Institute of Solid State Physics

University of Latvia

ANNUAL REPORT

2016

Riga 2016

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Riga, Institute of Solid State Physics, University of Latvia, 2017, p.136

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INTRODUCTION

The research in solid state physics at the University of Latvia restarted after World War II. The **Institute of Solid State Physics** (ISSP) of the University of Latvia was established on the basis of Laboratory of *Semiconductor Research* and Laboratory of *Ferro- and Piezoelectric Research* in 1978. 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 our 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 M EUR has increased our research activities, particularly extending the list of our research partners and scientists who come to work to our Institute from the leading European research centres.

Next step of CAMART was in 2015, when ISSP won Horizon 2020 Teaming project: "**The Excellence Centre of Advanced Material Research and Technology Transfer – CAMART^2"**. 169 proposals were submitted, however only 31 were selected to develop their Business Plans. Between them with a score 14,5 (from 15) was the only project from Latvia submitted by the ISSP 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 was elaborated, demonstrating the long - term science and innovation development strategy.

The Business Plan was highly estimated in second phase of Horizon 2020 Teaming project dedicated to the establishment of significantly stronger Centre of Excellence during 2017 – 2023.

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 15 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. New elections of the Council was in 2016.

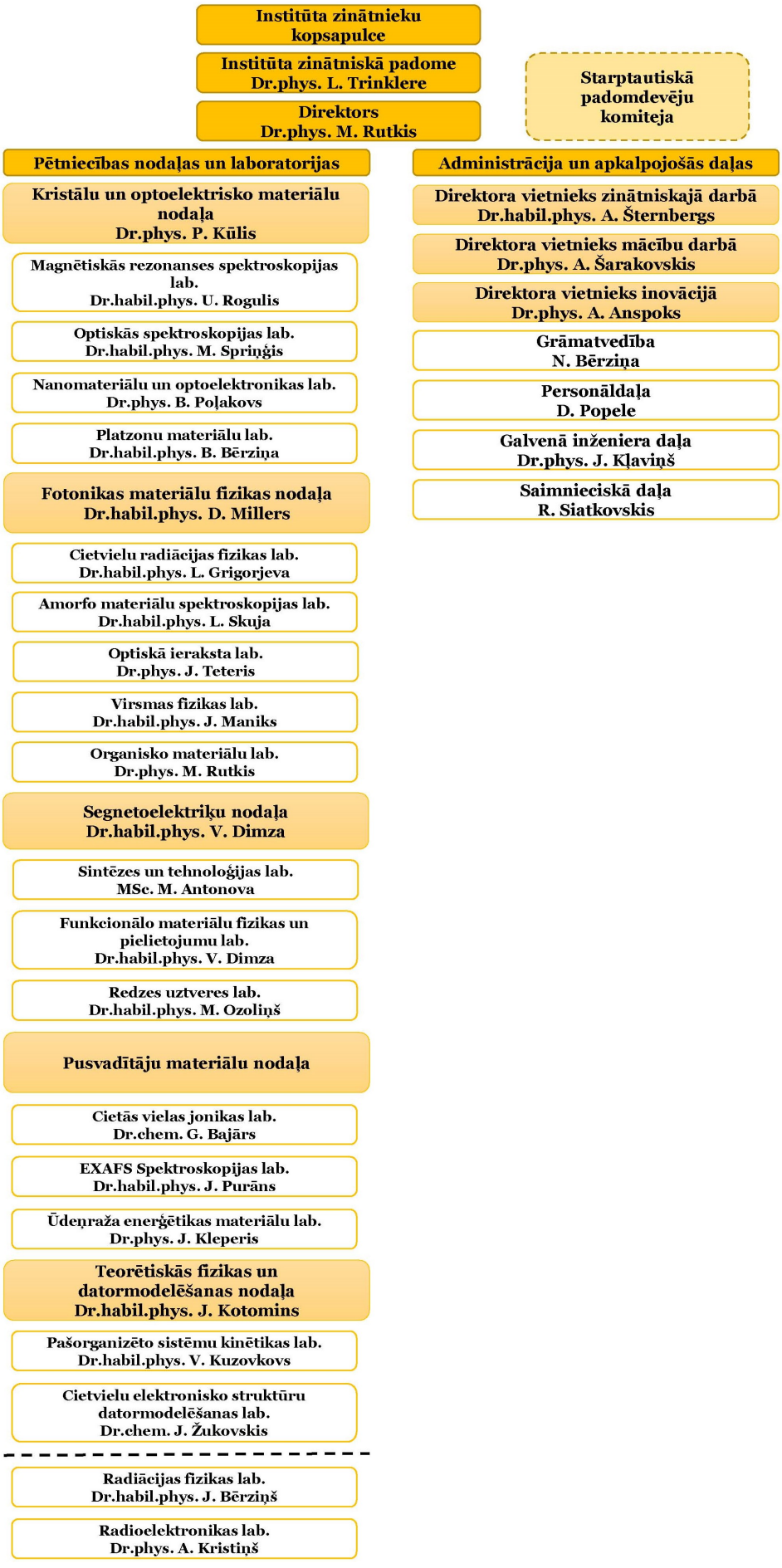
The Scientific Council in June 2016 elected new director - former deputy director for research of ISSP Dr. phys. Martins Rutkis.

Table 1

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2016

International Supervisory Board
Council of Institute *Dr.phys*. L.Trinklere
Director *Dr.phys*. A. M.Rutkis

RESEARCH DEPARTMENTS AND LABORATORIES	**ADMINISTRATION AND DOMESTIC SERVICES**


Institūta zinātnieku kopsapulce
Institūta zinātniskā padome
Dr.phys. L. Trinklere
Direktors
Dr.phys. M. Rutkis
Starptautiskā padomdevēju komiteja
Pētniecības nodaļas un laboratorijas
Kristālu un optoelektrisko materiālu nodaļa
Dr.phys. P. Kūlis
Magnētiskās rezonanses spektroskopijas lab.
Dr.habil.phys. U. Rogulis
Optiskās spektroskopijas lab.
Dr.habil.phys. M. Spriņģis
Nanomateriālu un optoelektronikas lab.
Dr.phys. B. Poļakovs
Platzonu materiālu lab.
Dr.habil.phys. B. Bērziņa
Fotonikas materiālu fizikas nodaļa
Dr.habil.phys. D. Millers
Cietvielu radiācijas fizikas lab.
Dr.habil.phys. L. Grigorjeva
Amorfo materiālu spektroskopijas lab.
Dr.habil.phys. L. Skuja
Optiskā ieraksta lab.
Dr.phys. J. Teteris
Virsmas fizikas lab.
Dr.habil.phys. J. Maniks
Organisko materiālu lab.
Dr.phys. M. Rutkis
Segnetoelektriķu nodaļa
Dr.habil.phys. V. Dimza
Sintēzes un tehnoloģijas lab.
MSc. M. Antonova
Funkcionālo materiālu fizikas un pielietojumu lab.
Dr.habil.phys. V. Dimza
Redzes uztveres lab.
Dr.habil.phys. M. Ozoliņš
Pusvadītāju materiālu nodaļa
Cietās vielas jonikas lab.
Dr.chem. G. Bajārs
EXAFS Spektroskopijas lab.
Dr.habil.phys. J. Purāns
Ūdeņraža enerģētikas materiālu lab.
Dr.phys. J. Kleperis
Teorētiskās fizikas un datormodelēšanas nodaļa
Dr.habil.phys. J. Kotomins
Pašorganizēto sistēmu kinētikas lab.
Dr.habil.phys. V. Kuzovkovs
Cietvielu elektronisko struktūru datormodelēšanas lab.
Dr.chem. J. Žukovskis
Radiācijas fizikas lab.
Dr.habil.phys. J. Bērziņš
Radioelektronikas lab.
Dr.phys. A. Kristiņš
Administrācija un apkalpojošās daļas
Direktora vietnieks zinātniskajā darbā
Dr.habil.phys. A. Šternbergs
Direktora vietnieks mācību darbā
Dr.phys. A. Šarakovskis
Direktora vietnieks inovācijā
Dr.phys. A. Anspoks
Grāmatvedība
N. Bērziņa
Personāldaļa
D. Popele
Galvenā inženiera daļa
Dr.phys. J. Kļaviņš
Saimnieciskā daļa
R. Siatkovskis

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff.** At end of 2016 there were 196 employees working at the Institute, 20 of 116 members of the research staff hold Dr.habil.degrees, 65 hold Dr. or PhD. At the end of 2016 there were 16 PhD students and 48 undergraduate and graduate students in physics, chemistry, materialscience and optometry programmes working at the ISSP.

Table 2

The Scientific Council of the Institute, elected in 2016

1. Laima Trinklere, Dr.phys., chairperson of the Council
2. Marcis Auzins, Dr.habil.phys., UL
3. Gunars Bajars, Dr.chem.
4. Jurģis Grūbe, PhD student
5. Mārtins Rutkis, Dr.phys.
6. Andrejs Silins, Prof., Dr.habil.phys.
7. Anatolijs Sharakovskis, Dr.phys.
8. Andris Sternbergs, Dr.habil.phys.
9. Anatolijs Truhins, Dr.habil.phys.
10. Andris Anspoks, Dr.phys.
11. Dmitrijs Bočarovs, Dr.phys.
12. Jānis Kleperis, Dr.phys.
13. Māris Knite , RTU profesors
14. Donāts Millers, Dr.habil.phys.
15. Aivars Vembris, Dr.phys.

The annual report summarizes the research activities of the ISSP in 2016. The staff of the Institute has succeed in 5 **national science grants** and in **one national cooperation project** with the total financing 264,4 thous. EUR

Since 2008 the budgetary increase of science was focused on scientific infrastructure financing and launching of National Research Programmes (NRP). One of the scientific priorities in Latvia is **materialscience**. ISSP became coordinating institution for the Materials NRP and collaborates as well in the NRP “Energetics” attracting 218,7 thous. EUR budget in 2016. The infrastructure financing for ISSP in 2016 was 1063,6 thous. EUR and it was partly used also for the salaries of the scientific and maintenance staff of the Institute. (Table 3).

At the end of 2016, more than 60 students, master's candidates and doctoral candidates worked in our Institute under the supervising of our scientists. The Institute has always strived to be actively involved in student teaching on all levels.

In **2016 two international conferences** have been organised:

1. International Young Scientist Conference "Developments in Optics and Communications 2016", April 21. – 22, 2016, Riga, Latvia;
2. Saules kauss 2016, May 25, Riga, Latvia.

Main awards, received at 2016:

No	Author	Award
1.	Dr hab.phys. Uldis Rogulis	The Member of Latvian Academy of Science
2.	Dr.phys. Aleksejs Kuzmins	The Member of Latvian Academy of Science
3.	Dr. phys Roberts Eglītis	E. Silins award (Latvian Academy of Science)
4.	Dr. phys Roberts Zābels	L. and M.Jansons award for young scientists in physics (Latvian Academy of Science)
5.	Dr. phys Jurģis Grūbe	award for new scientists (Latvian Academy of Science)

Table 3

INCOME OF ISSP, THOUSAND EUR, FROM 2008 -2016

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
2016	2 747,00	483,06	1 063,63	114,50	586,78	499,04

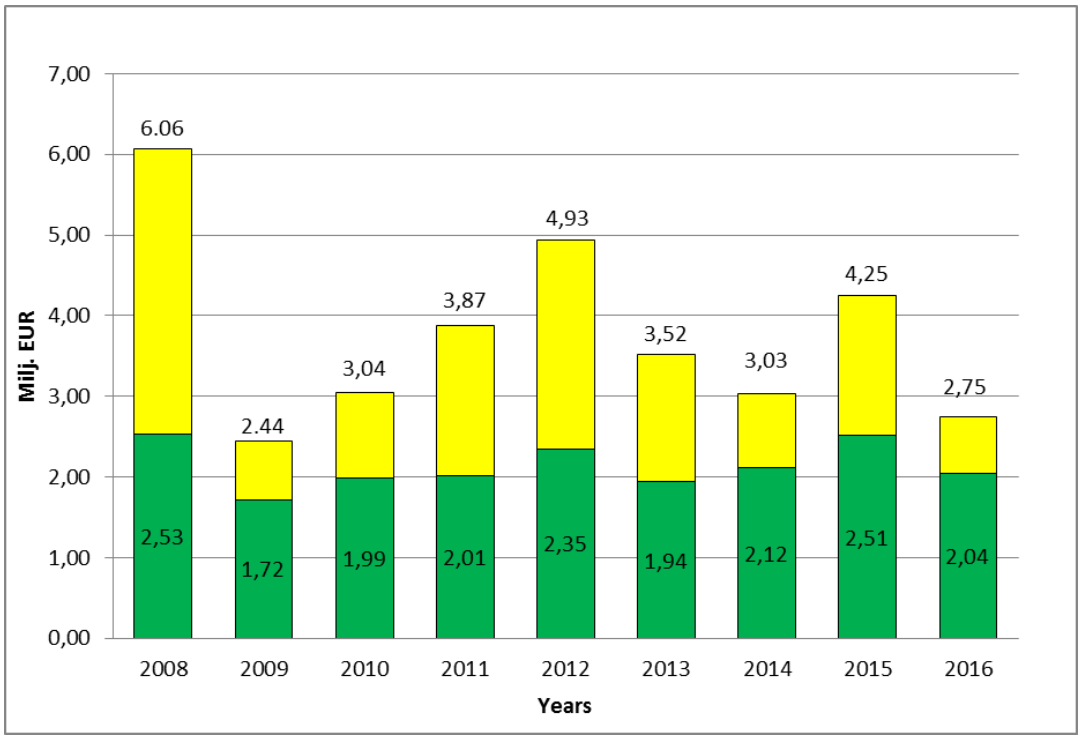


Fig.1. Total financing of the ISSP milj. EUR from 2008 to 2016

- *salaries*

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

- H2020 – WIDESPREAD-2015 project CAMART^2 – 124,4 thous. EUR;
- 4 EUROFUSSION projects – 230,6 thous. EUR;
- H2ESOT project – 51,0 thous. EUR.

Main achievements in 2016

1. The CAMART^2 project in Horizon 2020 Programme (Phase 2) was accepted. Next 7 years (2017 – 2023) ISSP together with partners from Sweden will receive 15 MEUR for increasing the level of commercialisation of research in Latvia, enhance collaboration between business and academia, paving the way for innovation –based economic grow, and diminishing the disparities between Latvia and well-performing member states
2. 121 SCI papers published by the staff of Institute;
3. 12 B.sc. thesis and 8 M.Sc. theses in physics, optometry, chemistry and materialscience were defended under the supervision of our scientists;
4. Ilze Dimanta was acquired degree of doctor of biology (PhD).

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 62 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
4. Assist. Dz. Bērziņš

PhD students
1. A. Antuzevičs
2. M. Ķemere

Students
1. J. Sperga
2. G. Priedītis

SCIENTIFIC VISITS ABROAD

E. Elsts (2 weeks in Lithuania)
M. Ķemere (2 days in Lithuania)
A. Antuzēvičs (2 days in Lithuania)

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)

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

RARE EARTH DOPED GLASS-CERAMICS CONTAINING $NaLaF_4$ NANOCRYSTALS

E. Elsts, G. Krieke, U. Rogulis, K. Smits, A. Zolotarjovs, J. Jansons, A. Sarakovskis, K. Kundzins

Oxyfluoride glasses $16Na_2O$-9NaF-$5LaF_3$-$7Al_2O_3$-$63SiO_2$ (mol%) activated with 3% terbium, dysprosium, praseodymium and neodymium fluorides have been prepared and studied by differential thermal analysis, cathodoluminescence, X-ray induced luminescence, X-ray diffraction, scanning electron microscopy and energy dispersive X-ray spectroscopy. We found out that the presence of crystalline phase enhances the X-ray induced luminescence intensity. X-ray induced luminescence is the most intense for the sample activated with terbium and treated at 700°C, whereas the praseodymium and neodymium activated samples have the fastest decay times.

OPTICAL DETECTION OF PARAMAGNETIC CENTRES: FROM CRYSTALS TO GLASS-CERAMICS

U. Rogulis

An unambiguous attribution of the absorption spectra to definite paramagnetic centres identified by the EPR techniques in the most cases is problematic. This problem may be solved by applying of a direct measurement techniques - the EPR detected via the magnetic circular dichroism, or briefly MCD-EPR. The present survey reports on the advantages and disadvantages applying the MCD-EPR techniques to simple and complex para-magnetic centres in crystals as well as glasses and glass-ceramics.

SYNTHESIS OF ZnO AND CdO-ZnO THIN FILMS BY EXTRACTION–PYROLYTIC METHOD

A. Cvetkovs, O. Kiselova, U. Rogulis, V. Serga, R. Ignatans

The extraction-pyrolythic method has been applied to synthesize the ZnO and CdO-ZnO thin films on glass and quartz glass substrates. According to the X-ray diffraction measurements, in the films the ZnO and CdO crystalline phases have been produced with an average size of 20-60 nm in the films. The thickness of the layers measured by a profilometer was up to 150 nm. The surface morphology measurements show that the surface may be rough and non-continuous. The SEM results confirm the dependence between the preparation procedure and the quality of the thin film.

LOCAL STRUCTURE OF GADOLINIUM IN OXYFLUORIDE GLASS MATRICES CONTAINING SrF_2 AND BaF_2 CRYSTALLITES

A. Antuzevics, M. Kemere, R. Ignatans

Gd^{3+} doped aluminosilicate oxyfluoride glasses and glass-ceramics containing SrF_2 and BaF_2 crystallites have been studied by differential thermal analysis (DTA), X-ray diffraction (XRD), transmission electron microscopy (TEM), photoluminescence (PL) and electron paramagnetic resonance (EPR) spectroscopy techniques. A pronounced EPR fine structure emerges after the heat treatment of the glass matrix. EPR spectra simulations indicate the formation of cubic, tetragonal and trigonal Gd^{3+} centres in the studied compositions.

SCIENTIFIC PUBLICATIONS

1. **E. Elsts**, G. Krieke, **U. Rogulis**, K. Smits, A. Zolotarjovs, J. Jansons, A. Sarakovskis, K. Kundzins, Rare earth doped glass-ceramics containing $NaLaF_4$ nanocrystals, Optical Materials 2016, vol. 59, p. 130-135, DOI: 10.1016/j.optmat.2016.01.005
2. **U. Rogulis**, Optical detection of paramagnetic centres: from crystals to glass-ceramics, Low temperature physics, 2016, v. 42, No. 7, pp. 689-693.
3. A. Cvetkovs, O. Kiselova, **U. Rogulis**, V. Serga, R. Ignatans, Synthesis of ZnO and CdO-ZnO thin films by extraction–pyrolytic method, Latvian Journal of Physics and Technical Sciences, 2016, vol. 53, pp. 57–66, DOI: 10.1515/lpts-2016-0021
9. **A. Antuzevics**, **M. Kemere**, R. Ignatans, Local structure of gadolinium in oxyfluoride glass matrices containing SrF_2 and BaF_2 crystallites, Journal of Non-Crystalline Solids, 2016, vol. 449, pp. 29-33.

LECTURES ON CONFERENCES

1. M. Kemere, U. Rogulis, S. Schweizer, F. Steudel, S. Loos, A. Ch. Rimbach, R. Ignatans, Luminescence and quantum efficiency of europium doped oxyfluoride glasses and glass-ceramics, Abstracts of the 12th International Young Scientist conference "Developments in Optics and Communications" DOC, 2016, p. 23.
2. J. Sperga, M. Kemere, U. Rogulis, J. Grube, Luminescence of europium and dysprosium co-doped oxyfluoride glasses, Abstracts of the 12th International Young Scientist conference "Developments in Optics and Communications" DOC, 2016, p. 17.
3. M. Kemere, J. Sperga, U. Rogulis, J. Grube, Luminescence properties of europium and dysprosium co-doped oxyfluoride glasses, 59th Scientific Conference for Young Students of Physics and Natural Sciences, Open Readings 2016, Vilnius, Lithuania, 2016, P3-05.
4. A. Antuzevics, M. Kemere, R. Ignatans, Structure of Gd^{3+} ions in oxyfluoride glass ceramics containing fluorite crystallites, Abstracts of the 12th International Young Scientist conference "Developments in Optics and Communications" DOC, 2016, p. 22.
5. A. Antuzevics, M. Kemere, R. Ignatans, Electron paramagnetic resonance study of Gd^{3+} ions in oxyfluoride glass ceramics, 59th Scientific Conference for Young Students of Physics and Natural Sciences, Open Readings 2016, Vilnius, Lithuania, 2016, P3-43.
6. A. N. Trukhin, A. Antuzevics, K. M. Golant, D.L. Griscom, Luminescence of Phosphorus Doped Silica Glasses, 11th International Symposium on SiO_2, Advanced Dielectrics and Related Devices, Book of abstracts, 2016, p.93-94. DOI: sciencesconf.org:sio2-2016:97199.

7. Uldis Rogulis, Meldra Ķemere, Stefan Schweizer, Franziska Steudel, Sebastian Loos, Charlotte Rimbach, Reinis Ignatāns, QUANTUM EFFICIENCY OF EUROPIUM LUMINESCENCE CENTRES IN OXYFLUORIDE GLASSES AND GLASS-CERAMICS, Abstracts of the 32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, p.14.
8. P. Savchyn, O.I. Aksimentyeva, H.Klym, I.Karbovnyk, E. Elsts, J. Jansons, A.I.Popov, COMPARATIVE STUDIES OF CATHODOLUMINESCENCE PROPERTIES OF ACCEPTOR-DOPED $BaZrO_3$ AND $SrTiO_3$, Abstracts of the 32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, p.52.
9. Jānis Sperga, Meldra Ķemere, Uldis Rogulis, Jurģis Grūbe, LUMINESCENCE OF EUROPIUM AND DYSPROSIUM CO-DOPED OXYFLUORIDE GLASSES, Abstracts of the 32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, p. 43.
10. Andris Antuzevičs, Andris Fedotovs, Dzintars Bērziņš, Uldis Rogulis, Reinis Ignatāns, Sonia Baldochi, MAGNETIC RESONANCE SPECTROSCOPY STUDIES IN BaY_2F_8 CRYSTAL, Abstracts of the 32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, p.39.
11. Andris Antuzevičs, Meldra Ķemere, Edgars Elsts, Reinis Ignatāns, Gd^{3+} LOCAL STRUCTURE IN GLASS MATRICES CONTAINING CaF_2, SrF_2, BAF_2 AND $NaLaF_4$ CRYSTALLITES, Abstracts of the 32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, p.17.
12. Andris Fedotovs, Uldis Rogulis, Meldra Ķemere, Dzintars Bērziņš, MAGNETIC CIRCULAR DICHROISM IN RARE EARTH ACTIVATED OXYFLUORIDE GLASS CERAMICS, Abstracts of the 32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, p.42.

MASTER THESIS

Ludmila Rodionova, „ Properties of point defects in barium yttrium fluoride crystal", Master thesis, Riga, LU, 2016

BACHELOR THESIS

Jānis Sperga, „ Luminescence of europium and dysprosium co-doped oxyfluoride glasses", Bachelor thesis, Riga, LU, 2016

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 Ba - containing fluoride structures (cubic fluorite type, tetragonal nanocrystals and rhombohedral $Ba_4Y_3F_{17}$) was studied. Along with the mentioned activities a research topic related to the luminescence processes in rare-earth (RE) doped oxyfluoride glass and glass ceramics was expanded. 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+}) $NaYF_4$, $NaLaF_4$ and Ba^{2+} containing 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. Novel Er^{3+} doped transparent glass ceramics containing hexagonal $Na(Gd,Lu)F_4$ nanocrystals were prepared from oxyfluoride glasses. A strong deviation of rare earth ion content in fluoride nanocrystals in comparison to the base glass has been observed. Preferential incorporation of Gd^{3+} over Lu^{3+} ions in the fluoride lattice leads to the stabilization of hexagonal $Na(Gd,Lu)F_4$ structure. A considerable enhancement of upconversion luminescence correlates with the formation of hexagonal solid solutions and is attributed to an efficient energy transfer between Er^{3+} ions.

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”).

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 (maternity leave)

Students
K. Jirgensons
E. Pavlovska

SCIENTIFIC VISITS ABROAD

G. Krieķe (6 days, Germany)

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

CRYSTALLIZATION AND UPCONVERSION LUMINESCENCE OF DISTORTED FLUORITENANOCRYSTALS IN Ba^{2+}CONTAINING OXYFLUORIDE GLASS CERAMICS

G. Krieke, A. Sarakovskis

Novel Er^{3+}-doped transparent glass ceramics were prepared from melt-quenched glasseswith general composition of Na_2O-NaF-BaF_2-YF_3-Al_2O_3-SiO_2. The phase composition of the annealedglass ceramics strongly depends on the BaF_2content in glass matrix. Crystallization of β-$NaYF_4$, cubic fluorite type, tetragonal nanocrystals and rhombohedral $Ba_4Y_3F_{17}$was observed. An introduction of BaF_2in the glass matrix suppresses the crystallization of β-NaYF4, promotes the formation of Ba^{2+}containing fluoride phases and reduces the cross-relaxation between Er^{3+}ions in fluoride crystals. Small rate of the nonradiative processes and low local symmetry of rhombohedrally disordered $Ba_4Y_3F_{17}$enables an efficient upconversion luminescence surpassing that of the glass ceramics containing β -$NaYF_4$nanocrystals.

OXYGEN INFLUENCE ON LUMINESCENCE PROPERTIES OF RARE-EARTH DOPED $NaLaF_4$

A.Tuomela, V.Pankratov, A.Sarakovskis, G.Doke, L.Grinberga, S.Vielhauer, M.Huttula

Luminescence properties of erbium and europium doped $NaLaF_4$ with different oxygen content have been studied.Vacuum ultraviolet (VUV) excitation luminescence spectroscopy technique has been applied by using synchrotron radiation excitation. It was found that oxygen impurity leads to significant degradation of Er^{3+} or Eu^{3+} emission under VUV excitation. The intensive O^{2-}– Er^{3+} charge transfer excitation band has been detected from oxygen abundant $NaLaF_4$ in the 150–165 nm spectral range. This band reveals a competing absorption mechanism in oxygen containing $NaLaF_4$. It is clearly demonstrated that one reason for the Er^{3+} emission degradation in oxygen abundant $NaLaF_4$ is strong suppression of 4f–5d transitions in Er^{3+} ion. The degradation of the Eu^{3+} emission under VUV excitation was explained by diminishing of F^-–Eu^{3+} charge transfer absorption band as well as by competing relaxation centers in the oxygen abundant $NaLaF_4$.

TEMPERATURE INFLUENCE ON $NaLaF_4:Er^{3+}$ GREEN LUMINESCENCE

Jurgis Grube

Er^{3+} doped $NaLaF_4$ is a promising material for up-conversion luminescence applications due to low phonon energy and multisite nature of the crystalline lattice. In this work, luminescence processes in $NaLaF_4:Er^{3+}$ materials have been studied at different temperatures. Spectra and decay kinetics of the green luminescence were measured under excitation to $^4F_{7/2}$ state. Analysis of the green luminescence excitation spectra, the luminescence spectra and the luminescence decay kinetics at different temperatures reveals that the observed single green uminescence spectra at room temperature are related to overlapping of the green luminescence excitation bands from erbium ions located at non-equivalent lattice sites. In addition, spectroscopic data obtained from the green and the infrared luminescence spectra at different temperatures suggest that both $^4S_{3/2}$ and $^2H_{11/2}$ states are involved in energy transfer between erbium ions, leading to concentration quenching of the green luminescence.

TEMPERATURE AND IMPURITY CONCENTRATION EFFECTS ON UPCONVERSION LUMINESCENCE IN $LaInO_3$ DOPED WITH Er^{3+}

Sarakovskis, A., Grube, J., Strals, K., Krieke, G., Springis, M., Mironova-Ulmane, N., Skvortsova, V., Yukhno, E.K., Bashkirov, L.A.

