmars Zarins, Aivars Vembris , Elina Misina , Martins Narels, Raitis Grzibovskis, Valdis Kokars

Small organic molecules with incorporated 4H-pyran-4-ylidene (pyranylidene) fragment as the π-conjugation system which bonds the electron acceptor fragment with electron donor part in the molecule - also well known as derivatives of 4-(dicyano-methylene)-2-methyl-6-[p-(dimethylamino)styryl]-4H-pyran (DCM) laser dye -have attracted considerable attention of scientists as potential new generation materials for organic

photonics and molecular electronics due to their low-cost fabrication possibility, flexibility and low-weight.

Six glassy derivatives of 4H-pyran-4-ylidene (pyranylidene) with attached bulky 2-(trityloxy)ethyl and tert-butyl groups are described in this report. Almost all of the synthesized compounds form good optical quality transparent amorphous films from volatile organic solvents and could be obtained in good yields up to 75%. Their light emission in solution and thin solid films is in the range of 600-700 nm, they are thermally stable and show glass transition in the range of 108-158oC. The amplified spontaneous emission threshold values of the neat films of the glassy pyranylidene derivatives vary from 155 to 450 □J/cm2 and their HOMO and LUMO energy levels are between of those of tris(8-hydroxy quinolinato) aluminium (Alq3). The photoluminescence quantum yields of the glassy compounds are in the range from 1% to about 8% and their electroluminescence properties have been investigated. Therefore, glassy pyranylidene derivatives could be a very potential low-cost solution processable materials for Alq3 hosted light-amplification and light-emitting application studies.

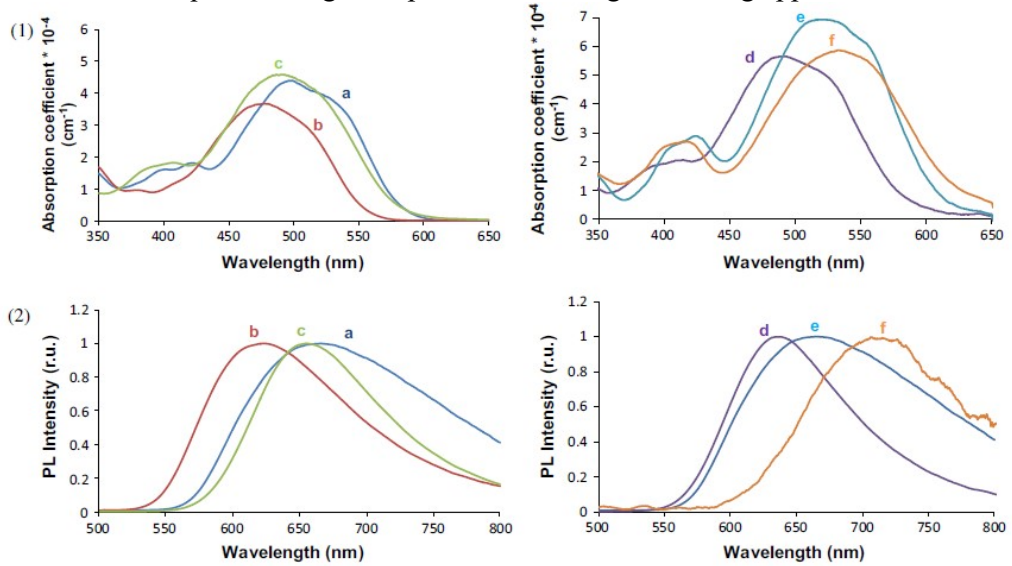


Fig. 1. Optical properties of the compounds in the solution and in the thin solid films (1) absorption and (2) photoluminescence of (a) ZWK-1TB, (b) DWK-1TB, (c) JWK-1TB, (d) MWK-1TB, (e) EWK-1TB, (f) JWK-1TBS.

Optical properties of **WK-1TB** compounds in pure thin film. □$_{abs}$ – wavelength of absorption maximum, □$_{PL}$ – wavelength of photoluminescence maximum, **PLQY** – photoluminescence quantum yield, □$_{ASE}$ – wavelength of amplified spontaneous emission, **FWHM** – full with of half maximum of amplified spontaneous emission band, **E$_{th}$** – irradiation threshold energy density at which amplified spontaneous emission appears

Compound	□$_{abs}$, nm	□$_{PL}$, nm	PLQY, %	□$_{ASE}$, nm	FWHM, nm	E$_{th}$, □J/cm^2
ZWK-1TB	498 ± 3	666 ± 3	3.4 ± 1	654 ± 1	25 ± 2	182 ± 9
DWK-1TB	477 ± 3	623 ± 3	7.7 ± 1	634 ± 1	30 ± 2	155 ± 7
JWK-1TB	490 ± 3	656 ± 3	4.8 ± 1	675 ± 1	20 ± 2	158 ± 8
MWK-1TB	486 ± 3	637 ± 3	3.1 ± 1	656 ± 1	13 ± 2	172 ± 8
EWK-1TB	515 ± 3	662 ± 3	1.6 ± 0.5	683 ± 1	13 ± 2	450 ± 22
JWK-1TBS	532 ± 3	710 ± 5	<0.5	-	-	-

In this report various physical properties of six 2-tert-butyl-6-methyl-4H-pyran-4-ylidene fragment containing derivatives with attached bulky 2-(trityloxy)ethyl groups were analyzed. Almost all of the compounds WK-1TB form good optical quality transparent amorphous films from volatile organic solvents and could be obtained in good yields in the last stage of synthesis. The thermal stability of obtained glasses is no lower than 242oC and their glass transition is above 108oC. The light absorption of the glassy pyranylidene compounds in solutions of dichloromethane in range from 450 nm

to 550 nm, but the light absorption in their solid state are in range from 500 nm to 600 nm and are mostly influenced by the electron acceptor fragment of the molecule. The amplified spontaneous emission threshold values of the pure films of the glassy pyranylidene derivatives were below 200 □J/cm2 and the PLQY up to about 8% which could both be improved by doping the glassy compound in a host. The HOMO and LUMO energy levels of all glassy compounds WK-1TB are between of those of Alq3 and almost all of them show electroluminescence properties, therefore, they could be used as dopants in Alq3 hosted electroluminescence layer for various light emitting application studies. Among the six investigated glassy compounds, 2-(2-(4-(bis(2-(trityloxy)ethyl)amino)styryl)-6-tert-butyl-4H-pyran-4-ylidene)malononitrile (DWK-1TB) could be obtained in highest yield (75%), had the highest glass transition (158oC). The pure film of DWK-1TB obtained from solution by spin-coating approach showed the highest PLQY (7.7 ± 1 %) and lowest ASE threshold value (155 □J/cm2). The above mentioned properties show that DWK-1TB could be a very potential material in different fields of organic photonics and molecular electronics.

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2. **Aivars Vembris**, Elmars Zarins, Valdis Kokars, Solid state solvation effect and reduced amplified spontaneousemission threshold value of glass forming DCM derivative in PMMA films, Journal of Luminescence 158 (2015) pp 441–446, http://dx.doi.org/10.1016/j.jlumin.2014.10.050
3. K. Traskovskis, E. Zarins, L. Laipniece, **A. Tokmakovs**, V. Kokars, **M. Rutkis**, Structure-dependent tuning of electro-optic and thermoplastic properties in triphenyl groups containing molecular glasses, Materials Chemistry and Physics, 155 (2015), pp 232-240, http://dx.doi.org/10.1016/j.matchemphys.2015.02.035
4. **M. Rutkis,** K. Traskovskis, Triphenylmethyl and triphenylsilyl based molecular glasses for photonic applications, SPIE Proceedings, 9360, 93600H-1, (2015), DOI: 10.1117/12.2080806
5. A. Gerbreders, A. Bulanovs, J. Mikelsone, K. Traskovskis, E. Potanina**, A. Vembris**, J. Teteris, Photoinduced mass transport in low molecular organic glasses and its practical application in holography, Journal of Non-Crystalline Solids, 421, (2015), pp 48–53. http://dx.doi.org/10.1016/j.jnoncrysol.2015.04.040
6. **E. Nitiss, A. Bundulis, A. Tokmakov, J. Busenbergs, E. Linina, M. Rutkis**, Review and comparison of experimental techniques used for determination of thin film electrooptic coefficients, Phys. Status Solidi A, 1–13 (2015) / DOI 10.1002/pssa.201532054
7. A. Bucinskas, G. Bagdziunas, A. Tomkeviciene, D. Volynyuk, N. Kostiv, D. Gudeika, V. Jankauskas, **M. Rutkis,** J. V. Grazulevicius, Structure-property relationship of isomeric diphenylethenyl-disubstituted dimethoxycarbazoles, RSC Adv., 2015,5, 49577-49589, DOI: 10.1039/C5RA09161F
8. A. Sternberg, L. Grinberga, A. Sarakovskis, **M. Rutkis**, 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International Conference on Functional Materials and Nanotechnologies (RCBJSF–2014–FM&NT), IOP Conf. Series: Materials Science and Engineering 77 (2015) 011001, doi:10.1088/1757-899X/77/1/011001
9. **E. Nitiss,** K. Bluss, J. Alnis, Numerical 2D and 3D Simulations of a Spherical Fabry-Pérot Resonator for Application as a Reference Cavity for Laser Frequency

Stabilisation, Latvian Journal of Physics and Technical Sciences, 3 (Vol. 52), 11.-20 (2015)

10. Elmars Zarins, **Aivars Vembris**, Elina Misina, **Martins Narels**, Raitis Grzibovskis, Valdis Kokars, Solution processable 2-(trityloxy)ethyl and tert-butyl group containing amorphous molecular glasses of pyranylidene derivatives with lightemitting and amplified spontaneous emission properties, Optical Materials 49 (2015) 129–137, http://dx.doi.org/10.1016/j.optmat.2015.09.004
11. E. Birks, M. Kundzins, **E. Nitiss**, R. Ignatans, M. Dunce, M. Antonova, A. Sternbergs, Study of Tetragonal Phase in 0.4Na1/2Bi1/2TiO3-(0.6-x)SrTiO3-xPbTiO3 Solid Solutions by Second-Harmonic Generation, Ferroelectrics, Volume 485, Issue 1, 26 August 2015, Pages 53-57, 10.1080/00150193.2015.1060106
12. G. Mozolevskis, A. Ozols, **E. Nitiss, E. Linina, A. Tokmakov, M. Rutkis**, Reduction of Electric Breakdown Voltage in LC Switching Shutters, Latvian Journal of Physics and Technical Sciences, Volume 52, Issue 5, 1 October 2015, Pages 47-57, DOI: 10.1515/lpts-2015-0028
13. J. Klavins, G. Mozolevskis, A. Ozols, **E. Nitiss, M. Rutkis,** Screen Printing of SU-8 Layers for Microstructure Fabrication, Latvian Journal of Physics and Technical Sciences, Volume 52, Issue 5, 1 October 2015, Pages 58-67, DOI: 10.1515/lpts-2015-0029

LECTURES ON CONFERENCES

***31th Scientific Conference of the Institute of Solid State Physics, University of Latvia, February 24-26, 2015*:**

1. R.Gržibovskis, A.Vembris**,** Limiting factors for energy level determination using scanning Kelvin probe tecnique Abstracts p.45
2. J. Perveņecka, R.Gržibovskis, A.Vembris, Energetical levels of DMABI chromophore consisting molecules, Abstracts p.46

11th International Young Scientist Conference „Developments in Optics and Communications" Riga, April 8-10, 2015:

1. Julija Pervenecka, Raitis Grzibovskis, Aivars Vembris, Optical and photoelectrical properties of DMABI chromophore consisting molecules, Book of Abstracts, p.47
2. M. Narels, A. Vembris, Amplified spontaneous emission of DCM derivative in PVK thin film, Book of Abstracts, p.18
3. Aivars Vembris, Organic solid state lasers,, Book of Abstracts, p.1

XVI International Forum on Thermoeletricity, May 18-23, Paris, 2015:

1. K. Pudzs, A. Vembris, J.Tjarve, M. Rutkis Thermo-electrical properties of tetrathiotetracene thin films doped with iodine

34th Annual International Conference on Thermoelectrics and 13th European conference on Thermoelectrics, June 28-July 2, Dresden, 2015:

1. K. Pudzs, A. Vembris, M. Rutkis, J.Tjarve, Electrical and thermo-electrical properties of tetrathiotetracene iodide thin films

Euro Nano Forum 2015, June 10-12, Riga, 2015:

1. J. Latvels, R. Grzibovskis, K. Pudzs, A. Vembris, Photovoltaic properties of bulk heterojunction system containing glass forming indandione derivative with attached bulky groups, Poster abstract, 1A-12

The 14th European Conference on Organised Films, June 29 - July 2, Genova, 2015:

1. J. Latvels, R. Grzibovskis, K. Pudzs, A. Vembris, Photovoltaic effect in bulk heterojunction system with glass forming indandione derivative DMABI-6Ph, Book of Abstracts p. 104.
2. A.Vembris, E.Zarins, V.Kokars, Stimulated emission of pyranyliden derivatives in amorphous thin films, Book of Abstracts, pp. 142.

Northern Optics & Photonics, Lappeenranta, Finland, June 2.-4., 2015:

1. E. Nitiss, M. Rutkis, A hybrid SOI/polymer waveguide modulator operating in the visible range, Book of Abstracts p. 91.

Baltic Polymer Symposium 2015, Sigulda, Latvia, September 16-18, 2015:

1. M. Rutkis, A. Šarakovskis, A. Šternbergs, National research program "Multifunctional materials and composites, photonics and nanotechnology", Programme and proceedings p. 19.

100% Climate Neutrality/ Solutions for crossing borders, October 6-7, Sonderborg, Denmark, 2015:

1. J. Latvels, R. Grzibovskis, K. Pudzs, A. Vembris, D. Blumberga, Innovative indandione containing materials for organic solar cells

10th International Conference on Functional Materials and Nanotechnologies (FM&NT 2015) , October 5 – 8, Vilnius, Lithuania, 2015:

1. M. Rutkis, K. Pudžs, A. Vembris, J. Tjarve, Development of tetrathiotetracene based thin films for thermo-electrical applications, Book of Abstract p.78

Riga Technical University 56th International Scientific Conference, October 14-16, Riga, Latvia, 2015:

1. K. Pudzs, A. Vembris, J. Busenbergs, M. Rutkis, Measurements of Seebeck coefficient of organic thin films, Book of Abstracts p. 32.
2. R.Grzibovskis, A.Vembris, K.Pudzs, Molecule ionization energy dependence on film thickness and morphology of two indandione derivatives, Book of Abstracts p. 32.

8th International Symposium on Flexible Organic Electronics (ISFOE15), July 6-9, Thessaloniki, Greece, 2015:

1. E. Zarins, A. Vembris, E. Misina, V. Kokars, Synthesis and physical properties of glassy triphenyl group containing derivatives of DCM laser dye, Thesis in book of abstracts, pp. 133.
2. V. Kokars, K. Siltane, E. Zarins, A.Ozols, P. Augustovs, A. Vembris, Synthesis and holographic properties of alkyl 2-cyanoacetate acceptor fragment containing push – pull type organic glasses, Thesis in book of abstracts, pp. 130

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REAEARCH AREAS

Materials

1. Production of new modified ferroelectric ceramics by doping with monoxides, developing binary or multicomponent solid solutions:
− complex lead-containing perovskite family with general chemical formulas PbB'1/2B''1/2O3 (where B'=Sc+3, Lu+3, Yb+3, Tm+3 etc.; B''= Nb+5, Ta+5) and PbB'1/3B"2/3O3, (where B'=Mg+2, Zn+2, Ni+2, Cd+2 etc., B"- Nb+5, Ta+5 and etc);
− modified (Pb,La)(Zr,Ti)O3 (PLZT);
− lead-free perovskite ceramics based on $(K_{0.5}Na_{0.5})NbO_3$, $(Na_{0.5}Bi_{0.5})NbO_3$, or $BaTiO_3$;
- $BiFeO_3$, $Bi(Fe_{0.5}Cr_{0.5})O_3$,$SrMnO_3$,
2. Thin films, multiferroic materials, inorganic functional and nanomaterials

Methods

1. Investigation of kinetic parameters of synthesis and sintering proceses;
2. X-ray diffraction, atomic force microscopy, piezo-response force microscopy, electron scanning microscopy with EDX option, EPR and Raman spectroscopies, dielectric impedance and hysteresis measurement tools, ellipsometry and reflectometry techniques;

Properties: electromechanical properties; piezoelectric properties and field induced deformation, electrocaloric effect, thermal expansion, optical (absorbtion, luminiscence), dielectric and magnetic properties, electronic structure**;**

Problems

1. Phase transitions (including field-induced ferroelectric phase transitions) and ordering effects in "ordinary" ferroelectrics and ferroelectric *relaxors* along with new compositions (including 3d elements doping of ABO_3 perovskites); replacement of lead-containing materials in various applications
2. investigation of electronic structure of prospective inorganic functional and nanomaterials using advanced synchrotron based methods.

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STRUCTURE AND DIELECTRIC PROPERTIES OF $Na_{1/2}Bi_{1/2}TiO_3$-$CaTiO_3$ SOLID SOLUTIONS.

E. Birks, M. Dunce, R. Ignatans, A. Kuzmin, A. Plaude, M. Antonova, K. Kundzins, and A. Sternberg

Structure and dielectric properties of poled and unpoled $Na_{1/2}Bi_{1/2}TiO_3$-$CaTiO_3$ solid solutions are studied, projecting the obtained concentration dependence of structure and dielectric properties on pure $Na_{1/2}Bi_{1/2}TiO_3$ as the end member of this solid solution group. X-ray diffraction patterns for $Na_{1/2}Bi_{1/2}TiO_3$-$CaTiO_3$ family of solid solutions reveal a majority of an orthorhombic Pnma phase, even for compositions approaching the end composition ($Na_{1/2}Bi_{1/2}TiO_3$). While structure of pure $Na_{1/2}Bi_{1/2}TiO_3$ can be considered as coexisting of rhombohedral and orthorhombic phases. The Rietveld analysis is unable to give preference between different symmetries describing the diffraction patterns. Features of dielectric permittivity, corresponding to the observed structural phase transition, are identified. It is discussed that R3c phase is responsible for appearance of the frequency-dependent shoulder of dielectric permittivity temperature dependence, characteristic for depoled $Na_{1/2}Bi_{1/2}TiO_3$.

LUMINESCENCE IN Er^{3+}-DOPED $0.4Na_{0.5}Bi_{0.5}TiO_3$-$(0.6-x)SrTiO_3$-$xPbTiO_3$ SOLID SOLUTIONS

Marija Dunce, Eriks Birks, Anatolijs Sarakovskis, Jurgis Grube, Maija Antonova, Andris Sternberg

Previously we have shown that a gradual transfer from relaxor to classical ferroelectric state, passing various intermediate states, occurs in $0.4Na_{0.5}Bi_{0.5}TiO_3$-$(0.6-x)SrTiO_3$-$xPbTiO_3$ (0.4NBT-(0.6-x)ST-xPT) solid solutions upon increasing of PT concentration from x=0.00 to x=0.25. X-ray diffraction patterns have indicated that coexistence of tetragonal and cubic phases is characteristic to the compositions of this group of materials, which are in the relaxor state. Whereas Raman spectra, which ar sensitive to a local symmetry in a crystallographic lattice, only weakly depend on the fact if a particular composition is in relaxor or in ferroelectric state. The aim of this work is to find out what is the influence of ferroelectric ordering on luminescence properties in Er^{3+}-doped $0.4Na_{0.5}Bi_{0.5}TiO_3$-$(0.6-x)SrTiO_3$-$xPbTiO_3$ solid solutions, comparing compositions in the relaxor and the ferroelectric states. Upon excitation at 980 nm ($^4I_{15/2}\rightarrow{}^4I_{11/2}\rightarrow{}^4F_{7/2}$), well-expressed up-conversion luminescence bands were observed in the green ($^4S_{3/2}\rightarrow{}^4I_{15/2}$ and $^2H_{11/2}\rightarrow{}^4I_{15/2}$) and in the red ($^4F_{9/2}\rightarrow{}^4I_{15/2}$) part of spectrum. For the compositions with higher PT concentrations a pronounced second optical harmonic signal was observed at 490 nm. For the compositions with PT concentration above x=0.15 the second optical harmonic intensity significantly exceeds the up-conversion luminescence intensity. Luminescence spectra and decay kinetics were studied for the compositions with different PT and Er^{3+} concentrations.

This work has been supported by the National Research Program in the framework of project "Multifunctional Materials and composites, photonics and nanotechnology ($IMIS^2$)".

INFLUENCE OF UNIAXIAL PRESSURE ON DIELECTRIC PROPERTIES AND AGING EFFECT OF BiFeO3 CERAMIC

Suchanicz, J., Bujakiewicz-Koronska, R., Dziubaniuk, M., Kalvane, A., Sternberg, A.

The external stress (0–1500 bar) dependence of dielectric properties and an aging effect of BiFeO3 ceramic has been investigated. The electric permittivity and dielectric losses first increased (up to about 700 bar) and next decreased with uniaxial pressure applied parallel to the ac field direction, while increased with the stress perpendicularly applied. It was suggested that combination of the de-aging, clamping of the domain walls, and the polarization reorientation mechanisms can be responsible for these changes. The aging effect is followed logarithmic law and is related to the relaxation of the domain structure towards an equilibrium configuration.

SrTiO3 AND Pr EFFECTS ON STRUCTURAL, DIELECTRIC AND FERROELECTRIC PROPERTIES OF Na0.5Bi0.5TiO3 CERAMIC

Suchanicz, J., Klimkowski, G., Sitko, D., Antonova, M., Sternberg, A.

[(Na0.5Bi0.5TiO3)0.7Sr0.3]1-xPrxTiO3(NBTS30P) $(0 \leq x \leq 0.025)$ ceramics were prepared by solid-state synthesis process. Their crystal structure, microstructure dielectric and ferroelectric properties were studied. XRD data show that all of the ceramics possess a single perovskite phase. SEM results confirm that the ceramics are well sintered and exhibit relative densities higher than 97%. The results also reveal that the microstructure of the different compositions do not show a significant variation. The praseodymium (Pr) substitution to NBTS30 results in a change of crystal structure from cubic to tetragonal at x D 0.025. At the same time, electric
permittivity decreases, the maximum is broadened and slightly shifted to lower temperature, polarization and coercive field decreases. It is also found that the frequency dependence of Tm(the temperature where electric permittivity is maximum) increases with increasing Pr. A possible origin for these observed effects is discussed.The results show that the investigated ceramics are promising lead-free materials for electronic applications.

EFFECTS OF Mn ADMIXTURE ON DIELECTRIC PROPERTIES OF FERROELECTRIC RELAXOR PLZT CERAMICS.

V.Dimza, A.Popov, L.Kundzina, M.Kundzins, K.Kundzins, A.Plaude, M.Livins

A study of PLZT 8/65/35 ceramics prepared by two-stage hot pressing from chemically co-precipitated raw materials with admixture of Mn_2O_3 in concentration series of 0.01, 0.1, 0.3, 1.0, and 3.0 % by weight is reported. The complex dielectric permittivity $\varepsilon^* = \varepsilon' - i\varepsilon''$ as function of frequency and temperature and polarisation loops P(E) are measured.
Admixture of Mn is found to restrain the Vogel-Fulcher law held in the unmodified PLZT compound producing essential change of the dependence of ε^* on temperature and frequency and of the shape of P(E). The observed effects are explained by gradual involvement of Debye and Maxwell-Wagner polarisation mechanisms in relaxation processes with the growth of the concentration of Mn admixture. A decrease of the $\varepsilon'(T)$ maximum value and shift of the maximum to higher temperatures is observed.
The observed effects are attributed to impacts of Mn^{2+} and Mn^{3+} ions: formation of oxygen vacancies paired with Mn2+ as dipoles and Jahn-Teller distortion prompted by Mn^{3+} ions.

THE PECULIARITIES OF INFLUENCE OF COPPER AND LANTANUM DOPANTS ON FERROELECTRIC AND RELAXOR PROPERTIES OF PLZT CERAMICS: THE INVESTIGATIONS BY DIELECTRIC AND RADIOSPECTROSCOPY (EPR, NMR) METHODS

I.P.Bykov, Yu.A. Zagorodniy, L.P.Yurchenko, V. V.Trachevsky, V.Dimza, L.Jastrabik, A.Dejneka

EPR, NMR and dielectric spectroscopy investigation of PLZT 8/65/35 relaxor ferroelectric doped by copper oxide from 0.05 to 3 wt% was performed at 300 K . Behaviour of the complex dielectric permeability $\varepsilon^* = \varepsilon' - i\varepsilon''$ and polarisation in relaxor electro-optical PLZT 8/65/35 ceramics modified by admixture of Cu is studied within the 20 – 400^{o}C range of temperatures at frequencies from 130 Hz to 106 Hz. The observed ESR spectra were shown to be the superposition of Cu^{2+} being in axial and cubic symmetry field. The axial symmetry spectrum is stipulated by Cu^{2+} substituted for Ti^{4+} with its excess charge compensation by La^{3+} in its nearest neighbour; meanwhile cubic symmetry centers are those with the compensation in distant spheres. The ^{207}Pb NMR spectra of studied compounds show that increase of copper concentration from 0.005 to3 wt% lead to a marked increase in the intensity of the spectrum in a low field region. NMR spectrum presents the superposition of the Pb ions occupying sites with different symmetry of local environment and covalence of the chemical bond Pb-O, with less symmetry and more covalent chemical bond leading to a greater paramagnetic contribution from the given Pb ion. Thus, increasing of the copper content is accompanied by a change in the nature of the chemical bond Pb-O and lead to deformations of the structure, which has a significant impact on the ferroelectric and relaxor properties of PLZT. Increase of up to 5% lanthanum, accompanied by a monotonic shift of the line spectrum of 207Pb NMR. Further increase of lanthanum causes a change in the line shape of the strong field, which means that a further increase of the lanthanum atoms takes place with lead with less component covalent chemical bond.This is supported by the dielectric spectroscopy investigations where it was found that increase of Cu content shift the maximums of $\varepsilon'(T)$ and $\varepsilon''(T)$ curves to a higher temperature, increase the remnant polarisation, polarisation of saturation and lead to increase of the coercive field.

PHOTOELECTRIC CURRENT AND DIELECTRIC PROPERTIES OF BARIUM-STRONTIUM NIOBATE CERAMICS UNDER UV AND VISIBLE IRRADIATION *)

K. Bormanis, A.I. Burkhanov, Luu Thi Nhan, S.V. Mednikov, and M. Antonova

The study is focused on the photocurrent kinetics and dielectric response to infra-low frequencies in $Sr_{0.75}Ba_{0.25}Nb_2O_6$ (SBN-75) relaxor ceramics under visible and shortwave radiation in the vicinity of the broad phase transition. The compound, either in ceramic or single crystal form has a heterogeneous structure containing polar and nonpolar phases coexisting over a wide range of temperature determining its high sensitivity to external agitations. An amorphous phase might also be present on grain boundaries in ceramics determining a difference in reaction to liht between ceramics and single crystals.

Results of the study of the kinetics of photocurrent and the infra-low frequency dielectric response at different temperatures are discussed as the effects of the defected structure of ceramics and non-equilibrium carriers on relaxation of polarisation in the range of the broad phase transition.

At kHz frequencies a weak photo-electric effect on ε' is detected only at $t > 100$ s, it is, at time intervals corresponding saturation of the $\varepsilon'(t)$ curve.

The change of dielectric response is found to be well described by function $y = y_0 - A \cdot \exp(-t/\tau)$ where A, y, and y_o correspond to dielectric parameters, τ – relaxation time. Effective dielectric permittivity $\varepsilon'_{eff}(E)$ and dielectric loss $\varepsilon''_{eff}(E)$, $\tan\delta_{eff}$ are determined at frequencies of 0.1, 1.0, and 10 Hz and different field intensities E. Anomalies on the $\varepsilon'_{eff}(E)$ and $\varepsilon''_{eff}(E)$ curves of SBN-75 are observed before and after illumination.

Effective parameters $\tan\delta_{eff}(E)$, ε'_{eff}, and ε''_{eff} obtained from polarisation loops before and after irradiation at frequencies below 10 Hz, the interval representative of relaxation of polarisation in the relaxor phase of the SBN-75 ceramics, show that irradiation mainly causes some decrease of the values of $\tan\delta_{eff}$ and ε''_{eff}.

Most likely the anomalies are due to relaxation of the space charge. Irradiation is shown to reduce the contribution of space charge at temperatures (i.e., near T_m) corresponding to the range of the relaxor phase. The decrease of dielectric loss at irradiation of the SBN-75 ceramics points to rise of unbalanced carriers compensating the space charge in the material.