Novel method for synthesis of $LaInO_3:Er^{3+}$ is reported and upconversion luminescence properties of the synthesized material at different temperatures (9-300 K) are studied. The samples were prepared by co-precipitation and subsequent heat treatment of lanthanum, indium and erbium hydroxides. It is shown that the excitation at 980 nm leads to a strong green upconversion luminescence in the material. At the concentrations above 0.1 mol % of Er^{3+} the energy transfer upconversion mechanism of the luminescence becomes evident. Further increase of Er^{3+} content in the material leads to higher red-to-green upconversion luminescence intensity ratio. The mechanisms responsible for the observed variation are discussed.

SCIENTIFIC PUBLICATIONS

Guna Krieke, Anatolijs Sarakovskis. Crystallization and upconversion luminescence of distorted fluoritenanocrystals in Ba^{2+}containing oxyfluoride glass ceramics. Journal of the European Ceramic Society, (2016), 36, pp.1715–1722.

A.Tuomela, V.Pankratov, **A.Sarakovskis, G.Doke**, L.Grinberga, S.Vielhauer, M.Huttula. Oxygeninfluence onluminescencepropertiesofrare-earth doped $NaLaF_4$. Journal of Luminescence, (2016), 179, pp.16–20.

Jurgis Grube. Temperature influence on $NaLaF_4:Er^{3+}$ green luminescence. Journal of Luminescence, (2016), 179, pp. 107–113.

Sarakovskis, A., Grube, J., Strals, K., **Krieke, G**., Springis, M., Mironova-Ulmane, N., Skvortsova, V., Yukhno, E.K., Bashkirov, L.A. Temperature and impurity concentration effects on upconversion luminescence in $LaInO_3$ doped with Er^{3+}. Fizika Nizkikh Temperatur, (2016), v.42, pp. 733-737.

POPULAR SCIENCE PUBLICATIONS

G. Krieķe. Īpaša stikla keramika padarīs siltumstarojumu redzamu. Ilustrētā zinātne, 2016, 11(132), lpp.13, (in latvian).

LECTURES ON CONFERENCES

32nd Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2016, February 17-19.

1. G.Krieķe, A.Sarakovskis. Up-conversion luminescence of erbium in barium containing oxyfluoride glass ceramics. Abstracts, p.16.

2. G.Zageris, J.Grube, A.Sarakovskis, G.Krieke. Pr^{3+} luminescence in oxyfluoride glass and glass ceramic containing $NaLaF_4$. Abstracts, p.44.

3. J.Grube. Luminescences processes in $NaLaF_4:Tm^{3+}$. Abstracts, p.123.

4. A.Sarakovskis. NRP $IMIS^2$ 2.project: Nanomaterials and nanotechnology. Abstracts, p.105.

57th International Scientific Conference of the Riga Technical University, Riga, Latvia, 2016, October 21.

A.Sarakovskis. Nanomaterials and nanotechnology.

6th International Congress on Ceramics. Dresden, Germany, 2016, August 21–25.

Krieke G., Sarakovskis, A., Springis, M. Sarakovskis, A., Highly efficient upconversion luminescence of erbium doped glass ceramics with β-$NaYF_4$ nanocrystals.

MASTER THESIS

Martins Osis. “Up-conversion luminescence of oxyfluoride glass ceramics doped with Ce^{3+}, Ho^{3+} and Yb^{3+}”, supervisor Anatolijs Sarakovskis.

BACHELOR THESIS

Girts Zageris. “Luminescence of Pr^{3+} in oxyfluoride glass and glass ceramics containing $NaLaF_4$ “, supervisor Jurgis Grube.

Ansis Ansbergs. “Luminescence of Eu^{3+} in oxyfluoride glass and glass ceramics“, 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 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;
- light-induced energy storage in material;
- estimation of practical applications of the materials for the UV light dosimeters, gas sensors, UV and visible light emitters;
- working out 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).
Institute of Inorganic Chemistry, Riga Technical University (Prof. J. Grabis).
Institute of Technical Physics, Riga Technical University (Profs. A.Medvid, M.Knite).

Lithuania.

Institute of Applied Research, Department of Semiconductor Optoelectronics, Vilnius University, Vilnius (Dr. P.Scaev),
Center for Physical Sciences and technology, Optoelectronics department, Vilnius (Drs R.Nedzinskas, S.Tumenas)

Taiwan

National Taiwan University, Taipei (Profs. Li-Chyong Chen, Kuei-Hsien Chen), National Sun Yat-Sen University, Department of Materials and Optoelectronic Science Kaohsiung, Taiwan (Drs. M. M. C. Chou, L. W. Chang)

Ukraine

Institute of Physics of National Academy of Science of Ukraine, Department of Physics of Biological Systems (Prof. Galina Dovbeshko).

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 and 350 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.

Structure of luminescence centers responsible for the 420 nm luminescence in AlN nanopowder was proposed consisting of defects based on nitrogen vacancy type defects, such as v_N and so-called F centers.

These studies were supported 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.

SCIENTIFIC PUBLICATIONS

1. **B.Berzina, V.Korsaks, L.Trinkler,** A.Sarakovskis, J.Grube, S.Bellucci, Defect-induces blue luminescence of hexagonal boron nitride, Diamond and related materials 68 (2016) 131-137.
2. **L.Trinkler**, A.Trukhin, **B.Berzina, V.Korsaks**, P.Ščaev, R.Nedzinskas, S.Tumėnas, M.M.C.Chou, L.Chang, C-A.Li, Luminescence properties of $LiGaO_2$ crystal, Optical materials 69 (2017) 449-459, http://dx.doi.org/10.1016/j.optmat.2016.11.012.

LECTURES ON CONFERENCES

32nd Scientific Conference of Institute of solid State Physics, University of Latvia, February 17-19, 2016, Riga, Latvia

1. Laima Trinkler, Baiba Berzina, Valdis Korsaks, Anatolij Trukhin, Luminescence properties of wide band gap material $LiGaO_2$, Abstract Book, p. 15.
2. Paula Jankovska, Valdis Korsaks, Laima Trinkler, Janis Kristaps Valjonoks, Baiba Berzina, Oxygen gas sensing properties of AlN and hBN powders, Abstract Book, p. 19.

The 9th International Workshop on Zink Oxide and related materials, Oct 30-Nov 2, 2016, NTU, Taipei, Taiwan

3. L.Trinkler, A.Trukhin, B.Berzina, V.Korsaks, P. Ščajev, R.Nedzinskas, S.Tumenas, M. M. C. Chou, L. Chang, C-A. Li, Luminescence Properties of $LiGaO_2$ Crystal, Abstract book, TP 33.
4. E. Pozingytė, A. Rimkus, S. Tumėnas, R. Nedzinskas, L. Trinkler, B.Berzina, C.-Y. J. Lu, Y.-T. T. Tu, M.M.C.Chou, and L. Chang, Photo-and Cathodoluminescence of epitaxial rock-salt ZnMgO thin films and ZnMgO/MgO Quantum Wells, Grown on (100) MgO Substrate, Abstract book, TP30.
5. M.-Y.Ho, M.C.Wan, V.Korsaks, S.-F. Lee, L.Trinkler, L. Chang, and M. M. C. Chou, Optical and Electric Propertiesof Cu-doped ZnO Films Grown on MgO (100) Substrate, Abstract book, TP17.

The 19th International Conference on Defects in Insulating Matertials, July 10 – 15, 2016, Lyon, France

6. Baiba Berzina, Valdis Korsaks, Laima Trinkler, and Paula Jankovska, Blue luminescence caused by natural defects in hBN and AlN, Additional abstract

DEPARTMENT OF CRYSTALS PHYSICS AND OPTOELECTRONIC MATERIALS

Head of Department Dr. phys. P. Kulis

LABORATORY OF NANOMATERIALS AND 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, electtical and other properties.
2. Engineering and synthesis of core-shell nanocrystals and nanowires, including 2D materials as shell material (transition metal dichalcogenides).
3. Development and implementation of nanomechanical tests for 1D nanostructures and simulations of their mechanical properties; prototyping of nanodevices.
4. Euroatom.

SCIENTIFIC STAFF

Dr. Habil. Phys. I. Tale
Dr. Phys. P. Kulis
Dr. Phys. J. Butikova
Dr. Phys. L. Dimitrocenko
Dr. Phys. B. Polyakov
Dr. Phys. A. Voitkans
Dr. Phys. S. Vlassov (visiting researcher)
M. Sc. J. Jansons

PhD Students

M. Sc. E. Butanovs
M. Sc. G. Marcins

Students

P. Krivolapova

COOPERATION

Latvia

Joint stock company "Alfa"
SIA "Groglass"
Institute of Biomedical Engineering and Nanotechnologies, Riga Technical University
G. Liberts Innovative Microscopy Center, University of Daugavpils

Estonia

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

MAIN RESULTS

COMPARATIVE ANALYSIS OF MECHANICAL TEST CONFIGURATIONS FOR GOLD NANOWIRES AND NANOPLATES

M. Antsov, B. Polyakov, M. Mets, S. Oras, M.Vahtrus, L. Dorogin, R. Lõhmus, S. Vlassov

Nanometer-sized materials, such as nanowires (NWs) and nanoplates (NPLs) are practically important materials for the wide range of emerging applications. Among one-dimensional (1-D) nanostructures, metal NWs possess unique physical properties associated with their highly anisotropic geometry as well as the size effects that suggests using NWs for nanoscale interconnects, sensors, transparent, conductive electrodes in photovoltaic and optoelectronic devices.

Three point bending test is one of most polpular nanomechanical characterization method for 1-D nanostructures, which allows to determine Young modulus and bending strenght. However, it has same weak points. Distribution of stresses is highly non-uniform with the most localized stress in the vicinity of clamping and probe regions. The boundary problem of three point bending test was discussed previously in number of works. Researchers focused mainly on question of "good" or "poor" nanowire end adhesion to substrate if nanowire simply deposited without any additional ends fastening (e.g. FIB welding). It was shown, that depending on nanowire or/and substrate surface quality or interface properties results of obtained Young modulus may differ significantly. The problem is comlicated if boundary condition is uncertain. The most known solution is nanowire ends welding by platinum or carbon using FIB assisted deposition. The drawback is Pt or C material deposition in proximity to the welded region, which may increase radius of nanowire and alter mechanical test results.

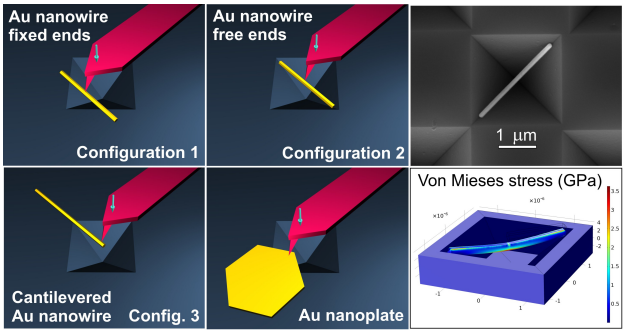


Fig. 3. Schematics of Au nanowire and nanoplate bending tests, SEM image of Au nanowire and corresponding FEM simulation.

In this study we utlized the opposite approach, where both nanowire ends are almost "free", and compared this configuration to the conventional fixed ends and cantilevered configurations. We have measured elastic modulus in all the three configurations and linked the results to the boundary effects of non-uniform mechanical stress by FEM modeling. Complementary measurements of elastic modulus of the Au NPLs have been carried out by nanoindentation in AFM. Additionally, plastic deformation and plastic yield were measured on Au NWs and Au NPLs, and compared to FEM modeling results.

COMPLEX TRIBOMECHANICAL CHARACTERIZATION OF ZnO NANOWIRES: NANOMANIPULATIONS SUPPORTED BY FEM SIMULATIONS

S. Vlassov, B. Polyakov, S. Oras, M. Vahtrus, M. Antsov, A. Šutka, K. Smits, L. M. Dorogin and R. Lõhmus

Nanowires (NWs) are among the most important objects in modern science and have a number of promising applications in nanotechnology. Plenty of prototype nanoelectromechanical systems (NEMS) based on NWs have already been demonstrated during the last few decades. The fabrication and functioning of NW-based devices are

tightly related to tribomechanical problems since they often involve the relative motion and mechanical interaction between a NW and other components.

In the present work, we had advanced the self-sensing approach by introducing a half-suspended NW configuration in combination with a pick-and-place manipulation, which enabled us to control the position and length of the adhered part of each NW. Experiments were performed inside a high resolution SEM on hexagonal ZnO NWs positioned over the trenches etched in a Si substrate and included measurements of the bending strength, static and kinetic friction. For the first time, kinetic friction was measured in the rotation regime. The calculation of static friction from the most bent state and the stress distributions in manipulated NWs were completely reconsidered. The new more realistic model was inspired by the concepts of fracture mechanics making use of finite element method (FEM) computations. On the basis of the present study, it can be concluded that the manipulation of suspended NWs have a number of strong advantages for nanotribological studies in comparison to manipulations on a flat substrate. A suspended configuration in combination with the pick-and-place technique allows us to perform multiple measurements on the same NW with a precisely varied contact area. Moreover, a suspended configuration enables us to avoid the tip wear caused by the tip/substrate contact, therefore assuring longer tip lifetime.

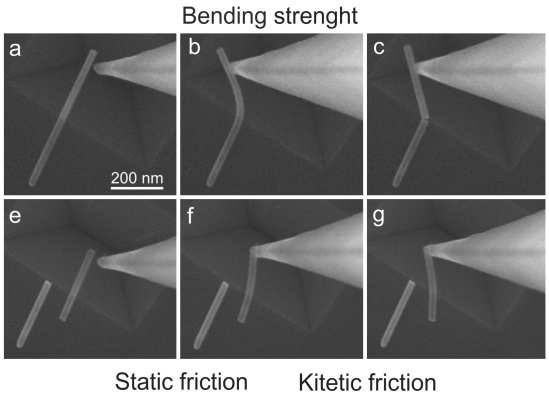


Fig. 2. Manipulation of half-suspended ZnO NW

SYNTHESIS AND CHARACTERIZATION OF ZnO-WS_2 CORE-SHELL NANOWIRES

B. Polyakov, A. Kuzmin, K. Smits, J. Zideluns, E. Butanovs, J. Butikova, S. Vlassov, S. Piskunov, and Y. F. Zhukovskii

Core−shell and multishell nanowires (NWs) are modern types of axially and radially heterostructured nanomaterials intensively explored during the last decades. The core−shell approach has several important advantages as compared to conventional two-dimensional (2D) material production technologies: it allows one, for example, to combine materials with lattice mismatch and even to initiate epitaxial growth of shell material on the core template. As a result, it is possible to significantly improve electrical, mechanical, and optical properties of NWs by proper combination of core and shell materials.

In this study epitaxial hexagonally shaped shell consisting of WS2 nanolayers was grown on {1Ī00} facets of prismatic wurtzite-structured [0001]-oriented ZnO nanowires for the first time. A synthesis was performed by annealing in a sulfur atmosphere of ZnO/WO3 core−shell structures, produced by reactive dc magnetron sputtering of an amorphous a-WO3 layer on top of ZnO nanowire array. The morphology and phase composition of synthesized ZnO/WS2 core−shell nanowires were confirmed by

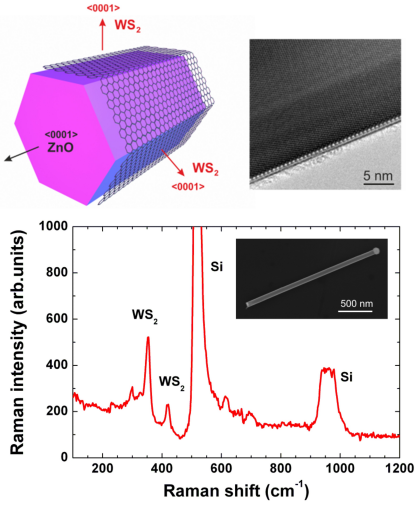


Fig. 1. Schematics of ZnO-WS2 core-shell nanowire, TEM image and Raman spectrum.

scanning and transmission electron microscopy (SEM and TEM), micro-Raman, and photoluminescence spectroscopy. Epitaxial growth of WS2(0001) layer(s) on {1Γ00} facets of ZnO nanowire is unexpected due to incompatibility of their symmetry and structure parameters. To relax the interfacial incoherence, we propose a model of ZnO/WS2 interface containing WS2 bridging groups inside and use first-principles simulations to support its feasibility.

SCIENTIFIC ARTICLES

1. M. Mets, M. Antsov, V. Zain, L. Dorogin, A. Aabloo, **B. Polyakov**, R Lõhmus. Structural factor in bending testing of fivefold twinned nanowires revealed by finite element analysis, Physica Scripta 91 (2016) 115701.
2. M. Vahtrus, A. Šutka, **B. Polyakov**, S. Oras, M. Antsov, N. Doebelin, R. Lõhmus. Effect of cobalt doping on the mechanical properties of ZnO nanowires, Materials Characterization 121 (2016) 40-47.
3. **B. Polyakov**, A. Kuzmin, K. Smits, J. Zideluns, **E. Butanovs, J. Butikova, S. Vlassov**, S. Piskunov, Y. F. Zhukovskii. Unexpected Epitaxial Growth of a Few WS2 Layers on {1-100} Facets of ZnO Nanowires, J. Phys. Chem. C, 120 (2016) 21451-21459.
4. **S. Vlassov, B. Polyakov**, S. Oras, M. Vahtrus, M. Antsov, A. Šutka, K. Smits, L. Dorogin, R. Lõhmus. Complex tribomechanical characterization of ZnO nanowires: nanomanipulations supported by FEM simulations. Nanotechnology 27 (2016) 335701 (10pp).

POPULAR SCIENCE ARTICLES AND BOOKS

1. **Jansons J.** No Latvijas Universitātes Fizikas institūta (1919) līdz Cietvielu fizikas institūtam (1978). – Rīga : LU Akadēmiskais apgāds, 2016. 196 lpp.
2. **Jansons J.** Fizikas profesoram Voldemāram Fricbergam (24.06.1926. – 02.08.1982.) – 90. – "Zvaigžņotā Debess" 2016. g. vasara (232), 31. – 37. lpp.
3. **Jansons J.** Fizikas profesors akadēmiķis Juris Ekmanis (2.XII 1941. – 9 IV 2016.). – "Zvaigžņotā Debess" 2016. g. vasara (232), 38. – 46. lpp.

PRESENTATIONS ON CONFERENCES

Organizing and participation COST MP1303 conference: "**The Second European Workshop on Understanding and Controlling Nano and Mesoscale Friction**", Riga, 4-7 July 2016:

Boris Polyakov, Sergey Vlassov, Mikk Antsov, Jelena Butikova, Edgars Butanovs, Janis Zideluns "2D TRANSITION METAL DICHALCOGENIDES AS A SOLID LUBRICANT FOR NANOWIRES MANIPULATION"

Annual ISSP conference (**the 32nd ISSP Scientific Conference**), Riga, 17-19 February 2016:

1. Edgars Butanovs, Boris Polyakov, Janis Zideluns, Alexei Kuzmin, Jelena Butikova "2D TRANSITION METAL DICHALCOGENIDE NANOCRYSTALS"
2. Janis Zideluns, Boriss Polakovs, Edgars Butanovs, Jelena Butikova, Aleksejs Kuzmins "METAL OXIDE NANOWIRE BASED HYBRID CORE-SHELL NANOMATERIALS"

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

Laboratory specializes in luminescence and other optical properties research in various complex oxides: single crystals, ceramics, nanopowders and coatings as well as other material characterization methods including microscopy (SEM, TEM), X-ray diffraction, electron-dispersive x-ray analysis, FTIR and others. 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, 10 ns); 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 were 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.phys. K.Smits

Students:
A.Zolotarjovs
A.Krumina
D.Olšteins
V. Liepiņa

SCIENTIFIC VISITS ABROAD

1. Dr,L.Grigorjeva, Estonia (5 days)
2. Dr.K.Smits, Germany, Cologne, (4 days).
3. L.Grigorjeva, Germany, Cologne, (4 days)
4. A.Zolotarjovs, Germany, Cologne, (4 days
3. Dr.K.Smits, France, PROMES, 2 weeks.
4. A.Zolotarjovs, France, PROMES, 2 weeks.
5. Dr.L.Grigorjeva, France, PROMES, 2 weeks.

COOPERATION

Latvia
Riga Technical University, Institute of Inorganic Chemistry (Dr.habil.sc.ing. Prof. J.Grabis).
LU Institute of Microbiology (M.Gavare, J.Liepiņš).
Institute of Chemical physics, UL (Dr. G.Kizāne, Dr.E.Pajuste).
Riga Technical University, Institute of Silicate Materials. Dr. A.Sutka
Estonia
Institute of Physics, Tartu (Dr.S.Zazubovich, Dr. I.Sildos))
Russia
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)
Serbia
Institute of Nuclear Sciences, University of Belgrade, Serbia

MAIN RESULTS

MULTICOLOR UPCONVERSION LUMINESCENCE OF $GdVO_4$:$Ln3^+$/$Yb3^+$ ($Ln3^+$ ¼ $Ho3^+$, $Er3^+$, $Tm3^+$, $Ho3^+$/$Er3^+$/$Tm3^+$) NANORODS

Tamara V. Gavrilovic, Dragana J. Jovanovic, Krisjanis Smits, Miroslav D. Dramicanin

Lanthanide-doped $GdVO_4$ nanorods that exhibit upconversion emission under 982 nm excitation have been prepared by a facile room-temperature chemical co-precipitation method followed by a subsequent annealing at temperatures of 600 ^oC, 800 ^oC and 1000 ^oC. Multicolor upconversion emission, including white, was achieved by tuning the concentrations of dopant lanthanide ions (Ho3+, Er3+, Tm3+ and Yb3+) in $GdVO_4$. It is found that four GdVO4 samples emit light with the white chromaticity coordinates of (0.326, 0.339), (0.346, 0.343), (0.323, 0.327) and (0.342, 0.340) respectively, under a single-wavelength NIR excitation. These coordinates are very close to the standard equal energy white light coordinates (0.333, 0.333) according to the 1931 CIE diagram. By varying dopant lanthanide concentrations in nanorods it is possible to produce upconversion emission with colors between red (0.504, 0.369), green (0.282, 0.577) and blue (0.142, 0.125) coordinates.

EFFECT OF POINT DEFECTS ON LUMINESCENCE CHARACTERISTICS OF ZnO CERAMICS

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

Photo- and thermally stimulated luminescence of ZnO ceramics are produced by uniaxial hot pressing. The luminescence spectra of ceramics contain a wide band with a maximum at 500 nm, for which oxygen vacancies VO are responsible, and a narrow band with a maximum at 385 nm, which is of exciton nature. It follows from luminescence excitation spectra that the exciton energy is transferred to luminescence centers in ZnO. An analysis of the thermally stimulated luminescence curves allowed detection of a set of discrete levels of point defects with activation energies of 25, 45, 510, 590 meV, and defects with continuous energy distributions in the range of 50–100 meV. The parameters of some of the detected defects are characteristic of a lithium impurity and hydrogen centers. The photoluminescence kinetics are studied in a wide temperature range

LUMINESCENT PEO COATINGS ON ALUMINUM

Aleksejs Zolotarjovs, Krisjanis Smits, Anete Krumina, DonatsMillers, and Larisa Grigorjeva

Results show the possibilities of pore filling approach to modify alumina coatings with various materials in order to enhance coating optical (or other) properties and develop new functional materials; as well as demonstrate novel alumina phase transition detection approach. Luminescent PEO coatings were produced on aluminum surface using pore-filling method. Three stage process was developed to modify alumina coating in order to enhance its luminescent properties. Eu3+ recharging to Eu2+ followed by significant (up to 10 times) total luminescence intensity increase was observed, Eu ion presence evaluated in final coating by measuring fast decay kinetics. Structure of obtained coatings was analyzed using XRD and FTIR spectroscopy indicating presence of η-alumina phase.

SCIENTIFIC PUBLICATIONS

1. Šutka, A., Järvekülg, M., Šutka, A., Heinmaa, I., Mäeorg, U., **Smits, K.**, Timusk, M. Mechanical reinforcement of electrospun poly(vinyl alcohol) by α-FeOOH nanowires (2016) Polymer Composites, . Article in Press.

2. Vlassov, S., Polyakov, B., Oras, S., Vahtrus, M., Antsov, M., Šutka, A., **Smits, K.**, Dorogin, L.M., Lõhmus, R. Complex tribomechanical characterization of ZnO nanowires: Nanomanipulations supported by FEM simulations (2016) Nanotechnology, 27 (33), art. no. 335701.

3. Rodnyi, P.A., Chernenko, K.A., **Zolotarjovs, A., Grigorjeva, L.,** Gorokhova, E.I., Venevtsev, I.D. Effect of point defects on luminescence characteristics of ZnO ceramics (2016) Physics of the Solid State, 58 (10), pp. 2055-2061.

4. **Zolotarjovs, A., Smits, K., Krumina, A., Millers, D., Grigorjeva, L.** Luminescent PEO coatings on aluminum.
(2016) ECS Journal of Solid State Science and Technology, 5 (9), pp. R150-R153.

5.Papan, J., Jovanović, D.J., Vuković, K., **Smits, K.,** Đorđević, V., Dramićanin, M. Europium(III)-doped A2Hf2O7 (A = Y, Gd, Lu) nanoparticles: Influence of annealing temperature, europium(III) concentration and host cation on the luminescent properties (2016) Optical Materials, 61, pp. 68-76.

6. Polyakov, B., Kuzmin, A**., Smits, K.**, Zideluns, J., Butanovs, E., Butikova, J., Vlassov, S., Piskunov, S., Zhukovskii, Y.F. Unexpected epitaxial growth of a few WS2 Layers on {1100} facets of ZnO nanowires (2016) Journal of Physical Chemistry C, 120 (38), pp. 21451-21459.
7. Gavrilović, T.V., Jovanović, D.J., **Smits, K.**, Dramićanin, M.D. Multicolor upconversion luminescence of GdVO4:Ln3+/Yb3+ (Ln3+ = Ho3+, Er3+, Tm3+, Ho3+/Er3+/Tm3+) nanorods (2016) Dyes and Pigments, 126, pp. 1-7.
8. E. Elsts , G. Krieke, U. Rogulis, **K. Smits, A. Zolotarjovs**, J. Jansons, A. Sarakovskis, K. Kundzins. Rare earth doped glass–ceramics containing NaLaF4 nanocrystals. Optical Materials 59 (2016) 130–135
9. A. Šutka, T.Käämbre, R. Pärna, N. Doebelin, M. Vanags, **K. Smits** and V. Kisand. Ag sensitized TiO2 and NiFe2O4 three-component nanoheterostructures: synthesis, electronic structure and strongly enhanced visible light photocatalytic activity. RSC Adv., (2016) DOI:10.1039/C6RA00728G.
10. A.N. Trukhin, **K. Smits**, J. Jansons, A. Kuzmin. Luminescence of polymorphous SiO2. Radiation Measurements 90 (2016) 6-13. DOI:10.1016/j.radmeas.2015.12.002

LECTURES ON CONFERENCES

LU CFI 31th Scientific Conference, 2016, 17-19. Febr. Riga, Latvia

1. D.Millers, K.Šmits, V.Vanks, L.Gigorjeva, R.Ignatāns, V.Dimza. Radiācijas inducēta optiskā absorbcija PLZT keramikā.
2. A.Zolotarjovs, A.Krūmiņa. Luminiscento īpašību izpēte ar Eu aktivētiem aluminija oksīda pārklājumiem uz aluminija.
3. L.Grigorjeva, F.Muktepavela, K.Šmits, A.Zolotarjovs, D.Millers. Luminiscences raksturīpašības ZnO nanopulveros un keramikās.
4. A.Krūmiņa, A.Zolotarjovs. Luminiscento pārklājumu izveide izmantojot plazmas elektroķīmisko oksidēšannas (PEO) metodi.
5. D.Olšteins, Dz.Jankoviča. Optimālās Er, Yb un Nb koncentrācijas ZrO_2 nanokristālos intensīvai augšup-pārveidotajai luminiscencei.

Transparent conductive materials (TCM-2016), 9-14 October,2016, Kret, Greece.

1. L.Grigorjeva, K.Smits, A.Zolotarjovs, E.Gorokhova, S. B. Eron'ko, P.Rodnyi, K.Chernenko. Electronic processes in doped ZnO nanopowders and transparent ceramics

UPCON 2016: Bright future for up-conversion , 09 - 11 Dec 2016. Wroclaw

1. L. Grigorjeva, K. Smits, D. Millers, A. Zolotarjovs, D. Jankovica. Efficiency of up-conversion luminescence of Yb/Tm doped fluorapatite nanopowders and ceramics

MASTER THESIS

A.Zolotarjovs. TSL un frakcionētās izspīdināšanas metodes defektu stāvokļu izpētei oksīdu materiālos.
LU Fiz.-mat.fakultāte, 2016

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.phys. M.Reinfelde
2. Dr. phys. J.Teteris
3. Dr. phys. A.Gerbreders
4. Dr. phys.U.Gertners

PhD Students

1. J.Mikelsone

Students

1. D.Damberga

COOPERATION

Latvia

1. Riga Technical University (prof. A.Ozols).
2. Daugavpils 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, 18.07.2016- 28.07.2016.

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.Mikelsone 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

1. **U.Gertners, M.Reinfelde, J.Teteris**, Light induced morphological processing of chalcogenide films, JOAM, **18** (2016) 24-28.
2. **M.Reinfelde**, L.Loghina, Z.G.Ivanova, **J.Teteris**, **U.Gertners**, S. Slang, M. Vlcek, Photoinduced surface relief grating formation in amorphous $As_{40}S_{60-x}Se_x$ thin films, JOAM, **18** (2016) 1-4.
3. A.Ogurcovs, Vj.Gerbreders, E.Tamanis, E.Sledevskis, **A.Gerbreders**, Photoelectrical and Gas-sensing Properties of Nanostructured ZnO/CuO Samples, Journ. of Nano- and Electronic Physics, **8** (2016) 04078.

LECTURES ON CONFERENCES

32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Rīga, Latvia, February 17-19, 2015.

1. J.Teteris, Hologrāfiskās litogrāfijas iespējas (Posibilities of holographic lithography), *LU CFI 32. zinātniskā konference*, Rīga, 2016.gada 17.-19.februāris*, 32st Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 17-19, 2016, Book of Abstracts, p.13.
2. J.Mikelsone, Tiešā ieraksta fotorezista izstrāde uz epoksīda polimēra bāzes (RTD of direct
   Photoresist on the base of epoxy polymer), *LU CFI 32. zinātniskā konference*, Rīga, 2016.gada 17.-19.februāris*, 32st Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 17-19, 2016, Book of Abstracts, p.47.

International Young Scientist Conference "Developments in Optics and Communications 2016", Riga, Latvia, March 21-23, 2016:

3. M.Reinfelde, Practical application of holography, Book of abstracts, p. 1
4. J.Mikelsone, J.Teteris, Direct holographic recording in azo-epoxy polymer films, Book of abstracts, p.9.

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. During 2016, near-infrared luminescence spectral. kinetics and polarization instrumentation and methods were developed, based on Hamamatsu liquid nitrogen-cooled photomultiplier.

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). Setup for measuring optical absorption changes of optical fibers ("solarization") under deep-UV ArF laser light.

Luminescence spectroscopy. Luminescence excitation by the following sources is available: diode-pumped solid state lasers (266 nm, 532 nm, 473nm, 671nm), 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 in 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). To facilitate wider access by all institute researchers, the spectrometer was transferred from laboratory room to the common-access laboratory.
Mass spectrometry: Dycor LCD-300 quadrupole mass-spectrometer, 1-300 a.m.u. with oil-free vacuum station.

MAIN RESULTS

DETECTION OF INTERSTITIAL OXYGEN AND CHLORINE IN AMORPHOUS SiO_2 BY LUMINESCENCE TECHNIQUES.

L.Skuja[1], K. Kajihara[2], K.Smits[1], A. Silins[1], H.Hosono[3]

Amorphous SiO_2 (a-SiO_2) consists of vertex-connected SiO_4 tetrahedra. The interstitial sites outside them are much larger in a-SiO_2 compared to the crystalline polymorphs of SiO_2. They can accommodate small gas molecules, either intentionally loaded (e.g., H_2 to prevent UV-solarization), or left from manufacturing processes by oxidizing $SiCl_4$ (Cl_2, O_2), or entering from environment (H_2O, O_2, N_2).
Chlorine impurities are detrimental to optical properties of a-SiO_2. Interstitial Cl_2 gives rise to absorption band at 3.8eV and increases damage to optical fibers by UV-light (solarization) or by ionizing radiation.
We have found that in the near-infrared region, alongside the photoluminescence (PL) detection of interstitial O_2 (0.976 eV band), a high sensitivity detection of interstitial Cl_2 molecules in SiO_2 is possible. At T<160 K a PL band at 1.27±0.04 eV, fwhm=0.4 eV and lifetime 7ms at T=14 K was observed. The PL spectrum shows a characteristic vibrational progression with >10 sub-bands with separations decreasing from 520 to 490 cm^{-1} towards lower energies. This feature allows to assign this PL band unambiguously to interstitial Cl_2. Estimate shows that concentrations less than 10^{14} Cl_2/cm^3 can be easily detected.

LUMINESCENCE OF SiO_2 AND GeO_2 CRYSTALS WITH RUTILE STRUCTURE. COMPARISON WITH α -QUARTZ CRYSTALS AND RELEVANT GLASSES.

A.N.Trukhin

Luminescence properties of SiO_2 in different structural states are compared. Similar comparison is made for GeO_2. Rutile and α-quartz structures as well as glassy state of these materials are considered. Main results are that for α-quartz crystals the luminescence of self-trapped exciton is the general phenomenon that is absent in the crystal with rutile structure. In rutile structured SiO_2 (stishovite) and GeO_2 (argutite) the main luminescence is due to a host material defect existing in as-received (as-grown) samples. The defect luminescence possesses specific two bands, one of which has a slow decay (for SiO_2 in the blue and for GeO_2, in green range) and an-other, a fast ultraviolet (UV) band (4.75 eV in SiO2 and at 3 eV in GeO2). In silica and germania glasses, the

luminescence of self-trapped exciton coexists with defect luminescence. The latter also contains two bands: one in the visible range and another in the UV range. The defect luminescence of glasses was studied in details during last 60–70 years and is ascribed to oxygen deficient defects. Analogous defect luminescence in the corresponding pure non-irradiated crystals with α-quartz structure is absent. Only irradiation of a α-quartz crystal by energetic electron beam, γ-rays and neutrons provides defect luminescence analogous to glasses and crystals with rutile structure. Therefore, in glassy state the structure containing tetrahedron motifs is responsible for existence of self-trapped excitons and defects in octahedral motifs are responsible for oxygen deficient defects.

SCIENTIFIC VISITS ABROAD

1. Anatoly Trukhin, Linards Skuja, International symposium on SiO_2, Advanced dielectrics and related devices, Nice, June 13-15, 2016 (France).
2. Linards Skuja, Visiting scientist in Laboratory of Irradiated Solids, Ecole Polytechnique, Univ, Paris Saclay, Palaiseau, France (France), October 1- 31, 2016.

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).

SCIENTIFIC PUBLICATIONS

1. **A.N. Trukhin**, Luminescence of SiO_2 and GeO_2 crystals with rutile structure. Comparison with α-quartz crystals and relevant glasses, Low Temperature Physics/Fizika Nizkikh Temperatur,, 42, 561 (2016).

2. **A.N.Trukhin**, K.Smits, J.Jansons, A.Kuzmin Luminescence of polymorphous SiO_2. Radiation Measurements, 90 p.6-13(2016) .

LECTURES IN CONFERENCES

International symposium on SiO_2, Advanced dielectrics and related devices, Nice, June 13-15, 2016 (France).

L.Skuja, K.Kajihara, K. Smits, H.Hosono Interstitial Chlorine Molecules in SiO_2 Glass, Abstracts, p. 89-90 (sciencesconf.org:sio2-2016:101362)

A.N.Trukhin, A.Antuzevičs, K.M.Golant, D.L. Griscom Luminescence of Phosphorus Doped Silica Glasses, Abstracts, p. 93-94 (sciencesconf.org:sio2-2016:97199)

International Workshop "LIGHTtalks: Power of Photonics" April 25, 2016, Riga, LATVIA

L.Skuja, Effect of interstitial gas molecules on perfomance of optical devices made from high purity glassy SiO_2, Book of Abstracts, p.11.

International Workshop "Metrology at nanoscale with diamonds", Riga Dec.16, 2016

Detection of interstitial oxygen in SiO_2-related materials.

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32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, Latvia, February 17-19, 2016:

1) L. Skuja, K. Kajihara, K.Smits, A. Siliņš, H. Hosono Detection of interstitial oxygen and chlorine in amorphous SiO_2 by luminescence techniques. Abstracts, p.102.

2) L.Trinklere, B.Berzina, V.Korsaks, A. Trukhin Luminescence properties of wide bandgap material $LiGaO_2$, Abstracts, p.15.

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 and coatings. Investigations include modification processes of structure and micro-mechanical properties in wide-gap ionic crystals induced by high dose irradiation with swift ions or laser treatment, and structural and mechanical characterization of complex nano-composite coatings for tribological and protective applications.
Other important area of interest is processes at grain boundaries in homogeneous as well as heterogeneous materials (nanopowders, oxide ceramics, superplastic alloys, nuclear materials etc.). These include investigation of interaction processes at interphase boundaries, such as adhesion, wetting and corrosion.
The main research topics in 2016 were:

- Effects of electronic and nuclear energy loss in formation of extended defects and modification of micro-mechanical properties of swift- ion- irradiated wide gap ion crystals (LiF).
- Investigations of structure and deformation behavior of high power DC magnetron sputtered a-C:Cu nanocomposite coatings for tribological applications and thin protective ALD oxide-based nanolaminate coatings.
- Structural and optical investigation of transparent ZnO-based ceramics.

LABORATORY EQUIPMENT

Nanoindenter G200 (Agilent, USA), Atomic force microscope CPII (Veeco Digital Instrum.), Optical microscope Nikon Eclipse L150

SCIENTIFIC STAFF

Dr.habil.phys., emeritus J.Maniks
Dr.phys. F.Muktepavela
Dr.phys. I.Manika
Dr.phys. R.Zabels

Students
B.sc. R.Grants

VISITORS FROM ABROAD

Prof.K.Schwartz, GSI, Darmstadt, Germany (1 week).

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)

Lithuania

Kaunas University of Technology, Department of Physics (Dr. L.Marcinauskas)

Estonia

Institute of Physics, University of Tartu (Dr. K. Kukli, T. Jogiaas)

Germany

GSI, Darmstadt, (Prof. K.Schwartz).

Spain

National Laboratory for Magnetic Fusion. Materials CIEMAT Avda, Madrid (Dr. Teresa Hernández).

Kazakhstan

L. Gumilyov Eurasian National University (Dr. A.Dauletbekova)

Russia

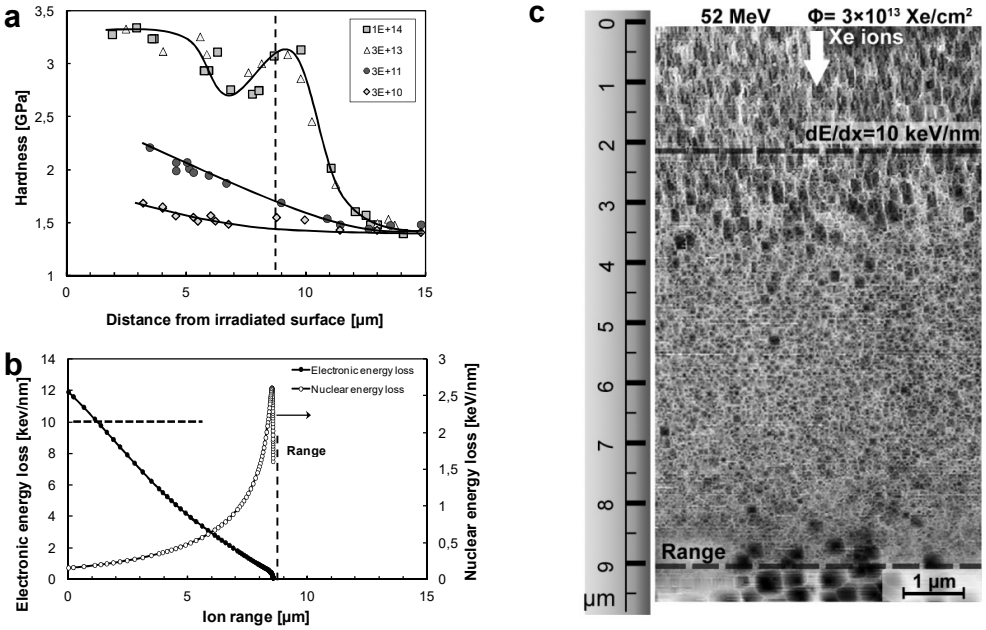
Institute of Solid State Physics RAN, Chernogolovka (Dr.V.Sursajeva)
National University of Science and Technology "MISIS, Moscow, (Prof. B. Straumal)
Research and Technological Institute of Optical Materials, Scientific Center "S.I. Vavilov State Optical Institute" St. Petersburg, Russia (Dr E. Gorokhova).

MAIN RESULTS

MeV-energy Xe ion-induced damage in LiF: The contribution of electronic and nuclear stopping mechanisms

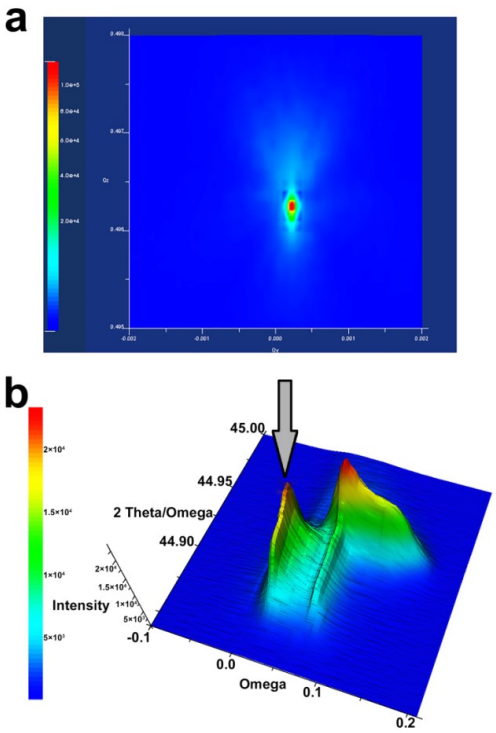
R. Zabels, I. Manika, K. Schwartz, M. Baizhumanov, R. Grants,
E. Tamanis, A. Dauletbekova, M. Zdorovets

The contribution of electronic and nuclear damage mechanisms in the modification of structure and micromechanical properties of LiF crystals irradiated with 52, 224, and



(a) Depth profiles of hardness obtained by indentation on cross-sections of 52 MeV Xe ion irradiated LiF crystals, (b) corresponding electronic and nuclear energy losses of 52 MeV energy Xe ions in LiF. (c) AFM micrograph of chemically etched cross-section of LiF irradiated to fluence 3×10^{13} ions/cm^2 with 52 MeV Xe ions.

450 MeV Xe ions at fluences 10^{10}–10^{14} ions cm^2 has been studied. The ion-induced formation of dislocations and hardening in LiF at fluences above 10^{10} ions/cm^2 has been observed. By comparison of depth profiles of hardness and calculated ion energy loss a joint contribution of electronic excitation and nuclear (impact) mechanisms to the ion-induced hardening can be seen. The electronic excitation mechanism dominates in the major part of the ion range while the impact mechanism prevails in a narrow zone at the end of the ion range. The comparison of the contribution of these mechanisms shows that the efficiency of hardening produced by electronic excitation mechanism is by an order of magnitude higher than that produced by the impact mechanism.



Ion-induced prismatic dislocation loops are the main cause of the hardening. At an electronic energy loss above the threshold of 10 keV/nm[1], an ordered dislocation structure is created. HRXRD measurements on heavily irradiated LiF crystals (at fluences above10^{12} Xe cm^{-2}) reveal a mosaic type substructure composed of nanosize domains tilted under low angles.

High resolution XRD reciprocal space maps of (a) pristine LiF crystal, (b) LiF irradiated with 450 MeV Xe ions, fluence 10^{13} ions/cm^2. Arrow marks the peak characteristic to the unirradiated LiF.

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1. **Zabels, R., Manika, I.,** Schwartz, K., Baizhumanov, M., **Grants, R.,** Tamanis, E., Dauletbekova, A., Zdorovets, M. MeV-energy Xe ion-induced damage in LiF: The contribution of electronic and nuclear stopping mechanisms. Phys. Status Sol.(b)., **253** (2016) (8) pp.1511-1516
2. K. Kukli, E. Salmi, T. Jõgiaas, **R. Zabels,** M. Schuisky, J. Westlinder, K. Mizohata, M.Ritala, M. Leskelä**.** Atomic layer deposition of aluminum oxide on modified steel substrates**.** Surface and Coatings Technology, **304** (2016) pp. 1–8.
3. M.Cemauskas, L.Marcinauskas, **R.Zabels**. Synthesis of nanostructured amorphous carbon-copper composite films by plasma-enhanced chemical vapour deposition, Thin Solid Films, **615** (2016) pp.195-201.
4. V. Mironovs, M. Lisicins, P. Onufrievs, **F. Muktepavela**, A. Medvids. Hardening of Steel Perforated Tape by Nd:YAG Laser, Key Engineering Materials, **721** (2016) pp.456-460.
5. A. Kjapsna, L. Dimitrocenko, I. Tale, A. Trukhin, R. Ignatans, **R. Grants**. Characterization of Crystalline Structure and Morphology of Ga_2O_3 Thin Film Grown by MOCVD Technique. Key Engineering Materials, **721** (2016) pp.253-257.

LECTURES AT CONFERENCES

XV Int. Conf. on Integranular and Interphase Boundaries in Materials (iib-2016). May, 23-27, Moscow, Russia

1. F. Muktepavela, E. Gorokhova, L. Grigorjeva, E.Tamanis, R. Zabels. Surface and grain boundary effects in luminescent properties of ZnO ceramics as functional material. Abstracts, p. 56.
2. F. Muktepavela, R. Zabels Deformation –induced wetting processes at phase boundaries in superplastic Pb-Sn eutectic. Abstracts, p. 157.

15th International Conference on Plasma Surface Engineering. September 12 - 16, 2016, Garmisch-Partenkirchen, Germany

3. P. Nazarovs, V. Mitin, R. Zabels, V. Kovalenko. Production and characterization of carbon-based nanocomposite tribological coatings obtained by High-power DC magnetron sputtering. Abstracts, PO p.303.

29th Symposium on Fusion Technology, September 5-9, 2016, Prague, Czech Republic

4. C.Soto, J. Echeberria, J.M. Martinez-Esnaola, T. Hernandez, M. Malo, A. Morono, E. Platacis, F. Muktepavela, C. Garciarosales. SiC-based sandwich material for Flow Channel Inserts in DCLL Blankets: manufacturing, characterization, corrosion tests. Abstracts, O3B p.48.

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5. T. Jogiaas, R. Zabels, H. Seemen, A. Tamm, K. Kukli, Atomic layer deposited thin films with gradient composition, Poster P-01-117.

IX Международная конференция Фазовые превращения и прочность кристаллов"(ФППК-2016) памяти академика Г.В.Курдюмова7-11 ноября 2016 года , Черноголовка Russia

6. Muktepavela F., Zabels R., Gorokhova E. “Microstructural factor in properties of ZnO:In ceramics ", Abstracts, p.1.

25th Int. Baltic Conf. of Enginering Materials &Tribology - Baltmattrib 2016, November 3-4, Riga, Latvia

7. V. Mironov, M. Lisicins, P. Onufrievs, F. Muktepavela, A. Medvids. Hardening of Steel Perforated Tape by Nd:YAG Laser. Abstract book.
8. A. Kjapsna, L. Dimitrocenko, I. Tale, A. Trukhin, R. Ignatans, R. Grants. Characterization of Crystalline Structure and Morphology of Ga_2O_3 Thin Film Grown by MOCVD Technique. Abstract book.

The 32nd Annual scientific conference of Institute of Solid State Physics, University of Latvia, February 17-19, 2016, Riga, Latvia

9. R. Zabels, V. Kovaļenko, P. Nazarovs. Interfacial plasticity of DC magnetron sputtered carbon/copper nanocomposite films, Abstracts, p.78.
10. R.Grants, R.Zabels, I.Manika, Nanoindentation and AFM study of depth-dependent damage in LiF irradiated with swift ^{12}C ions, Abstracts, p.124.
11. L. Grigorjeva, F. Muktepavela, K. Šmits, A. Zolotarjovs, D. Millers. Luminescence properties of ZnO nanopowders and ceramics, Abstracts, p.45.

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.
Oskars Vilītis	Dr.phys.
Aivars Vembris	Dr.phys.
Edgars Nitišs	Dr.phys.
Jānis Latvels	Dr.Eng.
Andrejs Tokmakovs	MSc.
Jānis Busenbergs	MSc.
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PhD students:

Elīna Laizāne	MSc.
Kaspars Pudžs	MSc
Raitis Gržibovskis	MSc
Igors Mihailovs	MSc.
Jūlija Perveņecka	MSc
Arturs Bundulis	MSc

Students:

Elza Lina Linina BSc

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;
- Thermo- electrical 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.

National Research Program in MultIfunctional Materials and composItes, photonicS and nanotechnology (IMIS^2) (2014-2017):

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

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

TETRATHIOTETRACENE THIN FILM MORPHOLOGY AND ELECTRICAL PROPERTIES

Kaspars Pudzs, Aivars Vembris, Janis Busenbergs, Martins Rutkis, Simon Woodward

Thermoelectric (TE) devices which can provide direct thermal to electrical energy conversion of low temperature waste heat (<200 °C) could potentially help reduce global warming if their widespread utilisation could be realized. Presently the materials used for efficient TE devices are expensive, often not widely available and normally contain unsustainable or toxic elements such as Te and Pb. Organic materials with good TE properties could be a solution to these issues. High-electrical conductivity materials are a prerequisite for TE generators. One class of candidates for TE devices are radical cation salts attained by oxidation of tetrathiotetracene (TTT, Figure 1A), such as ditetrathiotetracene triiodide. The TE performance of these salts is often compromised if non pristine TTT starting material is used and (low) electrical conductivity of the initial TTT is frequently the best indicator of its purity.

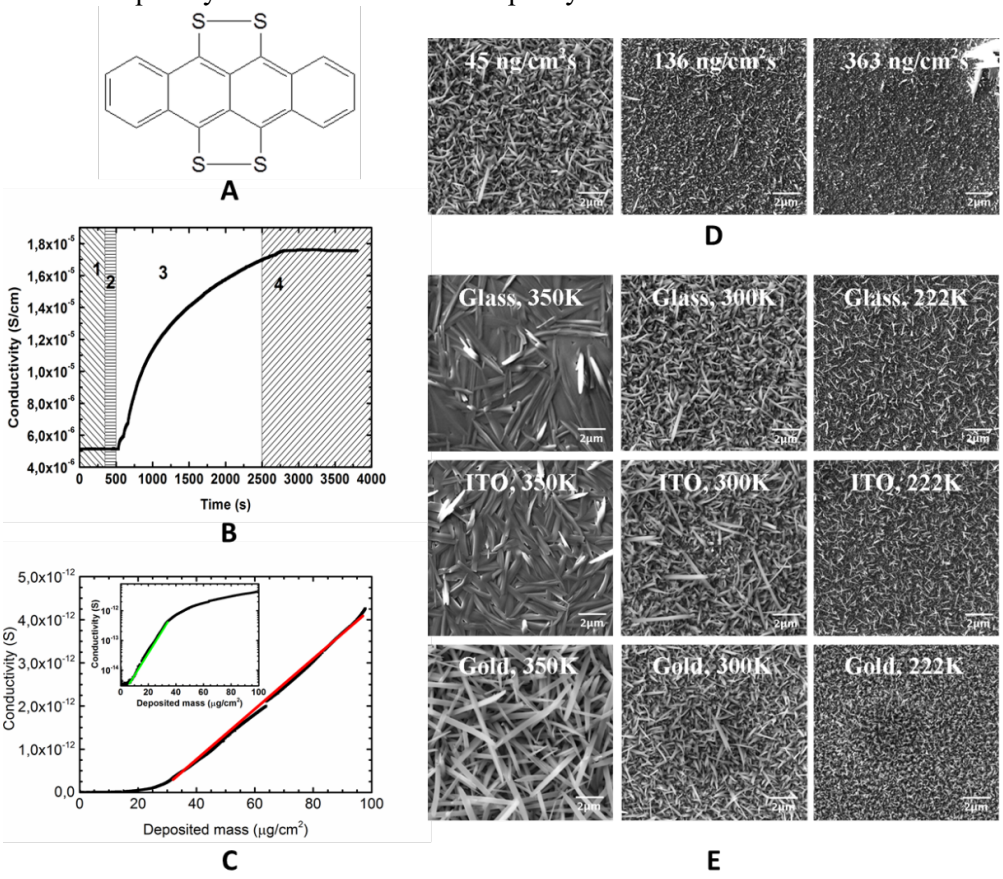


Figure 1 A - Chemical structure of tetrathiotetracene (TTT), B - Air impact on TTT thin film conductivity. 1 - Vacuum, 6·10-4 Pa, turbo pump decelerating, 2 - N_2 is inflated in the chamber, 3 – Chamber is exposed to the air, 4 – turbo molecular pump accelerating, vacuum. C - Linear and exponential electrical conductivity dependence on TTT thin film thickness, D - SEM images of the TTT thin films obtained at different evaporation rates on glass at 300 K, E - SEM images of the TTT thin films on different substrates at different temperatures during sublimation.