*) In cooperation with Volgograd State Architectural and Engineering University and with Volgograd State Technical University, Volgograd, Russia.

STRUCTURAL AND OPTICAL HOMOGENEITY IN LITHIUM NIOBATE CRYSTALS OF LOW PHOTOREFRACTIVITY *)

N.V. Sidorov, M.N. Palatnikov, N.A. Teplyakova, A.A. Yanichev, O.V. Makarova, O.Yu. Pikoul, and K. Bormanis

The structural and optical homogeneity of lithium niobate crystals ($LiNbO_3$) of stoichiometric, congruent ($LiNbO_{3cong.}$), and single-crystals of $LiNbO_3$ containing cation admixtures of Mg (0.078, 0.89 wt .%), Zn (0.03, 0.52, 0.62 wt .%), Cu (0.015 wt .%), B (0.12 wt .%), Gd (0.51 wt .%), Y (0.46 wt .%), Gd (0.23 wt .%): Mg (0.75 wt .%), Mg (0.86 wt .%): Fe(0.0036 wt .%), Ta (1.13 wt .%): Mg (0.011 wt .%), and Y (0.24 wt .%): Mg (0.63 wt .%) was studied by Raman scattering, photo-induced light scattering (PILS), laser conoscopy and optical spectroscopy. Having a low photorefractivity the crystals are promising materials for frequency and broadband converters of coherent optical radiation. Position of the optical absorption edge in modified crystals $LiNbO_3$: Y (0.46 wt. %) and $LiNbO_3$: Y (0.24 wt. %): Mg (0.63 wt. %) is found to match the absorption edge of congruent crystals. Disclosure of the PILS indicatrix of these crystals proceeds very fast - during the first second of laser irradiation, qualifying them as potential materials for holography, electro-optic modulators, and optical switches. A noticeable influence of the photorefractive effect on the conoscopic patterns is observed along with a smaller angle of the transmission curve in the $LiNbO_3$:Y(0.46 wt.%) and $LiNbO_3$:Y(0.24 wt.%):Mg(0.63 wt.%) crystals, as compared with a congruent crystal. indicates of a significantly lower optical homogeneity.

The asymmetry of the PILS indicatrix of $LiNbO_3$ crystal is shown to be the result of birefringence of the exciting laser radiation propagating perpendicular to the polar axis of the crystal, and the asymmetry of the Raman spectrum is the result of the presence of spontaneous polarization and birefringence. The shape of the PILS pattern depends on the difference between the values of refractive indices $\Delta n = n_o - n_e$ and the ratio of the energies E of the ordinary (n_o) and extraordinary (n_e) rays. If $En_o >> En_e$, the PILS picture is a round three-layer spot. With approximately equal energies the shape being a symmetrical number eight. At $En_o < En_e$ the PILS pattern is asymmetric.

*) In cooperation with I.V. Tananaev Institute of Chemistry and Technology of Rare Elements and Mineral Raw Materials of Kola Science Centre of RAS, Apatity, Russia and Far Eastern State University of Transportation, Khabarovsk, Russia.

SCIENTIFIC PUBLICATIONS

1. **E. Birks, M. Kundzinsh**, E. Nitiss, **R. Ignatans, M. Dunce, M. Antonova, A. Sternberg.** Study of tetragonal phase in 0.4Na1/2Bi1/2TiO3-(0.6-x)SrTiO3-xPbTiO3 solid solutions by second-harmonic generation. Ferroelectrics, 2015, vol. 485, p. 53-57.

2. **M. Dunce, E. Birks, R. Ignatans, A. Plaude, M. Antonova, A. Sternberg**. Dielectric and polarization properties of Na0.5Bi0.5TiO3-BaTiO3 solid solutions with Na and K niobates. Ferroelectrics, 2015, vol. 485, p. 80-88.

3. **M. Dunce, E. Birks**, J. Hagberg, J. Peräntie, **M. Antonova**, and **A. Sternberg**. Interpretation of the electrocaloric effect in Na1/2Bi1/2TiO3-SrTiO3-PbTiO3 solid solutions. Ferroelectrics, 2015, vol. 485, p. 143-152.

4.**V. Dimza, L. Kundzina, M. Kundzins, K. Kundzins, A. Plaude, M. Livins** & **M. Antonova** . Aging and Memory Effects in PLZT 8/65/35 Ceramics Modified with 3d Transition-Metal Ions, Ferroelectrics, 2015, vol.484(1), p.78-86.

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7. **K. Bormanis**, A.I. Burkhanov, Luu Thi Nhan, S.V. Mednikov, and **M. Antonova**. Photoelectric Current and Dielectric Properties of Barium-Strontium Niobate Ceramics under UV and Visible Irradiation. ID: 1061880 DOI:10.1080/00150193.2015.1061880. Ferroelectrics, 485, 1, 2015, 179-185.

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3. M. Dunce, E. Birks, J. Peräntie, J. Hagberg, M. Antonova, A. Sternberg. Phase transitions in $Na_{0.5}Bi_{0.5}TiO_3$-$(Sr_{0.7}Bi_{0.2})TiO_3$-$PbTiO_3$ solid solutions. *EMF-2015*, Porto, Portugal, June 28 – July 3, 2015, P6_10.
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5. V.Dimza, A.Popov, L.Kundzina, M.Kundzins, K.Kundzins, A.Plaude, M.Livins. Effects of Mn doping on dielectric properties of ferroelectric relaxor PLZT ceramics, EMRS 2015, Lille (France), 11.-15.05.2015.

DEPARTMENT OF FERROELECTRICS

Head of Department, Dr.habil.phys. V.Dimza

LABORATORY OF VISUAL PERCEPTION

Head of Division Dr.hab.phys. Prof. M.Ozolinsh

Human vision is a complex phenomenon. Its optical part is essential, however optical image stays only at the very beginning of the visual pathway and information processing in the cortex. We see with our brains, and as a result in some provocative cases it is very hard for us to accept the final outcome. Laboratory is a joint between colleagues in institute and Department of Optometry and vision science of the University. Most of Department's Master thesis have been accomplished due to collaboration between units. In 2015 more than 10 Bachelor's and Master's thesis have been completed under supervision of laboratory researchers.

RESEARCH PROBLEMS:

- investigation of smart optical materials and designs with controllable optical, electrooptic, refractive properties such as pjezooptic and electrooptic materials in order to accomplish effective radiation wavefront control, modification of light scattering and other optical characteristics;
- effect of aberrations in eye structures and appliances on retinal image formation and on the psychophysically detected human visual response, accomplishing adaptive optics compensation of optical objects aberration errors with fast control feedback;
- studies of binocular and stereovision, suppression and rivalry mechanisms of binocular vision, evaluation of suppression strength and depth effect on quality of vision binocular functions;
- fast eye kinematics studies for children and adults without and with several disorders of visual perceptions, eye kinematics studies in sport vision.
- evaluation of accommodation/convergence mechanisms reading print materials and for regular computer users;
- digital visual stimuli image processing determinant for analyse of the human visual response;
- multispectral material surface reflectance and emission analysis in visible and near IR and UV range, and its visual recognition by humans with normal and colour deficient vision;
- providing illumination and material visual appearance testing expertise and quality of products correspondence according to standards.

SCIENTIFFIC STAFF

Prof. Maris Ozolins
Prof. Ivars Lacis
Dr.phys. Sergejs Fomins
Dr.phys. Varis Karitans

Ph.D. students
Kaiva Juraševska
Olga Danilenko
Renars Trukša

SCIENTIFIC PROJECTS.

- LCScie State Programm VPP-15 Prog.„Designing of innovative multifunctional materials, signal processing and information technologies for competitive scientific advanced products" – IMIS2;
- Project funded by EU ERAF 2DP/2.1.1.1.0/10/APIA/VIAA/137: „Technologies for digital multispectral control of materials and quality improvement".
- ESF project Nr.2013/0021/1DP/1.1.1.2.0/13/APIA/VIAA/001 "Investigations and development of diagnostics of visual load and stress" .

PARTNERS ABROAD.

Spain	Universidad Complutense Madrid, Spain (Prof. M.C.Puel) Laboratorio de Optica, Universidad de Murcia, Spain (Prof. P. Artal)
Sweden	Chalmers TH, Sweden (Prof. L.Komitov)
Norway	Buskerud HØgskolan, Institutt for optometri (Prof. J.R.Bruenich).
Finland	Colour Research Laboratory, University of Eastern Finland (Prof.J.Parkkinen)
Germany	*Institut fur Arbeitsphysiologie an der Universität Dortmund*
The Netherlands	Utrecht University (Prof. R. van Ee)
France	Laboratoire Régional des Ponts et Chaussées de Clermont-Ferrand (Dr.M.Colomb)
Wales	University of Cardiff, The School of Optometry and Vision science (Dr. M.Rozanowska)

FOREIGN SCIENTIST VISITS IN LABORATORY

1. Prof. ***Brian Vohnsen***, University College Dublin, Ireland; 7.04. - 11.04.2015.
2. Prof. ***Galina Paramei***, Liverpool Hope University, England; 29.06. - 02.07.2015.

MAIN RESULTS

THE MEASUREMENT OF ISOCHROMATIC AREAS IN ALTERED COLOR VISION

Kaiva Jurasevska, Renars Truksa, Linda Broka, Maris Ozolinsh, and Gunta Krumina

Color vision tests are primarily designed for detecting the type and severity of the deficiency not for obtaining a comprehensive picture of the visual experience of a specific individual. Overuse of the visual system may result in vision fatigue and altered color perception. We have developed a tool for detecting individual isochromatic areas in color space among color vision deficient patients. Our modified derivative of the CAD (color assessment and diagnosis) test allows measuring the degree of vision function loss associated with color and shape perception. We have designed an algorithm which excludes artefacts in the test field background. The colored stimuli are chosen on mutually parallel lines in the CIE xy color space CRT gamut. Isochromatic areas for particular person with known color vision deficit are determined by comparing the results within and among the predefined lines. We were able to measure the chromatic sensitivity of color normal and color deficient patients and to determine individual protanopic, deiteranopic and tritanopic axes using psychophysical design.

Results from two deutan observers show that our method is valid for finding isochromatic areas within color deficient patients in CIE xy color space. Very high correlation with deutan isochromatic lines was obtained. The novelty of our method is the ability to acquire isochromatic area dimensions in opposite direction—above and below the corresponding confusion lines. In the future we aim to improve overall testing method and gather data from larger and more diverse sample size.
Supported by ESF-2013/0021/1DP/1.1.1.2.0/13/APIA/VIAA/001

"VARIANTOR" FUNCTIONAL SPECTRAL FILLTER THAT STIMULATES TRICHROMATS SEE AS DICHROMATS

Zane Jansone and Maris Ozolinsh

"Variantor" functional spectral filter helps people with normal color vision to understand what the world looks like to color deficient people and which color combinations are confusing for these people. In our study we tested the characteristics of these glasses: their spectrum of absorption; effectiveness of the color transfer and the patient response looking through the goggles on different color images. Their use was tested using color tests - Ishihara pseudoisochromatic plates and anomaloscope. The main goal was to test the "Variantor" effectiveness in everydays life. In our research participated observers: 1 thrichromat, a person with deiteroanomaly and a trichromatic person wearing glasses. During the studies (color discrimination of Ishihara plates) the results showed that person with "Variantor" response was much slower and it was more difficult to distinguish different color objects. Results showed that anomaloscope can't be applied to the test - are the patients trihromats or dichromats, because color stimuli used in anomaloscopes are monochromatic; and they belong to the spectrum range which is absorbed the filter.
Supported by ESF-2013/0021/1DP/1.1.1.2.0/13/APIA/VIAA/001.

SMART MODEL EYE ON BASE OF POLYMER DISPERSED LIQUID CRYSTALS AND CMOS SENSOR

Maris Ozolinsh, Paulis Paulins, and Varis Karitans

We report on developed model eye for studies of deterioration of image quality, optical system resolution, modulation transfer function in cataract eye lens using a polymer dispersed liquid crystal (PDLC) cell as smart media. The model allows the electrical field inducing of scattering that corresponds to various levels of cataract. Since now different media are used for alternating of scattering efficiency (i.e., no smart media, but model with alternate scattering – (Donnelly, 2005) in model eyes). Previously we have demonstrated the controlling of “cataract” scattering efficiency in visible by applying the AC electric field to a thin PDLC layer. The model eye is built using CMOS sensor built in PANASONIC Lumix LX1 camera with a sandwich element comprised of two glass plates with a light scattering PDLC layer filled between. The compound is built in a special adapter. The lens module (on the base of Sigma 24mm Olympus OM Filtermatic with effective f-number F = 2.8) is mounted on the platform of digital photocamera - horizontal sensor pixel pitch 1.4 _m, digital output 14-bit depth. Camera has full manual operation and allows to select exposure 1/4000 to 60 s. Applying the AC electric field up to 30V continuously diminishes scattering efficiency. Model eye properties were tested regarding to image point spread function PSF and image line spread function LSP, eye ”contrast vision function” in presence of simulated in PDLC light scattering. Light scattering effect on detectability of model eye lens aberrations using Shack-Hartman sensor is in progress.
Supported by “IMIS2”.

VISIBILITY OF PEDESTRIANS WEARING RETROREFLECTIVE SIGNS DURING EVENING DUSK TIME

Maris Ozolinsh and Natalja Davidenko

Human vision spectral and absolute sensitivity changes during the evening dusk time. Adaptation to decrease of solar illumination and switching to artificial ambient street illumination takes relatively long time stretch. That especially bothers car drivers still using of low beams, however the contrast of visibility of different road obstacles during this time span can appear insufficient. In order to improve these adverse viewing conditions pedestrians nowadays use retroreflective marks attached to the surface of wearing. We have studied observer visibility of such retroreflective signs during adaptation of eyes to mesopic and further to scotopic viewing conditions. Wearing with retroreflective signs was illuminated by diffuse ambient light sources with slowly changing intensity and by directed light beams of LED flood lights coincided with observers' sight line. The viewing distance was 50 m. We used different color wearing and white, yellow and red retroreflective marks. Comparing of recognition thresholds of retroreflective signs was carried out using pshychophysical forced choice paradigm – observer was obliged to answer are two signs oriented at angle -45^{o} or $+45^{o}$ according to vertical axis and those positions were chosen randomly in each trial. We obtained the data set of "high beam" illumination recognition thresholds for these retroreflective signs. We found better recognition thresholds by illumination with higher color temperature LED flood light and for higher wearing contrasts – darker surround and white retroreflectors.

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COLOUR INDUCED ENHANCEMENT OF PERCEPTION OF GLOBAL VERSUS LOCAL MOVEMENT

Maris Ozolinsh and Paulis Paulins

Local and global perception of moving objects was studied psychophysically and neurologically (Anstis and Kim, 2011; Zaretskaya et al., 2013). Authors hypothesise prevalence principles of perceptual "local" vs. "global" grouping that depends on stimuli geometry, lightness polarity, complexity. Previously elementary elements were gray-scaled and arranged in groups in various manners. We introduced: a)colour contrast between stimuli groups and between stimuli and background, b)viewing eccentricity of scene. We used spot doublets that can be perceived rotating around their symmetry centre ("local" motion) – organized at vertices of two squares that can be perceived sliding over each other along circular paths ("global" motion). Doublets were shown as red and green spots on yellowish background, further the colour saturation was minimized during trials. During onset of scene the local motion prevailed that further turned to global sliding of two squares. We measured with 2-AFC paradigm the time course of the first switching event to global motion in dependence of spot colour distances DK in La*b*space both for chromatic and achromatic scene and contribution of chromaticity into facilitation of switching. Facilitation of switching was observed increasing eccentricity of viewing continuously moving the fixation point from the doublet centre to centre of scene.

Supported by ESF-2013/0021/1DP/1.1.1.2.0/13/APIA/VIAA/001

"SMARTGLASS" OBSTACLES FOR DYNAMIC INDUCING OF LIGHT SCATTERING IN VISION RESEARCH EXPERIMENTS

Olga Danilenko, Maris Ozolinsh, Varis Karitans, and Paulis Paulins

We describe a technique that allows control of visual stimuli quality through the use of a setup with a polymer dispersed liquid crystal (PDLC) film positioned in the optical pathway of one or both human eyes. Nowadays, PDLC films allow alteration of the resolution and contrast limits of the transmitted light due to continuous change in the light scattering that is obtained by the application of an AC electrical field. In our experimental setup, the use of a wide-aperture up to area of 20x15 cm^2 PDLC sheet is combined with a flat-screen PC display or with a modified display emission block without its interference filter unit and with an installed individually controllable colored light-emitting diode (LED) backlight. In the latter case, the spatial structure of visual stimulus remains constant, but the PDLC switching-on timing for intensity, color, and contrast of visual stimuli control is done by a PC via an *Arduino* USB interface. *Arduino* applies a voltage to the backlight colored LEDs and the low voltage up to 30-80V to light-scattering PDLC sheet. Modifications to this setup can improve the resolution of the timing and screen stimulus intensity and color purity, and increase the flexibility of its application in visual research tasks. A particular use of PDLC scattering sheets involves the altering of the stimuli input strength of the eye in different binocular viewing schemes. In such applications, a restricted-optical-aperture PDLC element is mounted in a goggle frame, and the element is controlled by the application of low-voltage AC field. The efficacy of the setup is demonstrated in experiments of human vision contrast sensitivity adaptation studies. Studies allow to determine the characteristic time of the contrast sensitivity altering of 4s during adaptation phase and the same order of the characteristic time during recovery.

Supported by "IMIS2".

TIME COURSE AND INTEROCULAR TRANSFER OF SIZE AND CONTRAST ADAPTATION AFTEREFFECTS

Olga Danilenko,[1] Maris Ozolinsh, and Daniel H Baker

We performed psychophysical experiments to evaluate adaptation to size and contrast, and the dependence of these processes on stimulus texture. Stimuli were discs or rectangles presented against a mid-grey background, consisting of sine-wave or plaid patterns or areas of uniform luminance. In the adaptation phase for size adaptation experiments, a number of large disks (with diameter twice as that taken for a "standard") jittered in position (based on Baker & Meese, 2012; Perception, 41(S):33) in the left side of the visual field for up to 20 seconds. Target stimuli were then displayed, consisting of a fixed diameter standard in the adapted hemifield, and a comparison stimulus of variable size in the unadapted hemifield. Participants indicated which of the target stimuli appeared larger in size. By varying the adaptation period we obtained exponential time courses for size adaptation with a time constant of τ_{size}=7.1s (SE=±0.6s). Additional control experiments found no effect of the relative orientation of adaptor and target textures. Adapting to textured stimuli in the centre of the visual field produced a strong orientation-specific contrast sensitivity aftereffect with a time constant that was shorter than that measured for size adaptation (τ_{contr}=3.9s, SE=±0.2s). Similar values of time constant were observed during recovery from adaptation. For contrast sensitivity we also measured interocular transfer of adaptation by adapting and testing in the same eye or in different eyes. The latter case revealed a 75% reduction of the total adaptation depth, suggesting a strong monocular contribution to contrast adaptation.

Supported by "IMIS^2".

VALIDATION OF A METHOD FOR MEASURING THE RETINAL THICKNESS WITH SHACK–HARTMANN ABERROMETRY IN AN ARTIFICIAL EYE

Varis Karitans, Liene Jansone, Maris Ozolinsh and Gunta Krumina

In Shack–Hartmann aberrometry, it is assumed that a wave front emerges from a single point focused on a retina. However, the retina is a multi-layered structure and reflections may occur from several layers. This may result in several overlapping spot patterns on the CCD due to different vergences of the outgoing wave fronts. The amount by which these spot patterns are displaced may contain information about the retinal thickness. In this study, we perform simulations of formation of double spots in a living eye and also apply this method to measure the thickness of an artificial retina with a simple structure. We also compare the results obtained with artificial eye and compare them to the simulated data. We evaluate the recommended range of the lenslet parameters for analyzing the retinal thickness. We conclude that this method could be used in a living eye for estimating the total retinal thickness and to confirm retinal pathologies associated with significant increase in the retinal thickness like glaucoma, macular edema, etc.

Supported by ESF-2013/0021/1DP/1.1.1.2.0/13/APIA/VIAA/001

PUBLICATIONS.

1. **Kaiva Jurasevska, Renars Truksa**, Linda Broka, **Maris Ozolinsh**, and Gunta Krumina. The measurement of isochromatic areas in altered color vision. *Perception* **44**(4), p.459-460 (2015); WOS:000355889600027.

2. Ieva Timrote, Agnese Reinvalde, **Sergejs Fomins**, and Gunta Krumina. Peripheral vision effects central task performance under visual fatigue. *Perception* **44**(4), p.324-325 (2015); WOS:000362287800649.

3. Evita Kassaliete, **Ivars Lacis, Sergejs Fomins**, and Gunta Krumina. Reading and coherent motion perception in school age children. *Annals of Dyslexia* **65**(2), p.69-83 (2015); DOI: 10.1007/s11881-015-0099-6.

4. Ieva Timrote, Agnese. Reinvalde, **Sergejs Fomins**, and Gunta Krūmiņa. Visual search strategy changes between school-age and adulthood. *Perception* **44**(4) (2015), p.467(2015); WOS:000355889600051.

5.**Varis Karitans,** Liene Jansone, **Maris Ozolins**, and Gunta Krumina. Validation of a method for measuring the retinal thickness with Shack–Hartmann aberrometry in an artificial eye. *Journal of Modern Optics* **62**(8), p.662-675 (2015); DOI: 10.1080/09500340.2014.1003253.

6.**Maris Ozolinsh** and Paulis Paulins. Colour induced enhancement of perception of global versus local movement. *Perception* **44**(1), p. 224-225 (2015); WOS:000362287800449.

7. **Maris Ozolinsh** and Kristine Muizniece. Color difference threshold of chromostereopsis induced by flat display emission. *Front. Psychol.* **6**:337 (2015); doi: 10.3389/fpsyg.2015.00337.

PATENTS

EP2873364 - Multispectrally tested, printed colour vision test for the fine evaluation of the degree of deficiency. Sergejs Fomins and Maris Ozolinsh. Date of publ. 20.05.2015.

DEFENDED DOCTORAL THESIS

Juraševska, Kaiva „Development of a psychophysical pseudoisochromatic test and evaluation of color discrimination," def. 30.06.2015 (prom. Maris Ozolinsh).

PARTICIPANCE IN INT. CONFERENCES

- DOC-2015, Riga, Apr.2015.
- Northern Optics and Photonics - 2015, Lappeenranta, Finland, June 2015.
- Int.Conf. of Color Vission Society ICVS-2015, Sendai, Japan Jul.2015.
- Eur.Conf. of Visual Perception ECVP-2015, Liverpool, England, Aug.2015.
- 18-th Int. Conf.-School „Advanced Materials and Technologies – 2015", Palanga, Lithuania, Aug. 2016.
- Annual Conf. of Applied Vision Association AVA-2015, London Dec.2015.

DEPARTMENT OF SEMICONDUCTOR MATERIALS

Head of Department Dr.phys. A.Lusis

SHORT HISTORY

Semiconductor Material Department was established in University of Latvia at 1968. It was connected with semiconductor industry development in Soviet Latvia and growing demand for specialists educated in the field of semiconductor physics and electronics. Head of department was Andrejs Lusis, postgraduate student in that time and chairs department even today. Between first researchers there were Janis Klavins, Valdis Sternbergs, students Juris Lagzdonis, Janis Pinnis, Talivaldis Zamozdiks. In 1971 here was included the group of Aloizijs Patmalnieks (Inara Biele, Aris Veispals, Guntis Ramans). Investigations were related with CdS thin monocrystalline films, interface In/CdS, surface properties of epitaxial Si and MgO films. New direction, related with electrochromism, started on 1972. First electrochromic devices were obtained in 1994 by J.Klavins, T.Zamozdiks, O.Rode. On the end of 1970th the Semiconductor Material Department was largest and powerful scientific organization in previous Soviet Union, connected with electrochromic materials and devices. During 1979-1989 in Riga was organized annual Solid State Ionic conferences, collecting all scientists from USSR working in the field of electrochromism. The prosperity period of Department was 1981-1990, when were defended 12 doctoral dissertations, 23 university diploma works in physics and chemistry, 14 patent applications and published more than 200 scientific papers**.**

RESEARCH AREAS AND EXPERTISE

• Electrophysics and electrochemistry of specific semiconductor materials, mixed conductors, ion conductors (transition metal oxides, bronzes, metal hydrates, solid electrolytes, nanostructured and porous materials, composites etc.);
• Material preparation methods: thin and thick film technologies, sol-gel process, leaching, sonochemical processes, pyrolysis spray coating, electrochemical and electrophoretic deposition, functional coatings and multi layer electrochemical systems;
• Material characterization by spectroscopic methods (Raman scattering, Furrier IR, optical and Xray absorption, EXAFS), electrical and electrochemical impedance, Mott-Schottky plott, photoelectrochemical, AFM, TGA/DTA;
• Solid state ionics:
  - electro-, photo-, thermo-, chemo-, gaso-chromic phenomena in transition metal oxides;
  - structural and electronic phase transitions due to ion intercalation, lattice dynamics;
  - solid state reactions at interfaces electrode – solid electrolyte;
  - gases and ions sensing phenomena and detection technologies, odour removal;
• Hydrogen absorption and adsorption phenomena in hydrides (metals, alloys), nanopotous (zeolite) and few layer grapheme materials; development of new nano structured materials for hydrogen storage;
• Hydrogen production by electrolysis, photoelectrolysis, biomass fermentation; development of hydrogen generation equipment and reactors;
• Synthesis and research of polymer and composite proton conducting membranes for fuel cells and hydrogen separation; Tritium analysis.
• Development of cathode materials for Lithium and Sodium thin film batteries.

DEPARTMENT OF SEMICONDUCTOR MATERIALS

Head of Department Dr.phys. A.Lusis

LABORATORY OF SOLID STATE IONICS

Head of Laboratory Dr.chem. Gunars Bajars

RESEARCH AREA

Physics and electrochemistry of specific semiconductor materials, ion conductors, mixed ionic-electronic conductors (transition metal oxides, bronzes, solid electrolytes, nanostructured and porous materials and composites).
Materials for lithium and sodium ion batteries. Materials for photo-electrocatalysis.
Functional coatings and multi layer electrochemical systems. Functional fibers (glas and hemp) and textiles for technical application.

MAIN RESEARCH TOPICS

Ion transfer in solids, two phase interfaces and composites. Structural changes due to ion intercalation, lattice dynamics, structural and electronic phase transitions. Solid state reactions at electrode – solid electrolyte interface. Lithium and sodium intercalation materials and their application for thin film rechargeable battery. Doped titanium dioxide based materials for photo-electrocatalysis.
Nanostructuring methods and coating technologies for functionalization of fiber glass surfaces. Tritium release properties of neutron multiplier beryllium materials for fusion reactor development.

MATERIAL PREPARATION AND RESEARCH METHODS

Material preparation by solid and liquid state synthesis. Thin and thick film technologies: sol-gel, leaching and sonochemical processes, electrochemical and electrophoretic deposition, magnetron sputtering technique.

Material characterization by Raman spectroscopy, optical microscopy, voltammetry, chronopotentiometry, electrical and electrochemical impedance, photoelectrochemical methods, SEM, XRD and thermogravimetric analysis.

SCIENTIFIC STAFF:

Dr. chem.. G. Bajars
Dr. phys. J. Gabrusenoks
Dr. phys. G. Kucinskis
Dr. phys. A. Lusis
Dr.phys. E. Pentjuss

PhD students
K. Kaprans
Students
J. Mateuss
M. Rublans
Technicians
J. Balodis

SCIENTIFIC VISITS ABROAD

G. Kucinskis (4 month Max Planck Institute for Solid State Research, Stuttgart, Germany).

COOPERATION

Latvia

1. University of Latvia - Department of Chemistry (Dr. G. Kizane, Dr. G.Vaivars).
2. Riga Technical University - Institute of Inorganic Chemistry (Dr. A. Dindune).
3. Riga Technical University - Institute of Silicate Materials (G.Mežinskis).
4. Latvian Institute of Wood Chemistry (Dr.hab. G.Dobele, Dr.hab. J.Gravitis).
5. Association of Light Industry Enterprises (V.R.U.A).
6. Latvian Industrial Hemp Association (LIKA).
7. JSC "Valmiera Glass Fiber".
8. JSC "Sidrabe".

Germany

Max-Planck-Institut für Festkörperforschung (Stuttgart) – Prof. J.Maier.

Lithuania

University of Vilnius - Department of Physics (Prof. A.Orliukas, Dr. T.Salkus).

Taiwan

National Cheng Kung University – Department of Material Science and Enganeering (Prof. K.-Z. Fung).

MAIN RESULTS

MASS RECOVERY KINETICS OF HEATED, CARBONATED GLASS FABRIC IN ATHMOSPHERE WITH DIFFERENT HUMIDITY AND CO_2 CONCENTRATION

Evalds Pentjuss, Andrejs Lusis, Jeugenijs Gabrusenoks, Janis Balodis, Gunars Bajars

The Na-Al-Si glass fabric fibers contain Na^+ ions that diffuse to its surface and together with CO_2 and H_2O from atmosphere during long term storing create here the hydrated carbonate shell [1] with thickness of 1-2 um (SEM). Heating of fabric may leads to inverse process – decomposition of hydrated carbonate with evolving of CO_2 and H_2O. There are investigated the mass recovery kinetics (till 8000 h and more) of fabric samples (heated at different temperatures 1 h) in atmosphere with different CO_2 concentration and RH. At least during first 0,25 h in all tested cases the mass recovery follows (R^2>0,999) relation (1) [2]

$$A(t) = A_1(1-\exp(-t/t_1)) + A_2(1-\exp(-t/t_2)). \quad (1)$$

In (1) A_1 and A_2 are mass (or relative mass) constants, t_1 and t_2 - time constants. Experiments showed that $A_1 << A_2$ and characterize CO_2 and H_2O mass absorption limits (maximal, equilibrium or saturated state) when $t \to \infty$. Constant $t_1 << t_2$ and as a result CO_2 mass reach its saturated state at the beginning of 0,25 h interval, but H_2O mass do not reaches it till end of interval, and out of this interval begins to fall below the values predicted by relation (1). It indicates to some reordering appearance in crystals of carbonated shell that reduces water absorption increase. The values of A_1 and A_2 depend on sample heating temperature before and mass recovery atmosphere content. After long term storing (years) at room conditions the main or solely substance of shell is trona ($Na_3H(CO_3)_2.2H_2O$ (TGA)) having decomposition beginning temperature of 57 ^{0}C. Heating temperature increase of samples over mentioned value leads to sharp increase of A_1 and A_2 (as absorption sites) that have to be associated with absorption

sites number increase released by increasing evolving of CO_2 and H_2O during heating before. Value A_1 has a sharp (about 70 ^{0}C) and A_2 a wide and structured maximum extended up to about 160 ^{0}C. Both of them have correlation with its time constants relations *vs* heating temperature (as it suggests the time constants interpretation). It have to be occurs in the decomposed surface layer of trona crystals.
Mass restoring later 0,25 h falls below predicted by relation (1), that could be caused by decomposed crystal layer preparation to direct crystallization of absorbed water (necessary enough high RH 30-50 %). Direct water crystallization begins as second fast mass increase. In this case the owned mass is stable after artificial RH lowering in atmosphere. At a permanent 60-70 % RH there temporary (350 h) exists high mass absorption/desorption peak (may be formation of $Na_2CO_3.10H_2O$ and/or $Na_2CO_3.7H_2O$) and high free water content.
Proposed method employed big difference in CO_2 and water absorption time constants to separate its mass absorption using regression technique. The second gain is research object used in form of thin (1-2 μm), porous, crystalline shell on glass fibers with Ø 6μm, having good contact to surrounding atmosphere almost for every crystal that leads to absence of additional mass and heat transportation restrictions. There is necessary an additional research of method possibilities and to understand obtained results.

[1] Veal B.W., Lam D.J., Karim D.P. *Nuclear Technology* **51** (1980) 136.
[2] Pentjuss E, Lusis A, Bajars G and Gabrusenoks J 2013 *IOP Conf. Series: Materials Science and Engineering* **49** 012044 doi:10.1088/1757-899X/49/1/012044

ELECTROPHORETICALLY DEPOSITED TiO_2/Fe_2O_3 /REDUCED GRAPHENE OXIDE COMPOSITE MATERIAL AS ANODE FOR LITHIUM ION BATTERIES

Kaspars Kaprans, Janis Mateuss ,Anna Dorondo, Gunars Bajārs, Gints Kucinskis, Janis Kleperis

Lithium ion battery is an effective device for electrochemical energy storage in modern electronic devices such as cell phones, laptop computers and electric vehicles. It is important to develop anode materials for lithium ion battery with high reversible capacity, long cycle life and low cost.
One of the most promising materials for such purpose is graphene. In this study two metal oxide (Fe_2O_3 and TiO_2) additives have been coupled to the graphene oxide to improve its conductivity, rate capability and cycling stability. Electrophoretic deposition method was used to prepare sheets for anode material from water suspension and subsequent thermal reduction (500 °C and 700 °C) was applied. The morphology of the electrophoretically prepared Fe_2O_3/TiO_2/reduced graphene oxide films were examined by scanning electron microscopy, Raman spectroscopy and X-ray diffraction analysis. Electrochemical measurements were carried out by two electrode electrochemical cell with lithium foil as the counter electrode and $LiPF_6$ in ethylene carbonate and dimethyl carbonate mixture (volume ratio 1:1) as an electrolyte.
Thin film anode of TiO_2/Fe_2O_3/graphene oxide reduced at 700 °C showed the specific capacity 93 mAh·g^{-1} at a current density 50 mA·g^{-1} and specimen reduced at 500 °C showed 985 mAh·g^{-1} at a current density 110 mA·g^{-1}. Thin film anode of TiO_2/Fe_2O_3/reduced graphene oxide displays excellent performance with stable capacity retention after 100 charge/discharge cycles at a current density 0.8 A·g^{-1}. Folowing specimens were reduced at 700 °C showed specific capacities, TiO_2/reduced GO showed 116 mAh·g^{-1} at 20 mA·g^{-1} current, Fe_2O_3/reduced GO showed 39 mAh·g^{-1} at 30 mA·g^{-1}, TiO_2/Fe_2O_3/reduced GO showed 93 mAh·g^{-1} at 50 mA·g^{-1}, but specimen reduced un 500 °C showed specific capacities of 775 mAh·g^{-1} at current density 125 mA·g^{-1} for TiO_2/reduced GO, 232 mAh·g^{-1} at current density 1000 mA·g^{-1}.

Results show that TiO_2/Fe_2O_3 /reduced graphene oxide is a promising anode material for high energy and high power lithium ion batteries.

THE STUDY OF NANOSTRUCTURED BULK AND THIN FILM $LiFePO_4$ CATHODE MATERIALS FOR LITHIUM ION BATTERIES

G.Kucinskis, G.Bajars, K.Bikova, J.Kleperis

$LiFePO_4$ is a widely researched lithium ion battery cathode material often used in high power lithium ion batteries. However, despite numerous studies, the connection between intrinsic material parameters, grain structure and charging behavior (i.e. intra-particle and inter-particle lithium transport) has remained elusive. Additionally, new efficient ways of improving the rate capability of the cathode are necessary.
LiFePO4 lithium ion battery cathode material and its thin films have been studied. The possibilities of improving electrochemical properties and rate capability of LiFePO4 were analyzed by optimizing the synthesis conditions and experimenting with reduced graphene oxide electron-conducting additive. It was found that adding reduced graphene oxide at the earliest possible synthesis step benefits the rate capability and capacity of $LiFePO_4$ cathode.
Separately, electrophoretic deposition was studied as an alternative method for obtaining $LiFePO_4$/C/reduced graphene oxide electrodes. The grain structure and electrochemical properties of the obtained thin films were researched. The results show that the use of surfactant is crucial. Just by adding 0.4 volume % of a surfactant (TX-100), $LiFePO_4$ thin films with good rate capability and excellent cyclability were obtained. It was found that an increased amount of surfactant results in even higher deposition rates.
LiFePO4 thin films were obtained by pulsed laser deposition and magnetron sputtering. Their composition, structure, morphology and electrochemical properties were analyzed. The model of sequential LiFePO4 particle charge and discharge was studied. It was found that the (de)lithiation behavior is largely influenced by the strain effects within the thin film, as the volume expansion of $LiFePO_4$ is restricted by the specific grain structure. As a result of this restricted geometry, less pronounced memory effect was observed in thin films in comparison with the powder $LiFePO_4$ electrodes. Voltage hysteresis in thin films and powder material was observed during a partial charge and discharge cycle. However, it vanishes when both powder material and thin films have been cycled less than five percent of its overall capacity.

SCIENTIFIC PUBLICATIONS

1. **E.Pentjuss, A.Lusis, J.Gabrusenoks, G.Bajars** (2015) Environment humidity effect on the weight of carbonizes Na-Al-Si glass fabrics recovery. *IOP Conf. Ser.: Mater. Sci. Eng.* **77** 012021 doi:10.1088/1757-899X/77/1/012021
2. **A.Lusis, E.Pentjuss, G.Bajars**, U.Sidorovicha, G.Strazds (2015) A comparative study of natural fiber and glass fiber fabrics properties with metal or oxide coatings. *IOP Conf. Ser.: Mater. Sci. Eng.* **77** 012022 doi:10.1088/1757-899X/77/1/012022
3. I.Liepina, G.Bajars, **M.Rublans, J.Kleperis, A.Lusis, E.Pentjuss** (2015) Structure and photocatalytic properties of TiO_2-WO_3 composites prepared by electrophoretic deposition. *IOP Conf. Ser.: Mater. Sci. Eng.* **77** 012039 doi:10.1088/1757-899X/77/1/012039
4. **K.Kaprans, G.Bajars, G.Kucinskis,** A.Dorondo, **J.Mateuss, J.Gabrusenoks,** J.Kleperis, **A Lusis** (2015) Electrophoretic nanocrystalline graphene film electrode for lithium ion battery. *IOP Conf. Ser.: Mater. Sci. Eng.* **77** 012042 doi:10.1088/1757-899X/77/1/012042

5. **J.Gabrusenoks** (2015) Vibrational spectra of tungsten oxytetrachloride. *IOP Conf. Ser.: Mater. Sci. Eng.* **77** 012032 doi:10.1088/1757-899X/77/1/012032
6. M. Zubkins, R. Kalendarev, **J. Gabrusenoks**, K. Smits, K. Kundzins, K. Vilnis, A. Azens, J. Purans (2015) Raman, electron microscopy and electrical transport studies of x-ray amorphous Zn-Ir-O thin films deposited by reactive DC magnetron sputtering. *IOP Conf. Ser.: Mater. Sci. Eng.* 77 012035 doi:10.1088/1757-899X/77/1/012035
7. K.-Z. Fung, C.-T. Ni, S.-Y. Tsai, M.-H. Chen, A.F. Orliukas, **G. Bajars** (2015) Nanostructured $LiCoO_2$ cathode by hydrothermal process. *Ceramic Materials for Energy Applications IV: Ceramic Engineering and Science Proceedings* **35**, N 7, pp. 23-34.

DOCTOR THESIS

Gints Kucinskis

„The Study of Nanostructured Bulk and Thin Film $LiFePO_4$ Cathode Materials for Lithium Ion Batteries“.

MASTER THESIS

Karina Bikova

‘‘Electrophoretic deposition, physical and chemical properties of $LiFePO_4$ films”.

Anna Dorondo

‘‘Electrophoretic deposition, physical and chemical properties of graphene/metal oxide composite films”.

BACHELOR THESIS

Janis Mateuss

“Electrophoretic deposition and physico-chemical properties of graphene oxide composite”.

Marcis Rublans

“Structure, absorption and photocurrent measurements of electrophoretically deposited TiO_2-WO_3 semiconductors”.

LECTURES ON CONFERENCES

31st Scientific Conference of Institute of Solid State Physics, University of Latvia, February 24-26, 2015, Riga (Latvia):

1. G.Kucinskis, G.Bajars, J.Kleperis. Voltage hysteresis of $LiFePO_4$ lithium ion battery cathode material.
2. K.Bikova, G.Kucinskis, G.Bajars (2015) Electrophoretic deposition of $LiFePO_4$ on a steel electrode.
3. Dorondo, J.Mateuss, K.Kaprans, G.Kucinskis, G.Bajars, J.Kleperis. Electrophoretic deposition of nanoporous carbon material films from isopropanol and water suspensions.
4. Liepina, G.Bajars, M.Rublans, A.Lusis, E.Pentjuss, J.Balodis. Structure, optical and photocatalytic properties of TiO_2-WO_3 composites prepared by electrophoretic deposition.
5. Lusis, G.Bajars, I.Liepina, J.Gabrusenoks, J.Balodis, E.Pentjuss.Electrophoretic

deposition of TiO_2 nano particles coating on the glass fabric.

Smart and Green Interfaces Conference – SGIC2015, Belgrade, Serbia, March 30 – April 1, 2015, http://sgic2015.elexcomm.com/:

6. K.Kaprans, G.Bajars, A.Dorondo, J.Mateuss, G.Kucinskis, J.Kleperis, A.Lusis. Electrophoretically deposited nanostructured reduced graphene oxide as electrode material for lithium ion batteries.
7. M.Rublans, G.Bajars, I.Liepina, J.Gabrusenoks, A.Lusis, E.Pentjuss. Structure, optical and photocatalytic properties of TiO_2-WO_3 composite films prepared by electrophoretic deposition.
8. K.Bikova, G.Kucinskis, G.Bajars. Electrophoretic deposition of $LiFePO_4$ cathode for lithium ion batteries.

EuroNanoForum, Riga, Latvia, June 10-12, 2015, http://euronanoforum2015.eu/:

9. G.Kucinskis, G.Bajars, K.Bikova, J.Kleperis. $LiFePO_4$/C/reduced graphene oxide composite cathode for lithium ion batteries.
10. A.Lusis, G.Bajars, I.Liepina, J.Gabrusenoks, J.Balodis, E.Pentjuss, M.Rublans. Electrophoretic deposition of TiO_2 nanoparticles coating on the glass fabric.
11. E.Pentjuss, A.Lusis, J.Balodis, J.Gabrusenoks, G.Bajars. Absorption of water and carbon dioxide in carbonated glass fabric.

FM&NT-2015 Functional Materials and Nanotechnologies, Vilnius, Lithuania, October 5-8, http://www.fmnt.ff.vu.lt/:

11. G.Kucinskis, G.Bajars, K.Bikova, J.Kleperis $LiFePO_4$/C/reduced graphene oxide composite cathode for lithium ion batteries.

XXII Galyna Puchkovska International School-Seminar Spectroscopy of Molecules and Crystals, Sep. 27 – Oct. 4, 2015, Chynadiyovo, Zakarpattia, Ukraine

12. J. Gabrusenoks, M. Zubkins, G. Chikvaidze, J. Purans. Vibrational spectra of ZnO:Ir thin films.
13. J. Gabrusenoks. Lattice dynamics of CdWO4.

DEPARTMENT OF SEMICONDUCTOR MATERIALS

Head of Department Dr.phys. A.Lusis

LABORATORY OF EXAFS SPECTROSCOPY

Head of Laboratory Dr.habil.phys. Juris Purans

RESEARCH TOPICS

- X-ray Absorption Spectroscopy of functional materials and development of advanced EXAFS data analysis methodologies based on Molecular Dynamics and Reverse Monte Carlo methods.
- Confocal laser microscopy and Raman spectroscopy.
- The use of high performance computing for functional materials first principles and Molecular Dynamics simulations.
- Exchange interaction between radiation defects and transition metals ions in the dielectric crystals doped with the transition metals ions.

COOPERATION

Latvia
1. University of Latvia, Institute of Physics (M.M. Maiorovs).
2. Riga Technical University, Institute of Inorganic Chemistry (Dr. J. Grabis).

Czech Republic
1. Institute of Physics, AS CR, Prague (Prof. V Trepakov, Dr. A. Dejneka).

Estonia
1. Tartu University, Institute of Physics (Tartu, Estonia) (Prof. M. Brik, Dr. I. Sildos).

France
1. SOLEIL synchrotron center (Paris, France) (Dr. P. Roy, Dr. F. Baudelet, Dr. L. Nataf).
2. CRMCN/CNRS, Universite de la Mediterranee, UMR 6631 CNRS (Marseille, France) (Dr. D. Pailharey).

Germany
1. Karlsruhe Institute of Technology (Prof. P.Vladimirov).
2. HASYLAB (Hamburg) (Dr. A.Kalinko).

Italy
1. Trento University (Trento, Italy) (Prof. G. Dalba, Prof. P.Fornasini).
2. IFN-CNR, Institute for photonics and nanotechnologies (Trento, Italy) (Dr. F. Rocca).

Japan
1. Tokyo Institute of Technology, Tokyo (Prof. M. Itoh).

Russia
1. Joint Institute for Nuclear Research (Dubna) (Prof. A.M. Balagurov).
2. B. N. Yeltsin Ural Federal University (Ekaterinburg) (V. N. Churmanov, V. I. Sokolov, V. A. Pustovarov, V. Yu. Ivanov).
3. Department of Quantum Chemistry, St. Petersburg University, Russia (Prof. R. A. Evarestov).

Switzerland
1. Paul Scherrer Institute (Villigen) (Prof. M. Krack).

AWARDS

1. Dr. phys. Janis Timoshenko, Ludvigs and Maris Jansons Prize for the best work in physics awarded by Latvian Academy of Sciences. Work title: "Reverse Monte Carlo modelling of static and thermal disorder in crystalline materials". Supervisor: Dr.phys. A.Kuzmin

PARTICIPATION IN RESEARCH PROJECTS

Latvian:

1. ESF project "Innovative materials for transparent electronics and photonics", No. 2013/0015/1DP/1.1.1.2.0/13/APIA/VIAA/010.
2. Latvian Science Council Grant "XAFS studies of functional material local structure with femtometer accuracy", No.402/2012.
3. Latvian Science Council Grant "Local structure determination in functional materials from x-ray absorption spectra", Latvian Science Council Grant No.187/2012.
4. Latvian National Research Programme in Materials Science "Multifunctional materials and composites, photonics and nanotechnology" (IMIS2).

International:

1. "ODS steel with high creep strength", EUROfusion WPMAT - Advanced Steels (AS-2.3.2-05).
2. "When and how ODS particles are formed? - X-ray Absorption Spectroscopy and ab initio modelling of ODS steels", EUROfusion Enabling Research Project (CfP-WP15-ENR-01/UL-01) (2015-2017).
3. "Synthesis and study of photoluminescent and magnetic properties of perovskite-type $LaInO_3$ activated with Pr^{3+}, Nd^{3+} and Sm^{3+} for white LED applications", Latvian-Belorussian co-operation programme in science and techniques.

DIDACTIC WORK AT THE UNIVERSITY OF LATVIA

1. Course Fizi5028 "Structure and Description of Nanomaterials" at the University of Latvia (A.Kuzmin).

MAIN RESULTS

X-RAY ABSORPTION SPECTROSCOPY OF TIN TUNGSTATES

A. Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, R. Kalendarev

The atomic and electronic structure of tin tungstates, α-$SnWO_4$, α-$Sn_{1.03}W_{0.99}O_4$ and β-$SnWO_4$, was studied by the W L_3-edge X-ray absorption spectroscopy and first-principles linear combination of atomic orbital (LCAO) calculations based on the hybrid exchange-correlation density functional (DFT)/Hartree-Fock (HF) scheme. It was found that the crystal structure of both α-phases is built up of strongly distorted WO_6 octahedra, whereas that of β-$SnWO_4$ is composed of nearly regular WO_4 tetrahedra. In addition, there are distorted SnO_6 octahedra in both α- and β-phases. The metal-oxygen octahedra distortion is explained by the second-order Jahn-Teller effect. The influence of pressure on the structure of α-$SnWO_4$ and β-$SnWO_4$ was theoretically studied in detail based on the calculated equations of state. The compressibility of β-SnWO4 was found to be larger than that of α-$SnWO_4$. The existence of the insulator-to-metal transition was predicted in α-SnWO4 at about 16 GPa and was explained by a

symmetrization of metal-oxygen octahedra leading to a strong interaction of Sn 5s, W 5d and O 2p states and closing of band gap.
Room-temperature pressure-dependent (0-25 GPa) x-ray absorption spectroscopy at the W $L_{1,3}$-edges of α-$SnWO_4$ and β-$SnWO_4$ was performed using a dispersive setup and a high-pressure nanodiamond anvil cell. The detailed analysis of experimental x-ray absorption near-edge structure and extended x-ray absorption fine structure data suggests that upon increasing pressure, a displacement of tungsten atoms by about 0.2 Å toward the center of the WO_6 octahedra occurs in α-$SnWO_4$, whereas the coordination of tungsten atoms changes from tetrahedral to distorted octahedral in β-$SnWO_4$.

X-RAY ABSORPTION SPECTROSCOPY STUDY OF LOCAL DYNAMICS AND THERMAL EXPANSION IN ReO_3

J. Purans, P. Fornasini, S. E. Ali, G. Dalba, A. Kuzmin, and F. Rocca

The thermal expansion of polycrystalline ReO3 is studied in vacuum by x-ray diffraction from 300 to 600 K and by extended x-ray absorption fine structure (EXAFS) at the Re *L*3 edge from 30 to 600 K. A detailed EXAFS analysis is presented up to the sixth coordination shell around Re. The crystal thermal expansion is weak throughout the explored range, negative below 100 K, positive from 150 to 500 K, and negative again above 500 K. The analysis of mean square relative displacements obtained by EXAFS and of mean square displacements available from x-ray and neutron diffraction measurements confirms the presence of significant static disorder in the investigated samples. EXAFS results suggest that below 500 K in ReO3 at least some of the octahedral are slightly and disorderly rotated by an average angle _θ_, whose valued creases when the temperature increases. This explains why ReO3, in spite of the possibility of supporting rigid unit modes, shows a weak positive expansion at increasing temperatures, from 150 up to 500 K. Results are discussed and compared with recent experimental and theoretical work on materials characterized by negative thermal expansion.
DOI: 10.1103/PhysRevB

DETERMINATION OF METHEMOGLOBIN IN HUMAN BLOOD AFTER IONISING RADIATION BY EPR

M. Polakovs, N. Mironova-Ulman, A. Pavlenko, A. Aboltins

In the present work presents results of investigations of radiation influence on blood of patients examined by radio-isotopes diagnosis (Tc99m), blood of Chernobyl clean-up workers and human blood irradiated by LINAC using Electron Paramagnetic Resonance (EPR). The EPR spectroscopy reveals information on electronic states of transition metal ions, particularly Fe3+ in different spin states. It is shown that EPR spectra of blood of patients before examination has signal from metal-protein transferrin (g=4.3) and after administration of radio-isotope proves signal of Fe3+ (methemaglobin) in the high spin state (g=6.0). The EPR spectra of Chernobyl liquidator display number of signals including low and high state of ion Fe3+ (g = 2.0 and g= 6.0), and transferrin (g=4.3). The EPR spectra of irradiated human blood by LINAC (linear accelerator) have only signal Fe3+ (methemaglobin) in low-spin state with g = 2.0.

SCIENTIFIC PUBLICATIONS

1. **A.Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, R. Kalendarev,** External pressure and composition effects on the atomic and electronic structure of $SnWO_4$, Sol. Energy Mater. Sol. Cells 143 (2015) 627-634.
2. **J. Timoshenko, A. Anspoks, A. Kalinko, A. Kuzmin,** Local structure of nanosized tungstates revealed by evolutionary algorithm, Phys. Status Solidi A 212 (2015) 265-273.
3. **A.Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, R. Kalendarev,** L. Nataf, F. Baudelet, T. Irifune, High-pressure x-ray absorption spectroscopy study of tin tungstates, Phys. Scr. 90 (2015) 094003 (5pp).
4. B.Polyakov, R. Zabels, A. Sarakovskis, S. Vlassov, **A. Kuzmin,** Plasmonic photoluminescence enhancement by silver nanowires, Phys. Scr. 90 (2015) 094008 (4pp).
5. **N. Mironova-Ulmane, A. Kuzmin**, I. Sildos, Template-based synthesis of nickel oxide, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012025:1-5.
6. M. Polakovs, **N. Mironova-Ulmane**, A. Pavlenko, A. Aboltins, Determination of methemoglobin in human blood after ionising radiation by EPR, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012028:1-5.
7. **A.Cintins, A. Anspoks, J. Purans, A. Kuzmin, J. Timoshenko**, P. Vladimirov, T. Graning, J. Hoffmann, ODS steel raw material local structure analysis using X-ray absorption spectroscopy, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012029:1-6.
8. **I.Jonane, J. Timoshenko, A. Kuzmin**, EXAFS study of the local structure of crystalline and nanocrystalline Y_2O_3 using evolutionary algorithm method, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012030:1-5.
9. **K.Lazdins and A. Kuzmin**, Local structure and lattice dynamics of cubic Y_2O_3: an x-ray absorption spectroscopy study, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012031:1-5.
10. **V. Skvortsova, N. Mironova-Ulmane**, L. Trinkler, V. Merkulov, Optical properties of natural and synthetic beryl crystals, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012034:1-5.
11. **V. Skvortsova**, **N. Mironova-Ulmane,** L. Trinkler, Optical properties of irradiated topaz crystals, IOP Conf. Ser.: Mater. Sci. Eng. 80 (2015) 012008:1-5.
12. M. Zubkins, **R. Kalendarev**, J. Gabrusenoks, K. Smits, K. Kundzins, **K. Vilnis, A. Azens, J. Purans,** Raman, electron microscopy and electrical transport studies of x-ray amorphous Zn-Ir-O thin films deposited by reactive DC magnetron sputtering, IOP Conf. Ser.: Mater. Sci. Eng. 77 (2015) 012035:1-5.
13. **A.Kuzmin**, M. Zubkins, **R. Kalendarev**, Preparation and characterization of tin tungstate thin films, Ferroelectrics 484 (2015) 49-54.
14. **J.Purans**, P. Fornasini, S. E. Ali, G. Dalba, **A. Kuzmin,** F. Rocca, X-ray absorption spectroscopy study of local dynamics and thermal expansion in ReO_3, Phys. Rev. B 92 (2015) 014302:1-12.
15. V. N. Churmanov, N. B. Gruzdev, V. I. Sokolov, V. A. Pustovarov, V. Yu. Ivanov, **N. Mironova-Ulmane**, Low-temperature photoluminescence in $Ni_xMg_{1-x}O$ nanocrystals, Low Temp. Phys. 41 (2015) 233-235.
16. A.Antuzevics, U. Rogulis, A. Fedotovs, D. Berzins, V. Voronov, **J. Purans**, EPR study of Gd^{3+} local structure in ScF_3 - crystal with negative thermal expansion coefficient, Phys. Scr. 90 (2015) 115801.
17. **A.Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko**, The use of x-ray absorption spectra for validation of classical force-field models, Z. Phys. Chem. (2015), doi: 10.1515/zpch-2015-0664.
18. **J. Timoshenko, A. Anspoks, A. Kalinko, A. Kuzmin**, Local structure of cobalt tungstate revealed by EXAFS spectroscopy and reverse Monte Carlo/evolutionary algorithm simulations, Z. Phys. Chem. (2015), doi: 10.1515/zpch-2015-0646.

19. **J. Timoshenko, A. Anspoks, A. Kalinko, I. Jonane, A. Kuzmin**, Local structure of multiferroic $MnWO_4$ and $Mn_{0.7}Co_{0.3}WO_4$ revealed by the evolutionary algorithm, Ferroelectrics 483 (2015) 68-74.
20. **A.Anspoks, J. Timoshenko**, D. Bocharov, **J. Purans**, F. Rocca, A. Sarakovskis, V. Trepakov, A. Dejneka, M. Itoh, Local structure studies of Ti for $SrTi^{16}O_3$ and $SrTi^{18}O_3$ by advanced x-ray absorption spectroscopy data analysis, Ferroelectrics 485 (2015) 42-53.
21. **N. Mironova-Ulmane**, A. Sarakovskis, **V. Skvortsova**, Up-conversion and photoluminescence in Er^{3+} single crystal MgAl-spinel, Phys. Procedia 76 (2015) 106-110.
22. A. Volperts, G. Dobele, J. Ozolins, **N. Mironova-Ulmane**,Synthesis and Application of Nanoporous Activated Carbon in Supercapacitors, Mater. Sci. Appl. Chem. 31 (2015) 16-20.

DOCTOR THESES

1. Janis Timoshenko, "Reverse Monte Carlo modelling of structural and thermal disorder in crystalline materials", Latvian University, Riga, 2015.

BACHELOR THESES

1. A. Cintins, "Local structure analysis in ODS steel raw materials using x-ray absorption spectroscopy", Latvian University, Riga, 2015.
2. I. Jonane, "Yttrium oxide, iron fluoride and scandium fluoride local structures analysis using evolutionary algorithm", Latvian University, Riga, 2015.
3. K. Lazdins, "Application of molecular dynamics method to the interpretation of Y_2O_3 and FeF_3 x-ray absorption spectra", Latvian University, Riga, 2015.