In this paper the morphology of vacuum sublimed (7·10-6 mbar) tetrathiotetracene (TTT) thin films is shown to be strongly affected by the thermal deposition temperature (222-350 K) and rate of deposition. Mostly needle-like morphologies are identified by scanning electron microscopy. Optimal TTT purity (a pre-requisite for device preparation via subsequent oxidation) is evidenced by their initially low electrical

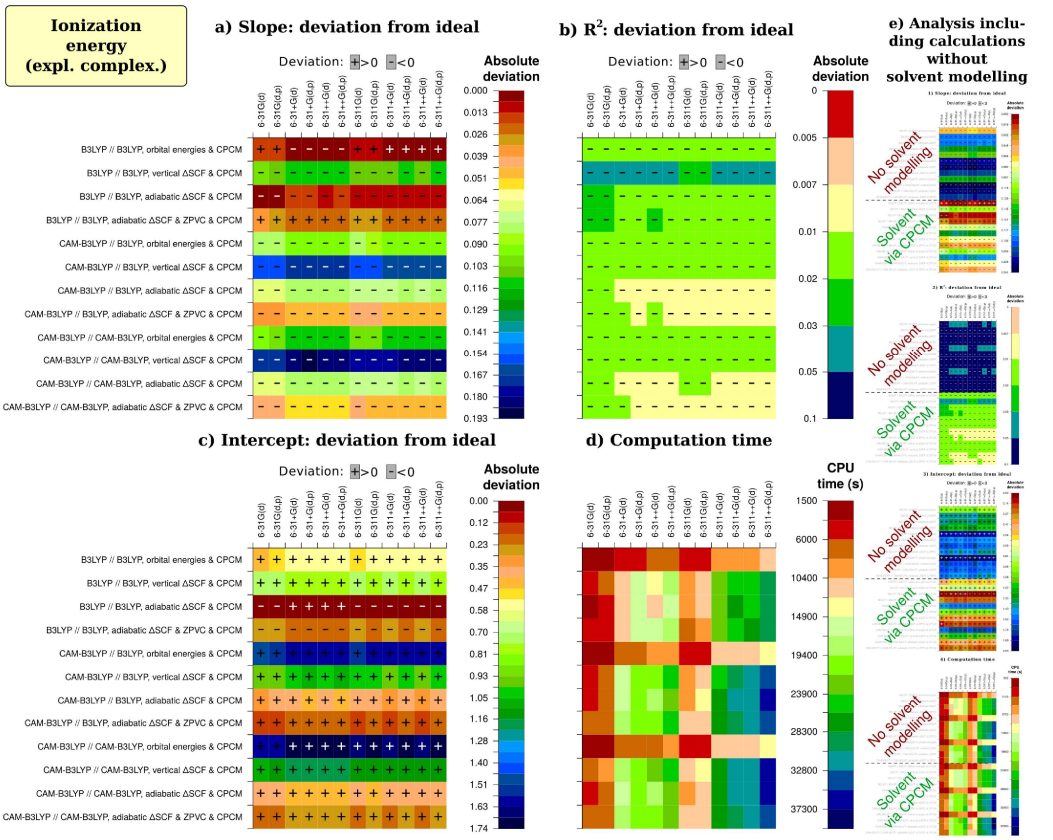
conductivity. Altering the TTT morphology, by variation of the evaporation parameters, strongly affects this base electrical conductivity. Four probe conductivity measurements and charge extraction by linear increasing voltage methods are used to characterize film electrical properties. In-plane conductivity of up to $7.03 \cdot 10^{-5}$ S/cm is achieved for pure TTT thin films. Subsequent aerial oxidation resulted in a 3.4-fold increase in electrical conductivity. (Figure 1B)

Threshold amounts of deposited TTT (>33 μg/cm2) are necessary to attain bulk material which has the highest electrical conductivity. As one can see from the logarithmic inset (Figure 1C), the conductivity increases exponentially up to 33 μg/cm2. One explanation for this is that this initial conductivity does not describe bulk material. If the initial deposition is not uniform but consists of small clusters of TTT forming a percolation network, the conductivity between the neighbouring clusters will be defined by tunnelling mechanism. We suggest two charge carrier transport mechanisms: Charge carriers tunnelling between TTT clusters take place at the beginning of film growth due to the formation of percolation network. Hopping mechanism becomes dominant at certain film thickness of material where bulk material conductivity occurs. The conductivity in the TTT films is anisotropic and depends on crystal size, packing density and alignment. It can be partially moderated by appropriate control of substrate type and temperature (Figure 1E) and TTT deposition rate (Figure 1D). Larger and more in-plane orientated crystals are favoured by increasing substrate temperature to 350 K. This increases the in-plane contribution to the electrical conductivity at the expense of the perpendicular component. Higher packing density and smaller crystals are favoured by increasing TTT deposition rates and lower temperatures. The improved packing of smaller poorly ordered TTT crystals provides higher in-plane conductivity than films with higher proportions of in-plane orientated larger crystals. Packing density has the pivotal role in the conductivity rather than crystallite size. Oxidation of TTT films offers the potential to access materials with useful electrical conductivities and this will be reported in due course.

RATIONAL COMPUTING OF ENERGY LEVELS FOR ORGANIC ELECTRONICS: THE CASE OF 2-BENZYLIDENE-1,3-INDANDIONES

Igors Mihailovs, Valdis Kampars, Baiba Turovska and Martins Rutkis

Device engineering in organic electronics, an active area of research, requires knowledge of energy levels of organic material (traditionally but ambiguously denoted HOMO and LUMO). These can be effectively determined by electrochemical investigation, but yet more effective would be quantum chemical (QC) computation of these quantities. However, there is no consensus on the computational method in the research community. Ongoing discussions often focus on choosing the right density functional method, but neglect other model parameters, in particular, the basis set. This study considers comparison of various methodologies and parameters for predicting ionization energy *I* and electron affinity *A*. Our aim was to outline a QC 'recipe' used in search of new structures with desired energy levels for application in the field of organic electronics. Validation of calculated results to electrochemically determined values through linear regression and factor analysis were used for compiling the recipe, ensuring trend-descriptive and resource-effective combination of QC model parameters. We explored a series of 1,3-indandione derivatives to reduce the need for too numerous calculations, as with this approach there should not be many factors of molecular composition to annihilate via the expansion of the compound set.



Results of factor analysis for ionization energy (including explicit complexation). Sign of deviation is indicated in each cell of the tables. Cell coloring represents the quality of results, with reddish brown corresponding to high precision mountains and dark blue – to deep discord seas. On slices (a) to (d) all studied factors are displayed but the most significant one (the inclusion of solvent in the computational model), effect of which can be overviewed on slice (e) as designed for better comprehension.

Accounting for solvation by the medium is found to be essential and hardly consuming any additional CPU time if basic CPCM (COSMO alike) is used; there is hardly any need to account for explicit complexation even with such a weakly basic solvent as acetonitrile, for electrode surface effects can dominate over advantages of such a simple approach. Counterpoise corrections were also to no advantage. Basis set extension with extra valence functions is found to be much more effective than by adding diffuse functions. Among explored methods, B3LYP/6-311G(d) + CPCM is the recommended one for ionization energy, providing experimental quality results suitable for screening purposes. CAM-B3LYP is deemed more efficient for electron affinity, though by far not achieving the desired quality. Correction by computed reference redox pair potential is also found to be overall advantageous. Interestingly, the stereotype of the ultimate need for diffuse functions to describe the electron affinity has been busted, with some support from literature. For the case of our molecules, geometry optimization with either functional yielded almost the same performance in *I* / *A* description.

STUDY OF STRUCTURE–THIRD-ORDER SUSCEPTIBILITY RELATION OF INDANDIONE DERIVATIVES

Arturs Bundulis, Edgars Nitiss, Igors Mihailovs, Janis Busenbergs, Martins Rutkis

In recent years nonlinear optical (NLO) organic materials have attracted a great interest due to their potential for applications in optical limiting, optical data storage and optical processing. In this regard, currently most of the effort is devoted towards finding organic NLO compounds with pronounced Kerr effect and two-photon absorption (TPA) as well as efforts to define guidelines which would allow to predict the third order NLO efficiency of organic molecules. In this paper we describe the results obtained during

measurement of third order nonlinearities of aminobenziliden-1,3-indandione (ABI) (see figure 1.A) derivatives which have shown to possess second order NLO properties. In our experiments, we investigated solutions in which the optical nonlinearity of an organic solute is determined with respect to organic solvent. The measurements were carried out employing the Z-scan, and two 1064 nm Nd:YAG lasers with picosecond (ps) and with nanosecond (ns) pulse widths, respectively, were used as excitation sources.

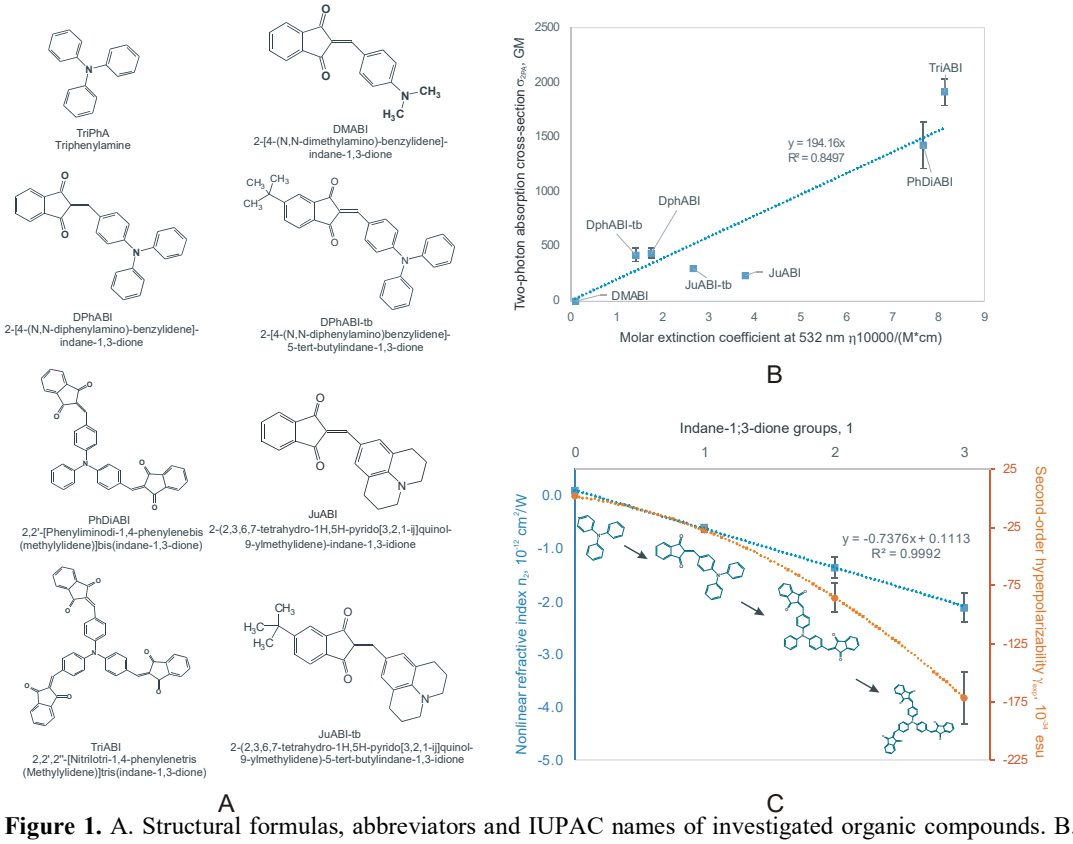


Figure 1. A. Structural formulas, abbreviators and IUPAC names of investigated organic compounds. B. Two-photon absorption cross-section values plotted as function from molar extinction coefficient. A correlation between both parameters can be observed. C. Nonlinear refractive index and second-order hyperpolarizability of TriPhA, DPhABI, PhDiABI and TriABI.

In the paper we demonstrate the influence of excitation source parameters for correct measurement of Kerr coefficient and TPA coefficient. Comparison of experimental results for chloroform from ns and ps data confirms that thermal effects can complicate determination of Kerr effect induced nonlinear refractive index. To avoid errors for Kerr effect measurements we would advise to choose appropriate laser pulse length and repetition frequency based on calculations of thermal diffusivity and sound wave to propagation time constants.

We showed the the correlation of the TPA cross-section and molar extiction coefficent values is expected but is not compulsory (see Figure 1.B), since the transition rules for two-photon transition are different to those of single photon. We also described the influence of different acceptor and donor groups on the third-order NLO properties of organic molecules containing aminobenziliden-1,3-indandione structural fragment. Firstly, by changing electron donor group the sign of optical Kerr coefficient also varies. For dimethylamino- group optical Kerr coefficient;Kerr was positive while for diphenylamino- or julolidyl- groups optical Kerr coefficient n2;Kerr was negative. Secondly, we concluded that introducing bulky tert-butyl group decreases the magnitude of optical Kerr coefficient. Lastly, by adding additional indane-1;3-dione groups to triphenylamino donor group optical Kerr coefficient changed linearly, while second-order hyperpolarizability increased nonlinearly (see Figure 1. C). This leads us to

believe that there is a synergistic interaction between each indane-1;3-dione branch. We also compared experimental and quantum chemical calculations for isotropically averaged molecular second-order hyperpolarizability real part. A linear correlation of both values was demonstrated, however experimental values were 3-6 times larger than the ones acquired from quantum calculations.

SCIENTIFIC PUBLICATIONS

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2. **Kaspars Pudzs, Aivars Vembris, Raitis Grzibovskis, Janis Latvels**, Elmars Zarins, Impact of the molecular structure of an indandione fragment containing azobenzene derivatives on the morphology and electrical properties of thin films, Material Chemistry and Physics 173 (2016) pp 117-125, doi:10.1016/j.matchemphys.2016.01.046
3. Elmars Zarins, **Andrejs Tokmakovs**, Valdis Kokars, Andris Ozols, Peteris Augustovs, **Martins Rutkis**, Triphenyl group containing molecular glasses of azobenzene for photonic applications, Optical Materials 53 (2016) pp 146–154, http://dx.doi.org/10.1016/j.optmat.2016.01.044.
4. **Raitis Grzibovskis, Aivars Vembris, Kaspars Pudzs**, Relation between molecule ionization energy, film thickness and morphology of two indandione derivatives thin films, Journal of Physics and Chemistry of Solids 95 (2016) 12–18, http://dx.doi.org/10.1016/j.jpcs.2016.03.010
5. Kaspars Traskovskis, Valdis Kokars, **Andrejs Tokmakovs, Igors Mihailovs, Edgars Nitiss,** Marina Petrova, Sergey Belyakov and **Martins Rutkis**, Stereoselective synthesis and properties of 1,3-bis(dicyanomethylidene)indane-5-carboxylic acid acceptor fragment containing nonlinear optical chromophores, Journal of Materials Chemistry C, 2016,4, 5019-5030, http://dx.doi.org/10.1039/C6TC00203J
6. **Raitis Grzibovskis, Aivars Vembris**, Study of the P3HT/PCBM interface using photoemission yield spectroscopy, Proc. SPIE. 9895 (2016) 98950Q, http://dx.doi.org/10.1117/12.2227823
7. **O. Vilitis, M. Rutkis, J. Busenberg**, D. Merkulov, Determination of contact potential difference by the kelvin probe (part I) I. Basic principles of measurements, Latvian Journal of Physics and Technical Sciences, 2016, 2, pp 48 – 57, http://dx.doi.org/10.1515/lpts-2016-0013
8. **Aivars Vembris**, Elmars Zarinsh, Valdis Kokars, Amplified spontaneous emission of pyranyliden derivatives in PVK matrix, Proc. SPIE. 9895 (2016) 989509-1-7, http://dx.doi.org/10.1117/12.2227841
9. Dalius Gudeika, Vita Zilinskaite, Juozas V. Grazulevicius, Roman Lytvyn, **Martins Rutkis**, **Andrey Tokmakov**, 4-(Diethylamino)salicylaldehyde-based twin compounds as NLOactive materials, Dyes and Pigments 134 (2016) 244 – 250, http://dx.doi.org/10.1016/j.dyepig.2016.06.047
10. **Igors N Mihailovs**, Valdis Kampars, Baiba Turovska and **Martins Rutkis**, Rational computing of energy levels for organic electronics: the case of 2-benzylidene-1,3-indandiones, RSC Advances, 2016, 6, 85242–85253, http://dx.doi.org/10.1039/C6RA16456K
11. **Arturs Bundulis, Edgars Nitiss, Igors Mihailovs, Janis Busenbergs**, and **Martins Rutkis**, Study of Structure–Third-Order Susceptibility Relation of Indandione Derivatives, J. Phys. Chem. C, 2016, 120 (48), pp 27515–27522, http://dx.doi.org/10.1021/acs.jpcc.6b07003

ABSTRACTS

32th Scientific Conference of the Institute of Solid State Physics, University of Latvia, February 17-19, 2016

1. Aivars Vembris, Optical and amplified spontaneous emission properties of DWK-1TB molecules in polymer matrix), Abstracts p.25
2. Jūlija Perveņecka, Aivars Vembris, Edgars Nitišs, Elza Liniņa, Preparation of microstructure in piramiliden derivatives containing su-8 films, Abstracts p.26
3. Raitis Gržibovskis, Aivars Vembris, Study of interface between two organic compounds using photoemisiion yield spectroscopy method, Abstracts p.27.
4. Kaspars Pudžs, Study of thermoelectric properties of organic thin films for infra-red radiation sensor application, Abstracts p.30
5. Arturs Bundulis, Edgars Nitiss, Janis Busenbergs, Martins Rutkis, Implementation of z-scan method for determinatio of non-linear optical material two-photon absorption and optical Kerr coefficients, Abstracts p.31

12th International young scientist conference "Developments in Optics and Communications", Riga, March 21-23

1. Kaspars Pudzs, Study of thermoelectric properties of organic thin films for infra-red radiation sensor application, Book of Abstracts pp.-5
2. Raitis Grzibovskis, Aivars Vembris, Kaspars Pudzs, Molecule ionization energy and morphology dependence on film thickness of two indandione derivatives, Book of Abstracts p.6
3. Jūlija Perveņecka, Aivars Vembris, Edgars Nitišs, Elza Liniņa, Preparation of microstructure and amplified spontaneous emission in piramiliden derivative containing SU-8 films, Book of Abstracts p.7

1ST NFFA EUROPE SUMMER SCHOOL, JULY 18-22, BARCELON, 2016

1. K. Pudzs. Fabrication process of electrodes for 3w methods measurements

14th European conference on Thermoelectrics, September 20-23, Lisbon, 2016

1. K. Pudzs, A. Vembris, M. Rutkis, J.Busenbergs, ZT value determination of tetrathiotetracene based organic thin films, Book of Abstracts p.235

16th Baltic Polymer Symposium, Klaipeda, Lithuania, September 21-24, 2016

1. Raitis Grzibovskis, Aivars Vembris, Kaspars Pudzs, Ionization energy studies of P3HT-PCBM interface using photoemission yield spectroscopy, Book of Abstracts p.68
2. Aivars Vembris, Elmars Zarins, Valdis Kokars, Stimulated emission of DCM derivatives in PVK matrix, Book of Abstracts p.13
3. J. Pervenecka, A. Vembris, E. Zarins, V.Kokars, Investigation of photoluminescence and amplified spontaneouse emission in bis-DCM derivates containing pure thin films, Book of Abstracts p.115

23rd International Conference on Spectral Line Shapes, June 19 -24, 2016, Toruń, Poland

1. G Revalde, J Alnis, E Nitišs, K Blušs, K Grundšteins, CRDS measurements of Acetone concentration.

DEPARTMENT OF FERROELECTRICS

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

LABORATORY OF PHYSICS AND APPLICATION OF FUNCTIONAL MATERIALS

Head of Laboratoy Dr.habil.phys. V.Dimza

LABORATORY OF SYNTESIS AND PROCESSING

Head of Laboratory M.chem. M.Antonova

REAEARCH AREAS
MATERIALS

1. Production of new modified ferroelectric ceramics by doping with monoxides, developing binary or multicomponent solid solutions:
− modified (Pb,La)(Zr,Ti)O_3 (PLZT);
− lead-free perovskite ceramics based on ($Na_{0.5}Bi_{0.5}$)NbO_3, (K,Na)NbO_3 and $BaTiO_3$;
- $BiFeO_3$, Bi($Fe_{0.5}Cr_{0.5}$)O_3 ,$SrMnO_3$,

METHODS

1. Investigation of kinetic parameters of synthesis and sintering processes;
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, equipment for measurement of electrocaloric effect, methods for measurement of electromechanical properties, luminescence;
Properties: electromechanical properties, electrocaloric effect, thermal expansion, optical (absorption, luminescence), dielectric and magnetic properties, electronic structure**;**
Problems
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; interpretation structure of NBT based materials, evaluation of electrocaloric effect.

SCIENTIFIC STAFF

Dr.habil.phys. V.Dimza, Dr.phys. K.Bormanis, Dr.phys M.Dunce, Dr.habil.phys. A.Sternberg, Mg.phys. Shirmane, Dr.phys. Ē.Birks, Dr.phys. V.Pankratovs, Dr.phys. M.Kundziņš, Mg.chem. M.Antonova, Mg.chem. A.Kalvane, Mg.phys. K.Kundzins, B.phys. M.Livinsh, Mg.phys. A.Plaude, Mg.phys. R.Ignatans, Mg.phys. L.Kundziņa

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Germany

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3. Darmstadt University of Technology (Dr. Joerg Zimmermann).
4. HASYLAB at DESY (Hamburg) (Dr. Aleksei Kotlov))

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2.Dr. Yuran Niu (Max IV, Lund, Sweden)

Denmark

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2. Aarhus University (Prof. Brian Bech Nielsen)

Estonia

Institute of Physics, Tartu University (Prof. Alexandr Lushchik, Prof. Ergo Nommiste)
Institute of Physics, Tartu University (Prof. Marko Kirm, Dr. Sebastian Vielhauer)

Finland

1. Uniiversity of Oulu (Prof. Marko Huttula)
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3. University of Oulu (Dr. Wei Cao)

Ukraine

1 Ivan Franko National University of Lviv (Prof. Anatoly Voloshinovskii, Prof. Vladimir Savchyn)
2 Poltava Quartz Glass Plant Ltd. (V. Panibratskiy)
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4. Taurida National V.I. Vernadsky University, Simferopol (A.V. Yatsenko).

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1 Fisk University, Tennessee (Prof. Arnold Burger)
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3 Lawrence Berkley National Laboratory (Dr. Gregory A. Bizarri)

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2 Vienna University of Technology, Institute of Atomic and Subatomic Physics (Prof. H.W. Weber).

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1. I.V. Tananaev Institute of Chemistry and Technology of Rare Elements and Mineral Raw Materials of Kola Science Centre of RAS, Apatity (M.N. Palatnikov, N.V. Sidorov).
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10. Southern Federal University, Research Institute of Physics and Physics Department, Rostov on Don, (I.P. Raevski, L. Reznichenko, I.A. Parinov).
11. Voronezh State Technical University, Voronezh

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MAIN RESULTS

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

J. SUCHANICZ, R. BUJAKIEWICZ-KORONSKA, M. DZIUBANIUK, A. KALVANE AND A. STERNBERG

The external stress (0–1500 bar) dependence of dielectric properties and an aging effect of BiFeO3 ceramic has bee n 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.

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 ε'(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.

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.

EFFECTS OF HIGH-INTENSITY LIGHT ON STRUCTURE AND MECHANICAL CHARACTERISTICS OF CERAMIC Nb_2O_5 AND $Nb_{2(1-y)}Ta_{2y}O_5$ PENTAOXIDES *)

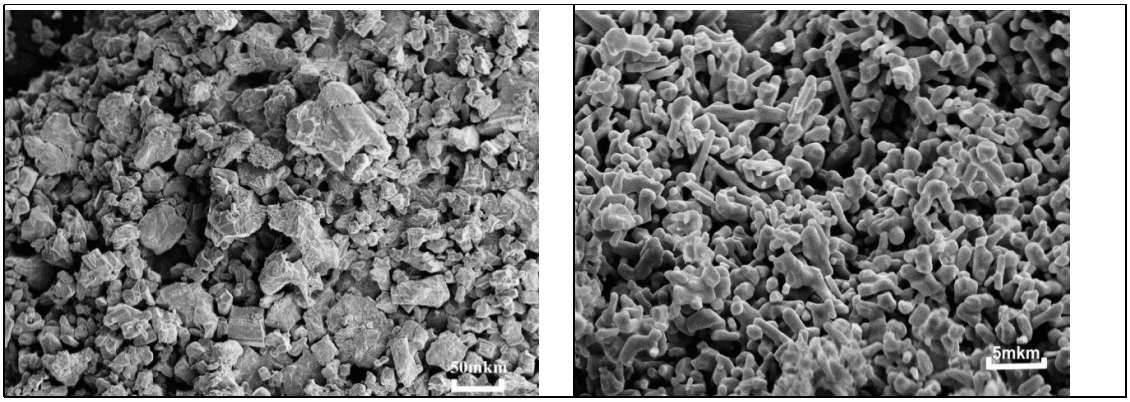
M.N. Palatnikov, O.B. Shcherbina, V.V. Efremov, N.V. Sidorov, and K. Bormanis

In mixtures of niobium and tantalum oxides co-precipitated from hydroxides the presence of one pentoxide affects the polymorphic transformations of the other (transformation of the low-temperature phase of niobium oxide L-Nb_2O_5 into the high-

temperature phase *H*-Nb_2O_5 is suppressed by tantalum pentoxide) and can be used to prepare mixed low-temperature polymorphs of niobium-tantalum pentoxides $Nb_{2(1-y)}Ta_{2y}O_5$ of low fluorine content.

The developed technological approaches to obtaining mixed $Nb_{2(1-y)}Ta_{2y}O_5$ oxides are shown to allow synthesis of $LiTa_yNb_{1-y}O_3$, $Li_xNa_{1-x}Ta_yNb_{1-y}O_3$ and $NaTa_yNb_{1-y}O_3$ solid solutions at lower temperatures the properties of the obtained solid solutions being different (for example, a higher value of the high-frequency permittivity and ion conductivity). The results are of great practical interest to comparative studies of the ways the structure and properties are affected by conditions under which the mixed niobium and tantalum pentoxides are prepared.

Mixed $Nb_{2(1-y)}Ta_{2y}O_5$ (y = 0.068, y = 0.111, y = 0.363) oxides of fluorine concentration of less than 0.05 wt.% and concentration of basic cation impurities not exceeding ~ $5 \cdot 10^{-4}$ wt.% have been obtained. The structure and mechanical properties of ceramic Nb_2O_5, $Nb_{2(1-y)}Ta_{2y}O_5$ ceramics co-precipitated from oxides, prepared by conventional techniques and by high-intensity light treatment are studied and compared.



a b

Figure 1. Microstructure of the $Nb_{2(1-y)}Ta_{2y}O_5$ ceramic prepared by a conventional ceramic processing technique: $y = 0.068$ (a) and $y = 0.363$ (b).

The changes of the polycrystalline structure in the $Nb_{2(1-y)}Ta_{2y}O_5$ ceramics series is shown depending on the tantalum concentration and the way of being prepared (Figure 1). Dependence of the modulus of elasticity and micro-hardness of $Nb_{2(1-y)}Ta_{2y}O_5$ ceramics on the particular features of microstructure are revealed. The treatment by high-intensity light significantly changes the structure of Nb_2O_5 and $Nb_{2(1-y)}Ta_{2y}O_5$ ceramics as manifested by changes somewhat improving mechanical characteristics of the materials, such as micro-hardness, strength, micro-fragility. High-intensity light treatment affects mostly the structure of Nb_2O_5 while the structure of $Nb_{2(1-y)}Ta_{2y}O_5$ at y = 0.363 is the least affected; perhaps because the structure of $Nb_{2(1-y)}Ta_{2y}O_5$ is "loosening" with rising the concentration of Ta_2O_5 having a higher melting point.

*) 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

SCIENTIFIC PUBLICATIONS

1.**M.Dunce**, **E.Birks**, J.Peräntie, J.Hagberg, **M.Antonova**, **R.Ignatans**, **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. (2016) Ferroelectrics, 498, pp. 94-101.