CONFERENCE PROCEEDINGS

1 CEIT-IK4, San Sebastián, SPAIN Dr. Carmen García-Rosales

Lectures at Conferences

1. 11th International Young Scientist conference Developments in Optics and Communications, Riga, Latvia, April 8-10, 2015.
   - "Temperature dependence of the local structure of Y_2O_3 from EXAFS analysis using evolutionary algorithm method", I. Jonane (Oral).

2. 588. WE-Heraeus Seminar "Element Specific Structure Determination in Materials on Nanometer and Sub-Nanometer Scales using modern X-Ray and Neutron Techniques", Bad Honnef, Germany, April 26-30, 2015.
   - "Local structure of transition metal tungstates revealed by EXAFS spectroscopy and reverse Monte Carlo - evolutionary algorithm simulations", J. Timoshenko (Poster).
   - "The use of x-ray absorption spectra for validation of classical force-field models", A. Kuzmin (Poster).

3. E-MRS 2015 Spring Meeting, May 11-15, Lille, France.
   - "Temperature-dependence of copper nitride lattice dynamics probed by EXAFS spectroscopy and evolutionary algorithm", J. Timoshenko (Oral).
   - "X-ray absorption spectroscopy study of high-pressure phase transition in Cu_3N", A. Kuzmin (Oral).

4. EuroNanoForum 2015, June 10-12, Riga, Latvia.
   - "Near field X-ray SPM: new tools for nanoscience ", J. Purans (Invited).
   - "Atomic structure relaxation in NiO nanoparticles studied by x-ray absorption spectroscopy in combination with molecular dynamics", A. Anspoks (Poster).
   - "Static disorder in nanocrystalline yttria probed by X-ray absorption spectroscopy", I. Jonane (Poster).
   - "First-principles study of the effect of uniaxial pressure on α-$SnWO_4$", A. Kuzmin (Poster).
   - "Study of Y_2O_3 nanoparticles by x-ray absorption spectroscopy", K. Lazdins (Poster).
   - "Template-based synthesis of Ni/NiO nanocomposites", N. Mironova-Ulmane (Poster).
   - "Study of iridium ions influence on optical properties of zinc-iridium oxide thin films" V. Skvortsova, M. Zubkins, R. Kalendarevs, G. Chikvaidze, J. Purans (Poster).
   - "Structural and optical properties of ZnO:Ir thin films deposited by reactive magnetron co-sputtering." M. Zubkins*, R. Kalendarev, K. Kundzins, J. Gabrusenoks, K. Vilnis, A. Azens, J. Purans(Poster).
   - "Nanoporous wood-waste based carbons for supercapacitors electrodes". Aleksandrs Volperts, Galina Dobele, Nina Mironova-Ulmane, Ilmo Sildos, Jurijs Ozolinsh (Poster).

5. XAFS-16, 23-28 August 2015, Karlsruhe, Germany.
   - "Disappearance of correlations in the atom motion upon hydrogen intercalation into ReO_3 lattice", J. Timoshenko (Oral).
   - "Local dynamics and phase transition in quantum paraelectric $SrTiO_3$ studied by Ti K-edge x-ray absorption spectroscopy", Andris Anspoks (Oral).
   - „Local structure of perovskites ReO_3 and ScF_3 with negative thermal expansion: interpretation beyond the quasiharmonic approximation", J. Purans (Poster).
   - "Pressure-induced insulator-to-metal transition in α-$SnWO_4$", A. Kuzmin (Poster).

6. RMC6, Budapest, Hungary 17-19 September, 2015.
   - "Reverse Monte Carlo/evolutionary algorithm approach for the analysis of EXAFS data from distant coordination shells of crystalline materials", J. Timoshenko (Oral).

7. FM&NT-2015, October 5-8, Vilnus, Lithuania.
   - "Validation of material models using x-ray absorption spectroscopy", Alexei Kuzmin (Invited).
   - "Effect of Iridium Ions on the Optical Spectra of Zinc-Iridium Oxide Thin Films", V. Skvortsova (Poster).
   - "Structural, optical and electrical properties of ZnO:Ir thin films deposited by reactive magnetron co-sputtering", M. Zubkins (Poster).
   - Supercapacitors with electrodes from wood-based nanoporous carbons. Volperts, G. Dobele, N. Mironova-Ulmane, Z. Zalane, A. Sametov, E. Skolnikov, D. Vervikishko, I. Sildos(Poster).

8. ICOM Budva, Montenegro 31st August to 4th September 2015, Budva, Montenegro
   - " Up-conversion luminescence in $LaInO_3:Er^{3+}$" Nina Mironova-Ulmane, Vera Skvorcova, Kristaps Strals, Guna Krieke, Anatolijs Sarakovskis, Leonid Bashkirov, Elena Juhno (Poster).

9. LUMDETR 2015 conference in Tartu, Estonia, September 20–25, 2015.
    - "Spectroscopic properties of neutron-irradiated magnesium aluminium spinel single crystals. N. Mironova-Ulmane, V. Skvortsova, A.Pavlenko, E. Feldbach, A. Lushchik, Ch. Lushchik, V. Churmanov, D. Ivanov, V.Ivanov

10. HBSM Tartu, Estonia, August 24–27, 2015
    - "Spectroscopic properties of erbium doped single crystal magnesium aluminum spinel". Nina Mironova-Ulmane, Andreijs Pavlenko, Anatolijs Sarakovskis, Vera Skvortsova, Laurits Puust, Ilmo Sildos, Maksim Sarychev, Vladimir Ivanov

11. REMAT 2015 conference, 26-28 October, 2015 , Ślęza/Wroclaw, Poland.
    - "Spectroscopic properties of LaInO3 doped Sm^{3+}, Sb^{3+} and Er^{3+}„ A. Sarakovskis, V.Skvortsova, G.Chikvaidze, N. Mironova-Ulmane*

DEPARTMENT OF SEMICONDUCTOR MATERIALS

Head of Department Dr.phys. A.Lusis

LABORATORY OF HYDROGEN ENERGY MATERIALS

Head of Laboratory Dr. Janis Kleperis

Laboratory of Hydrogen Energy Materials was established in 2006 when firstly in Latvia the National Research Programs were announced and research in hydrogen technologies were included in National Research Program in Energy. At the same time Researchers together with Entrepreneurs established Latvian Hydrogen Association. Laboratory was established from multi-discipline specialists and students: physics, chemists, biologists, economists and geographers. Different hydrogen energy materials and technologies are studied at our laboratory being applied to hydrogen as energy carrier - production, storage and usage.

RESEARCH TOPICS

- Ion transfer in bulk, through interfaces, on porous surfaces in different materials and composites as well as structural, photocatalytic activity changes due to ion intercalation.
- Application of electrochemical and photo-electrical methods (volt-amperic, galvanometric, potentiometric, impedances, Mott-Schottky for characterization of ionic systems, nanostructured and porous coatings and materials, composites.
- Application of Sievert type and thermogravimetric methods for investigation of porous materials and absorbing capacity of hydrogen gas.
- Synthesis and research of new materials for hydrogen technologies (electrodes for electrolysis and microbial fuel cells, structured nanomaterials for photoelectrolysis, hydrogen storage media, polymer membranes and membrane-electrode assemblies for fuel cells);
- Li, Mg, NH_3, ion intercalation materials and their application for thin film capacitors, batteries; the technologies for electricity generation from renewables (solar, wind, static electricity, water, algae and microorganisms);
- Gas sensors and sensor arrays for gas and odour monitoring; odour removal with adsorbents and corona discharge technologies;

METHODS AND LABORATORY EQUIPMENT

Facilities to obtain nanostructured materials:

- Spray pyrolysis method to obtain nano-crystalline materials, coatings - the facility itself is made with two spray guns, nitrogen as a carrier gas, the substrate can be heated up to 450 ° C (regulated heating/cooling speeds available) for samples with dimensions 40x40 mm.
- Electrochemical deposition method to obtain nanocrystalline thin film coatings, using VoltaLab 40 (PGZ301; Radiometer Analytical) potentiostat with software VoltaMaster 4 and/or self-made impulse power supply.
- Electrochemical anodizing method for obtaining self-organized nanostructured oxide layers on the metallic substrates; consisting from a DC power supply, digital thermometer and data logger with the opportunity to register current/potential/temperature changes during film growing process.

- Few layer graphene (FLG) sheet exfoliation method using graphite electrodes and self-built pulse generator; material washing/filtering facilities. Electrochemical exfoliation of graphene sheets from graphite electrode can be arranged simultaneously with reduction of graphene oxide, as well as with insertion of different ions and cations between the graphene sheets.

Facilities for the optical and photo-electrochemical studies of materials:

- Spectrometer HR4000 UV-NIR with the program SpectraSuite and UV + VIS + NIR light source DH-2000 for studying light transmission/scattering of materials, and emission spectra of different light sources;
- System to investigate photo-electrochemical properties of materials and coatings built from self-made electrochemical cell, light source (150 W high-pressure xenon lamp and/or 30 W LED flood light), light modulator and VoltaLab 40 (PGZ301; Radiometer Analytical) potentiostat with VoltaMaster 4 software.

Facilities to study physical and physico-chemical characteristics of the materials:

- Gas sorption analysis system PCTPro-2000 (SETARAM) with mass spectrometer RGAPro-100 (up to 100 mass/charge number units). The device is intended to study gas sorption/desorption characteristics for various materials (now available only hydrogen gas) and various gases (currently - hydrogen) following SIEVERT (volume change) method.
- Selective gas permeability studies in self-made differential pressure detection chamber for flat (membrane) samples and cylindrical (outer diameter 10 mm) samples.
- Conductivity measuring system to determine ionic conductivity of polymer membranes in the temperature range from RT to +80° C with sample holder BekkTech BT-512 and water thermostat bath.

SCIENTIFIC STAFF:

Dr.phys. J. Kleperis,
Dr.phys. G. Chikvaidze,
Dr.phys. J. Klavins,
Dr.phys. L. Grinberga,
Dr.phys. J. Hodakovska,
Dr.phys. M. Vanags,
Ass. Prof., Dr.chem. G. Vaivars,
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Prof., Dr.oec. B. Sloka

TECHNICAL STAFF:
L. Jekabsons
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PhD STUDENTS:
I. Dimanta
P. Lesnicenoks
A. Knoks

STUDENTS:
A. Volkovs
I. Grauduma
A. Rasnačs

COOPERATION:

Latvia

1. University of Latvia: Faculty of Physics and Mathematics, Faculty of Chemistry (Dr. G. Kizane, Prof. Dr. A.Vīksna), Faculty of Biology (Prof. I.Muiznieks, Prof. V. Nikolajeva), Faculty of Economics and Management (Prof. B.Sloka), Faculty of Earth Science and Geography (Dr. I.Steinberga)

2. Riga Technical University: Institute of Inorganic Chemistry (Dr. J. Grabis, Dr. E.Palcevskis, Dr. A. Dindune), Institute of Silicate Materials (G.Mežinskis), Institute of Technical Physics (Prof. M. Knite).
3. Latvia University of Agriculture, Research Institute of Agricultural Machinery;
4. Latvian Institute of Physical Energetics, Riga
5. Latvian Institute of Wood Chemistry (Dr.hab. G.Dobele, Dr.hab. J.Gravitis)
6. Latvian Hydrogen Association
7. JSC "Sidrabe"
8. JSC „Riga Electric Machine Building Works",
9. SME: SIA „EMU PRIM", IC „Plazma PL", SIA "Eko Osta", SIA "Multipla Energy", SIA "Ambiteh Group AG"
10. Riga City Council: Housing and Environment Department of Riga City Council, Riga, Riga Energy Agency

Estonia

1. Tartu University, Institute of Physics (Tartu, Estonia) (Dr. K.Mauring).

Germany

1. Kassel University (Prof. Jürgen Zick)

Lithuania

University of Vilnius - Department of Physics (Prof. A.Orliukas)
Lithuanian Institute of Energetic (Dr. D. Milcius, Dr. M.Lelis)

Norway

Institute for Energy Technology, Kjeller, Prof. Volodimir Yartis

Russia

1. Institute of Chemical Problems of Chemical Physics of the RAS (IPCP RAS), Chernogolovka, Moscow Region, Russia) (Prof. Y. Dobrovolski, Dr. A.E. Ukshe)

PARTICIPATION IN RESEARCH PROJECTS:

Latvian:

1. National Research Program IMIS^2 (2014-2017)", Sub-project coordinator Dr.phys. L.Grinberga;
2. National Research Program LATENERGI (2014-2017), Subproject No.4.3 "Research of methods for hydrogen production, storage and safety for application in national economy" Sub-project coordinator: Dr.phys. J. Kleperis
3. Research Cooperation Project of Latvian Council of Science „Synthesis and studies on controlled porosity composite thin layers and systems for energy storage and conversion applications (2014-2017)"; No 666/2014; Project coordinator: Dr.phys. J. Kleperis

International

1. COST action MP 1004 „(Hybrid Energy Storage Devices and Systems for Mobile and Stacionary Applications",(2011-2015); Representation Latvia and ISSP UL – J. Kleperis;
2. COST action MP1103" Nanostructured materials for solid-state hydrogen storage" (2011 – 2015) Representatives from Latvia and ISSP UL – L. Ginberga, J. Kleperis

DIDACTIC WORK AT THE UNIVERSITY OF LATVIA

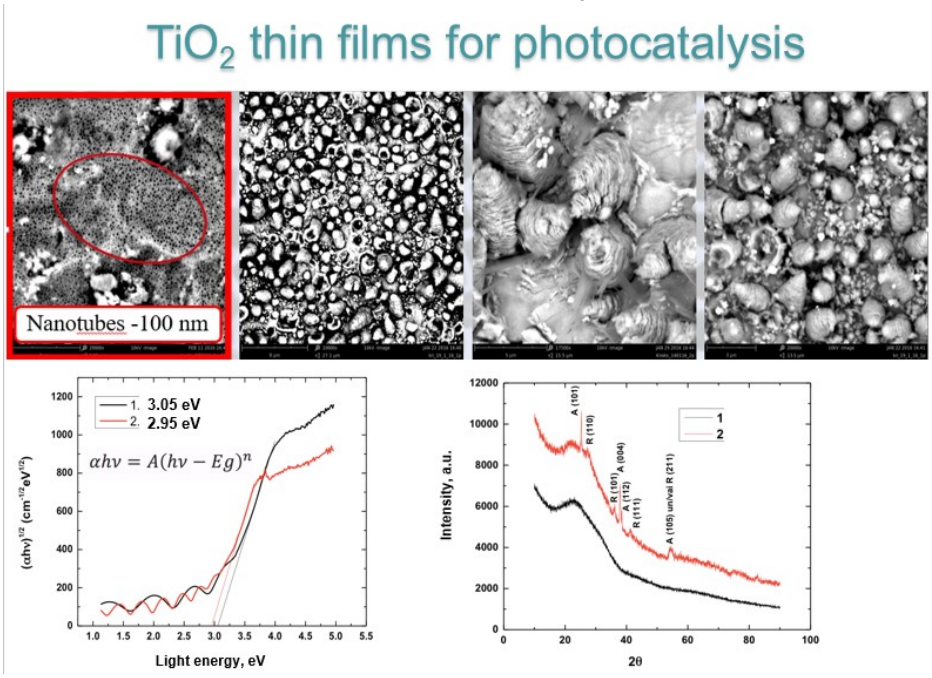
1. Master degree course "Solid State Ionics" at Faculty of Chemistry, UL – 4 credit points (G. Vaivars)
2. Course in Physics "Fundamentals of Physics and Mathematics" at the Riga Stradiņš University (M. Vanags).

RESEARCH AND DEVELOPMENT OF MATERIALS AND DEVICES FOR HYDROGEN ENERGY TECHNOLOGIES

G.Bajars, J.Chikvaidze, J.Hodakovska, L.Grinberga, A.Knoks, J.Kleperis, J.Klavins, A.Lusis, J.Straumens, G.Vaivars, M.Vanags, L.Jekabsons, A.Volkovs, P.Lesnicenoks, V.Nemcevs, I.Dimanta, A.Gruduls, B.Sloka, J.Dimants, P.Gurdziels, S. Ložkins, I.Grauduma, E.Laiviņa, K.Gauja, M.Zvīne, A.Januškēvica, V.L.Muzikants, M.K.Jurjāns

Hydrogen production studies

Photo-catalytic water splitting. Growing threat of global warming and high energy dependency on fossil fuels urges scientists all around the world to search for new technologies to reduce the use of fossil fuels in order to reduce carbon imprint. Materials with high photocatalytic activity are necessary - TiO_2 on ITO/glass substrate is synthesized using magnetron sputtering method, but on Ti metal grown with electrochemical anodization in NaF and H_2SO_4 and H_3PO_4 solution.



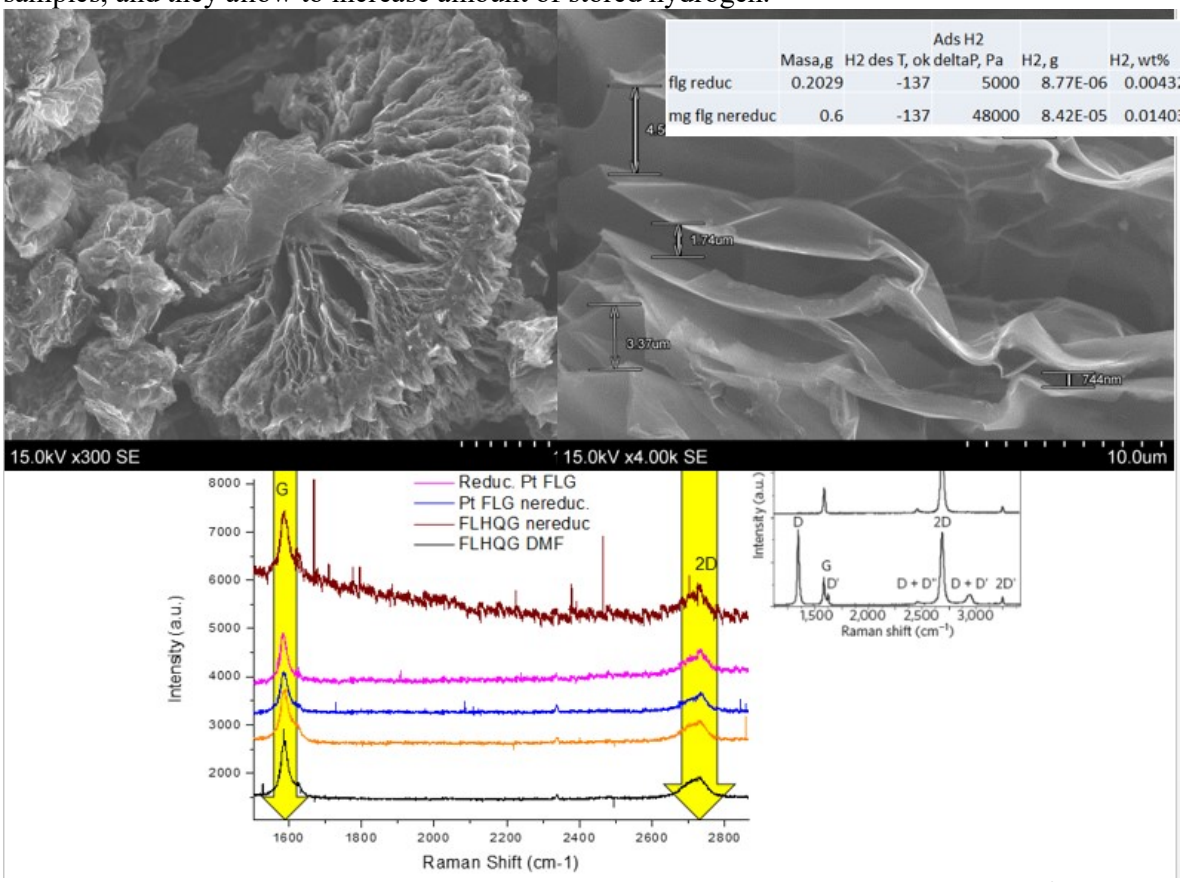
Magnetron sputtering is effective way of producing thin films with straightly regulated thickness and composition. Morphology of samples is studied with scanning electron microscope (Figure above) and profilometer, while the photo-physical properties are studied determining optical absorption spectrum forbidden gap (for sputtered thin films values 2.95 and 3.05 eV are found) and photoelectric properties in the three electrode cell measurements of photo-potential, short-circuit, and photo-current. Big potential is found in CO_2 photocatalytic reduction and turning into fuel, using sunlight. It is complicated reaction which needs optimal environment, materials and their structures. One of the best options is TiO_2 nanotubes. With development of nanotechnologies in the past decades there is made lots of research about those structures and their use in photocatalysis. In our work the reactor is built to check photocatalytic ability of the materials to convert CO_2 into methane in the presence of UV light and water vapor. First results showed that samples with larger surfaces and more pronounced catalytic activity must synthesized and used for next experiments.

Major drawback of CuO as photoelectrode in water photo electrolysis cell is its stability. In several research works the stability of CuO photoelectrode is enhanced with adding different impurities. The aim of our research is to demonstrate that changing the DC

component value during photoelectrolysis can increase the resilience of CuO coating. Cu2O layer is coated on stainless steel substrate with electrophoretic method, and after annealed at 450 °C for one hour. Structure and morphology of coatings are studies by XRD and SEM respectively; it is established that during annealing dominate CuO phase, so the firing process characterizes with transforming of Cu2O into CuO phase. Photo-electrochemical measurements showed that the maximum photocurrent is at obtained at -500 mV (with respect to reference electrode SCE). At -50 mV the dark current of CuO coating changes to the opposite polarity. Measurements of photocurrent stability at -500 mV indicate the decrease by 40% in 1 hour. Nevertheless, when photocurrent is measured with another mode (illuminates the sample at -500 mV - 10 seconds, darkness at -50 mV - 10 seconds), photocurrent did not significantly change its value during 1 hour, but after 5 hours it had fallen by only 5%. Further research is looking for an explanation to this effect.

Hydrogen storage studies

Hydrogen binding with carbon nanostructures. Synthesis of few layer graphene stacks (FLGS) with intercalated light metal elements was performed by our method of electrochemical exfoliation, by applying DC voltage to graphite work electrode, for 3 s and then flipping the polarity to 5 s – the electrolyte composition regulates what ions interact with graphite and also if they get bonded to FLGS surfaces and defects by Wan der Waals forces or by chemical bonds. FLGS modification with Li and Mg defect stabilizers, allow us to increase edge surfaces, by blocking graphene self-healing properties (Figure). Analysis of Raman spectra proves the presence of defects in our samples, and they allow to increase amount of stored hydrogen.

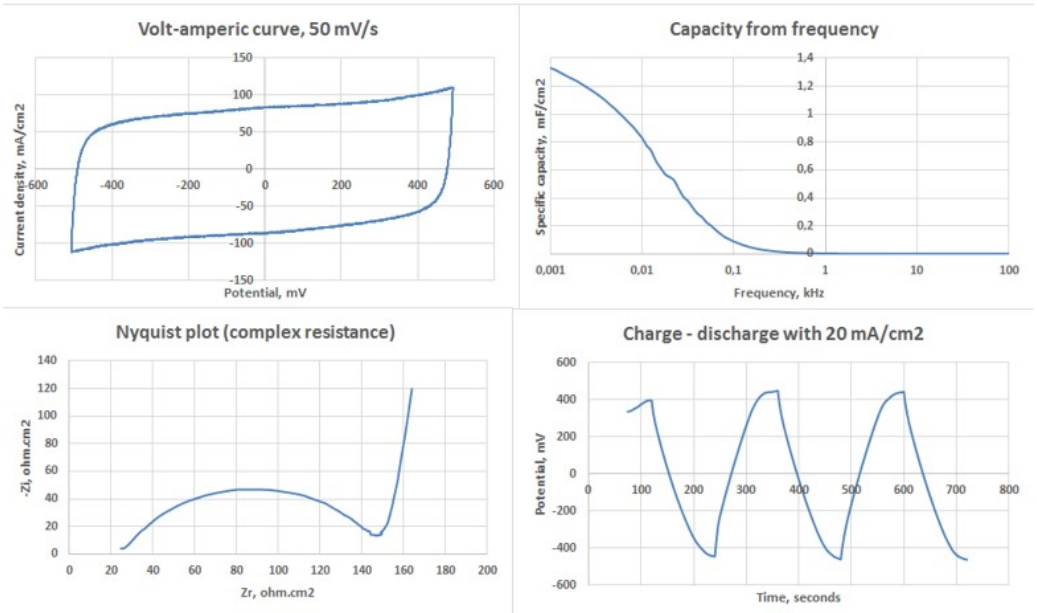


We have developed methodic for gas sorption measurements at temperatures +/-200 °C in powder type samples with volume 35–80 mm^3. This can be done using Sievert's method – constant volume canister to compare pressures. Large volume powder samples

allow to limit pressure difference measurement errors, which arises using small samples. Also the option to use similar volumes and reweighing of samples allow to limit measurement errors. Measurement device consists of reactor chamber itself, temperature control system (Keramserviss LTD), membrane and turbomolecular pump, masspectrometer, 500ml reserve gas cylinder, two pressure sensors (at the rector chamber and at the reserve 500ml gas chamber), data logger for pressure and temperature registration and two PC. Heating/cooling processes can be done linearly. Two gases, hydrogen and helium are applied to sample firstly calibrating sample volume, then measuring adsorption/desorption values in powder like sample. By choosing to work with larger samples – because of the small weight, volume of the reactor provides measurements with inertia to cooling and heating effects that is why some data analysis is required to determine hydrogen storage possibility and volume in such a material. Best obtained results calculated from PT curves gives values 0.14 wt% for hydrogen adsorption at -100 - -120 ^{o}C.

Few layer graphene stacks (FLGS) as electrode material for supercapacitor. Supercapacitor was built from symmetric FLGS powder electrodes (clean and also with Na^{+}, Mg^{2+} and Li^{+} impurities) and tested with different electrolytes (NaCl, $LiPF_6$, KOH, Na_2SO_4, NH_4Cl solutions with the concentration of 1M). Potentiostat Voltalab PGZ301 is used to measure impedance, volt-amperic curve and charge/discharge cycling with constant current.

Capacitor with FLGS powder electrodes having specific capacity 1.4 mF/cm^2

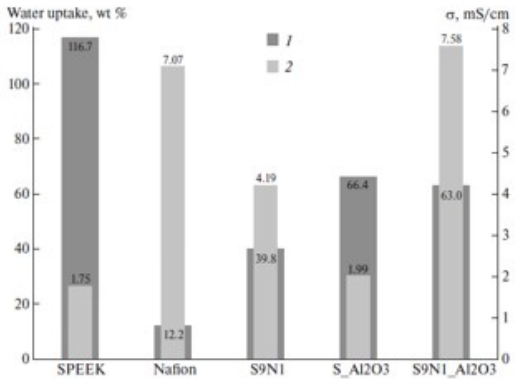


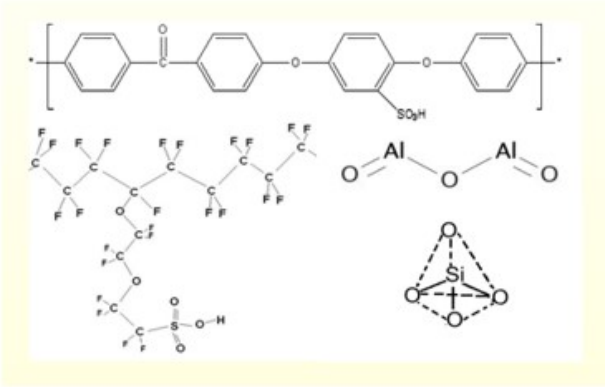
Studies of n membranes with proton conductivity

In alternative energy devices the medium temperature polymer electrolyte membrane (PEM) fuel cells are of growing importance. It resulted in rising interest in field of ionic liquids as components for polymer membranes due to higher membrane use temperature (100-200 ^{o}C) and electrochemical stability. Water absorbed inside the membrane provides proton conductivity but also possess some difficulties when membrane is operated at elevated temperatures. Impregnating membrane with ionic liquids (IL) as one of solutions is proposed. These composites are thermally stable and possess proton conductivity or adding inorganic hydrates (phosphated ZrO_2) with better dehydration stability at elevated temperatures. The IL might decrease the mechanical stability of the membrane at higher temperatures. But nanostructuring is important for stabilizing mechanical properties, which are crucial for application of polymer membrane in energy

devices. Sulfonated PEEK is suitable to be used in field of energetics. Exact amount of Ionic liquids and zirconium oxide nanoparticles have remarkable effect on membrane properties by varying membrane applications. Ionic liquids has great influence on physical and chemical properties of polymer membrane. In this study the zirconium oxide nanoparticles were successfully added to the SPEEK membrane stabilizing its' structure and properties. Zirconium oxide can be added to polymer membrane, but the optimization is needed to figure out the right amount of nanoparticles providing the best performance of membranes and studies are needed to find out how they bind with polymer and ionic liquids.

Next study was to create a material, which is able to work in dry atmosphere (relative humidity being significantly below 100%) at the same time retaining good proton conductivity. In this work, the properties of ternary membrane are studied. As the main component of membrane sulfonated poly(ether-ether-ketone) (SPEEK) is used: two other parts are Nafion and aluminum oxide nanopowder. SPEEK is one of the promising alternatives to Nafion for mid-temperature polymer fuel cells; it belongs to aromatic backbone polymer, and is comparably cheap and has good tuning possibilities. Aluminum oxide is hygroscopic oxide, so its main function is to increase water retention at higher temperatures, allowing membrane to operate more efficient at these working conditions. The choice of the third component was based on its ability to improve proton conductivity and water absorption. According to obtained results, three-component membrane made from SPEEK, Nafion and aluminum oxide in studied proportions (SPEEK : Nafion = 9 : 1, aluminum oxide 2 wt%) show promising results with highest proton conductivity at 70°C and RH = 40%. Average water uptake could lead to fewer geometrical dimension changes, at the same time providing sufficient water to ensure proton transport (Figure below).





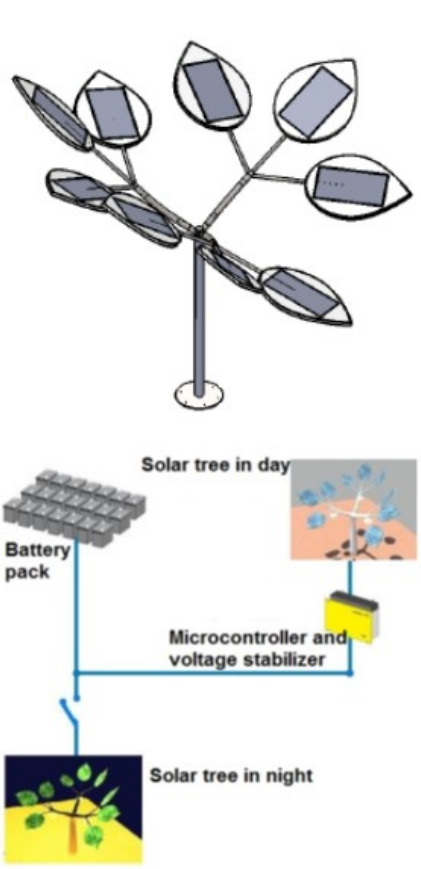
Renewable energy technologies - demonstration and publicity
Saules Kauss 2015 (a.k.a. Solar Cup 2015)

Solar Cup`s in Latvia is organized by ISSP UL already from 2008 for children students from schools in Latvia with aim to acquire knowledges about renewable energy technologies. In 2015 it was organized together with JSC "Sidrabe". In this contest participants are asked to prepare a land racing model 30 x 30 cm (because of the track size) or 30 x 30 x 20 cm large water racing models. Used power supply is only solar PV battery and must not exceed 120 x 100 mm and 2v, 500 mA to fit in folk racing class, but if model can fit on the track it can have a larger photo-voltaic panel surface and compete in master class. It is required for teams to provide a video of building/testing process of the models, to prepare answers on questions about renewable energy technologies and materials. Solar Cup 2015 took place on May 16, in the territory of "Sidrabe". For competition was registered 72 teams, which received from organizers the

solar batteries and motor sets (with support of EuroNanoForum 2015), and 15 larger PV panels (gift from "Sidrabe") for construction of solar energy radio-controlled models. To the event came 56 teams, each 2-3 participants, a total of 142 pupils and students from 26 different schools in Riga and Latvian regions (Figure below).

Exhibition Vide un Enerģija 2015 (a.k.a. Environment and Energy 2015)

ISSP UL already 11 years is participating in the international exhibition-trade "Environment and Energy" – the central event for industry professionals of renewable and environmental technologies in the Baltic States. The Environment and Energy trade fair presents solutions for upgrading energy, energy efficiency, environmental technology and infrastructure, as well as the efficient use of renewable energy resources. The leading companies of the sector are offering modern energy-efficiency technologies and the most efficient solutions for a wide range of customers – from devices and equipment for large companies and municipalities to solutions for medium and small enterprises, as well as economically favorable offers for every household. ISSP UL in 2015 provided possibility at stand to sit under the Solar tree (designer Tālivaldis Muzikants, ISSP implementation) and to talk about harvesting and storage of energy from the water, Sun, Wind, biomass; production of hydrogen, storage and usage of it - the methods and technologies, the availability in market and research in these directions. One from the SME partners of ISSP UL is Multipla Energy Ltd., engaged in the research and commercialization of alternative energy sources (solar, wind, biomass, etc.). The vertical axis wind turbine model focused on households, was demonstrated, as well as consultancies provided.



Frame structure of built Solar Tree (Golden Apple Tree) prototype is formed of metal tubes with different diameters and coated with polymer composite shell. The trunk holds three branches of the curved tubes which each diverges into three smallest branches with an overall height of construction 3 meters (Figure up). Each from the 9 smallest branches (ø30 mm) has a leave at the end with photovoltaic (PV) solar panel with peak power 20 W, area 52x29 cm^2, silicon single crystal cells with efficiency 13%, an open circuit voltage at optimal lighting 21 V, and short circuit current at peak power 1.22 A. All 9 PV solar panels are connected in parallel circuit, having total peak power 180 W, nominal voltage 12-15 V and current 9 A, what is directed through voltage stabilizer scheme to charge two 70 Ah lead-acid batteries connected parallel (voltage 12 V).

SCIENTIFIC PUBLICATIONS

1. Šutka, A., Lagzdina, S., Käämbre, T., Pärna, R., Kisand, V., **Kleperis, J.,** Maiorov, M., Kikas, A., Kuusik, I., Jakovlevs. Study of the structural phase transformation of iron oxide nanoparticles from an Fe2+ ion source by precipitation under various synthesis parameters and temperatures. Materials Chemistry and Physics, Volume 149, 15 January 2015, Pages 473-479; DOI: 10.1016/j.matchemphys.2014.10.048
2. Kaprans, K, Bajars, G., Kucinskis, G., Dorondo, A., Mateuss, J., Gabrusenoks, J., **Kleperis, J.,** Lusis, A. Electrophoretic nanocrystalline graphene film electrode for lithium ion battery. IOP Conference Series: Materials Science and Engineering Volume 77, Issue 1, 2015, Article number 012042. DOI: 10.1088/1757-899X/77/1/012042
3. Liepina, I., Bajars, G., Rublans, M., **Kleperis, J.**, Lusis, A., Pentjuss, E. Structure and photocatalytic properties of TiO2-WO3 composites prepared by electrophoretic deposition. IOP Conference Series: Materials Science and Engineering , Volume 77, Issue 1, 2015, Article number 012039. DOI: 10.1088/1757-899X/77/1/012039

4. Nikolajeva, V., Neibergs, M., Valucka, S., **Dimanta, I., Kleperis, J**. Application of pretreatment, bioaugmentation and biostimulation for fermentative hydrogen production from maize silage. Open Biotechnology Journal, Volume 9, Issue 1, 2015, Pages 39-48. DOI: 10.2174/1874070701509010039
5. **Vanags, M.,** Šutka, A., **Kleperis, J.**, Shipkovs, P. Comparison of the electrochemical properties of hematite thin films prepared by spray pyrolysis and electrodeposition. Ceramics International, Volume 41, Issue 7, 1 August 2015, Pages 9024-9029. DOI: 10.1016/j.ceramint.2015.03.272
6. Šutka, A., Millers, M., Döbelin, N., Pärna, R., **Vanags, M.**, Maiorov, M., **Kleperis, J.,** Käämbre, T., Joost, U., Nõmmiste, E., Kisand, V., Knite, M. Photocatalytic activity of anatase-nickel ferrite heterostructures. Physica Status Solidi (A) Applications and Materials Science, Volume 212, Issue 4, 1 April 2015, Pages 796-803, DOI: 10.1002/pssa.201431681
7. Sternberg, A., **Grinberga, L.,** Sarakovskis, A., Rutkis, M. 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International Conference on Functional Materials and Nanotechnologies (RCBJSF-2014-FM&NT), Physica Scripta, Volume 90, Issue 9, 2015, DOI: 10.1088/0031-8949/90/9/090301
8. Sternberg, A., **Grinberga, L.,** Sarakovskis, A., Rutkis, M., Preface, IOP Conference Series: Materials Science and Engineering, Volume 77, Issue 1, 2015, DOI: 10.1088/1757-899X/77/1/011001
9. Sternberg, A., **Grinberga, L.,** Guest editorial, Ferroelectrics, Volume 483, Issue 1, 2015, DOI: 10.1080/00150193.2015.1101936
10. Sarakovskis, A., Krieke, G., Doke, G., Grube, J., **Grinberga, L.,** Springis, M., Comprehensive study on different crystal field environments in highly efficient NaLaF4:Er3+ upconversion phosphor, Optical Materials, Volume 39, 1 January 2015, Pages 90-96. DOI: 10.1016/j.optmat.2014.11.004
11. Trukhin, A.N., Smits, K., Jansons, J., **Chikvaidze, G.,** Dyuzheva, T.I., Lityagina, L.M. Luminescence of coesite. Physica Scripta, Volume 90, Issue 9, 1 September 2015, Article number 094009. DOI: 10.1088/0031-8949/90/9/094009
12. Trukhin, A.N., Smits, K., Jansons, J., Berzins, D., **Chikvaidze, G.,** Griscom, D.L. UV and yellow luminescence in phosphorus doped crystalline and glassy silicon dioxide. Journal of Luminescence; Volume 166, 20 June 2015, Pages 346-355. DOI:10.1016/j.jlumin.2015.05.045
13. Ying, Q., Naidoo, S., **Vaivars, G.** Function of titanium oxide coated on carbon nanotubes as support for platinum catalysts. Physica Scripta, Volume 90, Issue 9, 1 September 2015, Article number 094021. DOI: 10.1088/0031-8949/90/9/094021
14. Ying, Q., Naidoo, S., **Vaivars, G.** Investigation of activities for Pt-M bimetallic nanoparticles catalysts on the oxygen reduction reaction. Ferroelectrics, Volume 484, Issue 1, 5 August 2015, Pages 101-107. DOI:10.1080/00150193.2015.1059729
15. Sprugis, E., Reinholds, I., **Vaivars, G.** Mechanical properties of composite SPEEK polymer membranes modified with ionic liquids. IOP Conference Series: Materials Science and Engineering; Volume 77, Issue 1, 2015, Article number 012043. DOI: 10.1088/1757-899X/77/1/012043

CONFERENCE PROCEEDINGS

1. P Lesničenoks, J Zemītis, J Kleperis, Georgijs Čikvaidze, Reinis Ignatāns. Studies of Reversible Hydrogen Binding in Nano-Sized Materials. Riga Technical University: Material Science and Applied Chemistry, 2015/31. doi: 10.7250/msac.2015.004

LECTURES ON CONFERENCES

1. LU 73. zinātniskā konference, Rīga, LU, 2015.gada janvāris-februāris; 73rd Scientific Conference of the University of Latvia. Environmental and Experimental Biology, January-February, 2015, Riga Latvia:

- Valucka S., Dimanta I., Kleperis J., Muižnieks I., Nikolajeva V. Analysis of biologically produced hydrogen in activated metal hydride alloys, oral report.

2. LU Cietvielu fizikas institūta 31 zinātniskā konference, Rīga, LU Cietvielu fizikas institūts, 2015.gada 24.-26.februāris; 31st Scientific Conference of Institute of Solid State Physics, University of Latvia, February 24-26, 2015, Riga, Latvia:

- Jānis Kleperis, Pēteris Lesničenoks, Ilze Dimanta, Līga Grīnberga. Ūdeņraža infrastruktūras attīstības aspekti – iegūšana, uzglabāšana, kvalitātes un drošības kontrole; Hydrogen infrastructure development aspects – production, storage, quality and safety control; oral.
- Justs Dimants, Ilze Dimanta, Biruta Sloka, Jānis Kleperis. Politika un standarti gāzveida degvielu uzpildes stacijām un ūdeņraža vieta tajos; Policy and standards of gaseous fuel filling stations and the place of hydrogen therein; oral.
- Ilze Dimanta, Sintija Valucka, Vizma Nikolajeva, Jūlija Hodakovska, Indriķis Muižnieks, Jānis Kleperis. Enterobacter aerogenes saražotā ūdeņraža uzglabāšanas iespējas dažādos metālhidrīdos; Enterobacter aerogenes produced hydrogen storing possibilities in various metal hydride alloys; oral.
- Ainārs Knoks, Jānis Kleperis, Līga Grīnberga. TiO_2 nanocaurulīšu augšanas īpatnības anodēšanas procesā; Features of anidized TiO_2 nanotube growth process; oral.
- Alberts Kristiņš, Irina Gvardina, Jānis Melderis, Jānis Straumēns, Jānis Kleperis, Pēteris Lesničenoks, Jānis Zemītis. Automātiskā starta-finiša kontroles iekārta un sacensību norises protokolsSaules mašīnu un laivu sacensībām; Automatic start-finish control unit and the venues protocol-software for race competitions of ssolar cars and boats; oral.
- G.Kučinskis, G.Bajārs, J.Kleperis. $LiFePO_4$ litija jonu bateriju katodmateriāla sprieguma histerēze; Voltage Hysteresis of $LiFePO_4$ Lithium Ion Battery Cathode Material, poster.
- A.Dorondo, J.Mateuss, K.Kaprāns, G.Kučinskis, G.Bajārs, J.Kleperis. Nanoporaina oglekļa materiālakārtiņu elektroforētiska uzklāšanano izopropanola un ūdens suspensijām; Electrophoretic deposition of nanoporous carbon material films from isopropanol and water suspensions, poster.
- Rihards Vaivods, Kārlis Lācis, Ainārs Knoks, Jānis Kleperis, Līga Grīnberga. TiO_2 nanostruktūru sintēze un pielietojumi ūdens attīrīšanai. Synthesis of TiO_2 nanostructures for water purification, poster.
- Antonija Dindune, Janis Ronis, Dagnija Valdniece,Vilma Venckutė,Antanas Orliukas. Litija jonu vadītāji sistēmā; Lithium ion condyctors in system $Li_4Ti_{1-x}P_2O_7$ (x=0; 0,06; 0,2), poster.
- Ilze Dimanta, Sintija Valucka, Vizma Nikolajeva, Jūlija Hodakovska, Indriķis Muižnieks, Jānis Kleperis. Enterobacter aerogenes saražotā ūdeņraža uzglabāšanas iespējas dažādos metālhidrīdos. Enterobacter aerogenes produced hydrogen storing possibilities in various metal hydride alloys, oral.
- Pēteris Lesničenoks, Līga Grīnberga, Jānis Kleperis. Materiālu ūdeņraža uzglabāšanai pētniecības metodes Kauņā un Rīgā. Materials for hydrogen storage - methods available in Kaunas (LT) and Riga (LV), oral.

- Jūlija Hodakovska, Jānis Kleperis. Trīs komponenšu membrānu pētījumi izmantošanai degvielas šūnās; Research of three-component membranes for polymer fuel cells, poster.
- Jānis Zemītis, Mārtiņš Vanags, Jānis Kleperis. Indija piejaukuma ferītā ietekmes izpēte uz struktūru, fizikālķīmiskajām īpašībām un fotoaktivitāti plānās kārtiņās; Impact of indium impurities in thin film ferrite on structure, physicochemical properties and photoactivity, poster.
- Roberts berķis, Artūrs Gruduls, Rasa Šmite, Raitis Šmits, Jānis Kleperis. Elektroenerģijas savākšana no piesārņotu ūdeņu baseiniem, izmantojot mikroorganismu baterijas; Electricity collection from waste water basins using microbial batteries. Poster.
- Amanda Dolgā, Ingars Lokoševičs, Pēteris lesničenoks, Jānis Kleperis. Sintezēto ceolītu struktūras un sastāva raksturošana un ūdeņraža adsorbcijas pētījumi tajos; Characterization of structure and composition of synthesized zeolites and hydrogen adsorption studies; poster.
- Gustavs Baumanis, Krišjānis Auziņš, Pēteris Lesničenoks, Jānis Zemītis, Jānis Kleperis. Reciklēta grafīta vairākslāņu grafēna pielietojums elektrovadošas tintes izstrādē; Application of multi-layer graphene from recycled graphite in the development of conductive ink; poster.

3. Smart and Green Interfaces Conference – SGIC2015, Belgrade, Serbia, March 30 – April 1, 2015, http://sgic2015.elexcomm.com/:

- K.Kaprans, G.Bajars, A.Dorondo, J.Mateuss, G.Kucinskis, J.Kleperis, A.Lusis. Electrophoretically deposited nanostructured reduced graphene oxide as electrode material for lithium ion batteries.

4. 4th International Conference "Multifunctional, Hybrid and Nanomaterials", 09.03.2015.-13.03.2015., Barselona, Spānija. https://elsevier.conference-services.net/programme.asp?conferenceID=3774&action=prog_categories

- Dimanta I., Valucka S., Nikolajeva V., Kleperis J., Muiznieks I. Fermentative bacteria produced hydrogen gas storage in metal hydride alloys.

5. EuroNanoForum, Riga, Latvia, June 10-12, 2015, http://euronanoforum2015.eu/:

- J.Kleperis, J.Gravitis, G.Vaivars, A.Gruduls, G.Bajars, A.Lusis. Advanced method of formation of heteropoly oxometalate nanocoating on electrodes for direct biomass conversion to energy; poster.
- A.Knoks, J.Kleperis, L.Grinberga. Anodization pre-treatment influence on growths facilities of TiO_2 nanotube arrays; poster.
- P.Lesničenoks, R. Merijs-Meri, J.Kleperis. Research of hydrogen storage in meso-porous large surface area materials for applications in automotive industry; poster.
- G.Vaivars, E.Āboltiņa, M.Markus, K.Krūkle-Bērziņa, A.Actiņš, A.Zicmanis. Nanostructuring approach in developing polymer membranes for advanced energy conversion devices; poster.
- J.Zemītis, M.Vanags, J.Kleperis, A.Šutka. Influence of IIIA group element impurities on the photo-electric properties of nanocrystalline hematite; poster.
- G.Kucinskis, G.Bajars, K.Bikova, J.Kleperis. $LiFePO_4$/C/reduced graphene oxide composite cathode for lithium ion batteries; poster;
- Dimanta I., Kleperis J., Valucka S., Nikolajeva V., Muižnieks I. Research of hydrogen collection from organic matter in dark fermentation process, poster;
- G.Vaivars, E.Āboltiņa, M.Markus, K.Krūkle-Bērziņa, A.Actiņš, A.Zicmanis. Nanostructuring approach in developing polymer membranes for advanced energy conversion devices; poster.

7. MRS 2015 Fall Meeting, Warsaw University of Technology (Poland), September 14 to 18, 2015: http://www.european-mrs.com/2015-fall-symposium-c-european-materials-research-society:

- Janis Kleperis, Peteris Lesnicenoks, Liga Grinberga, Georg Chikvaidze. The Studies of Hydrogen Adsorption in Nanoporous and Nanostructered Materials, poster;

8. FM&NT-2015 International conference on Functional Materials and Nanotechnologies, Vilnius, Lithuania, October 5-8, http://www.fmnt.ff.vu.lt/ :

-
- G.Kucinskis, G.Bajars, K.Bikova, J.Kleperis $LiFePO_4$/C/reduced graphene oxide composite cathode for lithium ion batteries, oral;
- E. Sprūģis, E. Āboltiņa, M. Markus, I. Reinholds, G. Vaivars. Mechanical properties of sulfonated polyetheretherketone composite membranes with ionic liquids and inorganic nanoparticles at elevated temperatures; poster.
- A.Knoks, L. Grinberga, J. Kleperis. Structural, optical and photo-electrochemical research of anodised TiO2 nanotube arrays; poster.
- P. Lesnicenoks, J. Kleperis, L.Grinberga. Research of advanced solid state hydrogen storage nanomaterials for sustainable energy applications; poster.
- J. Hodakovska, J. Kleperis. Research of Three-Component Proton Conductive Membranes for Fuel Cell Application; poster.

PATENTS

1. G.Cikvaidze, A.Kalle. Method for refining silicon using an electron beam. European patent application: EP 2 883 837 A1; Date of publication: 17.06.2015, Bulletin 2015/25; Applicant: Institute of Solid State Physics University of Latvia

BACHELOR'S AND MASTER'S THESIS

Artis Volkovs, Bachleor Thesis: Spectroscopic research of ion composition in corona discharge of water/air mixture, 2015, ISSP UL, Supervisors J.Kleperis; M.Vanags.
Staņislavs Ložkins, Bachleor Thesis: Synthesis and research of proton conduction composite materials based on Nafion polymer for applications in fuel cell, 2015, ISSP UL, Supervisor Jūlija Hodakovska.
Pēteris Lesničenoks. Master of Science Thesis: Research of meso-porous large surface materials for hydrogen storage application in car industry. 2015, Riga Technical University; Supervisors J. Kleperis; R. Merijs-Meri.
Jānis Zemītis. Master of Science Thesis: Research of influence of IIIA group element impurities on physical-chemical properties of Fe2O3 thin films. 2015, Riga Technical University; Supervisors J. Kleperis, M.Vanags, R. Merijs-Meri.

PhD THESIS

Mārtiņš Vanags, PhD Thesis: Synthesis and properties of nanostructured iron oxide; mechanisms of pulse electrolysis and photoelectrolysis, 2015, Riga Technical University, Supervisors J.Kleperis, A. Šutka.

DEPARTMENT OF THEORETICAL PHYSICS AND COMPUTER MODELLING

Head of Department Dr. hab. phys. Eugene Kotomin

RESEARCH AREA AND MAIN PROBLEMS

Our theoretical research interests are focused on six classes of problems related to:

- kinetics of diffusion-controlled processes, with emphasis on pattern formation and catalytic surface reactions;
- the atomic and electronic structure of numerous advanced materials, with emphasis on calculations of properties of defects, surfaces, metal/insulator interfaces;
- theoretical simulations and experimental studies of nanostructures and nanomaterials, *e.g.*, evaluation of their photocatalytic suitability;
- modeling of advanced functional materials for energy applications (fuel cells, ceramic membranes, Li batteries, fusion and fission reactors);
- gyrotron development for thermonuclear reactors

We combine several different techniques, including analytical formalisms and large-scale computer simulations (quantum chemical methods, stochastic simulations as well as Monte Carlo/cellular automata modeling) as described in our homepage http://www1.cfi.lu.lv/teor

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Dr. O. Dumbrajs (full member of Latvian Acad. Sci.)	Dr. D. Bocharov
Dr. D. Gryaznov	Dr. R. Eglitis (corr. member of Latvian Acad.Sci.)
Dr. E. Klotins	Dr. Yu. Mastrikov
Dr. hab. E. Kotomin (full member of Latvian Acad. Sci.)	Dr. S. Piskunov
Dr. hab. V. Kuzovkov	Dr. hab. Yu. Shunin
Dr. A. Popov	Dr. Yu. Zhukovskii
Dr. G. Zvejnieks	M.S. A. Chesnokov
M.S. J. Shirmane	M.S. A. Gopejenko
B.S. Moskina	M.S. J. Kazerovskis
	M.S. B.S. O. Lisovski
	M.S. A. Platonenko
	B.S. M. Sokolov

SCIENTIFIC VISITS ABROAD

1. Dr. hab. E. Kotomin, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (8 months), Photochemistry Center, Russian Academy of Sciences, Moscow, Russia (1week)
2. Dr. O. Dumbrajs, Fukui University, Japan (3 months)
3. Dr. A. Popov, Max Planck Institute, Stuttgart, Germany (1 week); Institute of Physics, University of Tartu, Estonia (3 weeks), CIEMAT, Spain (1 week)

4. Dr. D. Bocharov, Paul Scherrer Institut, Viligen, Switzerland (8 months), University of Duisburg-Essen, Germany (two weeks)
5. Dr. Yu. Mastrikov, Institut für Angewandte Materialien, Karlsruhe Institut für Technologie, Germany (2 weeks)
6. Dr. S. Piskunov, University of Duisburg-Essen, Germany (two months)
7. Dr. hab. Yu. Shunin, Laboratori Nationali di Frascati, Italy (1 month)
8. Dr. Yu. Zhukovskii, St. Petersburg State University, Russia (3 weeks), Institut für Angewandte Materialien, Karlsruhe Institut für Technologie, Germany (2 weeks)
9. M.S. A. Gopejenko, Institut für Angewandte Materialien, Karlsruhe Institut für Technologie, Germany (one month)
10. M.S. A. Chesnokov, University of Duisburg-Essen, Germany (2 weeks)
11. M.S. J. Kazerovskis, University of Ulm, Germany (10 months)
12. M.S. O. Lisovski, Uppsala University, Sweden (7 months)

INTERNATIONAL COOPERATION

Belarus	1. Institute of Nuclear Problems, Belarusian State University, Minsk (Prof. S. A. Maksimenko)
China	2. Beijing Institute of Technology, Beijing (Dr. H. Shi).
Estonia	3. Institute of Physics, University of Tartu (Prof. A. Lushchik)
Finland	4. Helsinki University of Technology, Espoo (Dr. T. Kurki-Suonio)
France	5. Laue-Langevin Institute, Grenoble, Prof. H. Schober)
Germany	6. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 7. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov) 8. Darmstadt University of Technology, Darmstadt (Prof. H von Seggern) 9. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk) 10. Max-Planck Institut für Plasmaphysik, Garching, (Prof. Dr. H. Zohm) 11. Institut für Angewandte Materialien (KIT), Karlsruhe (Prof. Dr. A. Möslang, Dr. P. Vladimirov) 12. Dept Theoretical Chemistry, Univ. Duisburg-Essen (Prof. Dr. E. Spohr)
Israel	13. Ben Gurion University, Beer Sheva (Prof. D. Fuks)
Italy	14. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Kazakhstan	15. Gumilyov Eurasian National University, Astana (Prof. A.T. Akilbekov)
Japan	16. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	17. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Norway	18. Center for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, FASE, Norway
Poland	19. Warsaw University, Department of Chemistry (Prof. A. Huczko, Prof. A. Dąbrowska) 20. Institute of Physics, Academy of Science, Warsaw (Prof. H. Szymczak)
Romania	21. University of Craiova (Dr. D. Constantinescu)
Russia	22. St. Petersburg State University, Petrodvorets (St. Petersburg) (Prof. R.A. Evarestov) 23. Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (Prof. P.N. Dyachkov) 24. Photochemistry Center, Russian Academy of Sciences, Moscow (Prof. A.A. Bagaturyants)
Spain	25. Centro de Investigaciones Energeticas Medioambientales y Tecnologicas (CIEMAT), Madrid (Dr. R. Vila)
UK	26. University College London (Prof. A.L. Shluger)

Ukraine	27. Ivan Franko National University, Lviv (Prof. O. I. Aksimentyeva, Prof. I. Bolesta, Dr. I. Karbovnyk)
USA	28. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

MAIN RESULTS

A. Electronic structure calculations for advanced materials

THERMODYNAMIC STABILITY OF STOICHIOMETRIC $BiFeO_3$

E.A. Kotomin,
E. Heifets, R. Merkle, J. Maier

$BiFeO_3$ (BFO) continues to attract great attention due to its multiferroic properties under ambient conditions. It was found also, that photocatalytic and photovoltaic properties of BFO are enhanced due to its ferroelectricity. Related perovskite solid solutions ($Bi_{1-x}Sr_xFeO_{3-\delta}$ and $Bi_{1-x}Sr_xFe_{1-y}Co_y O_{3-\delta}$) were proposed recently as cathodes for solid oxide fuel cells (SOFCs) operating at intermediate temperatures (> 600 ºC). Determination of thermodynamic stability conditions for BFO is important and represents the first step for future investigations of formation of intrinsic defects, surface structures and surface chemical reactions (e.g. oxygen reduction reaction), as well as formation of solid solutions, like the mentioned above cathode materials, their possible structures and stability. Also, the data on stability of BFO can be used to provide valuable information on conditions suitable to produce this and related materials. Based on first principles hybrid calculations performed *in close collaboration with Max Planck Institute for Solid State Research, Stuttgart* the phase diagram has been constructed (**Fig. 1**), which allows us to predict the stability region of stoichiometric $BiFeO_3$.