2.**E.Birks**, **M.Dunce**, **R.Ignatans**, A.Kuzmin, **A.Plaude**, **M.Antonova**, **K.Kundzins**, **A.Sternberg**. Structure and dielectric properties of $Na_{0.5}Bi_{0.5}TiO_3$-$CaTiO_3$ solid solutions. (2016) Journal of Applied Physics, 119, pp. 074102 (7).
3.**M.Dunce**, **E.Birks**, A.Kuzmin, **R.Ignatans**, **A.Plaude**, **M.Antonova**, **A.Sternberg**. X-ray Diffraction and Raman Spectroscopy Studies in $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ Solid Solutions. (2016) Ferroelectrics, 503, pp.52-59
4.**A.Plaude**, **R.Ignatans**, **E.Birks**, **M.Dunce**, **M.Antonova**, **A.Sternberg**. Structure and dielectric properties at phase transition of $Na_{1/2}Bi_{1/2}TiO_3$-$BaTiO_3$ solid solutions. (2016) Ferroelectrics, 500, pp. 47-53.
5.**K.Bormanis**, A.I.Burkhanov, **I.Smeltere**, **M.Antonova**, **A.Kalvane**, B.Garbarz-Glos. Dielectric properties of potassium–sodium niobate ceramics at low frequencies. (2016) Phase Transitions, pp. 1-6. Article in Press.
6.A.Molak, A.Leonrska, M.Kadziolka-Gawel, A.Szeremeta, R.Bujakiewicz-Koronska, **A.Kalvane**. Electric relaxation and Mn3+/Mn4+ charge transfer in Fe-doped $Bi_{12}MnO_{20}$ - $BiMn_2O_5$ structural self-composite. **Journal of Materials Science,** DOI: 10.1007/s10853-016-0515-2, http://dx.doi.org/10.1007/s10853-016-0515-2
7. R.Bujakiewicz-Koronska, L.Vasylechko, D.M.Nalecz, E.Markiewicz, **A.Kalvane**. X-ray and dielectric characterization of Co doped tetragonal BaTiO3 ceramics, **Phase Transitions,** DOI: 10.1080/01411594.2016.1252978. http://dx.doi.org/10.1080/01411594.2016.1252978 .
8. R.Bujakiewicz-Koronska, D.M.Nalecz, A.M.Majcher, E.Juszynska-Galazka, M.Galazka, L.Vasylechko, E.Markiewicz, D.Majda, **A.Kalvane**, K.W.Koronski. Structural, magnetic, dielectric and mechanical properties of (Ba,Sr)MnO3 ceramics, Journal of the European Ceramic Society. http://dx.doi.org/10.1016/j.jeurceramsoc.2016.10.033
9. E.M. Dutkiewicz, J. Suchanicz, V. Bovtun, K. Konieczny, P. Czaja, K. Kluczewska, B. Handke, M. **Antonova**, **A. Sternberg**. Raman spectra and anomalies of dielectric properties and thermal expansion of lead-free $(1-x)Na_{0.5}Bi_{0.5}TiO_3$-$xSrTiO_3$ (x = 0, 0.08 and 0.1) ceramics. Phase Transitions, (2016): DOI:10.1080/01411594.2016.1182167. Published online: 15 May 2016.
10. **K.Bormanis**, A.I.Burkhanov, **I.Smeltere**, **M.Antonova**, **A.Kalvane**, B.Garbarz-Glos. Dielectric properties of potassium–sodium niobate ceramics at low frequencies. Phase Transitions, DOI:10.1080/01411594.2016.1201822
Published online: 05 Jul 2016.
11. J. Suchanicz, M. E. Dutkiewicz, P. Jelen, B. Handke, M. Skolowski, **M. Antonova**, **A. Sternberg**. Influence of Sr addition on structural, dielectricand Raman properties of $Na_{0.5}Bi_{0.5}TiO_3$ ceramics. Integrated Ferroelectrics, 173:1, 59-64, DOI:10.1080/10584587.2016.1184498. Published online: 17 Jun 2016.

LECTURES ON CONFERENCES

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2. M.Dunce, E.Birks, R.Ignatans, M.Antonova, A.Sternberg, J.Peräntie, J.Hagberg. Nature of dielectric polarization and electrocaloric effect in poled and depoled $Na_{0.5}Bi_{0.5}TiO_3$ Joint RCBJSF-IWRF Conference, Matsue, Japan, 2016
3. А.В.Сопит, А.И.Бурханов, В.О.Семибратов, K.Bormanis, M.Antonova, A.Kalvane Характер диэлектрической нелинейности в керамике KNN с примесью тантала в зависимости от предыстории. Материалы Международной научно-технической конференции «Фундаментальные Проблемы Радиоэлектронного Приборостроения» (INTERMATIC – 2016), 21–25 ноября 2016 г., Москва, Под редакцией академика РАН А.С. Сигова. Proceedings of the International Scientific

and Technical Conference «Fundamental Problems of Radioengineering and Device Construction » (INTERMATIC – 2016), November 21–25, 2016, Moscow, Edited by A. Sigov, Part 3, pp. 58-61.
4. А.В.Жирков, А.И.Бурханов, К.Борманис, М.Антонова Процессы поляризации и переполяризации в сегнетокерамике (K0.5Na0.5)(Nb0.93Sb0.07)O3 в области размытых фазовых переходов. Материалы Международной научно-технической конференции «Фундаментальные Проблемы Радиоэлектронного Приборостроения» (INTERMATIC – 2016), 21–25 ноября 2016 г., Москва, Под редакцией академика РАН А.С. Сигова. Proceedings of the International Scientific and Technical Conference «Fundamental Problems of Radioengineering and Device Construction » (INTERMATIC – 2016), November 21–25, 2016, Moscow, Edited by A. Sigov, Part 3, pp. 11-13.
5.M.Palatnikov, O.Shcherbina, V.Efremov, N.Sidorov, and K.Bormanis. Effects of High-Intensity Light on the Structure and Mechanical Characteristics of Ceramic Niobium-Tantalum Pentoxides. Proceedings of conference «Physics of Lead-Free Piezoactive and Relative Mate (Analysis of Current State and Prospects of Development)» (LFPM- 2016), Rostov-on-Don, V. 2., pp. 103.-107.
6.N.V.Sidorov, M.N.Palatnikov, A.A.Kruk, A.A.Yanichev , B.N.Mavrin, K.Bormanis. Raman Studies of Stoichiometric and Congruent Lithium Niobate Crystals at Temperatures Within the 100-400 K Range. Proceedings of conference «Physics of Lead-Free Piezoactive and Relative Mate (Analysis of Current State and Prospects of Development)» (LFPM- 2016), Rostov-on-Don, V. 2., pp. 161.-167.

DEPARTMENT OF FERROELECTRICS

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

LABORATORY OF VISUAL PERCEPTION

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

Optical facilities of human visual sensor, its spatial and intensity detection of light input, electrical processing of further information flow, discrimination and decision making – all that work together in an astonishing manner to provide the ergonomic perception modality. Human vision really is a very 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 serves as a joint between colleagues in institute and Department of Optometry and vision science of the University of Latvia. Most of Department's Master thesis have been accomplished due to collaboration between units. In 2016 more than 8 Bachelor's and Master's thesis have been completed under supervision of laboratory researchers.

Research in laboratory is focused on following 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, modelling of the eye optical structures;
- 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;
- digital visual stimuli image processing determinant for analyse of the human visual response;
- studies of spectral and seasonal changes of ambient natural illumination, and the impact of the use of economic white LED diodes light sources for artificial illumination and for different displays and mobile devices on distortion of the normal circadian cycles;
- 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
Dr.phys. Sergejs Fomins
Dr.phys. Varis Karitans
Dr.phys. Paulis Paulins

Ph.D. students

Olga Danilenko

SCIENTIFIC PROJECTS.

- LCScie State Programm VPP-15 Progr.„Designing of innovative multifunctional materials, signal processing and information technologies for competitive scientific advanced products" – IMIS2;
- 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. H.M.Bueno)
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*
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. ***Harilaos Ginis***, Department of Research, Athens Eye Hospital, Athens, Greece; 7.04. - 11.04.2016.

MAIN RESULTS

SEASONAL ENVIRONMENTAL SPECTROPHOTOMETRY

Sergejs Fomins, Janis Kleperis, Maris Ozolinsh

The circadian rhythm is controlled by the light and blue light sensitive non-object forming visual system. Light properties impact human health promoting events as day-night cycle, mood, and perception. Latvian geographic location at latitude of 57 degrees north introduces substantial seasonal changes in both, illumination and environmental colorimetry. It is logically to propose that natural colorimetric gamut is shaped by the seasonal conditions. Unfortunately, illuminance or irradiance monitoring stations do not provide the circadian light properties. The annual irradiance data from the solar plantation at Institute of Solid State Physics, University of Latvia, is given in figures. Almost five times differences at winter and summer months. Our proposed methodology is based on the integral spectral measurements of the illumination information and hyperspectral acquisition of the environmental scenes. We use calibrated Ocean Optics spectrometer equipped with integrating sphere to continuously acquire the spectral information along the calendar year starting from the 2016th. The fragmentary results of the previous spectral data show substantial changes of thephotometric quantities of environmental light with less expressed changes of the circadian light. Multispectral analysis of the scenes acquired in previous years showed the reduction of the gamut at red and green components of visual

spectrum, while preserving the blue component of the scenes at winter time. However, at least one full annual cycle of circadian light data could provide the important new details relative to human physiology.

MANUALLY TUNABLE LENS BASED EYE MODEL

Varis Karitans, Jolanta Logina, Gunta Krumina

We report on the optical and geometrical properties of a new model eye based on a manually tunable polymer lens ML-20-35-NIR-HR. Using the translation and refraction matrix calculations position of the cardinal (principal, nodal and focal) planes were found. The primary principal plane H1 is located about 0.9 mm behind the cornea while the secondary principal plane H2 is located about 3 mm in front of the cornea. The distance between the principal planes and the corresponding nodal planes HN is about 9 mm. The primary focal length f1=-18.6 mm, the secondary focal length f2=27.5 mm. Regarding Zernike aberrations increased levels of both coma-x and coma-y can be observed. This may be due to the liquid polymer lens the shape of which has distorted slightly resulting in coma aberrations. As expected, the spherical aberration has the largest magnitude from all types of higher-order aberrations. A big advantage of the new model eye is that the adjustable element is the ocular lens like in a living eye. This new model eye has demonstrated potential for being used in ocular accommodation studies and retinoscopy training. If a gel like substance is used to simulate the vitreous humour it would also be possible to simulate vitreous floaters and to study the impact of refractive error on their appearance. However, there are shortcomings characteristic to the optical system of this model eye. Although the equivalent optical power and power tuning range of the model eye is comparable to the corresponding values of a living eye there are strong back-reflections because of deviations of the refractive indices and curvature of surfaces away from the real values. These diferences could be minimized by choosing optical media simulating liquids with refractive indicēs very close to those in a living eye. Supported by Latvian Project IMIS2.

THE COMPOUND MECHANISM OF ADAPTATION TO HIGH CONTRAST

Olga Danilenko, Maris Ozolinsh, Varis Karitans, and Varvara Zavjalova

Adaptation to high contrast stimuli results in set of two separate mechanisms that contribute to temporary loss in contrast sensitivity. The first mechanism is negative afterimage formatting on the retina level, while the second mechanism would be a contrast adaptation occurring in higher level of perception [1, 2]. Summary effect of such adaptation is depended on total time of exposure, the contrast of adaptive stimuli and external factors. A time course of such process was designed via phychophysical experiment. The build up of summary adaptation effect is successfully fitted by exponential approximation. The relaxation to basic level that ensues after the adaptation period is stopped is described by exponential decrease function with time constant equal 3.7 sec. The effect of external factors on summary adaptation is studied and separation of two underlying mechanisms is achieved by various methods. Similar adaptation process is studied with involvement of colour perception.

SLOPE OF THE ACCOMMODATIVE RESPONSE MEASURED WITH THE RETINAL BRIGHTNESS METHOD

Varis Karitāns, Natālija Fridrihsone, Evita Kassaliete, Aiga Švede, and Māris Ozoliņš

Inour study, we used the retinal brightness measurements to calculate the slope of the ccommodative response. During the experiment, a subject viewed a red checkerboard pattern the distance of which is varied between 0.25 m and 4 m. Light from an infrared laser enters the eye, and a photodetector measures the amount of light going out of the eye. A calibration curve plotting the amount of light versus known dioptric power is measured be means of a model eye with optical properties close to those of popular mathematical model of the eyes. By comparing the subjects' data and the data of the model eye, the accommodative response and its slope can be calculated. Five subjects were enrolled in the experiment. Two subjects were myopic, one subject was emmetropic, and two subjects were hyperopic. The refractive error wasn't corrected and the accommodative response was calculated as the stimulus power plus the refractive error. The results show that the emmetropic subject and one of the myopic subjects had a slope smaller than that in the hyperopic subjects and in the myopic subject who had worn the correction previously. These results are in agreement with studies relating the slope of the accommodative response to the refractive error (Millodot, 2015). The results also support the finding that adaptation to blur and reduced sensitivity to blur result in reduced accommodative response in myopes (Collins, Buehren, & Iskander, 2006; Rosenfield, Hong, & George, 2004). The study was supported by ESF project No 2013/0021/1DP/1.1.1.2.0/13/APIA/VIAA/001

COLORIMETRIC AND CIRCADIAN LIGHT CHARACTERISTICS OF LATVIAN SKY

Sergejs Fomins and Māris Ozoliņš

The light impacts the physiological function of organisms, particularly humans, through the blue light sensitive receptors in human retina. Melanopsin acting as a non-object vision pigment promotes day-night cycle regulation and related body functions as vigilance, body temperature, and also mood. At the moment, there is no research about circadian light properties in Latvian latitudes. However, the seasonal changes in day light properties, including physiologically relevant light, and vegetation are sufficient in northern latitudes. To identify the proportion and dynamics of circadian component in seasonal variations of light, we started continuous monitoring of radiometric data. Since 2012, total amount of radiation is available from the Solar cells plantation of Institute of Solid State Physics, University of Latvia (UL ISSP). To obtain spectral information, our team has developed the spectral radiometric system for continuous monitoring of the day light radiance information starting from April 2016. It consists of the calibrated visible range spectrometer equipped with optics for radiometric measurements. The averaged data are acquired in five minutes for full day night cycle. We provide measurements at 45 degrees' altitude in the northern part of the sky`s hemisphere. Acquired data show that clear skylight colorimetry is comparable to that of the Granada daylight database. Analysis of Granada spectral database (Hernández-Andrés, et al., 2001) showed linear behaviour for circadian light in proportion to luminance. Data acquired at UL ISSP in late spring period clearly indicated the non-linear ratios of circadian light to luminance. This result indicates the higher amounts of melanopsin regulating light at lower luminance in northern latitude compared to results calculated on the data of Hernández-Andrés et al. (2001).

PERCEPTUAL ADAPTATION STUDIES AT SIMULATION OF UNILATERAL CATARACT VISUAL CONTRAST DECREASE

Olga Danilenko, Maris Ozolinsh, and Varvara Zavjalova

Unilateral eye image deterioration due to electrically controlled light scattering was applied by a Smart Light adapter built into a Virtual Reality device allowing separation of eyes' optical visual pathways when observing stimuli on a high-resolution mobile phone display. Vision adaptation to high contrast slanted gratings was studied using a previously cited technique where during the post-adaptation test phase the eyes would perceive differently structured stimuli. This could initiate either a left-rotated or right-rotated grating of perceptual sense. The latter depends on positive adding or subtractive adding of binocular inputs, which could vary due to different depth of retinal aftereffects and cortical amplification. Colored stimuli have been applied that besides luminance pathways engaged in the game would also add parvocellular processing, so the resulting observer's psychophysically based decisions could be more variable. Supported by Latvian Project IMIS2.

BACKGROUND LUMINANCE EFFECT ON AFTERIMAGE LIGHTNESS AND SATURATION

Sergejs Fomins, Ieva Jekabsone, and Maris Ozolinsh

Aftereffects are the result of pigment bleaching and following adaptation. Acting on global scale background significantly changes the perception of chromatic spots and therefore the afterimages. White`s illusion is n example of the global processing with both color assimilation and contrast. Brighter backgrounds would assimilate the stimuli lightness. In our study we identify the effect of background luminance on perceived afterimages chromatic and lightness parameters in binocular and dichoptic viewing conditions. We use a 'chaser' type stimulus with circularly arranged twelve spots subtending 4 degrees. At each timestamp one point disappears for 300 ms allowing the afterimage to appear. The sequential short disappearance of spots produces the perception of afterimage rotation in clockwise direction. Eight stimuli colors are defined in the DKL color space with four coordinates falling on cardinal axes and other four in diagonal to them. Five background luminances range from 30 to 150 cd/m2, with third luminance identical to the stimulus. Results of three participants show insignificant changes in perceived afterimage saturation in dichoptic and binocular viewing. Parallel eye pupil tracking helps to identify the 2 log Trolands of retinal illumination on darkest background of our experiments. Nevertheless, the mesopic conditions are not met; darker backgrounds produce aftereffects of higher chromatic saturation in S-(L+M) direction. Supported by Latvian Project IMIS2.

BINOCULAR SUMMATION MODEL OF COLOUR IMAGES IN RESPECT TO PREVIOUS ADAPTATION

Olga Danilenko, Maris Ozolinsh, and Varvara Zavjalova

The main objective of this research is to determine the model in which human brain proceeds with fused image creation if the images for both eyes are different. Such conditions in visual system can be produced by outer blurring or underlying eye disease. The impact of visual adaptation was also studied as the factor that can affect perception. Visual stimuli were presented on a mobile cellphone screen and image separation was

achieved by Virtual Reality device. That provided presentation of different image for the left and right eyes during testing phase, while the adapting stimuli remained the same for both eyes. The stimuli were composed of tilted gratings which could be isohromatic or coloured. By using different types of stimuli we ensure that percieved images would be analysed by separate pathways as in magnocellular or parvocellular visual systems. Achromatic and yellow gratings of contrast Cm=0.5 for both eyes were used for adaptation that lasted up to 15 s. During a short successive test phase left(green) and right(red) eye stimuli were divergent - with the same spatial frequency, however gratings were spatially non-uniform and without slant symmetry. Mathematical addition of these images can result to anti- or clockwise oriented grating set. For colour stimuli the test stimuli contrast was randomly changed for green stimuli eye in the range up Cm<0.5. Observers task was to report the apparent orientation of viewed test stimuli. Furthermore, stimuli were analysed on computer screen by the means of image calculation and the model of binocular summation was created. Psychometric curves revealed the green stimuli contrast Cm overbend point at values Cm=0.10 for adaptation duration 15 s comparing to contrast threshold at achromatic experimental condition Cm=0.19 and approved the shift in these contrast values due to adaptation time. Supported by Latvian Project IMIS2.

RETINAL IMAGE QUALITY AND VISUAL STIMULI PROCESSING BY SIMULATION OF PARTIAL EYE CATARACT

Maris Ozolinsh, Olga Danilenko, and Varvara Zavjalova

Visual stimuli were demonstrated on a 4.3'' mobile phone screen inside a "Virtual Reality" adapter that allowed separation of the left and right eye visual fields. Contrast of the retina image thus can be controlled by the image on the phone screen and parallel to that at appropriate geometry by the AC voltage applied to scattering PDLC cell inside the adapter. Such optical pathway separation allows to demonstrate to both eyes spatially variant images, that after visual binocular fusion acquire their characteristic indications. As visual stimuli we used grey and different color (two oponent components to vision – red-green in L*a*b* color space) spatially periodical stimuli for left and right eyes; and with spatial content that by addition or subtraction resulted as clockwise or counter clockwise slanted Gabor gratings. We performed computer modeling with numerical addition or subtraction of signals similar to processing in brain via stimuli input decomposition in luminance and color opponency components. It revealed the dependence of the perception psychophysical equilibrium point between clockwise or counter clockwise perception of summation on one eye image contrast and color saturation, and on the strength of the retinal aftereffects. Existence of a psychophysical equilibrium point in perception of summation is only in the presence of a prior adaptation to a slanted periodical grating and at the appropriate slant orientation of adaptation grating and/or at appropriate spatial grating pattern phase according to grating nods. Actual observer perception experiments when one eye images were deteriorated by simulated cataract approved the shift of mentioned psychophysical equilibrium point on the degree of artificial cataract. We analyzed also the mobile devices stimuli emission spectra paying attention to areas sensitive to macula pigments absorption spectral maxima and blue areas where the intense irradiation can cause in abnormalities in periodic melatonin regeneration and deviations in regular circadian rhythms. Therefore participants in vision studies using "Virtual Reality" appliances with fixed vision fields and emitting a spike liked spectral bands (on basis of OLED and AMOLED diodes) different from spectra of ambient illuminators should be accordingly warned about potential health risks.

CHROMOSTEREOPSIS IN "VIRTUAL REALITY" ADAPTERS WITH ELECTRICALLY TUNEABLE LIQUID LENS OCULARS

Maris Ozolinsh, Kristine Muizniece, Paulis Paulins, and Janis Berzinsh

Chromostereopsis can be sight and feel in "Virtual Reality" adapters, that induces the appearance of color dependant depth sense and, finally, combines this sense with the source conceived depth scenario. Present studies are devoted to investigation the induced chromastereopsis when using adapted "Virtual Reality" frame together with mobile devices as smartphones. We did observation of composite visual stimuli presented on the high spatial resolution screen of the mobile phone placed inside a portable "Virtual Reality" adapter. Separated for the left and right eyes stimuli consisted of two areas: a) identical for both eyes color chromostereopsis part, and b) additional conventional color neutral random-dot stereopsis part with a stereodisparity based on the horizontal shift of a random-dot segment in images for the left and right eyes, correspondingly. The observer task was to equalize the depth sense for neutral and colored stimuli areas. Such scheme allows to determine actual observed chromostereopsis disparity value versus eye stimuli color difference. At standard observation conditions for adapter with +2D ocular lenses for mobile red-blue stimuli, the perceptual chromostereopsis depth sensitivity on color difference was linearly approximated with a slope SChS ≈ 2.1[arcmin/(Lab color difference)] for red-blue pairs. Additional to standard application in adapter the tuneable "Varioptic" liquid lens oculars were incorporated, that allowed stimuli eye magnification, vergence and disparity values control electrically. Supported by Latvian Project IMIS2.

LOCAL AND PERIPHERAL MOTION CONTRADICTION VIEWED IN MOBILE DEVICES IN DEPENDENCE OF STIMULI COLOR AND INTENSITY CONTENT

Maris Ozolinsh

Visual timuli were organized in a similar way as in the original Shapiro-Meilstrup illusion (Shapiro et al.,2008,Meet.of Soc.Neurosc.811.3; Meilstrup&Shadlen,2008, Meet.of Soc. Neurosc.460.11) using two sets of identical basic contradictional movement perception sources that were shifted horizontally. Back layer of elements contains global motion sources - two clockwise spinning disks on neutral background. Disks consist of centro-symmetrical radial rays which luminance was modulated in sinus mode along the disc circumference. Spinning speed was 0.15rps. Frontal stimuli layer contains two sets of concentrically allocated six circular apertures in neutral background rotating with the same speed however counter-clockwise. The latter motion assumed as perceived local movement. Apertures were arranged concentrically with centres collocated to back layer disk centres. Observers should make judgements (Tobserv=2sec): movement of disks seems jumbled; spinning perceived continuous however either counter- or clockwise. Psychophysically viewing eccentricity of subjective equivalence were determined where local counter-clockwise perceived movement equalizes to global clockwise movement. Stimuli varied in colour (all greyscale; spinning disks blue), in luminance and in contrast. As reference the value of eccentricity was chosen corresponding to subjective perception equilibrium between controversial motions - detected as ca.4deg for greyscale stimuli of contrast 100%. In our experimental isoluminant conditions, eliminating of red-green colours from global motion sinusoidal pattern strengthened the global clockwise motion perception dominance. So shift from peripherally observed global motion perception to central vision local motion dominance occurs at smaller observance eccentricity. That would be explained by the fact that lack of the longwave radiation in sinosoidally

modulated pattern increases the relative excitation strength of retinal receptive fields and further legs of neural pathways of blue input. The global motion perception dominance in case of stimuli containing only blue shifts toward central vision that characterises by low S cone density.

SIMULTANEOUS PRESENCE OF STEREODISPARITY AND CHROMOSTEREOPSIS OBSERVING "VIRTUAL REALITY" IMAGES

Kristīne Muižniece and Maris Ozolinsh

Chromostereopsis is a visual illusion whereby an impression of depth is conveyed in two-dimensional color images, usually a combination of blue with red. Chromostereopsis and its minimum color difference on blue-red line to distinguish depth sense have been studied previously [1,2] however no data on chroomostereopsis induced stereodisparity numerical values was published previously. We did observation of composite visual stimuli presented on the high spatial resolution screen of the mobile phone placed inside a portable "Virtual Reality" adapter. Separated for the left and right eyes stimuli consisted of two areas: a) identical for both eyes color chromostereopsis part, and b) additional conventional color neutral random-dot stereopsis part with a stereodisparity based on the horizontal shift of a random-dot segment in images for the left and right eyes, correspondingly. Observer task was to compare and to equalize depth sense in color and neutral random-dot parts using the constant stimuli psychophysical force choice method where the parameters were: color difference ΔE in CIE xy color space on blue-red, blue-green and green-red lines in stimuli color part, and a pixel shift of the central segment in neutral random-dot segment part. Supported by Latvian Project IMIS2.

MODEL EYE INCORPORATING A MANUALLY TUNABLE POLYMER LENS AND MICROFLUIDICSC FOR SIMULATION OF VITREOUS FLOATERS

Varis Karitans

There is a wide variety of mathematical model eyes with optical and geometrical parameters close to the average values of a living eye. However, there are very few real model eyes. One such model has optical and geometrical properties very close to that of a real eye and includes many features for extensive fundus and tear-film examination. Another model eye was designed to mimic behaviour of the tear-film. We report on a model eye incorporating a manually tunable lens and microfluidics chamber for simulation of vitreous floaters has been described. Aberrations correspond to average values in population and diffraction effects could be observed. Supported by Latvian Project IMIS2.

PUBLICATIONS IN CITED JOURNALS

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PARTICIPANCE IN INT. CONFERENCES

- Congress of the Optical Society of America (OSA) "Imaging and Applied Optics" - 2016, Heidelberg, Germany.
- 2nd World meeting „Visual and Physiological Optics 2016" VPO-2016, Antverpen.
- 3rd International Symposium on Visual Physiology, Environment, and Perception (VISPEP), Riga 2016.
- Advanced Materials and Technologies AMT-2016, Palanga.
- Annual Conf. of Applied Vision Association AVA-2016, London Dec.2016.
- International Symposium on Color Vision „Seeing Colors-2016", Regensburg.
- SPIE Photonics Asia 2016, Beijing.
- Developments in Optics and Communications DOC-2017, Riga.

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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 multilayer electrochemical systems. Functional fibers (glass 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. E. Pentjuss Dr.phys. A. Vitins	**PhD student** K. Kaprans **Student** J. Mateuss **Technician** J. Balodis

SCIENTIFIC VISITS ABROAD

G. Kucinskis, Max Planck Institute for Solid State Research, Stuttgart, Germany (12 month).

COOPERATION

Latvia

1. University of Latvia - Department of Chemistry (Dr. G.Vaivars).
2. Institute of Chemical Physics of the University of Latvia (Dr. G.Ķizāne, Dr. E.Pajuste).
3. Riga Technical University - Institute of Inorganic Chemistry (Dr. A. Dindune).
4. Riga Technical University - Institute of Silicate Materials (G.Mežinskis).
5. Latvian Institute of Wood Chemistry (Dr.hab. G.Dobele, Dr.hab. J.Gravitis).
6. JSC "Sidrabe" (G.Pipkevich).

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, Tainan – Department of Material Science and Engineering (Prof. K.-Z. Fung).

Russia

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

PARTICIPATION IN RESEARCH PROJECTS:

Latvian:

1. Latvian National Research Program in Materials Science "Multifunctional materials and composites, photonics and nanotechnology" (IMIS2).
2. 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", No 666/2014.

International:

MP1106 "Smart and green interfaces - from single bubbles and drops to industrial, environmental and biomedical applications".

MAIN RESULTS

THERMAL DECOMPOSITION OF TRONA OF CARBONISED GLASS FIBER FABRICS

Evalds Pentjuss, Janis Balodis, Jeugenijs Gabrusenoks, Gunars Bajars

There are continued research to elucidate the using of glass fiber fabrics containing shell of trona ($Na_2CO_3 \cdot NaHCO_3 \cdot 2H_2O$) crystals on its elementary filaments at elevated temperatures and different atmospheric condition [1,2]. The other motivation of experiments is small sizes (below one μm in two directions) of trona crystals that increase

attitude of surface to volume and facilitate assured investigation of surface phenomena. The samples of fabric were preheated at different temperatures up to 155^0C. There was used the earlier defined relation (1) to characterize the kinetic of CO_2 and H_2O mass adsorption from atmosphere, that in force at least of 0.25 h after heating and were determined the related time and mass constants and its dependence on preheating temperature [2].
Analysis of obtained relations showed the steep adsorption increase of CO_2 and H_2O after known decomposition beginning of trona at 57^0C and until approach to its approximate maximum values at about 70 and 80^0C, accordingly. This adsorption increase is associated with derive the new absorption sites from degradation of crystals surface and increase its area. Before the adsorption maximum is reached, the adsorption sites are fulfilled. Desorption of CO_2 and H_2O and number of free absorption sites increase along temperature, that leads to form a maximum and decrease of absorption. The mass loss of samples over 100^0C is determined by decomposition and desorption processes.
The identical adsorption rise beginning at preheating temperature of 57^0C and domination of water adsorption over CO_2 (more than one order) indicates to decomposition of crystallized water and releasing of CO_2, adsorbed in structure defects and pores. In this stage of experiments there are no signs that indicate to evolving CO_2 chemically bonded in crystals below about 150^0C.
Supported by "IMIS2".