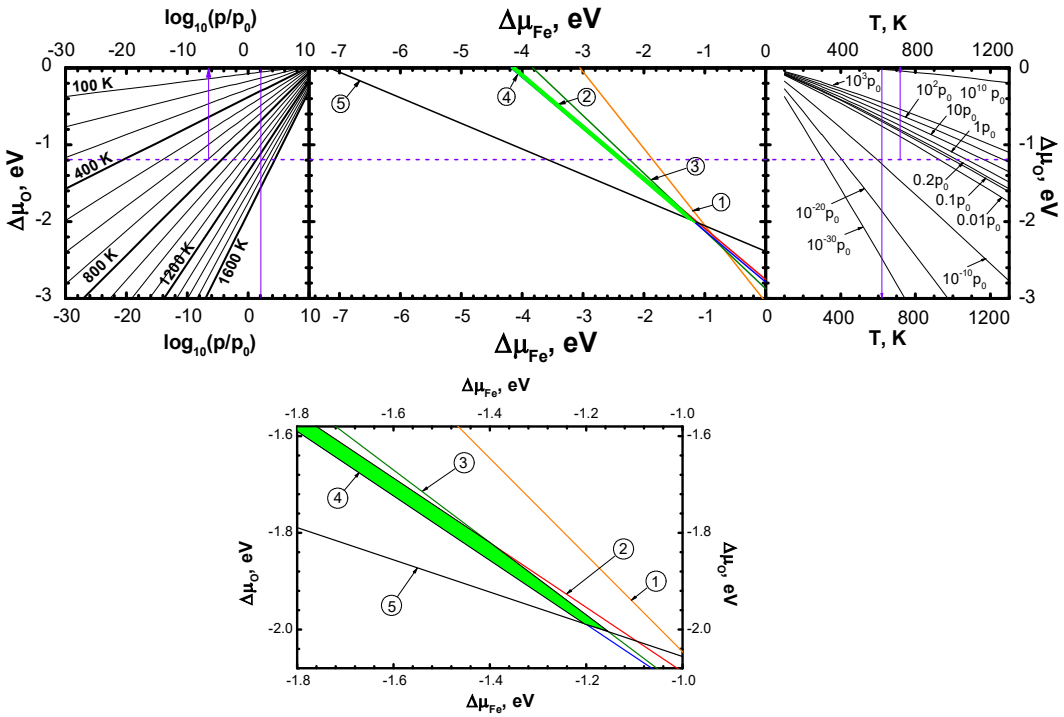


Figure 1. (a) Phase diagrams for $BiFeO_3$ based on hybrid density functional calculations with all electrons on Fe ions included explicitly. The numbered lines in the central panel describe conditions of forming of: 1) FeO ; 2) Fe_2O_3 ; 3) Fe_3O_4 ; 4) Bi_2O_3 ; 5) Bi metal. Green area marks the region of $BiFeO_3$ stability. Side panels serve to convert values of

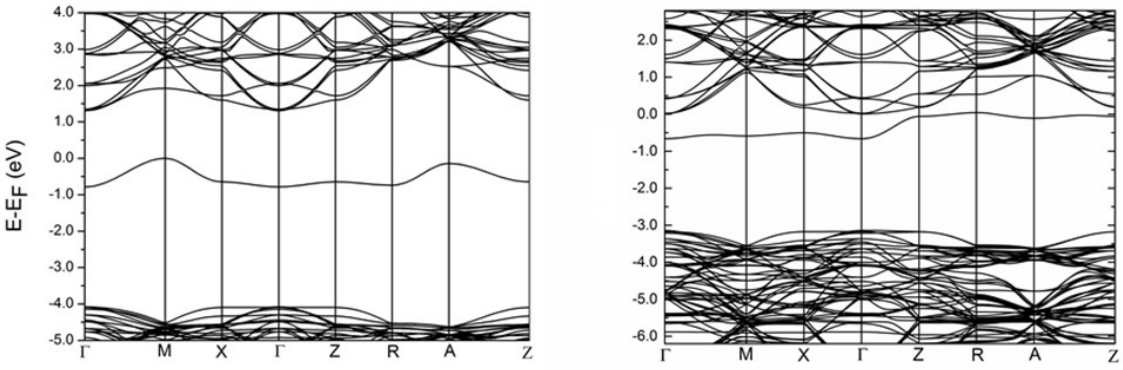
oxygen chemical potential to easily observable values of temperature T and oxygen partial pressure p_{O_2}. (b) Enlargement of the region marked by a rectangular from (a). for more details on applied technique. The variation of chemical potential for Fe atoms is defined as the deviation of Fe atoms chemical potential from value in metallic iron ($\Delta\mu_{Fe} \approx \mu_{Fe} - E_{Fe}$), which is the standard state for the iron and approximated by the total energy of Fe atom in Fe metal. Similarly, the variation of O atom chemical potential is calculated with respect to the total energy of O atom in O_2 molecule

THERMODYNAMIC PROPERTIES OF NEUTRAL AND CHARGED OXYGEN VACANCIES IN $BaZrO_3$ BASED ON FIRST PRINCIPLES PHONON CALCULATIONS

D. Gryaznov, E.A. Kotomin, M. Arrigoni, J. Maier, T. S. Bjørheim

ABO_3-type perovskite structured oxides comprise a broad family of technologically important materials, which display a wide range of functional properties, such as ferroelectricity, magnetism, their combination (multiferroics), piezoelectricity, high-temperature superconductivity, mixed ionic-electronic conductivity and electro-optic effects. Oxygen vacancies are common point defects in these materials and were shown to influence a variety of properties, *e.g.*, mechanical and optical properties, as well as ionic conductivity.

The structural, electronic and thermodynamic properties of neutral (V_O^x) and positively doubly charged ($V_O^{\bullet\bullet}$) oxygen vacancies in the $BaZrO_3$ are addressed by first principles phonon calculations (Fig. 2). The calculations have been performed *in close collaboration with Max Planck Institute for Solid State Research, Stuttgart, and Centre for Materials Science and Nanotechnology, University of Oslo*, using two complementary first principles approaches and functionals; the linear combination of atomic orbitals (LCAO) within hybrid Hartree-Fock and density functional theory formalism (HF-DFT), and the projector augmented plane wave approach (PAW) within DFT and PW basis set. Phonons are shown to contribute significantly to the formation energy of the charged oxygen vacancy at high temperatures (~1 eV at 1000 K), due to both its large distortion of the local structure, and its large negative formation volume. For the neutral vacancy the resulting lattice distortions, and thus the contributions from phonons to the free formation energy, are significantly smaller. As a result, phonons affect the relative stability of the two defects at finite temperatures and the charge transition level for oxygen vacancies (+2/0) is predicted change from 0.42 to 0.83 eV below the conduction band bottom as temperature increases from 0 K to 1000 K.



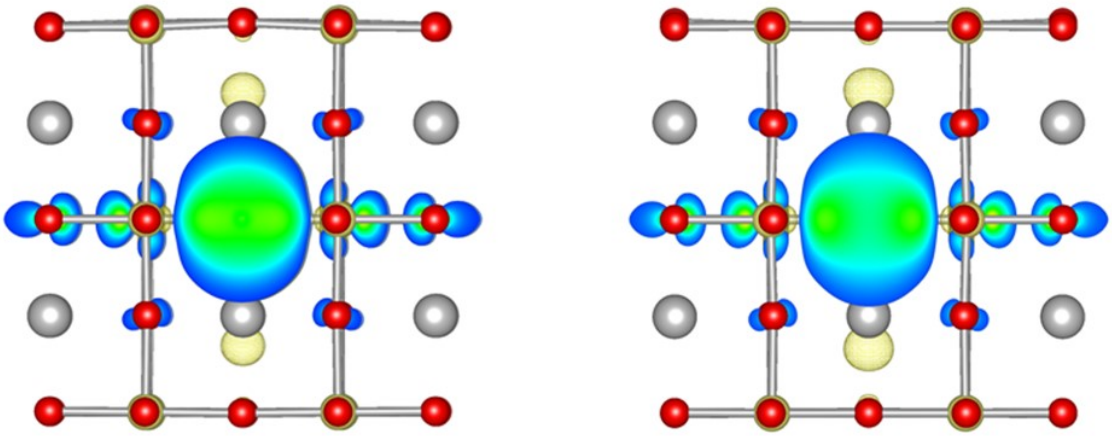


Figure 2 Top: Band structure of the 2×2×2 $BaZrO_3$ supercell with a $v_O^{\bullet\bullet}$ calculated with CRYSTAL (left) and VASP (right); bottom: electronic charge density of $v_O^{\bullet\bullet}$ projected on the defect level obtained with CRYSTAL using the ghost BS (left) or leaving vacuum (right). The isosurface threshold level is set to 0.002 e/a_0^3; only points with an electron charge density value greater than the threshold are shown and they lie inside the isosurface (the larger the value, the warmer the color).

HYDRATION ENTROPY OF $BaZrO_3$: FIRST PRINCIPLES PHONON CALCULATIONS

E.A. Kotomin, T. S. Bjørheim, R. Merkle, J. Maier

Oxide crystals display solid state protonic conduction at temperatures up to 1000 °C, and may thus be used as electrolytes in the intermediate temperature solid oxide fuel cells, electrolysers and H_2 gas separation membranes. Acceptor-doped barium zirconate, *e.g.,* $BaZr_{1-x}Y_xO_3$, is the most promising candidate material for practical applications to date, with a protonic conductivity of ~10^{-2} S/cm at 600 °C.

The impact of phonons on the hydration and defect thermodynamics of undoped and acceptor (Sc, In, Y and Gd) doped $BaZrO_3$ has addressed by means of first principles supercell calculations, *in collaboration with Max Planck Institute for Solid State Research, Stuttgart, and Centre for Materials Science and Nanotechnology, University of Oslo*. In contrast to previous, similar investigations, we evaluate contributions from all phonon modes, and also pressure/volume effects on the phonon properties. The calculations are performed at the GGA-level with the PBE and RPBE functionals, which both predict for $BaZrO_3$ a stable cubic perovskite structure (**Fig. 3**). Both functionals also give similar defect entropies for undoped, and Sc- and In-doped $BaZrO_3$. For all dopants, the vibrational formation entropy of the fully charged oxygen vacancy ($v_O^{\bullet\bullet}$) is significantly lower than that of the protonic defect ($OH_O^{\bullet}$), which therefore also is the dominant contribution to the entropy of hydration, in addition to loss of H_2O(g). The large, negative vibrational formation entropy of $v_O^{\bullet\bullet}$ stems both from local structural relaxations, and contraction of the entire supercell and corresponding blue-shift of the phonon spectrum. Neglect of the phonon contribution to the vacancy free formation energy leads to a significant error (120 kJ/mol at 1000 K). The formation volume and vibrational formation entropy of both $OH_O^{\bullet}$ and $v_O^{\bullet\bullet}$ become more negative with increasing dopant size. The calculated hydration entropies, and the trend of more negative entropies in the order Y < Gd < In < Sc, are in good agreement with experimental results, lending support to the applicability of the adopted method.

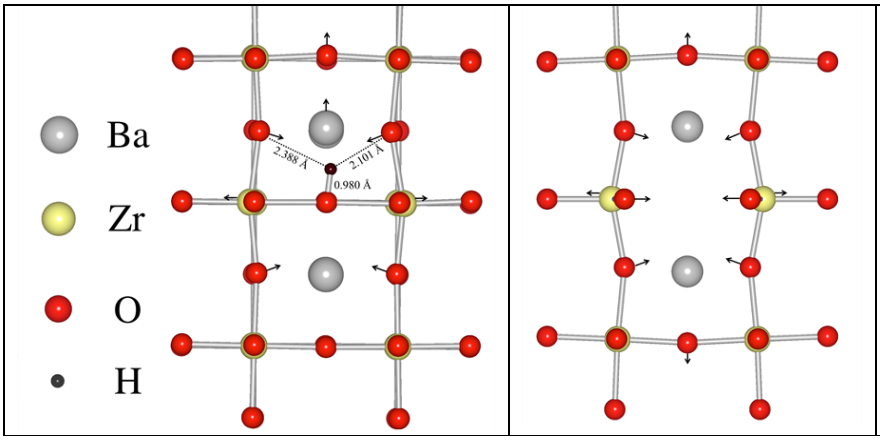


Figure 3. Atomic structure of $OH_O^{\bullet}$ and $V_O^{\bullet\bullet}$ in a 3×3×3 supercell calculated with PBE and full volume relaxations. The structures are projected along the (0 0 1) direction and show the major atomic relaxations around the defects.

WATER INTERACTION WITH PERFECT AND FLUORINE-DOPED Co_3O_4 (100) SURFACE

Yu.A. Mastrikov, E.A. Kotomin, G.A. Kaptagay, T.M. Inerbaev, A.T. Akilbekov

The increasing consumption of energy has stimulated intensive research of different kinds of renewable energy resources. This includes research of spinel-type tri-cobalt tetra oxide (Co_3O_4) as a cathode material for water splitting at ambient temperatures as a result of the oxygen evolution reaction (OER). The interaction of H_2O with transition-metal oxide surfaces plays also important role in catalysis, surface chemistry, gas sensors, photochemistry, and electrochemistry. One of the main characteristics of the OER is the overpotential.

Whereas the atomic scale mechanisms of the OER is complicated and not fully studied, insights into the thermodynamics of the reaction can be obtained using the recently developed schemes based on the first principles calculations. Theoretical investigations of water adsorption on perfect and fluorine-doped Co_3O_4 (100) surface have been performed *in collaboration with L.N. Gumilyov Eurasian National University, Astana*, by means of the plane-wave periodic density functional theory (DFT) calculations combined with the Hubbard-*U* approach and statistical thermodynamics (**Fig. 4**). We demonstrated the positive effect of fluorine-doping of the Co_3O_4 (100) surface and calculated oxygen evolution reaction overpotential based on the Gibbs free-energy diagram of perfect and F-doped surfaces.

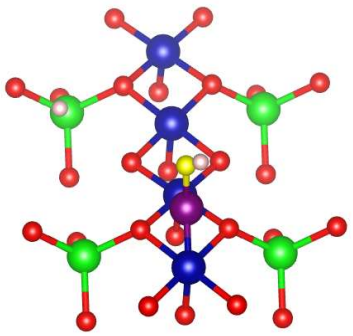


Figure 4. Top view of dissocation geometry on the Co_3O_4 (100) $Co_{0.5}$-terminated surface. Color coding: Co_{5c}^{O}, blue; Co_{4c}^{T} , green; Co_{2c}^{T} ,purple; water O, yellow; H atom, white.

C-, N-, S-, AND Fe-DOPED TiO_2 AND $SrTiO_3$ NANOTUBES FOR VISIBLE-LIGHT-DRIVEN PHOTOCATALYTIC WATER SPLITTING: PREDICTION FROM FIRST PRINCIPLES

A. Chesnokov, S. Piskunov, O. Lisovski, D. Bocharov, Yu.F. Zhukovskii, E. Spohr, M. Wessel

Water splitting under the influence of solar light on semiconducting electrodes inserted in aqueous electrolyte is a potentially clean and renewable source for production of hydrogen fuel. Its efficiency depends on relative position of the band gap edges (the visible light interval between infrared and ultraviolet ranges of electromagnetic spectrum corresponds to gap widths 1.5-2.8 eV) accompanied by a proper band alignment relative to both reduction (H^+/H_2) and oxidation (O_2/H_2O) potentials (4.44 eV and 5.67 eV, respectively) which must be positioned inside the band gap. Some metal oxides are capable of driving the water-splitting reaction when irradiated with sunlight, and both titania and strontium titanate are among these materials. Band gaps of cubic perovskite-type $SrTiO_3$ and TiO_2 anatase-type bulk were experimentally found to be 3.2 eV for both materials, which corresponds to photocatalytic activity under ultraviolet light possessing only ~1% efficiency of sunlight energy conversion.

In collaboration with Department of Theoretical Chemistry, University of Duisburg-Essen, Germany, we have performed large-scale *ab initio* ground-state calculations on the single-wall anatase-structured TiO_2(001) and cubic $SrTiO_3$(110) nanotubes, with fixed number of atomic layers as well as chiral indexes (*n*,0) for both NTs, respectively, doped by C, N, S, or Fe atoms and co-doped by pair of N and S atoms. We have constructed also both periodic and cluster models of doped TiO_2 NTs, for which either *CRYSTAL09* code or *NWChem* code have been applied, respectively. For both types of calculations, we have used the formalism of localised Gaussian-type functions (GTFs), which form the basis set (BS) of localised atomic orbitals for each chemical element as implemented in both types of codes where crystalline and molecular orbitals are constructed within either CO LCAO or MO LCAO approaches.

Noticeable growth of photocatalytic efficiency can be achieved by essential adjustment of band edges for titania bulk through nanoscale transformation of its morphology to anatase-type nanotubes formed by folding of nanothin (001) TiO_2 sheets consisting of 9 atomic layers and six-layer (110) $SrTiO_3$ sheets, both possessing (*n*,0) chiralities, accompanied by partial substitution of pristine atoms by C_O, Fe_{Ti}, N_O and S_O simple dopants as well as N_O+S_O co-dopant (in the case of TiO_2 NTs). In the former case, the band gap can be reduced down to 2.2 eV (**Fig. 5**) while its efficiency is increases up to ~15%. Efficiency of $SrTiO_3$(110) nanotubes for visible-light photocatalytical applications has been found to be much lower.

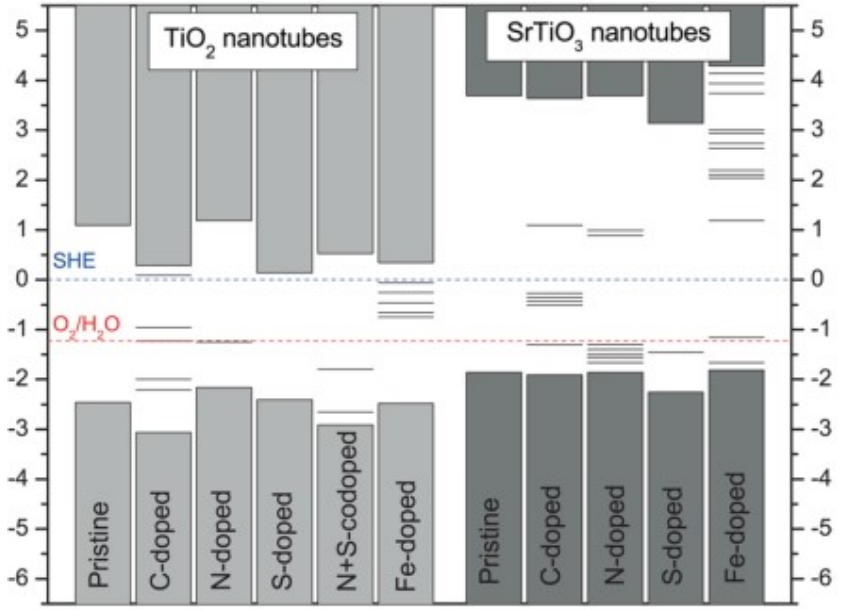


Figure 5. Schematic representation of the band edges and midgap states of periodic, pristine and doped TiO_2 and $SrTiO_3$ nanotubes. Blue and red horizontal dashed lines correspond to the redox potentials for H^+/H_2 and O_2/H_2O dissociation, respectively. Zero of the energy scale corresponds to the standard hydrogen electrode (SHE).

The differences between the edges of band gap (VB and CB) as well as the highest occupied and lowest unoccupied impurity levels inside the band gap (HOIL and LUIL, respectively) induced in doped nanotubes must preserve the proper disposition of these levels relatively to the redox potentials, so that $\varepsilon_{VB} < \varepsilon_{HOIL} < \varepsilon_{O_2/H_2O} < \varepsilon_{H^+/H_2} < \varepsilon_{LUIL} < \varepsilon_{CB}$, thus reducing the photon energy required for dissociation of water molecule.

ENERGETIC STABILITY AND PHOTOCATALYTIC ACTIVITY OF $SrTiO_3$ NANOWIRES: *AB INITIO* SIMULATIONS

Yu.F. Zhukovskii, A.V. Bandura, R.A. Evarestov

First principles periodic calculations based on the density functional theory within the localized atomic orbital approach (DFT-LCAO) using the hybrid exchange–correlation potential PBE0 have been performed *in close collaboration with Department of Quantum Chemistry, St. Petersburg State University (Russia)*, in order to simulate the structural and electronic properties of both stoichiometric (**Fig. 6**) and nonstoichiometric [001]-oriented four-faceted $SrTiO_3$ (STO) nanowires (NW) of cubic structure. Their diameters have been varied from 0.3 up to 2.4 nm with a corresponding consequent change of NW cross-section from 2×2 to 5×5 extension of the lattice constant in bulk.

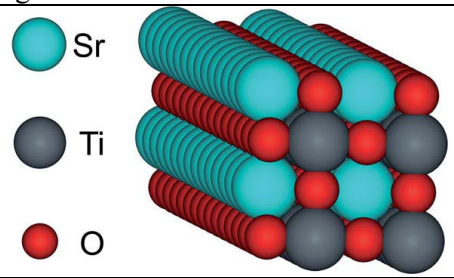


Figure. 6. Axonometric image of stoichiometric [001]-oriented $SrTiO_3$ nanowire terminated by both SrO {100} and {010} as well as TiO_2 {100} and {010} facets with 2×2 extension of the thinnest possible 1×1 nanowire (5 atoms per UC). Left panel contains labels of constituent atoms.

Energetic stability of STO NW (both stoichiometric and non-stoichiometric) has been found to increase with the decrease of their formation energies together with the increase of NW diameter. The electronic structure calculations have shown that the width of the band gap changes in STO NWs of different structural types as compared to that in bulk being consequently reduced with the growth of NW diameter although the character of

such a decrease depends on the morphology of the nanowire. Analysis of these changes shows that stoichiometric and non-stoichiometric TiO_2-terminated strontium titanate nanowires can be quite promising candidates for further applications in photocatalytic processes under solar irradiation whereas SrO-terminated NWs are rather not suitable for this purpose.

THE ELECTRONIC STRUCTURES OF MONO- AND BI-ATOMIC CHAINS OF IV, III–V AND II–VI GROUP ELEMENTS CALCULATED USING THE DFT LCAO AND LACW METHODS

S. Piskunov, Yu.F. Zhukovskii, P.N. D'yachkov, V.A. Zaluev

Within the current trends of miniaturization of electronic devices, the problems of interconnects between nanodevices attract growing interest in the stability, band structure, and conductivity of the nanowires. The thinnest possible nanowire is established to be a single-atom width chain. Using the first principle non-relativistic linear combination of atomic orbitals (LCAO) and relativistic linearized augmented cylindrical wave (LACW) methods, the band structures of the covalent and partially ionic $A^N B^{8-N}$ single atom width chain have been calculated *in close collaboration with Kurnakov Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow*. Both methods show that the chains of C, Si, Ge, Sn, and Pb are metallic. However, there is a great difference between the relativistic and non-relativistic band structures. The π bands crossing the Fermi level are orbitally doubly degenerate in the non-relativistic model. The relativistic LACW calculations demonstrate that the spin and orbital motion of electrons are coupled, thereby splitting the π bands (**Fig. 7**).

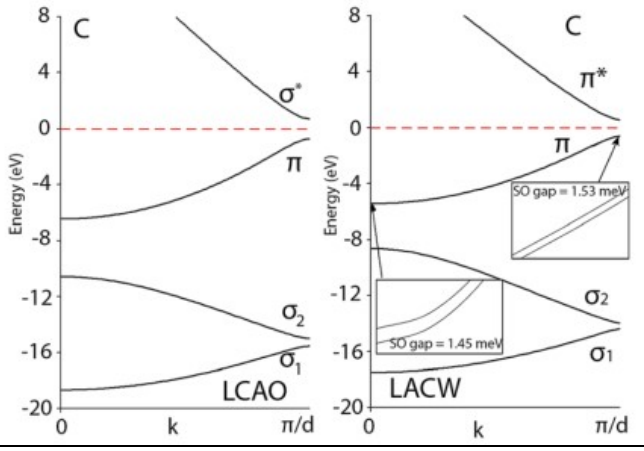


Figure 7. Non-relativistic LCAO and relativistic LACW band structures of polyynic carbine filament presented in left and rright panels, respectively. Insets demonstrate splitting of the π bands.

The spin–orbit gaps are equal to 1.5 meV, 28 meV, 0.22 eV, 0.45 eV, and 4 eV for the C, Si, Ge, Sn, and Pb chains, respectively. The mass–velocity corrections result in a lowering of all the valence band levels. In the carbon and silicon chains, the corrections are possibly negligible (2–5 and 10–30 meV, respectively), while in the Ge, Sn, and Pb chains the low-energy shifts are equal to 0.6, 2.2, and 3.7 eV, respectively, due to these effects. The Darwin corrections are several times smaller in comparison to the mass–velocity contributions. The transition from the covalent chains to the partially ionic ones is accompanied by a drastic change in the band structure. The C chain with all bond lengths equal has a metal type electronic structure while the BN chain is an insulator with an energy gap equal to 6–8 eV.

The differences between the covalent and partially ionic chains are explained by the presence of the antisymmetric components of the electron potential in the latter case. The transition from the BN chain to the AlP, GaAs, and InSb ones is accompanied by a

gradual decrease in the gaps; for example, the AlP chain is a semiconductor. According to the LCAO calculations, the GaAs chain is a semiconductor, but it is a metal according to the relativistic LACW method. The InSb chain possesses a metal type band structure, but the spin–orbit interaction splits the π states, forming the two π^+ and π^- sub-bands, and noticeably complicates the band structure and density of states in the vicinity of the Fermi level.

In the case of compounds from the same horizontal row in the periodic table, the transition from the $A^{III}B^{V}$ chains to the $A^{II}B^{VI}$ ones is accompanied by a sharp increase in the band gap. The calculations indicate the metallic nature of the InSe chain, but the CdTe one is an insulator. Among the atomic $A^{N}B^{8-N}$ chains, there are compounds with different electrical properties: from metals to semiconductors and insulators.

AB INITIO SIMULATIONS ON FRENKEL PAIRS OF RADIATION DEFECTS IN α-Al_2O_3

A. Platonenko, S. Piskunov, Yu.F. Zhukovskii, E.A. Kotomin

Corundum (α-Al_2O_3) is important radiation-resistant material with potential applications for components of diagnostics, breeder blanket and in future fusion reactors as coating to avoid the light gases permeation. Induced changes in structural and optical properties of radiation-exposed α-Al_2O_3 crystalline materials are mainly associated with oxygen vacancies V_O and complementary Frenkel pairs of defects (O_i+V_O). Despite technological importance of corundum crystalline structures, electronic, defects have not yet comprehensively studied theoretically. The main reasons for this are the following: the complicated atomic structure of α-Al_2O_3 (**Fig. 8**) as well as the semi-covalent and semi-ionic chemical bonding. In this study, we have consequently performed *ab initio* calculations on (*i*) perfect corundum structure, (*ii*) that containing single point defects, such as neutral O vacancy V_O and interstitial oxygen atom O_i, (*iii*) that containing Frenkel pair O_i+V_O, as well as (*iv*) that containing dumbbell O_i+O_{reg} pair in the case of α-Al_2O_3 structures containing either single O_i impurity or Frenkel pair.

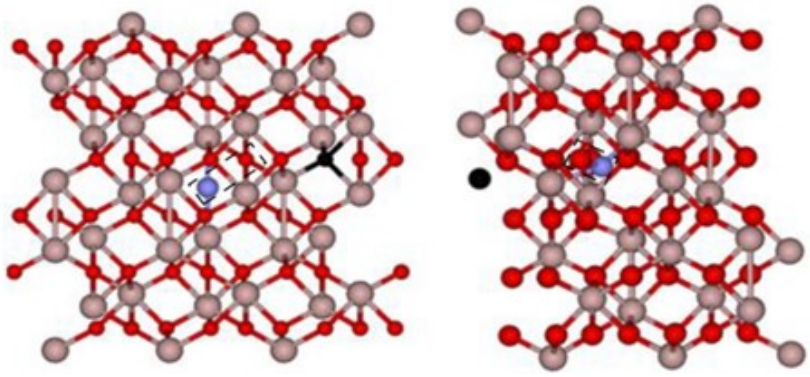


Figure 8. Images of Frenkel pair in initial and optimized corundum structures (left and right panels, respectively). V_O vacancy is shown as a black ball while the interstitial O_i atom is shown as a blue (dark grey) one. Configurations of dumbbell are shown as a dotted rectangle.

Using optimization procedure, we have determined equilibrium locations and configurations of V_O, O_i, and O_i+V_O inside corundum lattice. After relaxation of the ideal supercell structure, the optimized $d_{Oi\text{-}VO}$ distance has been found to be ~4.5 Å while the formation energy of Frenkel pair has achieved 11.7 eV. The interstitial O_i atom, both single and a component of O_i+V_O pair, spontaneously forms a dumbbell with the adjacent atom in the regular oxygen sublattice ($d_{Oi\text{-}V_O}$ = 1.404 Å) with the induced charge -1.1 *e*. On the whole, possibilities of supercell model for proper description of Frenkel pairs with changing inter-defect distance and space orientation inside corundum crystal are rather limited. In order to simulate well-separated Frenkel pairs of varying length as well as charged and excited defects, a cluster model will be used in the next studies,

which also excludes artifacts caused by the periodic network of defect-defect interactions.

FIRST PRINCIPLES HYBRID DFT CALCULATIONS OF $BaTiO_3/SrTiO_3$ (001) INTERFACE

S. Piskunov and R.I. Eglitis

We performed *ab initio* calculations for $BaTiO_3/SrTiO_3$ (001) interfaces taking into account non-stoichiometric compositions. Using B3PW hybrid exchange-correlation functional inside the density functional theory (DFT) we demonstrate that charge redistribution in the interface region weakly affects the electronic structure of the studied material (**Fig. 9**).

The key effect found at $BaTiO_3/SrTiO_3$ (001) interfaces is strong dependence of the band gap on the external BaO or TiO_2 (001) termination. This effect is much stronger, than the dependence of the interface band gap on the number of augmented layers upon the substrate.

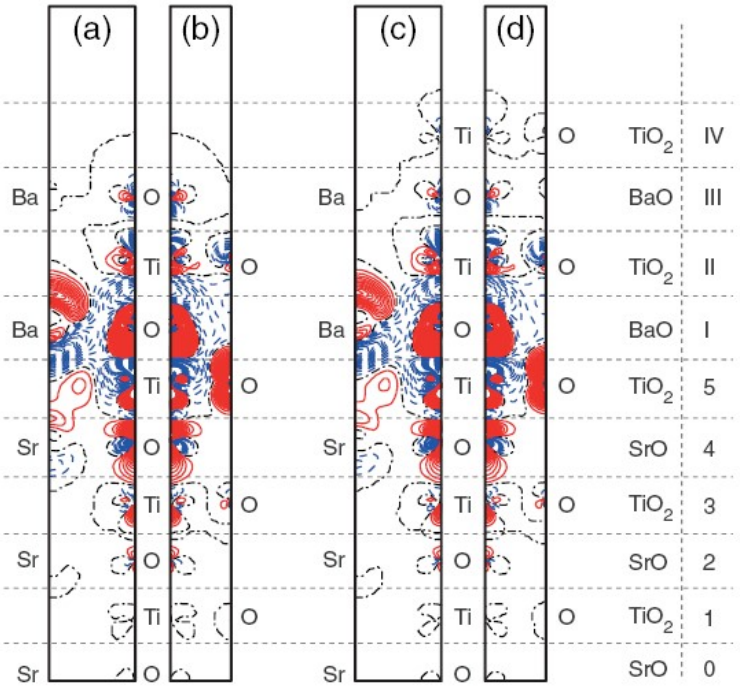


Figure 9. Difference electron charge density maps calculated for BTO/STO (001) heterostructures: (a) (110) cross-section for N_{BTO} = 3, (b) (100) cross-section for N_{BTO} = 3, (c) (110) cross-section for N_{BTO} = 4, (d) (100) cross-section for N_{BTO} = 4. Red solid (dark gray), blue dashed (light gray) and black dashed-dot isolines describe positive, negative and zero values of the difference charge density, respectively. Isodensity curves are drawn from -0.025 to +0.025 e Å^{-3} with an increment of 0.0005 e Å^{-3}. Right-side bar shows the atomic monolayers from which atoms are originated. STO and BTO monolayers are numbered beginning from the center of slab (0 means the central monolayer of the symmetrical slab unit cell). Monolayers are numbered separately for STO (001) substrate and for BTO (001) nanofilm using Arabic and Roman numbers.

FROM DETERMINATION OF THE FUGACITY COEFFICIENTS TO ESTIMATE OF HYDROGEN STORAGE CAPACITY: A CONVENIENT THEORETICAL METHOD

R. I. Eglitis, P. Fu, R. Jia, C.-P. Kong, , H.-X. Zhang

The equation of state (EOS) from virial expansion (VE) was used to pave the way for determining the fugacity coefficients of the hydrogen fluid at arbitrary temperature and pressure. The fugacity coefficients from our VE method have more physical meaning than the empirical values. In this way, the hydrogen storage capacity of a novel material model have been estimated *in a close collaboration with Beijing Institute of Technology, China*, using a few density functional theory (DFT) calculations with the aid of a continuum model.

The efficient continuum model can provide a more accurate estimation of the hydrogen storage capacity than the direct DFT calculations. Furthermore, the expensive grand canonical ensemble (μ_{NT}) simulations combining with the quantum mechanics methods (*i.e.*, QM/MD-μ_{NT}) are unnecessary within this method. The hydrogen fluid can be handled with our VE method at the temperature in the range of 160-773 K. The hydrogen storage capacity and the detailed thermodynamic information of a designed novel material can thereby be estimated using this method with relatively high accuracy and low computing cost. As an example, the hydrogen storage capacities of the expanded bilayer graphene systems were calculated. Our theoretical results are in an excellent agreement with experimental results.

CNTs- AND GNRs-BASED ELECTROMAGNETIC AND SPINTRONIC DEVICES: MODELS AND SIMULATIONS

Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N.Yu. Burlutskaya, T.D. Lobanova-Shunina, S. Bellucci

Fundamental electromagnetic and electromechanical properties of CNTs, graphene nanoribbons (GNR) and nanofibers (GNF), CNT- and graphene-based aerogels (CNTBA, GBA), CNT- and graphene-based 3D-nanofoams and carbon-based polymer nanocomposites are essential for various nanotechnology applications, *e.g.*, for engineering new classes of ultra-light, highly conductive nanomaterials with exceptional mechanical strength, flexibility, and elasticity. These nanomaterials are the basis for unique nanoelectronic devices and nanosensors. Particular properties of carbon-based nanoporous systems in dependence on porosity extent, morphology and fractal dimension allow finding practically useful correlations between their mechanical and electrical properties. Electromagnetic properties of CNTs and GNRs nanostructures with functionalized atomic groups and their various interconnects with the essential concentration of 'dangling bonds' are very sensitive to local external perturbations. The induced changes of local electronic density of states lead to the correlated changes of current and spin states. Models of nanocarbon spintronic devices are developed as memory nanodevices, particularly, based on magneto-resistance phenomena. Models of nanocomposite carbon-based materials and nanodevices are proposed (**Fig. 10**).

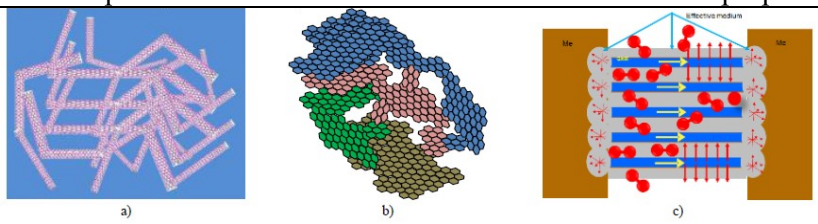


Figure 10. A set of models: a) structural model of CNTBA; b) model of GBA; c) GNRs-based gas nanosensor device.

The main objective of the current study is to demonstrate the implementation of advanced simulation models to ensure a proper description of the electronic properties, electrical conductivity, electromagnetic and electromechanical phenomena of

functionalized CNT- and GNR-based nanostructures of different morphologies and their interconnects for nanosensor and nanomemory systems. The sensitivity of the local electronic density of states to external influences (mechanical, chemical, magnetic, *etc*.) on the fundamental electromagnetic properties of CNTs, GNRs and their metal interconnects are analyzed from the point of view of nanosensor applications. We develop prospective models of nanocarbon-based nanomaterials and nanodevices which are based on various interconnects and interfaces.

B. Kinetics of processes with self-organization

EFFECTS OF PRESSURE, TEMPERATURE AND ATOMIC EXCHANGES ON PHASE SEPARATION DYNAMICS IN Au/Ni(111) SURFACE ALLOY: KINETIC MONTE CARLO STUDY

G. Zvejnieks, A. Ibenskas, E.E. Tornau

Instability of the Au/Ni(111) surface alloy has been studied under different CO gas pressure, p, and temperature limits, using the kinetic Monte Carlo simulations. We have analyzed the reaction front dynamics and formation of Au clusters, using the model which takes into account surface adatom pair- and three-body interactions, CO adsorption and desorption, catalytic carbonyl formation reaction, Au and Ni adatom diffusion and their concerted exchange. Variation of interaction parameters has allowed us to identify three possible reaction front propagation limits with different pressure dependencies (**Fig. 11**):

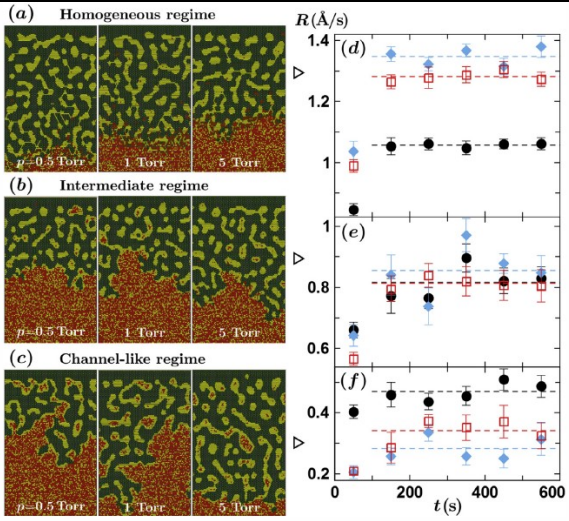


Figure 11. Lattice snapshots (90×40) at different pressures of CO gas and corresponding step-flow rates.

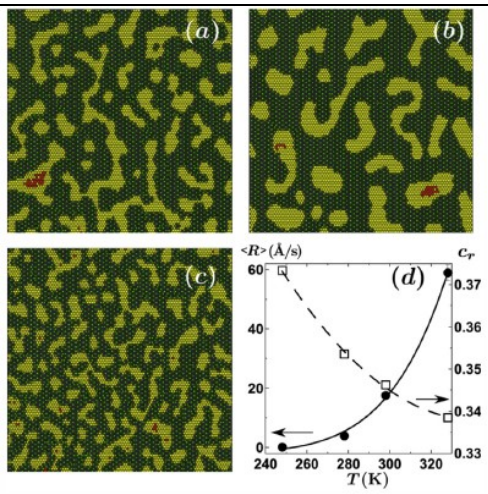


Figure 12. Lattice fragments (100×100) of Au islands at: (a) T=248 K, (b) T=328 K, (d) average SFR (solid line) dependence on temperature.

(*i*) slow channel-like flow in agreement with experimental data (Step Flow Rate – SFR, R, increases with p), (*ii*) intermediate regime (weak pedependence), and (*iii*) fast homogeneous flow (R decreases with p).

We have found that only Au-Ni exchange, contrary to both Ni-CO and Au-CO exchanges, significantly reduces the number of screened Ni atoms inside the Au clusters and stimulates the occurrence of Ni-free Au clusters. The size of Au islands depends on both pressure and temperature. At a fixed temperature it decreases with pressure due to an increased SFR. In the high temperature limit, despite the SFR exponential increase with temperature, the cluster size increases due to an enhanced Au mobility (**Fig. 12**).

ON CANONICAL QUANTIZATION OF ELECTRON-HOLE ACOUSTIC PHONON CRYSTALLINE SYSTEMS

E. Klotins

Methods of quantum electrodynamics are elaborated with application to consistent relativistic theory of open quantum systems. The study is motivated by developments of light-matter interaction which has excited interest in the description of important quantum systems for which interactions between the charged particles play a major role.
Special attention is paid to dielectrics and their interaction with electromagnetic (optical) radiation. The physical model includes spatially periodic structure of atoms supporting quasiparticles categorized as electrons, holes and accoustic phonons each having a complex influence on its neighbors and represents a challenge for extensively developing theory of condensed state. Particular problems are addressed to birth and annihilation of these quasi-particles, interacting both with the radiation and the acoustic oscillations of the ionic subsystem (phonons).
Obtained results include transition from the macroscopic description to the quantum kinetics for the constituting quasi-particles in a unified framework of nonstationary and nonequilibrium distribution functions. Rationale of these results is clues to dynamic effects induced by fempto-second light pulses and the relaxation of quasiparticles. Extensions that embody more complex models and higher order energy derivatives are available as advancement.

C. Plasma Physics

NON-STATIONARY OSCILLATIONS IN GYROTRONS REVISITED

O. Dumbrajs, H. Kalis

Development of gyrotrons requires detailed understanding of different regimes of gyrotron oscillations. It is known that in the planes of the generalized gyrotron variables: cyclotron resonance mismatch and dimensionless current or cyclotron resonance mismatch and dimensionless interaction length complicated alternating sequences of regions of stationary, periodic, auto modulation, and chaotic oscillations exist. In the past, these regions were investigated on the supposition that the transit time of electrons through the interaction space is much shorter than the cavity decay time. This assumption is valid for short and/or high diffraction quality resonators. However, in the case of long and/or low diffraction quality resonators, which are often utilized, this assumption is no longer valid. In such a case a different mathematical formalism has to be used for studying nonstationary oscillations. One example of such formalism has been described in our paper (**Fig. 13**).

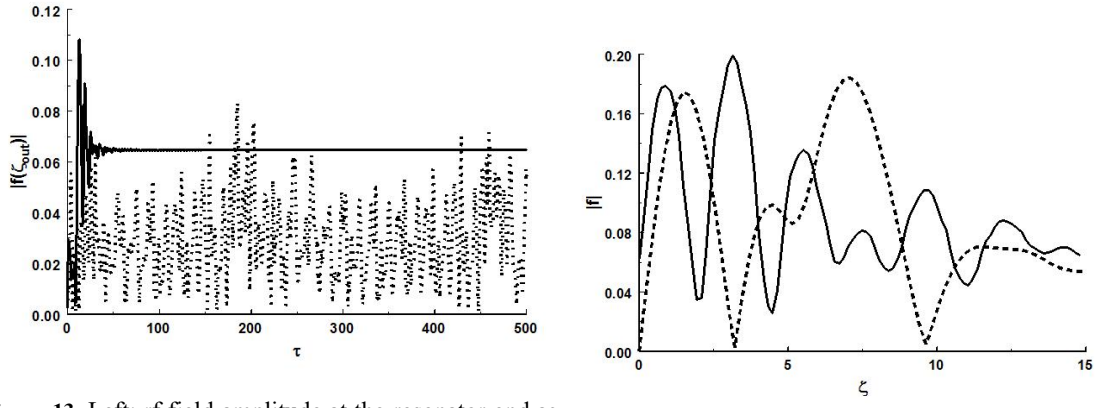


Figure 13. Left: rf field amplitude at the resonator end as

cavity. The solid curves were obtained when $t_{decay} >> t_{transit}$ ($t_{decay} \sim Q/\omega, t_{transit} = L/v_z$, Q is the quality factor, ω is the oscillation frequency, L is the interaction length, and v_z is the longitudinal velocity). (1) and (2) and the dashed curves when $t_{decay} \approx t_{transit}$.

FIELD FORMATION IN THE INTERACTION SPACE OF GYROTRONS

O. Dumbrajs,G.S. Nusinovich

For gyrotron applications in plasma installations, one of the most important factors is the gyrotron efficiency. To maximize the interaction efficiency, it is necessary not only to optimize such operating parameters as the magnetic field, beam voltage and current, but also the axial profile of the electromagnetic (EM) field in the interaction space.
In *collaboration with Institute for Research in Electronics and Applied Physics, University of Maryland*, we have performed a study of the effect of the profile of an irregular waveguide serving as a resonator on the axial structure of the EM field. Specific attention has been paid to the profile of the uptaper connecting the regular part of a resonator to the output waveguide (**Fig. 14**). Conditions of applicability of the nonuniform string equation, which is widely used in gyrotron designs for finding the axial structure of the EM field, were also discussed, as well as the occurrence of reflections from a smooth uptaper and the analogy between the nonuniform string equation and the stationary Schrödinger equation.

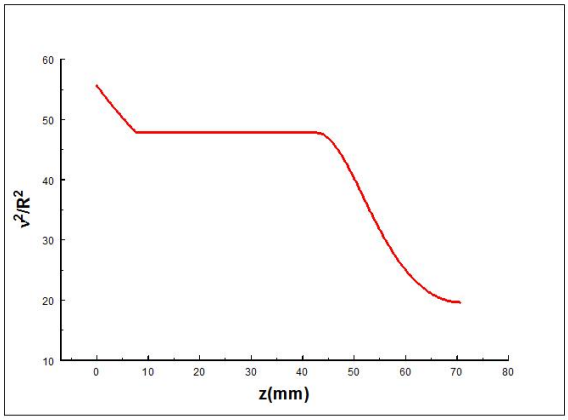


Figure 14. The well of the gyrotron potential in contrast to ordinary quantum mechanics potentials has no wall on the right hand side.

BIFURCATIONS AND FAST-SLOW DYNAMICS IN A LOW-DIMENSIONAL MODEL FOR QUASI-PERIODIC PLASMA PERTURBATIONS

O. Dumbrajs, D. Constantinescu, V. Igochine, K. Lackner, H. Zohm

Oscillations of plasma's parameters (saw teeth, edge localized modes, frequently interrupted regime of neoclassical tearing modes) are observed when some large scale plasma instabilities do not lead to an immediate termination of a discharge. The understanding of such phenomena is an important tool in controlling the whole reaction. There are many fundamental approaches to the subject, but, despite the huge theoretical and experimental efforts, these phenomena are not fully understood. We have focused on a low dimensional model which describes the dynamics of the plasma pressure gradient and of the amplitude of the magnetic field displacement.
Our low-dimensional model is given by

$$\begin{cases} \frac{d^2}{dt^2}\zeta = (p'-1)\cdot\zeta - \delta\cdot\frac{d}{dt}\zeta \\ \frac{d}{dt}p' = \eta\cdot(h - p' - \zeta^2\cdot p') \end{cases}$$

where ζ is the amplitude of the magnetic field displacement, p' is the plasma pressure gradient at the plasma edge, t is time, δ is dissipation/relaxation of the instability responsible for the ELM burst, η is diffusion and h is input power in the system. The first equation describes the evolution of the magnetic field perturbation and relaxation dynamics. The second equation describes power balance in the system including the effect of unstable modes.

This system is important both from a mathematical and a practical point of view. It was introduced in order to explain the quasiperiodic plasma dynamics observed in fusion experiments in Tokamaks. The system has some similar properties with the Lorenz system (dissipativity and symmetry). It is a fast-slow system. We have analyzed the stability of the equilibrium points studying some bifurcations of the system (pitchfork and Hopf bifurcations).

D. Experimental Studies

EXCITATION OF DIFFERENT CHROMIUM CENTRES BY SYNCHROTRON RADIATION IN MgO:Cr SINGLE CRYSTALS

A.I. Popov, E. Shablonin, A. Lushchik, S. Dolgov, A. Kotlov

Role of impurities, especially at their high concentrations, in the processes of the relaxation of the electronic excitation is still hot topic in radiation solid state physics. The excitation spectra for the emission of chromium-containing centres have been measured at 10 K using synchrotron radiation of 4–32 eV in MgO single crystals with different content of Cr^{3+} (5 to 850 ppm) and Ca^{2+} impurity ions. Both virgin crystals and the samples preliminarily irradiated with x-rays at 295 K have been studied.

Some typical spectra measured at DESY-synchrotron radiation facility are shown in **Fig. 15**

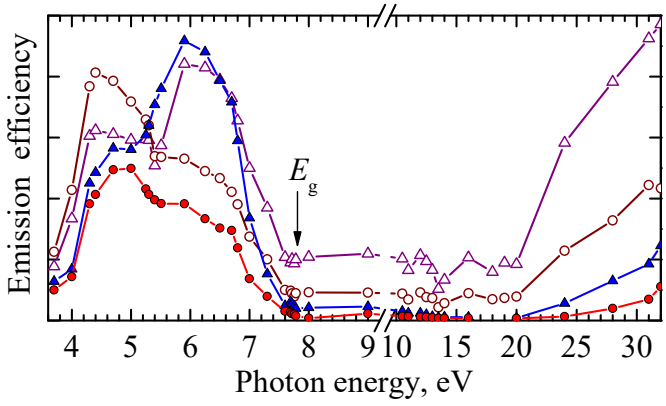


Figure 15. Excitation spectra of the emissions at 1.6 eV (▲, △) and 1.42 eV (●, ○) measured at 10 K for virgin (▲, ●) and x-irradiated (△, ○) MgO:Cr (850 ppm) crystals

The role of complex chromium centres containing two Cr^{3+} cations and a vacancy (sometimes nearby a Ca^{2+} ion) in the luminescence processes and the transformation/creation of structural defects has been analysed. According to **Fig. 15**,

the influence of preliminary X-irradiation on the excitation spectra for the emissions at 1.42 or 1.6 eV related to pair chromium centres at $h\nu > E_g$ is nearly the same as for R- and N-emission. However, below 7 eV the spectra difference for virgin and x-irradiated samples of MgO:Cr (850 ppm) is more complicated. It is worth noting that even a prolonged irradiation with $h\nu \sim 20$ eV at 10 K causes the recharging of some Cr^{3+} into Cr^{2+}. The intensity of Cr^{3+}-emission considerably decreases with a crystal cooling from 77 to 10 K. In our opinion, the effect is caused by the attenuation of the emission related to ^{54}Cr isotope with nuclear spin $I = 0$, while MgO:Cr (850 ppm) contains also ~80 ppm of ^{53}Cr ($I = 3/2$) ions the emission of which can be observed at 10 K.

FTIR STUDIES OF SILICON CARBIDE 1D-NANOSTRUCTURES

A. I. Popov,Karbovnyk, P. Savchyn, A Huczko, M Cestelli Guidi,

Stable 1D silicon carbide (SiC) nanostructures have been prepared *via* combustion synthesis route which is widely used for the fabrication of various nanomaterials. The examination of the raw reaction product (in the form of a powder) has shown that it actually consists of a mixture of SiC nanowires, distributed in diameter range from tens of nanometers to 100 nm, C nanocrystallites and remaining Si. In order to obtain pure SiC nanowires, wet-chemistry three-stage protocol was used. Structural studies have indicated that the obtained modification of SiC is 3*C* polytype with a cubic unit cell. The IR spectroscopy has been performed at SINBAD infrared beamline of Daphne Light synchrotron facility. IR absorption and reflection spectra for as-obtained and purified SiC nanowires have been compared with the spectra of commercially available SiC nanomaterials (**Figs. 16, 17**). Principal vibrational modes have been identified. Reflectivity spectrum has been reconstructed by modelling of the dielectric function (**Figs. 18, 19**).

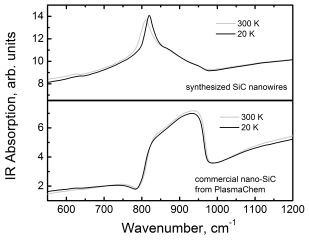


Figure 16. IR absorption spectra of SiC nanowires (upper part) as compared to the IR spectra of commercial SiC nanopowder.

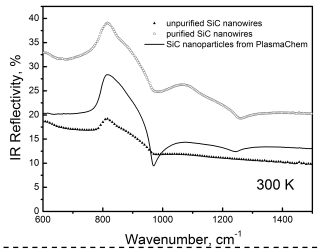


Figure 17. IR reflectivity of purified/unpurified SiC nanowires and commercial SiC nanopowder at 300 K.

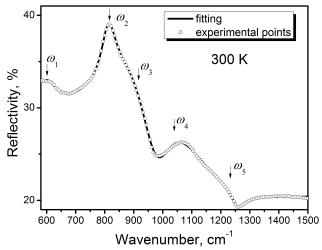


Figure 18. Experimental and calculated IR reflectivity of SiC nanowires. Arrows indicate the identified vibrational modes.

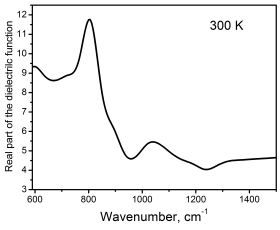


Figure 19. Real part of the dielectric function calculated for SiC nanowires in the frame of the factorized model.

The obtained frequencies of main vibrational modes of SiC nanowires are summarized in Table 1.

ω_{1TO}, cm^{-1}	ω_{1LO}, cm^{-1}	ω_{2TO}, cm^{-1}	ω_{2LO}, cm^{-1}	ω_{3TO}, cm^{-1}	ω_{3LO}, cm^{-1}	ω_{4TO}, cm^{-1}	ω_{4LO}, cm^{-1}	ω_{5TO}, cm^{-1}	ω_{5TO}, cm^{-1}
596	596	812	813	917	975	1018	1082	1258	1258

Obtained results show clear effect of nanostructure's morphology on the both IR absorption and reflectivity. In particular, vibrational modes, mostly depending on the morphology, were detected.

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29. I. Karbovnyk, P. Savchyn, A. Huczko, M. Cestelli Guidi, C. Mirri, and **A.I. Popov**, FTIR studies of silicon carbide 1D-nanostructures. - *Materials Science Forum*, 2015, 821-823, p. 261-264.

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1. **Yu.N. Shunin**, Spintronic Nanomemory and Nanosensor Devices (Lambert Academic Publishing, Saarbrücken), 2015, p. 2-49.

Non-SCI papers

1. S. Bellucci, F. Micciulla, **Yu.N. Shunin**, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and A. Capobianchi, Memory nanodevices based on carbon nanotube-Fe-Pt interconnects: Electromagnetic simulations and magnetically stimulated nanotube growth. - *J. Mater. Sci. Eng. B*, 2015, 5, p. 120-134.
2. **Yu.N. Shunin**, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, CNTs- and GNRs-based electromagnetic and spintronic devices: Models and simulations. - *Proc. Internat. Conf. „Physics, Chemistry and Application of Nanostructures (Nanomeeting-2015, Minsk, Belarus)"* (Eds. V.E. Borisenko, S.V. Gaponenko, V.S. Gurin, and C.H. Kam; World Scientific, New Jersey, London, Singapore, Beijing, Shanghai, Hong Kong, Taipei, Chennai), 2015, p. 207-210.
3. **Yu.N. Shunin**, S. Bellucci, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, and T. Lobanova-Shunina, Nanocarbon electromagnetics in CNT-, GNR- and aerogel-based nanodevices: models and simulations. - *Computer Modelling & New Technologies*, 2015, 19(1A), p. 35-42.
4. **Yu.N. Shunin**, S. Bellucci, **Yu.F. Zhukovskii**, T. Lobanova-Shunina, N. Burlutskaya, and V.I. Gopeyenko, Modelling and simulation of CNTs- and GNRs-based nanocomposites for nanosensor devices. - *Computer Modelling & New Technologies*, 2015, 19(5A), p. 14-20.
5. D. Fink, A. Kiv, **Yu.N. Shunin**, N. Mykytenko, T. Lobanova-Shunina, A. Mansharipova, T. Koycheva, R. Muhamediev, V. Gopeyenko, N. Burlutskaya, **Yu.F. Zhukovskii**, and S. Bellucci, The nature of oscillations of ion currents in the ion track electronics. - Computer Modelling & New Technologies, 2015, 19(6), p. 7-13.

PRESENTATIONS AT SCIENTIFIC CONFERENCES, MEETINGS, AND WORKSHOPS

I. 31th ISSP Conference (Riga, Latvia, February, 2015).

1. **O. Dumbrajs**, "Applications of girotrons for studies of particles in nuclear and solid state physics". Abstract: p. 21.
2. **A. Platonenko**, **S. Piskunov**, **Yu.F. Zhukovskii**, and **E.A. Kotomin**, "Ab initio simulations on neutral point defects and Frenkel pairs in corundum". Abstract: p. 40.
3. **A. Gopejenko**, **Yu.F. Zhukovskii**, P.V. Vladimirov, **E.A. Kotomin**, **Yu.A. Mastrikov**, V.A. Borodin, and A. Möslang, "Ab initio calculations of Y, O and V_{Fe} diffusion barriers inside fcc-Fe lattice". Abstract: p. 41.
4. **A. Chesnokov**, **O. Lisovski**, **D. Bocharov**, **S. Piskunov**, and **Yu.F. Zhukovskii**, "Connection between electronic structure of TiO_2 nanotubes and their morphology: Ab initio study". Abstract: p. 42.
5. **M. Sokolov, Yu.A. Mastrikov,** and **E.A. Kotomin,** "Optimization of the electron charge density integration parameters using the Bader method". Abstract: p. 74.