1. Pentjuss, E., Lusis, A., Bajars, G. and Gabrusenoks, J. (2013) Investigation of carbonized layer on surface of NaAlSi glass fibers. *IOP Conf. Series: Materials Science and Engineering*, **49** 012044 doi: 10.1088/1757-899X/49/1/012044.
2. Pentjuss, E., Lusis, A., Gabrusenoks, J. and Bajars, G. (2015) Environment humidity effect on the weight of carbonized Na-Al-Si glass fabrics recovery after heating. *IOP Conf. Series: Materials Science and Engineering*, **77** 012021 doi:10.1088/1757-899X/77/1/012021.

NANOSTRUCTURED α-Fe_2O_3 AND TiO_2 COMPOSITE ENWRAPPED BY REDUCED GRAPHENE OXIDE WITH EXCELLENT CYCLABILITY AND RATE CAPABILITY AS ANODE MATERIAL FOR LITHIUM ION BATTERIES

Kaspars Kaprans, Janis Mateuss, Anna Dorondo, Gunars Bajars

Two metal oxides, α-Fe_2O_3 and rutile phase TiO_2 with a particle diameter 50 nm and 21 nm respectively, were mixed with graphene oxide. Electrophoretic thin film deposition procedure from water suspension under potentiostatic mode was performed and the following composite thin films on a stainless steel substrate were obtained: α-Fe_2O_3/rGO, TiO_2/rGO, α-Fe_2O_3/TiO_2/rGO. Subsequently reduction of graphene oxide was performed. Thickness of acquired thin films was in the range of 2-6 μm. Electrochemical properties of all samples were studied by chronopotentiometry, cyclic voltammetry and electrochemical impedance spectroscopy. Gravimetric capacity was calculated for each synthesized material. Values of gravimetric capacity as well as rate capability after charge/discharge cycles were figured out. Structure and morphology investigations for each sample were performed by SEM, AFM, XRD and Raman spectroscopy.
Our synthesized composite material α-Fe_2O_3/TiO_2/rGO showed excellent electrochemical properties for application as lithium ion battery anode material compared with a α-Fe_2O_3/rGO and TiO_2/rGO and as well as previously synthesized material containing α-Fe_2O_3 with a main particle diameter of about 150 nm. The results showed that the obtained

composite material is a promising anode material for high energy and high power lithium ion batteries.
Supported by Research Cooperation Project of Latvian Council of Science No 666/2014.

SCIENTIFIC PUBLICATION

P. Lesnicenoks, M. Zvine, A. Januskevica, V. L. Muzikants, M. K. Jurjans, **K. Kaprans**, A. Volperts, **G. Kucinskis, G. Bajars**, G. Dobele, J. Kleperis (2016) Nanostructured carbon materials as promoters of energy storage. *Bulgarian Chemical Communications, Volume 48, Special Issue E2 2016,* pp. 365-372.

LECTURES ON CONFERENCES

32nd Scientific Conference of Institute of Solid State Physics, University of Latvia, February 17-19, 2016, Riga, Latvia:

- J.Gabrusenoks, M.Zubkins, G.Chikvaidze, J.Purans, A.Plaude. Vibrational spectra of ZnO:Ir thin films.
- E.Pentjuss, A.Lusis, J.Gabrusenoks, J.Balodis, G.Bajars. Mass recovery kinetics of heated Na-Al-Si glass fibric in atmospheres with different humidity and CO_2 concentration.
- R.Kovaldins, I.Reinholds, G.Kizane, J.Zicans, J.Gabrusenoks. Structural and mechanical property analysis of radiochemical cross-linked multi-layered carbon nanotube – poliolefinnanocomposit material.
- J.Mateuss, K.Kaprans, A.Dorondo, G.Bajars, G.Kucinskis, J.Kleperis. Graphene/ TiO_2/Fe_2O_3 composite electrophoretic deposition and comparison of physico-chemical characteristics for use in Li-ion batteries.
- M.Rublans, G.Bajars, A.Lusis, E.Pentjuss, J.Balodis, J.Gabrusenoks. Structure, optical and photocurrent measurements of TiO_2-WO_3 composites prepared by electrophoretic deposition.
- V.L.Muzikants, G.Kucinskis, M.K.Jurjans, G.Bajars. Carbon nanomaterial use in lithium ion batteries for cathode and anode creation.
- M.Zubkin, R.Kalendarev, J.Gabrusenoks, A.Plaude, K.Vilnis, A.Azens, J.Purans. Structure, optical and electrical properties of ZnO:Ir and Zn-Ir-O thin films deposited by reactive magnetron sputtering.

The 1st International Conference "Nanomaterials and Radiation Effects" of the Institute of Chemical Physics of the University of Latvia, 16th February 2016, Riga,Latvia:

- E.Pajuste, G.Kizane, A.Vitins, I. Igaune, JET contributors. Release and desorption of tritium from beryllium materials of the first wall of the vacuum vessel of the Joint European Torus (JET).

International Workshop 'LIGHTtalks: Power of Photonics', April 25, Riga, Latvia:

- J.Purans, M.Zubkin, J.Gabrusenoks, G.Cikvaidze, R.Kalendarev, A.Azens, A.Zitolo, K.Pudzs, A.Anspoks. Amorphous ZnO based thin films.

Smart and Green Interfaces Conference jointly with COST MP1106 Annual Meeting, May 4-6 Athens, Greece:

- G.Bajars, E.Pentjuss, A.Lusis, J.Gabrusenoks, J.Balodis. Mass recovery kinetics of heated carbonated glass fabric in atmosphere with different humidity and CO_2 concentration.
- G.Bajars, K.Kaprans, J.Mateuss, A.Dorondo, G.Kucinskis, J.Kleperis. Investigation of electrophoretically deposited metal oxide and reduced graphene oxide composite as anode materials for high performance lithium ion batteries.

The 22nd International Conference on Plasma Surface Interactions in Controlled Fusion Devices (22nd PSI), May 30 - June 3, 2016, Rome, Italy:

- E.Pajuste, G.Kizane, A.Vitins, I. Igaune, JET contributors. Tritium distribution and desorption from plasma facing beryllium materials of ITER-Like-Wall at JET.

12th international symposium of system with fast Ionic transport (ISFFIT-12), 2016, July 3-7, Kaunas, Lithuania

- K.Kaprans, J.Mateuss, A.Dorondo, G.Bajars, G.Kucinskis, J.Kleperis. Electrophoretically deposited TiO_2/Fe_2O_3 /reduced graphene oxide composite material as prospective anode for lithium ion batteries.

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.
- Magnetron sputtering of transparent conducting oxides (TCO).
- The use of high performance computing for functional materials first principles and Molecular Dynamics simulations.
- Confocal laser microscopy and Raman spectroscopy.
- 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).

USA
1. Yeshiva University, New York, USA (Dr. J. Timoshenko)

PARTICIPATION IN RESEARCH PROJECTS

Latvian:
1. Latvian Science Council Grant "XAFS studies of functional material local structure with femtometer accuracy", No.402/2012.
2. Latvian Science Council Grant "Local structure determination in functional materials from x-ray absorption spectra", Latvian Science Council Grant No.187/2012.
3. 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).

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

MAIN RESULTS

NEGATIVE THERMAL EXPANSION In PEROVSKITE-TYPE MATERIALS

J.Purans, A. Kuzmin, I. Jonane, A. Kalinko, J.Timoshenko

We propose an approach beyond the quasiharmonic approximation for interpretation of EXAFS and XRD data and for ab initio calculations of electronic and vibration properties of materials with negative thermal expansion. Ab initio electronic structure and lattice dynamics calculations for cubic and distorted ScF_3 were performed using the linear combination of atomic orbitals (LCAO) method. The band gap obtained in calculations for ScF_3 is equal to 10.54 eV and agree well with the expected value. The calculated infrared spectra of F displaced (FD) cubic ScF_3 allow us to predict that its mean Sc{F{Sc angle withinNTE deviates from 180 degree.
Strontium titanate is a model quantum paraelectric in which, in the region of dominating quantum statistics, the ferroelectric instability is inhibited due to nearly complete compensation of the harmonic contribution into ferroelectric soft mode frequency by the zero-point motion contribution. The enhancement of atomic masses by the substitution of 16O with 18O decreases the zero-point atomic motion, and low-T ferroelectricity in $SrTi_{18}O_3$ is realized. In this study we report on the local structure of Ti in SrTi16O3 and $SrTi18O_3$ investigated by Extended X-ray Absorption Fine Structure measurements in the temperature range 6 – 300 K.

THE USE OF X-RAY ABSORPTION SPECTRA FOR VALIDATION OF CLASSICAL FORCE-FIELD MODELS

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

Extended X-ray absorption fine structure (EXAFS) spectroscopy and molecular dynamics (MD) simulations are two complementary techniques widely used to study the atomic structure of materials. Their combined use, known as the MD-EXAFS approach, allows one to access the structural information, encoded in EXAFS, far beyond the nearest coordination shells and to validate the accuracy of the interaction potential models. The use of the MD-EXAFS method for a validation of several force-field models was demonstrated on an example of the cubic-perovskite $SrTiO_3$ and hexagonal wurtzite-type ZnO crystals.

LOCAL STRUCTURE AND LATTICE DYNAMICS OF COPPER NITRIDE

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

X-ray diffraction and x-ray absorption spectroscopy at the Cu K-edge were used to study the atomic structure in microcrystalline, nanocrystaline and amorphous copper nitride (Cu_3N). Extended x-ray absorption fine structure (EXAFS) spectroscopy combined with reverse Monte Carlo (RMC) and evolutionary algorithm (EA) modelling was used to advance the understanding of the local structure and lattice dynamics of Cu_3N. The RMC/EA-EXAFS method was provided us a possibility to probe correlations in the motion of neighboring atoms and allowed us to analyze the influence of anisotropic motion of copper atoms in Cu_3N. Textured nanocrystalline Cu_3N films were obtained using dc magnetron sputtering on substrates heated at about 190°C, whereas amorphous films having strongly disordered structure already in the second coordination shell of copper were deposited in the absence of heating. We found that the nearest interatomic distance Cu–N in thin films did not change significantly upon substrate heating and is close to that in bulk Cu_3N, indicating strong bonding between copper and

SCIENTIFIC PUBLICATIONS

1. **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. 230 (2016) 537-549.
2. 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. 230 (2016) 551-568.
3. V.I. Sokolov, V.A. Pustovarov, V.N. Churmanov, N.B. Gruzdev, M.A. Uimina, I.V. Byzov, A.V. Druzhinin, **N. Mironova-Ulmane**, Luminescence and optical spectroscopy of charge transfer processes in solid solutions $Ni_cMg_{1-c}O$ and $Ni_xZn_{1-x}O$, J. Lumin. 169 (2016) 641-644.
4. J. Timoshenko, **A. Kuzmin, J. Purans**, Disappearance of correlations in the atom motion upon hydrogen intercalation into ReO_3 lattice, J. Phys.: Conf. Ser. 712 (2016) 012003:1-4.
5. D. Bocharov, M. Krack, A. Kalinko, **J. Purans**, F. Rocca, S.E. Ali, **A. Kuzmin**, Ab initio molecular dynamics simulations of the Sc K-edge EXAFS of scandium

trifluoride,
J. Phys.: Conf. Ser. 712 (2016) 012009:1-4.

6. **J. Purans**, S. Piskunov, D. Bocharov, A. Kalinko, **A. Kuzmin**, S.E. Ali, F. Rocca, Local structure of perovskites ReO_3 and ScF_3 with negative thermal expansion: interpretation beyond the quasiharmonic approximation, J. Phys.: Conf. Ser. 712 (2016) 012013:1-4.
7. D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, **A. Kuzmin, J. Purans**, E. Kotomin, Interpretation of the U $_{L3}$-edge EXAFS in uranium dioxide using molecular dynamics and density functional theory simulations, J. Phys.: Conf. Ser. 712 (2016) 012091:1-4.
8. **A. Kuzmin, A. Anspoks**, A. Kalinko, J. Timoshenko, **R. Kalendarev**, L. Nataf, F. Baudelet, T. Irifune, P. Roy, Pressure-induced insulator-to-metal transition in α-$SnWO_4$, J. Phys.: Conf. Ser. 712 (2016) 012122:1-4.
9. **A. Anspoks,** J. Timoshenko, **J. Purans**, F. Rocca, V. Trepakov, A. Dejneka, M. Itoh, Local dynamics and phase transition in quantum paraelectric $SrTiO_3$ studied by Ti K-edge x-ray absorption spectroscopy, J. Phys.: Conf. Ser. 712 (2016) 012101.
10. A.N. Trukhin, K. Smits, J. Jansons, **A. Kuzmin**, Luminescence of polymorphous SiO_2, Rad. Meas. 90 (2016) 6-13.
11. **N. Mironova-Ulmane, V. Skvortsova, A. Pavlenko**, E. Feldbach, A. Lushchik, Ch. Lushchik, V. Churmanov, D. Ivanov, V. Ivanov, E. Aleksanyan, Luminescence and EPR spectroscopy of neutron-irradiated single crystals of magnesium aluminium spinel, Rad. Meas. 90 (2016) 122-126.
12. **I. Jonane, K. Lazdins,** J. Timoshenko, **A. Kuzmin, J. Purans**, P. Vladimirov, T. Gräning, J. Hoffmann, Temperature-dependent EXAFS study of the local structure and lattice dynamics in cubic Y_2O_3, J. Synchrotron Rad. 23 (2016) 510-518.
13. E. Birks, M. Dunce, R. Ignatans, **A. Kuzmin**, A. Plaude, M. Antonova, K. Kundzins, A. Sternberg, Structure and dielectric properties of $Na_{0.5}Bi_{0.5}Ti_{O3}$-$CaTiO_3$ solid solutions, J. Appl. Phys. 119 (2016) 074102:1-7.
14. P. Gamaletsos, A. Godelitsas, T. Kasama, **A. Kuzmin**, M. Lagos, T. J. Mertzimekis, J. Göttlicher, R. Steininger, S. Xanthos, Y. Pontikes, G. N. Angelopoulos, C. Zarkadas, A. Komelkov, E. Tzamos, A. Filippidis, The role of nano-perovskite in the negligible thorium release in seawater from Greek bauxite residue (red mud), Sci. Rep. 6 (2016) 21737 (13 pp).
15. P. Onufrijevs, P. Ščajev, K. Jarašiūnas, A. Medvid, V. Korsaks, **N. Mironova-Ulmane**, **M. Zubkins**, H. Mimura, Photo-electrical and transport properties of hydrothermal ZnO, J. Appl. Phys. 119 (2016) 135705 (7 pp).
16. A.M. Balagurov, I.A. Bobrikov, S.V. Sumnikov, V.Yu. Yushankhai, J. Grabis, **A. Kuzmin, N. Mironova-Ulmane**, I. Sildos, Neutron diffraction study of microstructural and magnetic effects in fine particle NiO powders, Phys. Status Solidi B 253 (2016) 1529-1536.
17. P.S. Vachhani, O. Šipr, A.K. Bhatnagar, R.K. Ramamoorthy, R.J. Choudhary, D.M. Phase, G. Dalba, **A. Kuzmin**, F. Rocca, Local structure and magnetization of ferromagnetic Cu-doped ZnO films: No magnetism at the dopant?, J. Alloys Compd. 678 (2016) 304-311.
18. **A. Kuzmin,** A. Kalinko, **A. Anspoks,** J. Timoshenko, **R. Kalendarev**, Study of copper nitride thin film structure, Latvian J. Phys. Tech. Sci. 53 (2016) 31-37.
19. J. Timoshenko, **A. Anspoks,** A. Kalinko, **A. Kuzmin**, Local structure of copper nitride revealed by EXAFS spectroscopy and reverse Monte Carlo/evolutionary algorithm approach, Phys. Scr. 91 (2016) 054003 (11pp).

20. **A. Kuzmin**, V. Pankratov, A. Kalinko, A. Kotlov, L. Shirmane, A. I. Popov, UV-VUV synchrotron radiation spectroscopy of $NiWO_4$, Low Temp. Phys. 42 (2016) 543-546.
21. A. Kalinko, **A. Kuzmin**, P. Roy, R. A. Evarestov, Synchrotron-based far-infrared spectroscopy of nickel tungstate, Low Temp. Phys. 42 (2016) 552-555.

22. D. Bocharov, P. Žguns, S. Piskunov, **A. Kuzmin, J. Purans**, Electronic structure of cubic ScF_3 from first-principles calculations, Low Temp. Phys. 42 (2016) 556-560.

23. **N. Mironova-Ulmane, V. Skvortsova,** A.I. Popov, Optical absorption and luminescence studies of fast neutron-irradiated complex oxides for jewellery applications, Low Temp. Phys. 42 (2016) 584-587.

24. A. Sarakovskis, J. Grube, K. Strals, G. Krieke, M. Springis, **N. Mironova-Ulmane, V. Skvortsova,** E.K. Yukhno, L.A. Bashkirov, Temperature and impurity concentration effects on upconversion uminescence in $LaInO_3$ doped with Er^{3+}, Low Temp. Phys. 42 (2016) 576-579.

25. S. Piskunov, P. A. Žguns, D. Bocharov, **A. Kuzmin, J. Purans**, A. Kalinko, R. A. Evarestov, S. E. Ali, F. Rocca, Interpretation of unexpected behavior of infrared absorption spectra of ScF_3 beyond the quasiharmonic approximation, Phys. Rev. B 93 (2016) 214101:1-9.

26. D. Bocharov, M. Chollet, M. Krack, J. Bertsch, D. Grolimund, M. Martin, **A. Kuzmin, J. Purans**, E. Kotomin, Analysis of the U L_3-edge X-ray absorption spectra in UO_2 using molecular dynamics simulations, Prog. Nucl. Energy (2016), DOI: 10.1016/j.pnucene.2016.07.017.

27. **I. Jonane,** J. Timoshenko**, A. Kuzmin**, Atomistic simulations of the Fe K-edge EXAFS in FeF_3 using molecular dynamics and reverse Monte Carlo methods, Phys. Scr. 91 (2016) 104001 (6pp).

28. E. K. Yukhno, L. A. Bashkirov, P. P. Pershukevich, S. V. Slonskaya, **N. A. Mironova-Ulmane**, A. G. Sharakovskis, Excitation and photoluminescence spectra of solid solutions based on lanthanum indate $LaInO_3$ of a perovskite structure doped with Nd^{3+} and Cr^{3+} ions, Glass Phys. Chem. 42 (2016) 379-385.

29. B. Polyakov, **A. Kuzmin**, K. Smits, J. Zideluns, E. Butanovs, J. Butikova, S. Vlassov, S. Piskunov, Y. F. Zhukovskii, Unexpected epitaxial growth of a few WS_2 layers on {1-100} facets of ZnO nanowires, J. Phys. Chem. C 120 (2016) 21451-21459.

30. **A. Kuzmin, A. Anspoks**, A. Kalinko, A. Rumjancevs, J. Timoshenko, L. Nataf, F. Baudelet, T. Irifune, Effect of pressure and temperature on the local structure and lattice dynamics of copper(II) oxide, Phys. Procedia 85 (2016) 27-35.

31. O. Šipr, J. Vackář, **A. Kuzmin**, Including atomic vibrations in XANES calculations: polarization-dependent damping of the fine structure at the Cu K edge of (creat)2CuCl4, J. Synchrotron Rad. 23 (2016) 1433-1439.

32. A. Kalinko, A. Bauer, J. Timoshenko, **A. Kuzmin**, Molecular dynamics and reverse Monte Carlo modeling of scheelite-type AWO4 (A=Ca, Sr, Ba) W L3-edge EXAFS spectra,Phys. Scr. 91 (2016) 114001 (9pp).

33. K. A. Cherednichenko, Y. Le Godec, **A. Kalinko**, M. Mezouar, V. L. Solozhenko, Orthorhombic boron oxide under pressure: In situ study by X-ray diffraction and Raman scattering, J. Appl. Phys. 120 (2016) 175901:1-8.

34. A. M. Balagurov, I. A. Bobrikov, S. V. Sumnikov, V. Yu. Yushankhai, **N. Mironova-Ulmane**, Magnetostructural phase transitions in NiO and MnO: neutron diffraction data, JETP Letters 104 (2016) 88–93.

35. M. Dunce, E. Birks, **A. Kuzmin,** R. Ignatans, A. Plaude, M. Antonova, A. Sternberg, X-ray diffraction and Raman spectroscopy studies in Na1/2Bi1/2TiO3-SrTiO3-PbTiO3 solid solutions, Ferroelectrics 503 (2016) 52-59.

CONFERENCE PROCEEDINGS

1. V. Skvortsova, N. Mironova-Ulmane, M. Zubkins, R. Kalendarevs, G. Chikvaidze, J. Purans. Optical Absorption Spectra of Zinc-Iridium Oxide Thin Films. Proceeding of the International Conference Actual Problem of Solid State Physics (SSP-2016), 2016 Minsk, Belarus ,"Kovcheg", vol. 1, p. 223-225.
2. N. Mironova-Ulmane, A. Kuzmin, V. Skvortsova, G. Chikvaidze, M. Pärs, I. Sildos, J. Grabis, A. Dindune, M. Maiorov. Vibrational Spectroscopy of MnO. Proceeding of the International Conference Actual Problem of Solid State Physics (SSP-2016), 2016 Minsk, Belarus ,"Kovcheg", vol. 1, p. 18-20.

LECTURES AT CONFERENCES

1. VII International Scientific Conference "ACTUAL PROBLEMS OF SOLID STATE PHYSICS" (SSP-2016), Minsk, October 25-28, 2016, Belarus
- "Vibrational Spectroscopy of MnO" N.Mironva-Ulmane (invite)
- "Absorption Spectra of Zinc-Iridium Oxide Thin Films" N.Mironva-Ulmane (oral)

2. 20th International Conference on Solid Compounds of Transition Elements (SCTE-2016), April 11-15, Zaragoza, Spain.
- "Raman and Infrared Spectromicroscopy and Magnetic Properties of Manganese Oxides" N.Mironova-Ulmane (Poster).

3. 3rd ODISSEUS Workshop & 3rd International Workshop on ODS Materials, April 19-22, Dresden, Germany.
- "Validation of force-field models based on x-ray absorption spectra", A. Kuzmin (Poster).

4. E-MRS 2016 Spring Meeting, May 2-6, Lille, France.
- "Effect of temperature, pressure and size on the local structure and lattice dynamics of copper (II) oxide", A. Kuzmin (Poster).

5. 13th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and International Workshop on Relaxor Ferroelectrics (RCBJSF-IWRF), Matsue, June 19-23, 2016, Japan.
    - "Local structure of $SrTiO_3$ and $EuTiO_3$ studied by X-ray absorption spectroscopy", A.Anspoks (oral)
6. 2- Belarus-Baltic Forum" COOPERATION - A CATALYST OF INNOVATION GROWTH
   6 - 7 October 2016, Minsk
    - "Electron Paramagnetic Resonance for dosimetry and dating" N. Mironova-Ulmane (oral)

7. International Conference. Superstripes, Ischia, Italy, 22-29.06.2016.
    - "Anharmonisity and EXAFS studies beyond the quasiharmonic approximation" J.Purans (invite)

8."6th International Symposium on Transparent Conductive Materials (TCM2016) Chania Greece 09.10-16.10.2016 J.Purans (invite)
    - "The Structure and properties of amorphous p-type ZnO-IrO_2 thin films (**Oral**)

9. International Conference To-Be Meeting Spring, 2016, Warwick, UK,
"Local structure and properties of amorphous ZnO-IrO_2 thin films" (poster)

10. 12 Int. Meeting on Electrochromism IME Aug 28 - Sept 1, 2016, Delft, The Netherlands,
"HiPIMS Deposition of Tungsten Trioxide Thin Films" (**poster.**).

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 – hydrogen 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 sensing materials for hydrogen gas detection.

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:

- FTIR analysis of the organic and inorganic materials, crystals, semiconductors, chemistry, biology etc. with Infrared Fourier Vacuum Spectrometer Bruker VERTEX 80v equipped with Hyperion 2000 Infrared Microscope and Liquid He cryostat (Spectral range: 10000 cm-1 to 10 cm^{-1}; Spectral resolution: 0.1 cm^{-1}; Microscope spatial resolution: 20 μm; Temperature region from 4 K to RT).
- 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:

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Bch: A. Rasnačs

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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 "Ambiteh Group AG"; SIA "Saules Dizains"
10. Riga City Council: Housing and Environment Department of Riga City Council,
11. Riga, Riga Energy Agency

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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

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).

MAIN RESULTS

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

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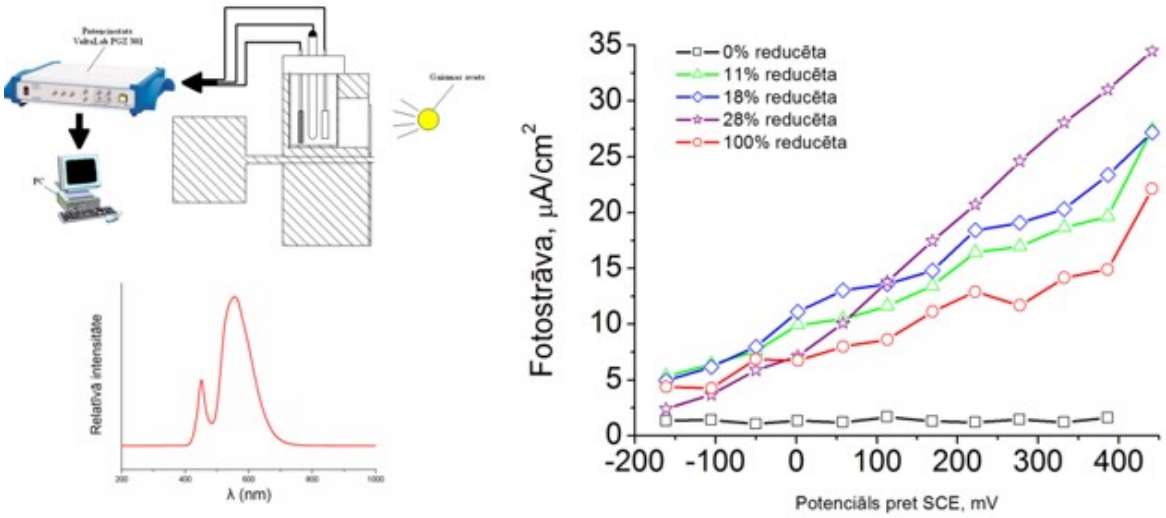
Hydrogen production studies

Photo-catalytic water splitting. Materials with high photocatalytic activity to split water are researched to prevent growing threat of global warming and reduce energy dependency from burning fossil fuels. Self-organized layers of TiO_2 nanotubes are grown onto Ti metal foil with electrochemical anodization method in NaF and H_2SO_4 and H_3PO_4 solution. To obtain crystalline TiO_2, thermal annealing is needed. It is possible to synthesize crystalline TiO_2 directly by irradiation the Ti metal with Nd:YAG laser. Properties of gained samples were investigated using various methods. Morphology by microscopy, structure with Raman spectroscopy and XRD, photoactivity determined from photocurrent measured in three electrode electrochemical cell and calculated charge density. Obtained results clearly showed that synthesis method and parameters influenced morphology, structure and photoactivity of samples. Simple method of electrochemical reduction for improvement of hematite photo activity is prpoposed. Thin ferric oxyhydrate layers were synthesized by anodic electroplating method in 0,02 M $FeCl_2$ solution on FTO glass substrates, and were afterwards reduced with negative potential to ferric monoxide into the same solution and a Cu counter electrode. After rinsing and heat treatment (1h, 400 °C) the layer material changed to Fe_2O_3 (hematite) phase, which was confirmed by X-ray diffraction analysis. For comparative measurements pure hematite layers were also obtained without reducing them after synthesis. Photo-electrochemical results in 1M NaOH solution revealed that both, electrical potential reduced and Cu counter electrode reduced layers, produces several times higher photocurrent than pure hematite layers, only photocurrent threshold voltage was shifted to anodic potentials for layer reduced with Cu counter electrode. Reducing ferric oxyhydrate layer electrochemically it reduces to iron monoxide. Reduction reaction is more active on grain boundary surfaces, which marks out grain boundaries, improving morphology of the layer surface. Potentially the copper counter electrode reduced layer is doped with copper, which improves both the surface morphology and optical properties, by modifying the width of forbidden gap and location of it in the absolute potential scale.



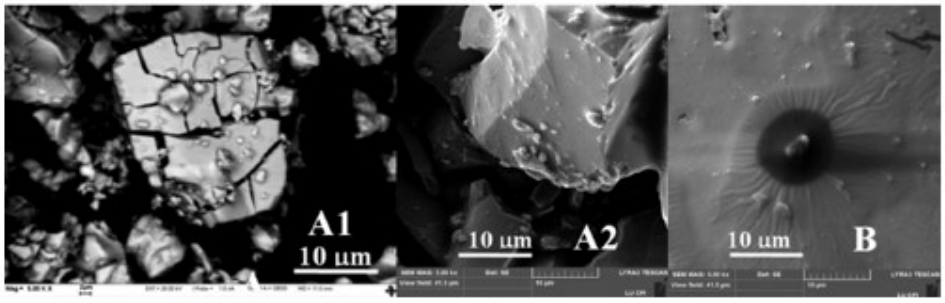
Biological hydrogen production. Biological production of hydrogen by bacterial anaerobic fermentation of widely available renewable resources is a promising and advantageous area. Currently hydrogen from liquid culture medium is collected in the gaseous state, since dissolved hydrogen is in equilibrium with gas phase and tends to release from solution if partial pressure of H_2 decreases. One alternative for hydrogen storage, that is also the safest method, is hydrogen storage in metal hydride alloys. We investigated various powdered metals and alloys (Pd, $LaNi_5$, AB_5, AB_2) forming hydrides to test for their facility to collect hydrogen directly from liquid phase. Differential thermogravimetric method, vacuum extraction and mass spectrometry were used to measure mass changes and hydrogen concentration produced by anaerobic bacteria fermentation process using crude glycerol as substrate. SEM analysis demonstrated that bacteria attached to the material surface. Storage effect was strongest with Pd, AB_5 and AB_2. It appeared that if the sample contained metal that absorbs hydrogen released in fermentation process, the concentration of hydrogen in the gaseous phase at the end of the process will be lower, total amount of captured hydrogen was higher comparing to samples without metal hydride alloys. The presence of powdered Pd or hydride-forming alloys in cultivation medium did not impede glycerol consumption: it was fully degraded during 24 h of fermentation. Concomitantly, the highest amount of absorbed H_2 was measured by the weight loss of hydride-forming materials in TG experiments after 18 h of glycerol fermentation.

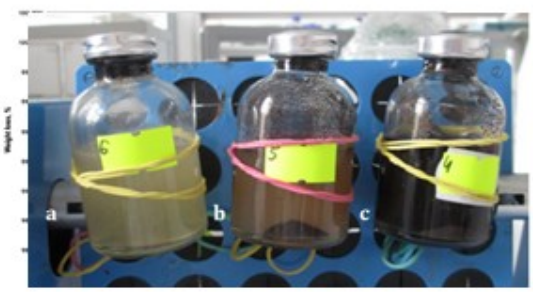
2016

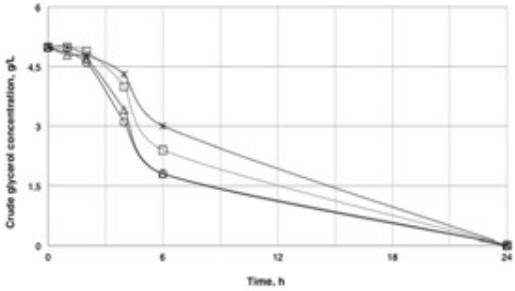
International Journal of Hydrogen Energy
Volume 41, Issue 22, 15 June 2016, Pages 9394–9401

Metal hydride alloys for storing hydrogen produced by anaerobic bacterial fermentation

I. Dimanta[a, b], J. Kleperis[b], I. Nakurte[c], S. Valucka[a], V. Nikolajeva[a], Z. Rutkovska[a, b], I. Muiznieks[a]







Hydrogen and Energy storage studies

Application of self-synthesized graphene an activated carbon. In order to reduce global climate change by limiting CO_2 emissions, it is necessary to switch from continuous power (electricity) production by burning fossil fuels (coal, oil, gas) to the unsteady energy generation from local renewable energy sources (sun, wind, water in rivers). Therefore nowadays reliable energy storage systems are critically needed to store and supply power in continuous manner. Electricity and hydrogen are two comparable energy carriers, and in order to be able to meet humanity's demand for energy, electricity storage and hydrogen storage methods are researched. Low scale electrochemical energy storage systems are electrochemical capacitors (also supercapacitors) and rechargeable batteries. Pristine and intercalated carbon nanostructures have attracted significant research interest for supercapacitors as electrode materials due to their developed structures with large specific area. Two different nanostructured carbon materials were tested – activated carbon (AC) from Latvian alder wood (Latvian institute of Wood Chemistry) and few layer graphene stacks (FLGS) – pristine and intercalated with Na, Mg and Li. In order to obtain FLGS, the electrochemical exfoliation was performed, using graphite industrial waste rod as working electrode. Different pulse sequences, amplitudes and filling factors were used to find optimal parameters of exfoliation process. Important step is purification of processed raw material – single sheets are lightest and can be easy separated with centrifuge or sedimentation. To guaranty higher degree of reduction of FLGS, filtered material was annealed in Ar/H_2 (95:5) gas flow at 300°C for 3 hours. Cyclic voltammetry results confirms that from the tested separators – "Celgard 2400" membrane, "Rossmann"

rayon/cellulose fabric and "Whatman" glass fibre filter - the last two show higher current values (1 M solution of NH_4Cl is used as electrolyte in all cases). The dependence from membrane material could indicate insufficient ionic transport through the separator. Comparing the hydrogen adsorption performance of activated carbon (AC) from Latvian alder wood with few layer graphene stacks FLGS intercalated with Li (Fig.7) it can be seen that activated carbon (brown line) starts to adsorb hydrogen at temperature of approx. 230 K. Calculated value of absorbed hydrogen mass in AC sample approaches 1.3 wt% and is promising value for further research and potential applications.

2016 Bulgarian Chemical Communications, Volume 48, Special Issue E (pp. 365 - 372) 2016

Nanostructured carbon materials as promoters of energy storage

P. Lesnicenoks[1,2], M. Zvine[3], A. Januskevica[3], V.L. Muzikants[3], M.K. Jurjans[3], K. Kaprans[1], A. Volperts[4], G. Kucinskis[1], G. Bajars[1], G. Dobele[4], J. Kleperis[1*]

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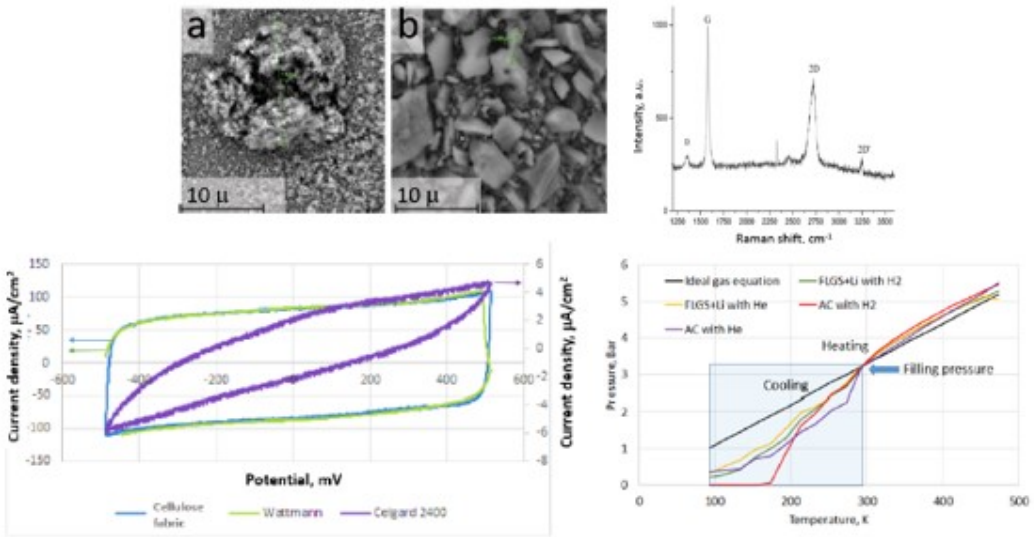

Studies of membranes with proton conductivity

Polymer fuel cell technologies for energy production are of interest due to their comparably low working temperature, possible CO_2 emission reduction. There are a lot of possible challenges lying ahead of the technology to become competitive price-wise with the existing technologies in hydrogen production, energetics, and one of such branches is developing a good material for proton conductive membrane. Some of the criteria are proton conductivity, thermal, chemical and mechanical stability from technical point of view, and price and lifetime from the consumers' point of view. Even though polymer-based materials for fuel cell technology are in research for quite a long time and great variety of materials were developed during last five decades, still there are not many materials that could compete with Nafion or similar fluorine-based. The question of finding alternative material is one of the most actual due to Nafion's high price and some other issues like methane permeability. To obtain polymer Poly(ether-ether-ketone) (PEEK) solution in N-Methyl-2-pyrrolidone (NMP) was cast on glass plate, and resulting membrane was washed and then dried. Five samples from two polymers (SPEEK and Nafion) and one inorganic compound (aluminium oxide) additive were prepared in

different proportions to find composite membrane material that is less dependent on relative humidity and has a good ionic conduction. It was found that three-component membrane made from SPEEK, Nafion and aluminium oxide in proportions SPEEK : Nafion = 9 : 1, aluminium oxide - 2 wt %.

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2016

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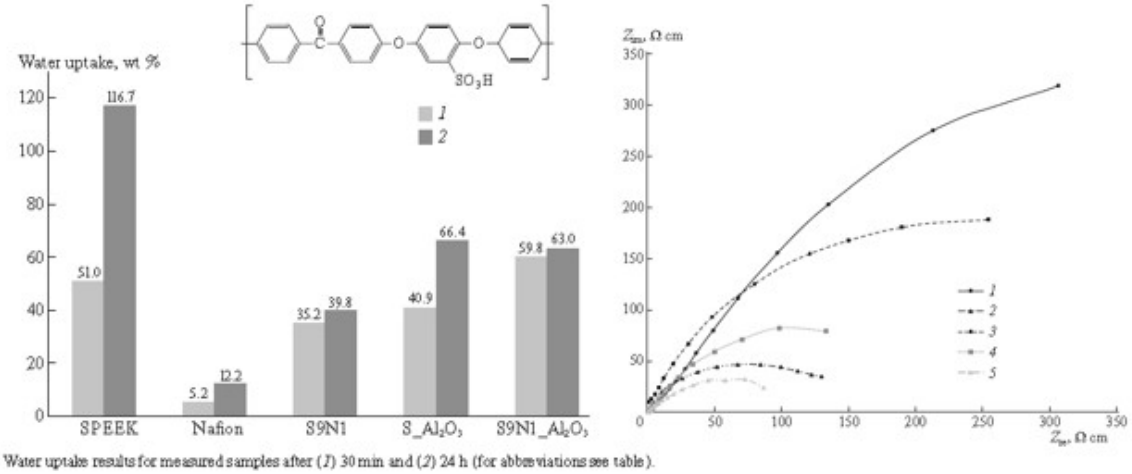
POLYMER MEMBRANES

Sulfonated Poly(ether-ether-ketone) and Nafion Composite Membrane with Aluminium Oxide Additive for Fuel Cell Applications[1]

J. Hodakovska and J. Kleperis
Institute of Solid State Physics, University of Latvia, 8 Kengaraga Street, Riga, LV-1063 Latvia

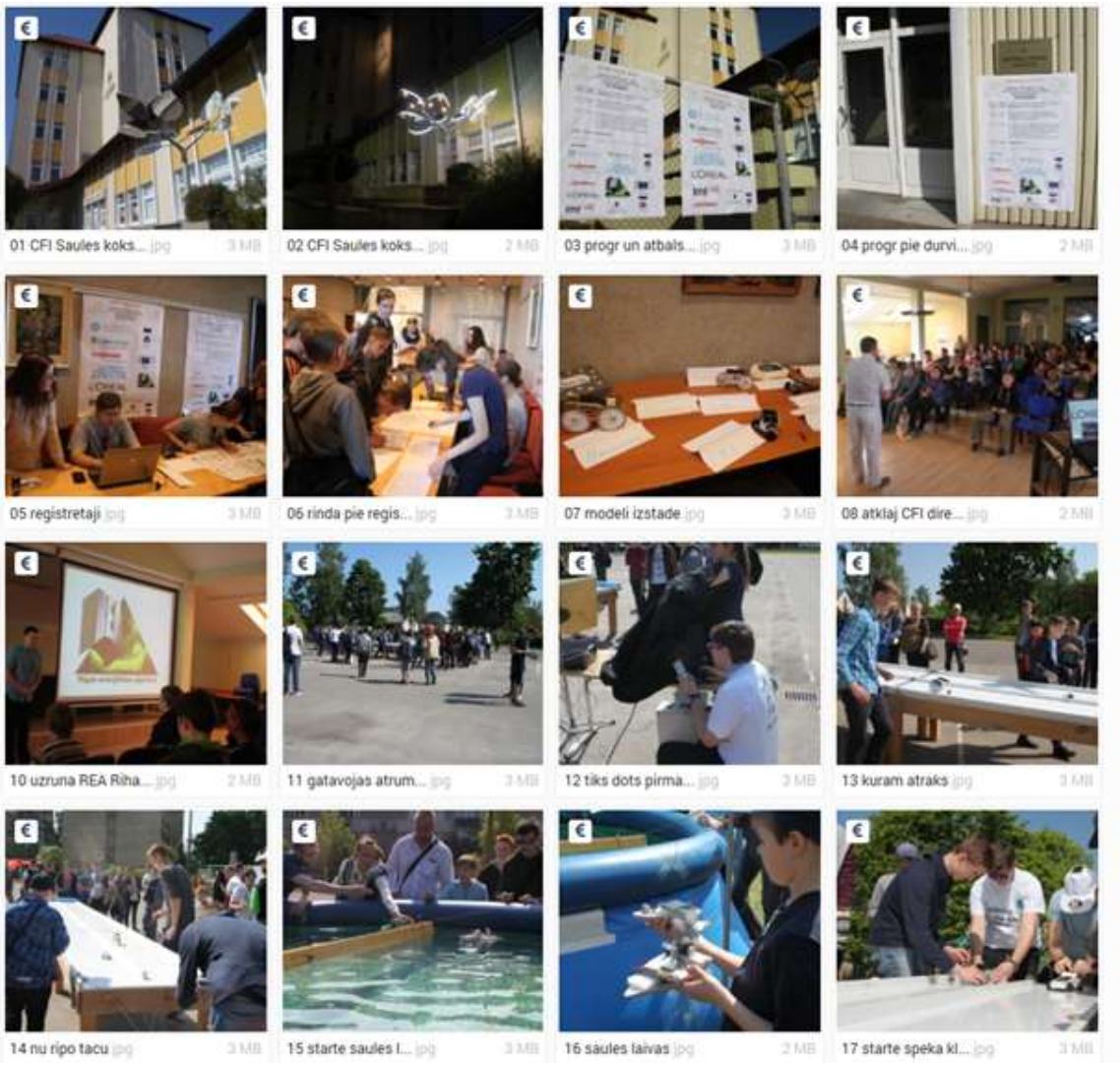


Water uptake results for measured samples after (*1*) 30 min and (*2*) 24 h (for abbreviations see table).

Renewable energy technologies - demonstration and publicity

Saules Kauss 2016 (a.k.a. Solar Cup 2016)

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 2016 main support was received from ISSP UL. Solar Cup 2016 took place on May 21, in the territory of ISSP UL. For competition came registered 43 teams, which received from organizers the solar batteries and motor sets (with support of ISSP UL). To the event came 56 teams, each 2-3 participants, a total of 93 pupils and students from schools of Aloja, Rēzekne, Rīga, Carnikava, Jelgava, Madona, Mālpils, Naukšēni, Kalēti, Priekuļi, Rauna, Rūjiena, Sigulda, Smiltene, Valmiera, Suntaži and Vecpiebalga.



Exhibition Vide un Enerģija 2016 (a.k.a. Environment and Energy 2016)

ISSP UL already 12th year 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. At the stand of ISSP UL in 2016 in evaluating the potential and inexhaustibility of the solar energy, young Artis Volkovs, Arturs Gruduls, and Martins Vanags, together with their elder colleagues, the designer Jānis Straumens and engineer Vladimir Nemtsev, under guidance of Janis Kleperis installed the electro-hinged hub motor in the tricycle's own rear wheel mounted on their own. To produce electricity by turning the pedals to the bike generator. The additional electric energy for the tricycle is given by two 100 W monocrystalline silicon solar panels that are located on the tricycle roof. Visitors to the exhibition "Environment and Energy

2016" will be able not only to look at the Latvian invention, but also to ride through the Hall of the Exhibition Center, using the accumulated solar energy.

Latvian LOréal scholarships for Women in Science awarded in 2016 with the support of the UNESCO Latvian National Commission and the Latvian Academy of Sciences

The world needs science, and the Science needs women, because women in science are able to change the world. On May 18, 2016, the Latvian Academy of Sciences awarded L'ORÉAL Scholarships for Women in Science in 2016. One of the three Latvian winners was the scientific assistant of the Institute of Solid State Physics at the University of Latvia, Ilze Dimanta, Ph.D., student of Biology. The Ilze scholarship is given to the study "Use of Hydride-based Materials for Collecting Hydrogen from Microorganisms and Designing a New Type Bioreactor". Microorganisms produce valuable energy carriers - hydrogen gas, by recycling various industrial processes by-products. A new application for the accumulation of hydrogen produced by microorganisms is gas-absorbing metal alloys.

SCIENTIFIC PUBLICATIONS

1. **I.Dimanta, J. Kleperis**, I. Nakurte, S. Valucka, V. Nikolajeva, Z. Rutkovska, I. Muiznieks. Metal hydride alloys for storing hydrogen produced by anaerobic bacterial fermentation. International Journal of Hydrogen Energy, Vol. 41, Issue 22, 15 June 2016, pp. 9394–9401. DOI:10.1016/j.ijhydene.2016.04.064.
2. **J.Hodakovska, J. Kleperis**. Sulfonated poly(ether-ether-ketone) and Nafion composite membrane with aluminium oxide additive for fuel cell applications (2016) Polymer Science - Series A, 58 (2), pp. 167-171. DOI: 10.1134/S0965545X16020103.
3. **N.Jekabsons**, S. Upnere, **J. Kleperis**. Numerical and experimental investigation of H-darrieus vertical axis wind turbine (2016) Engineering for Rural Development, 2016-January, pp. 1238-1243.
4. A.Tuomela, V. Pankratov, A. Sarakovskis, G. Doke, **L. Grinberga**, S. Vielhauer, M. Huttula, Oxygen influence on luminescence properties of rare-earth doped $NaLaF_4$ (2016) Journal of Luminescence, Volume 179, 1 November 2016, Pages 16-20, DOI: 10.1016/j.jlumin.2016.06.021
5. Zane Kleinmane, **Arturs Gruduls**, Vizma Nikolajeva, **Janis Kleperis**. Anodic biofilm vitality during operation of microbial fuel cells at various load conditions. Journal of Biotechnology > 2016 > 231 > Supplement > S105-S106 DOI 10.1016/j.jbiotec.2016.05.368
6. **J.Kleperis**, V. V. Solovey, V. V. Fylenko, **M. Vanags**, **A. Volkovs**, **L. Grinberga**, A. Shevchenko, M. Zipunnikov. Self-Sufficient PV-H_2 Alternative Energy Objects. Проблемы машиностроения Том 19, № 4 (2016) 62-68.

7. **J.Kleperis, B. Sloka, J. Dimants, I. Dimanta, J. Kleperis Jr.** Solution to Urban Air Pollution–Carbon Free Transport. Baltic Journal of Real Estate Economics and Construction Management 4 (1), 32-47. doi: 10.1515/bjreecm-2016-0003
8. **J.Kleperis**, Fylenko **V.V., Vanags M., Volkovs A., Lesnicenoks P., Grinberga L.**, Solovey V.V. Energy Storage Solutions for Small and Medium-Sized Self-Sufficient Alternative Energy Objects. Bulgarian Chemical Communications, 2016, Volume 48, Special Issue E2 (pp. 290 - 296)
9. **P.Lesnicenoks** P., Zvine M., Januskevica A., Muzikants V.L., Jurjans M.K., Kaprans K., Volperts A., Kucinskis G., Bajars G., Dobele G., **Kleperis J**. Nanostructured Carbon Materials as Promoters of Energy Storage. Bulgarian Chemical Communications, 2016, Volume 48, Special Issue E2 (pp. 365 - 372).
10. A.Volperts A., Dobele G., Zhurinsh A., Zalane Z., Ozolinsh J., **Kleperis J**., Vervikishko D., Shkolnikov E. Supercapacitor Electrodes from Activated Wood Charcoal. Bulgarian Chemical Communications, 2016, Volume 48, Special Issue E2 (pp. 337 - 341).
11. **Peteris Lesnicenoks, Liga Grinberga, Laimonis Jekabsons,** Andris Antuzevičs, Astrida Berzina, Maris Knite, Gatis Taurins, Šarnas Varnagiris, **Janis Kleperis**. Nanostructured carbon materials for hydrogen energetics. Journal of VBRI Press - Advanced Materials Letters, 2016. DOI: 10.5185/eamc2016 See more at: http://www.vbripress.com/aml/articlesinpres/details/674/#sthash.fuGNfdmf.dpuf

CONFERENCE PROCEEDINGS

1. Muzikants T., **Vanags M., Volkovs A., Gruduls A., Kleperis J.** Solar Tree as Light Pole and Aesthetic Pleasure in Urban Environment. Materials of Conference “XV International Scientific Conference "RE & IT - 2016" RENEWABLE ENERGY & INNOVATIVE TECHNOLOGIES”, Smolyan (Bulgaria), June 5-8, 2016, p. 152-156.
2. N. Mironova-Ulmane, A. Kuzmin, V. Skvortsova, **G. Chikvaidze**, M. Pärs, I. Sildos, J. Grabis, A. Dindune, M. Maiorov. Vibrational Spectroscopy of MnO. Proceeding of the International Conference Actual Problem of Solid State Physics (SSP-2016), 2016 Minsk, Belarus ,”Kovcheg”, vol. 1, p. 18-20.

ARTICLES IN POPULAR SCIENCE JOURNALS

1. J. Kleperis, Ūdeņradis ir visur, arī LU Cietvielu fizikas institūtā. Enerģija un Pasaule (2016.g. jūnijs - jūlijs, nr. 3 (98)), lpp. 58-61. Hydrogen is everywhere – also at ISSP UL. Journal Energy & World, June-July 2016; p.58-61.
2. J. Kleperis, Ieskats LU CFI Ūdeņraža enerģētikas materiālu laboratorijas 10 darbības gados. Enerģija un Pasaule (2016.g. augusts - septembris, nr. 4 (99)), lpp. 52-57. 10 years of Hydrogen Energy Materials Laboratory; Journal Energy & World, August-September 2016; p.52-57.
3. J.Barbans, A.Barisa, J.Kleperis. Klimata pārmaiņas Latvijā un pasaulē. Ilustrētā Zinātne, 2016.g. septembris; Climate Changes in Latvia and World. Journal Illustrate Science, September 2016.

LECTURES ON CONFERENCES

1. 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:

- Peteris Lesnicenoks, Liga Grinberga, Janis Straumens, Janis Kleperis. Reactor and methodic for gas sorption/desorption research in various materials with PVT (Sievert's) method in temperature interval +/-200 °C.
- Ieva Grauduma, Ainars Knoks, Janis Kleperis. Nanostructured titania for reduction of carbon dioxide.
- Janis Kleperis, Liga Grinberga, Julia Hodakovska, Martins Vanags, Georgijs Chikvaidze, Peteris Lesnicenoks, Ainars Knoks. How hydrogen energy materials laboratory is embedding new structure and research directions of ISSP UL?
- Janis Kleperis, Janis Berzins, Peteris Lesnicenoks. Thermo-chemical battery from insoluble liquids for collection of waste heat.
- Ainars Knoks, Liga Grinberga, Janis Kleperis. Allotropic modification, crystallinity and photo-activity of titanium dioxide.
- Martins Vanags, Artis Volkovs, Arturs Gruduls. Ferrous oxy-hydrate reduction techniques for improving the physical and photo electrochemical properties of thin layer hematite.
- Elizabete Laiviņa, Klaudija Gauja, Mārtiņš Zubkins, Ainārs Knoks, Jānis Kleperis. Physical and photoelectric properties of magnetron sputtered titanium dioxide.
- Peteris Lesnicenoks, Janis Kleperis, Maris Knite, Liga Grinberga. Carbon nanostructures and other materials for hydrogen sensor.
- Madara Zvīne, Anna Januškeviča, Pēteris Lesničenoks, Gatis Tauriņš, Jānis Kleperis. Research directions 2016-2024 of hydrogen energy materials laboratory.
- Valters Liberts Muzikants, Gints Kucinskis, Miks Krisjanis Jurjans, Gunars Bajars. Carbon nanomaterial use in lithium ion batteries for cathode and anode creation.
- Martins Vanags, Artis Volkovs, Janis Kleperis Stabilization mechanisms of CuO photoelectrode.
- Julija Hodakovska, Stanislavs Lozkins, Janis Kleperis. Sulfonated poly(ether-ether-ketone) and Nafion composite doping with hygroscopic oxides.
- Stanislavs Lozkins, Julija Hodakovska, Janis Kleperis. Nafion polymer modification with hygroscopic alumina and silica nanopowders for application in fuel cells.

J.Kleperis in 2016 - participation in 3 conferences with invited plenary reports:

- 13th International Conference of Young Scientists on Energy Issues (CYSENI 2016) May 26-27, Kaunas (Lithuania);
- 13-го Совещания с международным участием "Фундаментальные проблемы ионики твердого тела" (27 июня - 1 июля 2016 г.) (Russia);
- Nordic Energy Council conference Connecting Energy Challenges with Energy Research (Lithuania Energy Institute, 17th June, 2016, Lietuva, Kleperis J. "Urban planning and low carbon transport").

3. Scientific Conference "Renewable Energy & Innovative Technologies" (RE&IT 2016), June 10-11, 2016, Smolyan (Bulgaria):

- Muzikants T., Vanags M., Volkovs A., Gruduls A., Kleperis J. Solar Tree as Light Pole and Aesthetic Pleasure in Urban Environment. Materials of Conference "XV International Scientific Conference "RE & IT - 2016" RENEWABLE ENERGY & INNOVATIVE TECHNOLOGIES", Smolyan (Bulgaria), June 5-8, 2016, p. 152-156.
- Kleperis J., Fylenko V.V., Vanags M., Volkovs A., Lesnicenoks P., Grinberga L., Solovey V.V. Energy Storage Solutions for Small and Medium-Sized Self-Sufficient Alternative Energy Objects. Bulgarian Chemical Communications, 2016, Volume 48, Special Issue A2 (pp. 290 - 296)
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4. Global Graphene Forum(GGF) - a three-day international event organised by International Association of Advanced Materials, Linkoping University and VBRI Press AB during 23 - 25 August 2016 on the Baltic Sea from Stockholm-Helsinki-Stockholm by the Viking Line Cruise, M/S Mariella.