II. 9th International Conference on Materials Science & Engineering, BRAMAT2015 (Brasov, Romania, March, 2015).

6. **R. I. Eglitis**, "Towards a practical rechargeable 5 Volt Li ion battery using $Li_2CoMn_3O_8$ as a battery cathode material". Abstract: p. 24.
7. **R. I. Eglitis**, "Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ and $CaTiO_3$ perovskite (001), (011) and (111) surfaces". Abstract: p. 25.
8. **R.I. Eglitis**, H. Shi, and R. Jia, "Large scale ab initio calculations of the diffusion and aggregation of F centers, as well as bulk and nano-surface H centers in CaF_2, BaF_2 and SrF_2". Abstract: p. 282.

III. 49th Russian School on Condensed State Physics (St. Petersburg, Russia, March, 2015).

9. **A. Platonenko, S. Piskunov, Yu.F. Zhukovskii,** and **E.A. Kotomin**, "Ab initio simulation of point defects and Frenkel pairs in corundum crystal". Abstract: p. 168.

IV. 4th International Conference "Multifunctional, Hybrid and Nanomaterials (Barcelona, Spain, March, 2015).

10. **A.I. Popov,** V.P. Savchyn, **A. Moskina**, E. Elsts, and **R.I. Eglitis**, "Comparative studies of cathodoluminescence properties of $BaZrO_3$, $SrTiO_3$ and KBr crystals". Abstract: P3.289.

V. PSI Nuclear Materials Workshop (Meiringen, Switzherland, March, 2015).

11. **D. Bocharov,** M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J. Purans, and **E.A. Kotomin**, "Simulation of chromia-doped uranium dioxide".

VI. 13th International Conference "Information Technologies and Management", IT&M'2015 (Riga, Latvia, April, 2015).

12. **Yu.N. Shunin,** D. Fink, S. Bellucci, A.E. Kiv, T. Lobanova-Shunina, **Yu.F. Zhukovskii**, and V.I. Gopeyenko, "Nanotechnology and health nanodiagnostic tools". Abstract: p. 15-17.

13. **Yu.N. Shunin**, S. Bellucci, T. Lobanova-Shunina, **Yu.F. Zhukovskii**, N. Burlutskaya, and V.I. Gopeyenko,"Models and simulations of CNTs- and GNRs-based electromagnetic and spintronic devices". Abstract: p. 18-20.

14. **A. Gopejenko**, **Yu.F. Zhukovskii**, P.V. Vladimirov, V.A. Borodin, **E.A. Kotomin, Yu.A. Mastrikov,** and A. Möslang, "Ab initio calculations of Y, O and V_{Fe} migration barriers inside fcc-Fe lattice". Abstract: p. 21.
15. **Yu.F. Zhukovskii**, R.A. Evarestov, and A.V. Bandura, "Photocatalytic efficiency of $SrTiO_3$ nanowires: ab initio modeling". Abstract: p. 22-23.
16. **A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov**, and **Yu.F. Zhukovskii**, "Correlation between morphology of TiO_2 nanotubes and their photocatalytic abilities: ab initio study". Abstract: p. 28-29.
17. **A. Platonenko**, **Yu.F. Zhukovskii**, **S. Piskunov**, and **E.A. Kotomin**, "Ab initio simulations on interstitial oxygen atom in corundum". Abstract: p. 31.

VII. International Workshop "Advanced Methods of Oxide Materials Characterization" (Riga, Latvia, April, 2015).

18. **D. Gryaznov** and **E.A. Kotomin**, "Hybrid density functional calculations on bulk and surface properties of $(La,Sr)FeO_3$".
19. **A.I. Popov**, "VUV luminescence spectroscopy of perovskites".

VIII. E-MRS 2015 Spring Meeting (Lille, France, May, 2015).

20. **R.I. Eglitis**, "Towards a practical rechargeable 5 V Li ion battery". – Abstract: A.9.15.
21. **A. Chesnokov**, **O. Lisovski**, **D. Bocharov**, **S. Piskunov**, and **Yu.F. Zhukovskii**, "Ab initio simulations on pristine and doped TiO_2 anatase (101) nanotubes". – Abstract: B/P1.7.
22. G. Kaptagai, T.M. Inerbaev, A.T. Akilbekov, **Yu.A. Mastrikov**, and **E.A. Kotomin**,"Theoretical modeling of water adsorption on the fluorine-doped Co_3O_4 (111) surface". – Abstract: B/P2.23.
23. V.P. Savchyn, O.I. Aksimentyeva, Yu.Yu. Horbenko, I. Karbovnyk, and **A.I. Popov**, "Cathodoluminescence study of polystyrene–$BaZrO_3$ hybrid composites". – Abstract: C/P1.54.
24. **D. Bocharov**, M. Chollet, M. Krack, A. Kuzmin, J. Bertsch, D. Grolimund, and M. Martin, "Theoretical modeling of pristine and chromium-doped UO_2". – Abstract: F.1.4.
25. **Yu.F. Zhukovskii**, **A. Platonenko**, **S. Piskunov**, and **E.A. Kotomin**, "Ab initio computer simulations of radiation defects in corundum". – Abstract: G.2.2.
26. V.M. Lisitsyn, L.A. Lisitsyna, **E.A. Kotomin**, **A.I. Popov**, and J. Maier, "The peculiarities of the excitonic mechanism of defect formation and stabilisation in fluorides". – Abstract: G.2.3.
27. A.Ch. Lushchik, Ch.B. Lushchik, **A.I. Popov**, K. Schwartz, E. Shablonin, O. Sidletskiy, and E. Vasil'chenko, "Influence of complex impurity centers on radiation damage in wide-gap metal oxides". – Abstract: G.5.3.
28. **V.N. Kuzovkov**, **E.A. Kotomin**, **A.I. Popov**, and R. Vila, "Kinetics of radiation-induced colloid formation in Al_2O_3 and NaCl crystals". – Abstract: G.6.4.
29. **S. Piskunov** and **R.I. Eglitis**, "Ab initio calculations of F center in $SrZrO_3$ bulk and (001) surfaces as well as $SrTiO_3/BaTiO_3$ and $SrZrO_3/PbZrO_3$ (001) interfaces". – Abstract: G/P.3.
30. **Yu.A. Mastrikov**, P.V. Vladimirov, V.A. Borodin, **A. Gopejenko**, **Yu.F. Zhukovskii**, **E.A. Kotomin**, and A. Möslang, "Interaction of yttrium and oxygen with vacancy clusters within bcc-Fe matrix". – Abstract: G/P.11.

31. **A.I. Popov**, **E.A. Kotomin**, and J. Maier, “Analysis of the self-trapped hole center mobility and recombination in alkali halides and complex metal halides”. – Abstract: G/P.20.
32. I. Bolesta, I. Karbovnyk, I. Rovetskii, S. Velgosh, and **A.I. Popov**, “Morphological evolution of nanostructures in long-term annealed CdI_2 crystals”. – Abstract: H/9P.39.

33. M. Arrigoni, T.S. Bjørheim, **E.A. Kotomin**, and J. Maier, “First principles thermodynamics of oxygen vacancies in ultrathin films of $BaZrO_3$”. – Abstract: M.11.3.
34. E. Heifets, **E.A. Kotomin**, R. Merkle, and J. Maier, “Ab initio study of $BiFeO_3$ stability.” – Abstract: M/P.13.
35. **Yu.A. Mastrikov**, **E.A. Kotomin**, R. Merkle, M.M. Kuklja, and J. Maier, “Ab initio modelling of oxygen vacancies formation and migration in the bulk and on the surface of complex perovskites for solid oxide fuel cell cathodes”. – Abstract: M/P.31.
36. V. Dimza, **A.I. Popov**, L. Kundzina, M. Kundzins, K. Kundzins, M. Livins, and M. Antonova, “Effects of Mn doping on dielectric properties of ferroelectric relaxor PLZT ceramics”. – Abstract: M/P.61.
37. A.U. Abuova, **E.A. Kotomin**, **Yu. A. Mastrikov**, T.M. Inerbaev, and A.T. Akilbekov, “$LaMnO_3$ (001) surface doping with Ag and its catalytic effect on the oxygen reduction”. – Abstract: N/P1.9.
38. A. Usseinov, **E.A. Kotomin**, A.T. Akilbekov, **Yu.F. Zhukovskii**, J. Purans, and F. Abuova, “Hydrogen migration and stability in ZnO: Ab initio calculations”. – Abstract: N/P2.27.
39. **E.A. Kotomin**, M.M. Kuklja, D. Fuks, **Yu.A. Mastrikov**, and J. Maier, “Structural stability of complex perovskites for solid oxide fuel cells from first principles calculations”. – Abstract: N/P2.35.
40. **R.I. Eglitis**, “Point defects as well as (001), (011) and (111) surfaces in ABO_3 perovskites”. – Abstract: O/P.18.

IX. International Conference NANOMEETING-2015 (Minsk, Belarus, May, 2015).

41. **Yu.N. Shunin**, **Yu.F. Zhukovskii**, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "CNTs- and GNRs-based electromagnetic and spintronic devices: Models and simulations".

X. 227th Electrochemical Society Meeting (Chicago, USA, May, 2015).

42. T.S. Bjoerheim, **E.A. Kotomin**, and J. Maier, "Defect chemistry of CeO2 surfaces from first principles and space charge theory". - Abstract: 1775.

XI. MMA2015 (Sigulda, Latvia, May, 2015).

43. **O. Dumbrajs** and H. Kalis, “On numerical simulation of nonstationary oscillations in gyrotrons”.

XII. Platform for Advanced Scientific Computing Conference PASC15 (Zurich, Switzerland, June, 2015).

44. **D. Bocharov**, M. Krack, and A. Kuzmin, "EXAFS spectra interpretation using molecular dynamics and DFT simulations". – Abstract: M/P.13.

XIII. EuroNanoForum-2015 (Riga, Latvia, June, 2015).

45. A.V. Bandura, R.A. Evarestov, and **Yu.F. Zhukovskii**, “Comparative analysis of four-faceted [001]-oriented nanowires formed from TiO_2 rutile and $SrTiO_3$ cubic phases: Ab initio simulations”.
46. **A. Chesnokov**, **O. Lisovski**. **S. Piskunov**, **D. Bocharov**, and **Yu.F. Zhukovskii**, “Photocatalytic properties of doped TiO2 nanotubes: Prediction from first principles”.

47. **R.I. Eglitis**, “Ab initio calculations of point defects as well as (001), (011) and (111) surfaces in ABO3 perovskites”.
48. **Yu.N. Shunin,** V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, S. Bellucci, and **Yu.F. Zhukovskii**, “Electromechanical properties of carbon-based nanocomposites for pressure and temperature nanosensors”.

XIV. 20th International conference on Solid State Ionics (Keystone Colorado, USA, June, 2015).

49. **E.A. Kotomin, Yu.A. Mastrikov,** R. Merkle, M.M. Kuklja, and J. Maier, "First principles calculations of formation and migration of oxygen vacancies in the bulk and on surface of complex perovskites for solid oxide fuel cell cathodes". Abstract: D4.04.
50. T.S. Bjorheim, **E.A. Kotomin**, and J. Maier, "Defect chemistry of CeO_2 surfaces from first principles and space charge theory". Abstract: D8.07.
51. M.M. Kuklja, **E.A. Kotomin**, D. Fuks, **Yu.A. Mastrikov**, and J. Maier, "Structural stability of complex perovskites for solid oxide fuel cells from first principles calculations". Abstract: A2.01.
52. M. Arrigoni, **E.A. Kotomin**, J. Maier and T.S. Bjorheim, "First principles thermodynamics of oxygen vacancies in ultrathin films of $BaZrO_3$". Abstract: A2.04.

XV. 11th International Conference on Diffusion in Solids and Liquids DSL-2015 (Munich, Germany, June, 2015).

53. **V.N. Kuzovkov** and **E.A. Kotomin**, "Static and dynamic screening effects in diffusion-controlled self-assembly of charged nanoparticles". Abstract: p. 153.

XVI. 27th Joint Russian-German Workshop on ECRH and Gyrotrons (Greifswald, Germany, June, 2015).

54. **O. Dumbrajs** and G.S. Nusinovich, “Field formation in the interaction space of gyrotrons”.

XVII. 28th International Conference on Defects in Semiconductors (Helsinki, Finland, July, 2015).

55. **D. Gryaznov**, R. Merkle, and **E.A. Kotomin**, "Hybrid density-functional calculations on oxygen vacancy behaviour in complex perovskite oxides". Abstract: p.22.
56. **R.I. Eglitis**, Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ and $CaTiO_3$ perovskite (001), (011) and (111) surfaces. Abstracts: p.30.
57. **R.I. Eglitis**, H. Shi and R. Jia, First principles calculations of the diffusion and aggregation of F centers, as well as bulk and surface H centers in CaF_2, BaF_2 and SrF_2. Abstracts: p.30.
58. **R.I. Eglitis** and **S. Piskunov**, First principles hybrid DFT calculations of F centers in $SrZrO_3$ bulk and (001) surfaces, as well as $SrTiO_3$/$BaTiO_3$ and $SrZrO_3$/PbZrO3 (001) interfaces. Abstracts: p.30.
59. **R.I. Eglitis,** Towards a practical rechargeable 5 Volt Li ion battery. Abstracts: p.30.

XVIII. 16th International Conference on X-ray Absorption Fine Structure XAFS16 (Karlsruhe, Germany, August, 2015).

60. **D. Bocharov**, M. Krack, A. Kalinko, J. Purans, F. Rocca, S.E. Ali, and A. Kuzmin, ”Ab initio molecular dynamics simulations of the Sc K-edge EXAFS of scandium trifluoride”. Abstract: p. 107.
61. J. Purans, **S. Piskunov**, **D**. **Bocharov**, A. Kalinko, A. Kuzmin, and F. Rocca, ”Local structure of perovskites ReO_3 and ScF_3 with negative thermal expansion: interpretation beyond the quasiharmonic approximation”. Abstract: p. 141.
62. **D. Bocharov**, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, A. Kuzmin, J. Purans, and **E.A. Kotomin**, ”Interpretation of the U L3-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations”. Abstract: p.153.

XIX. 6th International Conference Diffusion Fundamentals (Dresden, Germany, August, 2015).

63. J.R. Kalnins, **E.A. Kotomin**, and **V.N. Kuzovkov**, "Effective diffusion coefficient in one-dimensional heterogeneous solids: a comparison of continuous and discrete lattice models". Abstract: p.27.
64. **V.N. Kuzovkov, E.A. Kotomin, A.I. Popov**, and R. Vila, "Diffusion-controlled kinetics of metallic colloid formation in irradiated Al_2O_3, MgO and NaCl crystals". Abstract: p.30.
65. **V.N. Kuzovkov**, **G. Zvejnieks**, and **E.A. Kotomin**, " Diffusion and self-assembly of charged nanoparticles in polar media: a competition between short-range and long-range interactions". Abstract: p.31.

XX. 40th International conference on Infrared, Millimeter and Terahertz Waves (Hong Kong, August, 2015).

66. **O. Dumbrajs,** E.M. Khutoryan, and T. Idehara, “Hysteresis and frequency tenability of gyrotrons”.

XXI. JA-EU-US RF Heating Technology Workshop (Tokyo, Japan, August – September, 2015).

67. **O. Dumbrajs,** E.M. Khutoryan, and T. Idehara, “Hysteresis and frequency tenability of gyrotrons”.

XXII. Solid state electrochemistry workshop (Roggensburg, Germany, September, 2015).

68. **E.A. Kotomin**, **D. Gryaznov**, **and Yu.A. Mastrikov**, "Defects in complex perovskites for electrochemical applications".

XXIII. E-MRS 2015 Fall Meeting, Symposium J (Ferroic perovskites for advanced materials) (Warsaw, Poland, September, 2015).

69. **D. Gryaznov**, M. Arrigoni, **E.A. Kotomin**, and **A.I. Popov**, "Hybrid DFT calculations of the electronic and phonon properties of defects in perovskite oxides". Abstract: J6.

XXIV. 3rd International School-Conference on Atomistic Simulations of Functional Materials (Moscow, Russia, October 2015).

70. **E.A. Kotomin,** "Ab initio calculations of defects in complex perovskites for energy applications".

XXV. 11th International Conference "Functional Materials and Nanotechnologies" FM&NT-2015 (Vilnius, Lithuania, October, 2015).

71. **Yu.N. Shunin**, S. Bellucci, **Yu.F. Zhukovskii,** T. Lobanova-Shunina, N Burlutskaya, and V.I. Gopeyenko, "Modeling and simulation of CNTs- and GNRs-based nanocomposites for nanosensor devices". Abstract: p. 45.

XXVI. COST Action CM1104 "Reducible oxides" meeting (Salzburg, Austria, October, 2015).

72. **E.A. Kotomin, Yu.A. Mastrikov**, M.M. Kuklja, D. Fuks, and J. Maier, "Structural stability of complex perovskites for solid oxide fuel cells: first principles calculations". Abstract: p. 15

73. **Yu.A. Mastrikov, E.A. Kotomin,** R. Merkle, M.M. Kuklja, and J. Maier, "Ab initio modeling of oxygen vacancy on LSCF surface". Abstract: p. 16

XXVII. First Workshop on Research into Nuclear Fuel in Europe and Materials Modeling and Simulation for Nuclear Fuels Workshop (Karlsruhe, Germany, November, 2015).

74. M. Krack, **D. Bocharov**, and A. Kuzmin, "Analysis of U L3-edge X-ray absorption spectra for uranium dioxide based on molecular dynamics simulations". Abstract: P.5.3.

XXVIII. Advances in Materials and Processing Technologies conference AMPT (Madrid, Spain, December, 2015).

75. M. Krack, **D. Bocharov**, and A. Kuzmin, "Structural and electronic properties of chromium doped uranium dioxide". Abstract: RE 7.

LABORATORY OF RADIATION PHYSICS

Head of laboratory Dr. habil. phys. J.Berzins

RESEARCH AREA AND MAIN PROBLEMS

The following main investigations are
developed in the laboratory:
- experimental and theoretical investigation of nuclear structure at medium and high excitation energies;
- development of the nuclear spectroscopy methods for the identification of radioactivity and nuclear materials in Latvia;
- development of gamma spectrometric methods for investigation of radionuclides, their migration in the environment, soils and ground waters in the most potentially polluted regions of Latvia;
- application of the liquid scintillation methods for the monitoring of tritium content in environment and drinking waters of food industry;

INTERNATIONAL PROJECTS:

Participation in the project **„Investigation of nuclear structure via (n,γ), (d,p) and (d,t) nuclear reactions"** with Institute of Nuclear Physik (Rzez, Czech Republic), Technical University Munich, Institute Laue -Langevin (Grenoble, France).

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Dr.hab. M.Balodis
Dr. L.Simonova
Dr. T. Krasta
Dr. D.Riekstina
Dr. O.Veveris

SCIENTIFIC VISITS ABROAD

Dr. hab. J. Berzins, European Commission Euratom, Brussels, Belgium (2 days)
Dr. D. Riekstina, Int. Conf . on Radiation and Appl. in various Fields of Research, June 8-12, 2015, Budva, Montenegro.
Dr. D. Riekstina, 25th. Seminar on Activation Analysis and Gamma Spectroscopy (SAAGAS), Aachen, Germany, 23.-25. February 2015
Dr. D. Riekstina, 25th. Seminar on Activation Analysis and Gamma Spectroscopy (SAAGAS), Aachen, Germany, 23.-25. February 2015

COOPERATION

Latvia
1. University of Latvia, Institute of Chemical Physics (Dr. G. Kizane)
2. Institute of Silicate Materiuals, Riga Technical University (Dr. hab.ing.V. Svinka)

USA
1. Mississippi University (Prof. A.Afanasjev).

Germany

1. Technical University Munich (Prof. T. von Egidy, Dr. H.-F. Wirth)

France

1. Institute Laue-Langevin, Grenoble, France (Dr. M. Jentchel).

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2. Department of Physics, Acadia University, Wolfville, NS (Dr.S.Barkanova)

Czech Republik

1. Nuclear Research Institute, Řež (Dr. I.Tomandl).

Denmark

Riso National Laboratory, Roskilde, (Dr. S. Nielsen)

MAIN RESULTS

STUDY OF ^{186}Re NUCLEAR LEVEL STRUCTURE

T. Krasta, J. Bērziņš, L. Simonova

The doubly-odd ^{186}Re nucleus (Z=75, N=111) is situated on the very edge of the deformed nuclei region with 150≤A≤190. It is a close neighbour to the ^{188}Re nucleus which was an object of our previous studies [1,2]. Experimental and theoretical studues of ^{188}Re structure allowed us to establish coexistence of axially-symmetric and non-axial states related with high j orbits. A comparison of ^{186}Re and ^{188}Re level structures would provide valuable information about nuclear shape phase transition in odd-odd nuclei of the A~190 region.

The ^{185}Re$(n_{th},\gamma)^{186}$Re reaction measurements have been performed at the high flux reactor of ILL. The target was made of metallic rhenium powder with enrichment to 97% of ^{185}Re. Secondary γ-ray spectra of ^{186}Re have been measured in the energy range from 100 keV to 2 MeV with the high-resolution crystal-diffraction spectrometer GAMS5. Evaluation of spectra in the first, second, and third reflection orders allowed to determine energies and intensities of more than 500 γ-lines assigned to ^{186}Re. Obtained γ-line energies have higher precision than those of the earlier crystal-diffraction measurements [3], especially in the energy range above 300 keV.

The present model-independent level scheme of ^{186}Re [4] includes ~50 levels with excitation energies up to 1 MeV. Most of intense γ-line energies obtained in our GAMS5 measurements have been assigned to transitions linking these levels. It allowed to determine energy values for all earlier known ^{186}Re levels with higher precision. Work at further development of the ^{186}Re level scheme is in progress using new spectroscopic information obtained both in our thermal neutron capture measurements, as well as that of the ^{187}Re$(p,d)^{186}$Re reaction measurements [5] performed with Munich Q3D spectrograph. Especial attention is given to positive parity level system which is less confident and where one has many unresolved structure problems.

Both ^{186}Re, and ^{188}Re have the same ground state configuration $K^{\pi}=1^{-}$ (p:5/2[402]-n:3/2[512]). Just like in the case of ^{188}Re, structure of the ^{186}Re levels has been interpreted in terms of proton orbits 5/2[402], 9/2[514], and neutron orbits 1/2[510], 3/2[512], 7/2[503], 9/2[505], 11/2[615] using the results of theoretical calculations in the frameworks of axially-symmetric two-quasiparticle plus rotor model. However, due to the two neutron difference, the level scheme of ^{186}Re is essentially different from that of its heavier neighbour. The most prominent differences are: absence of the low-lying $K^{\pi}=0^{+}$ band, and presence of the long-living $K^{\pi}=8^{+}$ isomeric level in the level scheme of ^{186}Re.

Unlike his neighbour, the ^{186}Re nucleus has strong axially-symmetric deformation (ε_2=0.21, ε_4=0.07). It is manifested also by the lower moment of inertia parameter, and lessened impact of valence particle spin polarization on residual NN-interaction. However, the effects due to presence of high j valence particle orbits is observed in

^{186}Re as well. For instance, one can reproduce the $K^{\pi}=8^{+}$ (p:5/2[402]+n:11/2[615]) isomeric state at 149.81 keV only by rising the mean field spin-orbital interaction parameter μ value for the N=6 shell. Therefore, in order to reproduce correctly single-particle states of transitional nuclei at A~190, where high j orbits are of utmost importance, one should use the Woods-Saxon potential. Or apply more advanced theory based on the relativistic mean field approach which accounts for spin-orbital interaction innately.

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RESULTS OF THE RADIONUCLIDE MONITORING IN THE VICINITY OF SALASPILS NUCLEAR REACTOR (1997- 2015)

D.Riekstina, J.Berzins, T.Krasta, J.Rudzitis

The now decommissioned Salaspils nuclear research reactor (SNR) near Riga was in operation from 1961 to 1998 which could have caused a pollution of the closest surrounding territory with artificial radionuclides. Within time lapse, nuclear reactor's first circuit water contains the products of neutron activation of micro impurities, the radioactive substances of metal coating corrosion, and also the nuclear fuel fission products. The last ones diffuse in the water through micro splits of the fuel ambient shells. The use of beryllium (Be) cassettes for neutron reflection in the reactor core resulted in the production of tritium which has leaked into basin water and further from the first circuit water in the environment. The aim of presented work is to provide an assessment of the accumulation of artificial radionuclides: Cs-137, Co-60, and H-3, as well as their migration in the soil and ground waters in the vicinity of the shut-down SNR.

The activity monitoring of γ and β radionuclides in the ground waters around SNR was started in 1990. For that purpose**,** 19 control-wells (at depth from 4 to 9 m) have been made at distances ca. 5 to 50 m from the reactor tank and special sewage basins. The tritium monitoring of ground waters is carried out since 1997. The high-resolution gamma-spectrometry method was used to measure concentrations of Co-60 and Cs-137 in the water. The first radionuclide characterizes neutron activation products, the second – fission products. The measurements of H-3 activity in water [1] were carried out with the liquid scintillation spectrometer Packard TRI-CARB 2100 and Hidex 300SL using the scintillation liquid OptiPhase HiSafe 3Ô.

The monitoring was continued also after the transfer of the fuel ambient shells to the storage-well. It has been found that the content of Co-60 in water has significantly decreased since walls of the storage-well do not contain activation products. In the end of 2014, a water leakage from the waste storing basins to ground water has been established due to corrosion of the storage basin walls. The frequency and thoroughness of the ground water monitoring measurements has been increased. We present the obtained dynamics of radionuclide concentration in ground waters of the SNR territory in dependence on time and location.

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NATURAL RADIOACTIVITY IN CLAY AND BUILDING MATERIALS USED IN LATVIA

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This paper presents the results of natural radionuclide concentration and activity index study in materials used for construction in Latvia. Special attention is given to clay and clay ceramics. Concentrations of K-40 and Th-232, U-238 radioactivity were determined using gamma-spectrometry method. In some building wares, maximal concentration of K-40 was 1440 Bq/kg, and of U-238 – 175 Bq/kg. In granite, established maximal concentration of Th-232 was 210 Bq/kg. It was found that radionuclide content in different period clay deposits can differ more than two times, and up to five times in different clay ceramics. The results obtained are compared with analogous data from the other Baltic and North European countries.

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LABORATORY OF ELECTRONIC ENGINEERING

Head of Laboratory *Dr. phys.* A. Kristins

MAIN PROBLEMS

1. Implement developing and manufacturing of unique measuring and monitoring apparatus and systems, which:
   - provide authorised access on the base of Touch Memory™ elements and Proximity Cards to different objects, including
     - ⇒ entrance check-points (entrance gates, access control systems, systems for multilevel parking buildings etc.);
     - ⇒ computers and programmes;
     - ⇒ car and other technical devices (anti-theft systems);
   - execute electronic documentation functions (Touch Memory™ -based electronic invoices, credit cards and so on);
   - test power units (high-voltage switches, automatic disconnecting switches, power-transformers);
   - determine a content of heavy metals (As, Cd, Co, Cu, Fe, Hg, Tl, Ni, Pb, Sn, Zn, Bi, Mn) in liquids, ground, food-stuffs;
   - check various environment parameters (temperature, lighting, humidity, radiation level);
   - control temperature and lighting at the different objects (housings, hothouses, production storehouses);
   - are used in medicine and for determining of agricultural production parameters (digestion systems, fluorimetres, fall number determinators).
   - drive and management of automatic devices.
2. Provide physical measuring and manufacturing process automation.
3. Also solve the other problems, not afore-mentioned.

SCIENTIFICAL STAFF

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4. P.Kalinikovs

COOPERATION

Latvia

1. Joint-stock company *Augstsprieguma tīkls*
2. „*Fonons*" Ltd
3. Riga Technical University
4. *AlphaMedia* Ltd
5. *Loks* Ltd,
6. „*ADI Kartes*" Ltd
7. *GROG* Ltd
8. *Energoremonts Rīga* Ltd
9. *"LDZ apsardze"* Ltd.

Estonia

1. Tallinn University of Technology
2. Competence Centre ELIKO

OUR CLIENTS

1. Latvijas Krājbanka;
2. Latvijas Pasts;
3. *LatRosTrans*; Ltd;
4. Latvijas Kuģniecība ;
5. Latvijas Gāze;
6. Latvian Environment Agency;
7. Latvian Hydrometeorological Agency;
8. Latvijas Dzelzceļš;
9. *Augstceltne* Ltd;
10. CSDD (Road Traffic Safety Directorate);
11. *Avantime Amusement Technology* Ltd;
12. Joint-stock company *Latvenergo;*
13. Latvia's Ministry of Foreign Affairs;
14. *Nienhaus & Lotz Lettland* Ltd;
15. *Godske Latvian Textile* Ltd;
16. *VAIDE* Ltd;
17. *Flexoplastic* Ltd

etc.

LECTURES ON CONFERENCES

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