- Peteris Lesnicenoks, Liga Grinberga, Laimonis Jekabsons, Andris Antuzevičš, Astrida Berzina, Maris Knite, Gatis Taurins, Šarūnas Varnagiris, Janis Kleperis. Nanostructured carbon materials for hydrogen energetics. Advanced Materials Letters, 2017, 8(1) 02-07. VBRI Press. DOI: 10.5185/amlett.2016.7088.

5. "15th International Symposium on Metal-Hydrogen Systems"; Interlaken, Switzerland 17-21 August, 2016.

ar referātu "Experiments with various hydride-forming alloys for biologically produced hydrogen storage":

- Ilze Dimanta et al. "Experiments with various hydride-forming alloys for biologically produced hydrogen storage".
-

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;

PATENTS

1. G.Cikvaidze, A.Kalle. Method for refining silicon using an electron beam. 02.11.2016 Bulletin 2016/44; European Patent EP 2 883 837 B1. Applicant: Institute of Solid State Physics University of Latvia

BACHELOR'S AND MASTER'S THESIS

Anete Gutmane, Bachleor Thesis: The solar energy available in Latvia and its accumulation potential, 2016, University of Liepaja, Supervisor M.Vanags (ISSP UL).

PHD THESIS

Ilze Dimanta, PhD biol. Thesis: Use of Hydride-based Materials for Collecting Hydrogen from Microorganisms and Designing a New Type Bioreactor. 2016, Faculty of Biology, University of Latvia; Supervisor Indrikis Muiznieks, Advisor J.Kleperis (ISSP UL).

DEPARTMENT OF THEORETICAL PHYSICS AND COMPUTER MODELLING

Head of Department Dr. hab. phys. Eugene Kotomin

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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 3D and 2D advanced materials, with emphasis on calculations of properties of defects, surfaces, metal/insulator interfaces;
- theoretical simulations and experimental studies of 1D and 0D advanced nanomaterials, *e.g.*, evaluation of their photocatalytic suitability;
- modeling of advanced functional materials for energy applications (fuel cells, ceramic membranes, 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

STAFF

Laboratory of kinetics in self-organizin.g systems	**Laboratory of computer modeling of electronic structure of solids**
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. Gopejenko
M.S. A. Chesnokov	M.S. O. Lisovski
M.S. J. Shirmane (Pankratova)	M.S. A. Platonenko
B.S. A. Moskina	B.S. M. Sokolov

SCIENTIFIC VISITS ABROAD

1. Dr. hab. E. Kotomin, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (6 months), Photochemistry Center, Russian Academy of Sciences, Moscow (1 week)
2. Dr. O. Dumbrajs, University of Fukui, Japan (3 months)
3. Dr. D. Gryaznov, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (1 week).
4. Dr. A. Popov, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (1.5 weeks), Institute of Physics, University of Tartu, Estonia (1.5 weeks)
5. Dr. Yu. Mastrikov, Institut für Angewandte Materialien, Karlsruhe Institut für Technologie, Germany (2 weeks).
6. Dr. S. Piskunov, Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (2.5 months); University of Duisburg-Essen, Germany (2 weeks).
7. Dr. hab. Yu. Shunin, Laboratori Nazionali di Frascati, Italy (1 month).
8. Dr. Yu. Zhukovskii, St. Petersburg State University, Russia (2 weeks); Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (1 week).
9. M.S. O. Lisovski, University of Duisburg-Essen, Germany (6.5 months).

INTERNATIONAL COOPERATION

China	1. Beijing Institute of Technology, Beijing (Dr. H. Shi).
Estonia	2. Institute of Physics, University of Tartu (Prof. A. Lushchik)
Finland	3. Helsinki University of Technology, Espoo (Dr. T. Kurki-Suonio)
France	4. Laue-Langevin Institute, Grenoble, Prof. H. Schober)
Germany	5. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 6. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov) 7. Darmstadt University of Technology, Darmstadt (Prof. H. von Seggern) 8. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk) 9. Max-Planck Institut für Plasmaphysik, Garching, (Prof. Dr. H. Zohm) 10. Institut für Angewandte Materialien (KIT), Karlsruhe (Prof. Dr. A. Möslang, Dr. P. Vladimirov) 11. Dept Theoretical Chemistry, Univ. Duisburg-Essen (Prof. Dr. E. Spohr)
Israel	12. Ben Gurion University, Beer Sheva (Prof. D. Fuks)
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Kazakhstan	14. Gumilyov Eurasian National University, Astana (Prof. A.T. Akilbekov)
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Lithuania	16. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Norway	17. Center for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, FASE, Norway (Dr. T. Bjørheim)
Poland	18. Warsaw University, Department of Chemistry (Prof. A. Huczko, Prof. Dąbrowska) 19. Institute of Physics, Academy of Science, Warsaw (Prof. H. Szymczak)
Romania	20. University of Craiova (Dr. D. Constantinescu)

Russia	21. St. Petersburg State University, Petrodvorets (St. Petersburg) (Prof. R. A. Evarestov) 22. Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (Prof. P.N. D'yachkov) 23. Photochemistry Center, Russian Academy of Sciences, Moscow (Prof. A.A. Bagaturyants)
Spain	24. Centro de Investigaciones Energeticas Medioambientales y Tecnologicas (CIEMAT), Madrid (Dr. R. Vila)
UK	25. University College London (Prof. A.L. Shluger)
Ukraine	26. Ivan Franko National University, Lviv (Prof. O. I. Aksimentyeva, Prof. I. Bolesta, Dr. I. Karbovnyk)
USA	27. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

MAIN RESULTS

A. Electronic structure calculations for advanced materials

FIRST PRINCIPLES COMPUTER MODELING OF COMPLEX PEROVSKITES FOR FUEL CELL AND PERMEATION MEMBRANE APPLICATIONS

Yu.A. Mastrikov, E.A. Kotomin

L.F. Liotta,

Institute for the Study of Nanostructured Materials (ISMS)-CNR, University of Palermo, Italy

Environmentally friendly solid oxide fuel cells operated at intermediate temperatures, 800-1000 K (IT-SOFC), are internsively investigated due to their potential high efficiency in energy conversion. Currently, the two most promising cathode materials for cathodes and permeation membranes are (Ba,Sr)(Co,Fe)O_3 (BSCF) and (La,Sr)(Co,Fe)O_3 (LSCF).

Comparing these materials, BSCF shows better performance but has several shortcomings, including irreversible transformation into hexagonal phase and carbonate formation in CO_2-containing atmosphere. In turn, LSCF is more stable and thus, being further doped with metal on *B*-sublattice, could serve as a promising candidate for IT-SOFC cathode. (La,Sr)(Co,Fe)O_3 (LSCF) perovskites are well known promising materials for cathodes of solid oxide fuel cells. In order to reduce cathode operational temperature, doping on *B*-sublattice metals was suggested.

Indeed, as it was experimentally shown recently, doping with low Pd content increases oxygen vacancy concentration which is one of factors controlling oxygen transport in fuel cells.

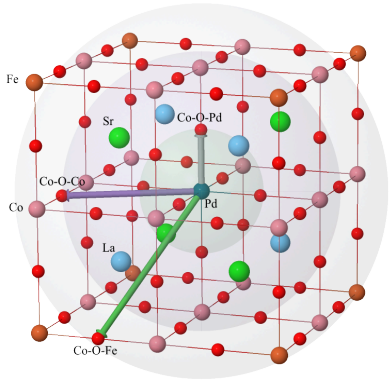

Figure 1. Model of $La_{0.5}Sr_{0.5}Co_{0.5}Fe_{0.25}Pd_{0.25}O_3$ supercell. Three nonequivalent types of oxygen positions are indicated: Co-O-Pd (25%), Co-O-Co (50%), Co-O-Fe (25%).

In this study, we modeled this material using fist principles DFT calculations combined with a supercell model. The charge density redistribution, density of states, and local lattice distortion around Pd ions are analyzed and reduction of the vacancy formation energy confirmed.

AB INITIO CALCULATIONS OF SURFACE SEGREGATION ENTROPY OF OXYGEN VACANCIES AND PROTONS IN $BaZrO_3$ CRYSTALS AND THIN FILMS

E.A. Kotomin,

M. Arrigoni, J. Maier,
Max Planck Institute for Solid State Research, Stuttgart, Germany

T.S. Bjørheim
Centre for Materials Science and Nanotechnology, Department of Chemistry, University of Oslo, Norway

The perovskite $BaZrO_3$ has attracted considerable attention in the recent decade due to its high temperature proton conducting properties, and possible application as electrolyte in intermediate temperature fuel cells and electrolyzers. We performed, for the first time, ab initio calculations of the phonon contribution to the defect thermodynamics of the ZrO_2 terminated (001) surface of $BaZrO_3$. The approach allows us to determine both the *segregation enthalpy* and *entropy* of defects, appled for two fundamental *d*- vacancies (effects in $BaZrO_3$: fully charged oxygen $v_O^{\bullet\bullet}$ and protonic $OH_O^{\bullet}$ defects).

The calculations show that both defects exhibit favorable segregation enthalpies of -65 and -125 kJ/mol, respectively. Further, the vibrational formation entropy of the surface $v_O^{\bullet\bullet}$ vacancy is significantly higher than that of bulk $v_O^{\bullet\bullet}$ vacancy, due to smaller local structural relaxations of the surface defect, leading to a finite surface segregation entropy of 53 J/molK. $OH_O^{\bullet}$, on the other hand, displays nearly identical vibrational spectra at the surface and in the bulk, and the segregation entropy is therefore negligible.

Hence, phonons not only stabilize the surface $v_O^{\bullet\bullet}$ vacancies compared to the bulk defect thermodynamically at high temperatures, but also affect the relative stability of $v_O^{\bullet\bullet}$ and $OH_O^{\bullet}$ at the surface. Finally, we applied a simplified space charge model to the (001) surface, and show that neglect of phonons results in underestimated surface concentration of $v_O^{\bullet\bullet}$ vacancies.

We studied also possible confinement effects on the atomic and electronic structure, and phonon properties of neutral ($v_O^{\times}$) and fully charged ($v_O^{\bullet\bullet}$) oxygen vacancies in $BaZrO_3$ (001) ultra-thin films.

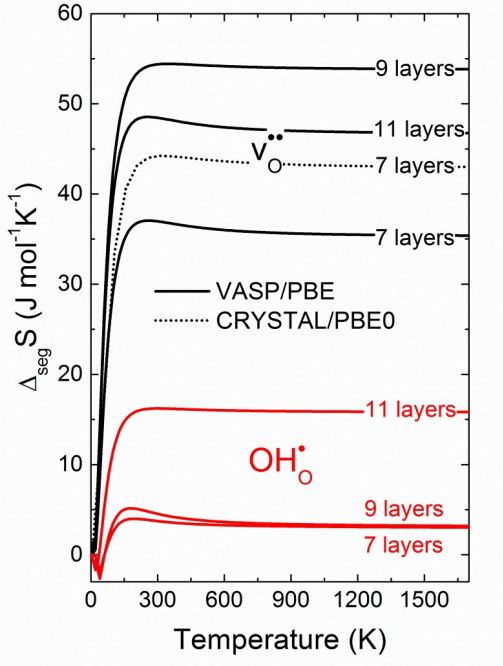

Figure 2. The vibrational contribution to the Gibbs free energy of $v_O^{\bullet\bullet}$ and $OH_O^{\bullet}$ calculated with 7, 9 and 11 atomic layer thick slabs of the ZrO_2 terminated (001) surface of $BaZrO_3$. For $v_O^{\bullet\bullet}$ vacancies, the calculations were performed with both VASP/PBE (solid black) and CRYSTAL/PBE0 computer codes (dotted black) for comparison.

First principles phonon calculations were performed also as a function of film thickness (from 3- to 7-atomic planes) using two complementary DFT methods. The calculations reveal that for both types of vacancies, the confinement effect is very short-range; for films containing 5 planes or more, the $v_O^{\bullet\bullet}$ vacancy properties are predicted to be similar to those observed in the bulk material.

Hybrid Density Functional Theory – Hartree-Fock calculations of oxygen vacancies and protons in complex perovskite oxides

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M. Arrigoni, J. Maier
Max Planck Institute for Solid State Research, Heisenbergstrasse 1, Stuttgart, Germany

Among fuel cells with ceramic electrolytes, those based on proton-conducting oxides (protonic ceramic fuel cells, PCFC) attract increasing interest. In particular, proton-conducting ceramic electrolytes, such as acceptor-doped $BaZrO_3$ discussed above, offer a higher ionic conductivity compared to standard zirconia or ceria oxygen ion conductors, in particular in the temperature range below 700 °C.

The main limiting factors in such cells are (*i*) the manufacturing of a thin electrolyte membrane with non-blocking grain boundaries, and (*ii*) optimization of cathode materials for application on a proton-conducting electrolyte. For cathodes on oxygen ion conducting electrolytes it has been shown that - in addition to a sufficient electronic conductivity - the cathode should be also conducting for oxygen ions to allow the oxygen reduction reaction to extend beyond the gas/cathode/electrolyte three-phase boundary.

Analogously, for PCFC the cathode should exhibit a certain proton concentration and corresponding proton conductivity. However, a proton conductivity in the range of 10^{-5} S/cm at operation conditions (*i.e.* much lower than that of the electrolyte) was estimated to suffice for this purpose.

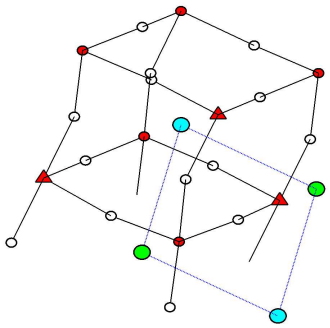

Figure 3. The schematic three-dimensional section of La0.5Sr0.5FeO3 structure; O = white circles, Fe = red, La = green, Sr = cyan. Fe ions in 4+ oxidation state are indicated by triangles

Using hybrid density functionals, detailed ab initio calculations based on the linear combination of atomic orbitals (LCAO) formalism were performed for vacancies and protons in La1-xSrxFeO3-δ perovskites serving as cathode material in PCFC. The atomic and electronic structure of different defect configurations and the role of Fe oxidation state are analyzed in detail. The energetics of the reduction and hydration reactions was stadied. The hydration energy is found to be markedly smaller than in the case of Ba(Zr1-xYx)O3, and the role of material's basicity is discussed as a decisive factor

First principles calculations of *F* centers in $SrZrO_3$ perovskite bulk and ZrO_2-terminated (001) surface

R.I. Eglitis, S. Piskunov

.Using a supercell model and B3PW hybrid exchange-correlation functional in the framework of the density functional theory (DFT), as implemented in the CRYSTAL computer code, we performed *ab initio* calculations for *F* center located in the $SrZrO_3$ bulk and on the ZrO_2-terminated (001) surface. According to results of performed relaxation of atoms around the defect, the two nearest Zr and four Sr atoms are repulsed, but all O atoms are attracted towards both bulk and (001) surface *F*-center. Displacements of atoms surrounding the bulk *F* center are found to be smaller than those around the (001) surface *F*-center while the ZrO_2-terminated (001) surface optical band gap (4.63 eV) is smaller than this value in the bulk (5.60 eV).

The *F* center bands for bulk and (001) surface in $SrZrO_3$ calculated using 3×3×3 and 3×3×1 supercells are located 1.12 and 0.93 eV under the conduction band bottom, respectively. The O vacancy in the $SrZrO_3$ bulk attracts 1.25*e*, and even less, only 1.10 *e* on the ZrO_2-terminated (001) surface. Performed calculations reveal significant enhancement of the chemical bond covalency among the $SrZrO_3$ bulk *F* center and its nearest Zr atoms of 0.24 *e* in comparison with the ideal

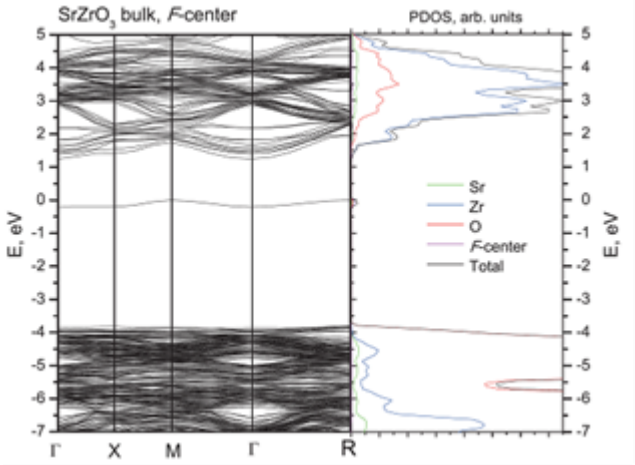

Figure 4. B3PW-calculated band structure for the $SrZrO_3$ bulk containing the isolated *F*-center (left plot) as well as total and projected DOS (right plot).

$SrZrO_3$ perovskite Zr-O chemical bond covalency of 0.10 *e*. Observed defect formation energy for the *F*-center located on the ZrO_2-terminated (001) surface 7.52 eV is somewhat smaller than in the $SrZrO_3$ bulk 7.55 eV. Difference of these formation energies may trigger the segregation of the *F*-center from the $SrZrO_3$ bulk towards the ZrO_2-terminated (001) surface.

AB INITIO MODELING OF $PbBO_3/SrBO_3$(001) HETEROSTRUCTURES (B = Ti, Zr)

R.I. Eglitis, S. Piskunov, Yu.F. Zhukovskii

We performed *ab initio* calculations for both $PbTiO_3/SrTiO_3$(001) and $PbZrO_3/SrZrO_3$(001) heterostructures. For PbO and TiO_2-terminated $PbTiO_3$ (001) thin films of different thickness, augmented on the $SrTiO_3$ (001) substrate, the magnitudes of atomic relaxations Δz increase

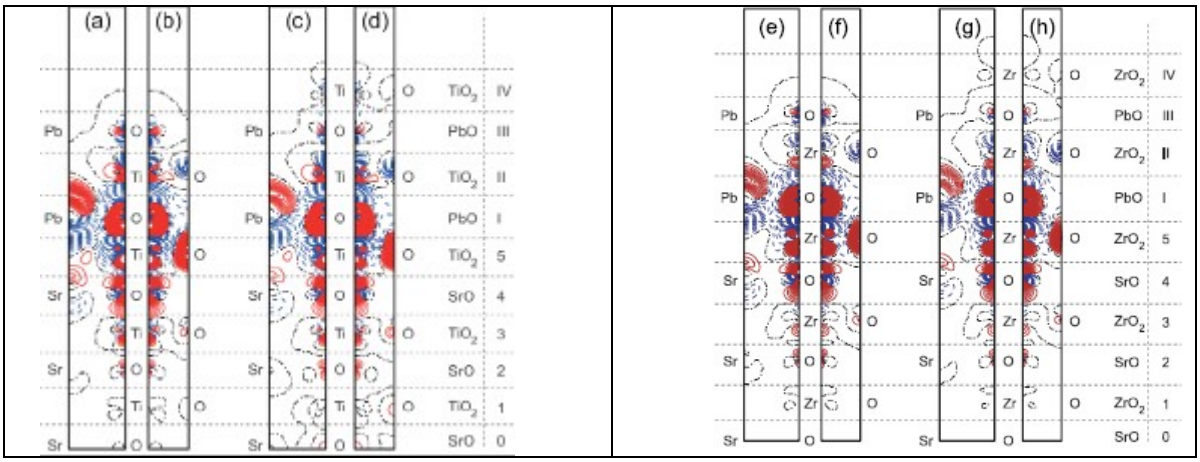

Figure 5. Difference electron charge density maps calculated for $PtTiO_3/SrTiO_3(001)$ and $PtZrO_3/SrZrO_3(001)$ heterostructures: (a) (110) cross-section for N_{PTO}= 3, (b) (100) cross-section for N_{PTO} = 3, (c) (110) cross-section for N_{PTO} = 4, (d) (100) cross-section for N_{PTO} = 4, (e) (110) cross-section for N_{PZO} = 3, (f) (100) cross-section for N_{PZO} = 3, (g) (110) cross-section for N_{PZO} = 4, (h) (100) cross-section for N_{PZO} = 4. Red solid (dark gray), blue dashed (light gray) and black dash-dot isolines describe positive, negative and zero values of the difference charge density, respectively. Isodensity curves are drawn from -0.025 to +0.025e $Å^{-3}$ with an increment of 0.0005*e* $Å^{-3}$. Right-side bars in both plots show the atomic monolayers from which atoms are originated.

as a function of the number of monolayers. For both terminations of the augmented $PbTiO_3$ (001) nanothin film, all upper, third and fifth monolayers are displaced inwards (Δz is negative), whereas all second, fourth and sixth monolayers are displaced outwards (Δz is positive). Qualitatively similar behaviour of $PbZrO_3(001)$ nanothin films above strontium zirconate substrate have been observed in $PbZrO_3/SrZrO_3(001)$ heterostructures.

The B3PW hybrid exchange-correlation functional, as implemented in CRYSTAL computer code, has been used for calculations of the band gaps in various $PbTiO_3/SrTiO_3$ (001) heterostructures (irrespectively on the number of augmented PTO nanolayers) which always were found to be smaller than the band gaps for the $PbTiO_3$ and $SrTiO_3$ bulk. For both terminations, their band gaps are found to be reduced (Figure 6) due to the increased number of $PbTiO_3(001)$ monolayers. The band gaps of PbO-terminated augmented $PbTiO_3(001)$ films are always larger than those for TiO_2-terminated $PbTiO_3(001)$ nanofilms. For each monolayer of the $SrTiO_3(001)$ substrate, the charge magnitudes are always more than several times larger, than for each monolayer in the augmented $PbTiO_3$ (001) thin film.

The 2D interfaces inside considered perovskite (001) heterostructures have been also checked as electrode materials potentially suitable for photocatalytic applications, *e.g.*, for visible-light-driven dissociation of water molecules in aqueous electrolytes. Their efficiency depends on relative position of the band gap edges ε_{VB} and ε_{CB} (the visible-light interval between the infrared and ultraviolet ranges of solar spectrum corresponds to band gap widths ~1.5–2.8 eV) accompanied by a proper alignment of the valence and conduction bands (ε_{VB} and ε_{CB}) as well as occupied and unoccupied induced levels (ε_{HOIL} and ε_{LUIL}) relative to both reduction (ε_{H^+/H_2}) and oxidation (ε_{O_2/H_2O}) potentials (-4.44 eV and -5.67 eV, respectively). The latter must be positioned inside the band gap between mentioned levels:

$$\varepsilon_{VB} < \varepsilon_{HOIL} < \varepsilon_{O_2/H_2O} < \varepsilon_{H^+/H_2} < \varepsilon_{LUIL} < \varepsilon_{CB},$$

in order to satisfy photocatalytic conditions.

As follows from DOS plots (Figure 6), $PbTiO_3/SrTiO_3(001)$ heterostructures containing even-layer, 4 UC-thick $PbTiO_3$ (001) nanothin film can be considered as potential candidates for hydrogen production. Nevertheless, the band gap of heterostructure containing 4 UC-thick

film (~3.4 eV) corresponds to ultraviolet light range, being too wide for sunlight energy conversion (15-17%). To overcome this shortcoming, such a photoelectrode must be doped, both by metal and non-metal atoms.

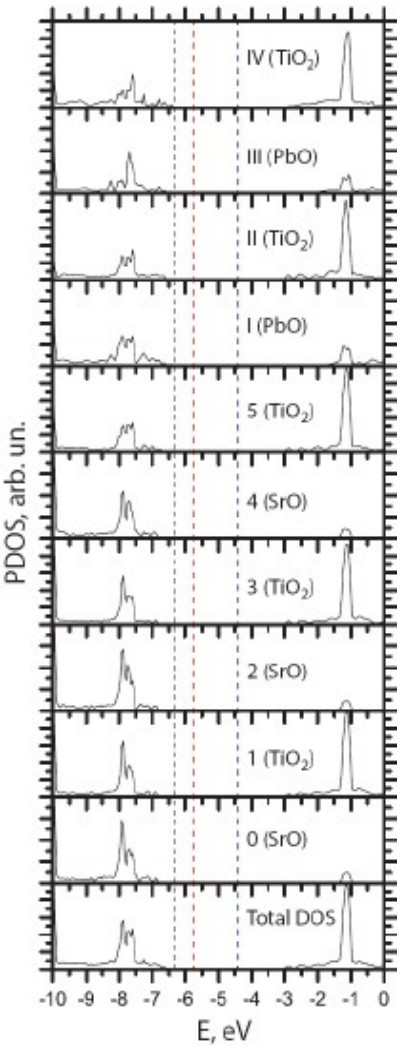

Figure 6. Layer by layer projected density of states of four unit-cell-thick $PbTiO_3/SrTiO_3$ (001) heterostructure. Energy scale is plotted regarding the vacuum level. Black vertical line corresponds to the Fermi level of heterostructure while red and blue lines describe oxidation and reduction electrochemical potentials (the latter is usually defined as the standard hydrogen potential SHE).

N- AND S-DOPED ANATASE-STRUCTURED TiO_2 (101) NANOTUBES FOR VISIBLE-LIGHT-DRIVEN PHOTOCATALYTIC WATER SPLITTING: PREDICTION FROM FIRST PRINCIPLES

O. Lisovski, A. Chesnokov, S. Piskunov, D. Bocharov, Yu.F. Zhukovskii

E. Spohr, M. Wessel

Department of Theoretical Chemistry, University of Duisburg-Essen, Germany

Choice of anatase-structured model for energetically stable six-layered TiO_2(101) nanotube (NT) with (-12,12) chirality (Figure 7a) is justified by a compromise between minimal formation energy and a number of atoms in the NT supercell. A nanotube of such a configuration consists of 144 atoms per unit cell (or 432 sites for Ti atoms). Four possible N or S monodopant sites are shown for non-equivalent oxygen atoms (Figure 7b).

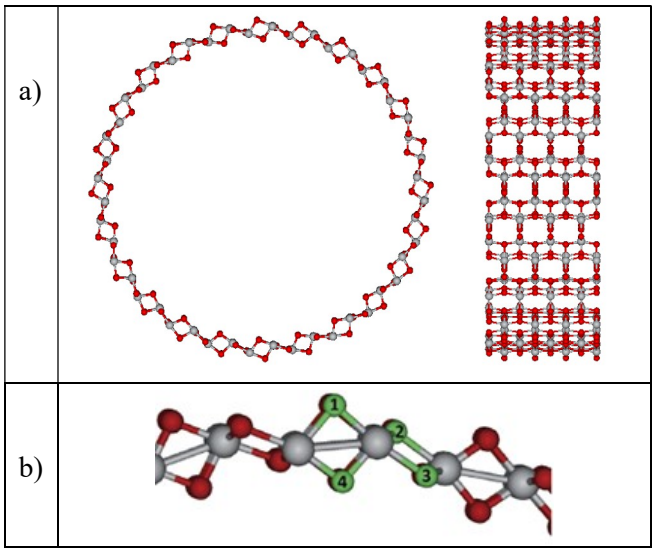

Figure 7. Schematic image of a 6-layer TiO_2(101) NT (a) with chirality indexes (-12,12): (top and lateral views). Ti atoms are shown in grey, O atoms in red, while outer substitutional atoms in yellow. The "basic" UC of (101) nanotube is repeated by 6 roto-translational symmetry operators. Numbered oxygen atoms shown as green (b) present different substitutional sites for N or S monodopant atoms.

In all cases sulphur dopants show a trend to be displaced from their initial substitution positions. Obviously, it is easier to follow such displacement from initial *S*1 and and S4 positions (Figure 7b). For sulphur substitutes, formation energies almost do not depend on S concentration, unlike N dopants, for which this dependence is noticeable, excluding external *N*1 site. Doping at *S*1 and *S*4 promotes the highest photocatalytic enhancement, reducing the gap between the ε_{LUIL} and ε_{HOIL} states, from 4.19 eV to 3.14 eV (3.12 eV) *vs*. 3.08 eV (3.07 eV) for 1.4% (2.8%) defect concentrations, respectively. It means that S-induced occupied levels have been found to be lower at 1.4% concentration. Unlike S-doped NTs, N dopants do not induce visible shift in positions of the VB top and CB bottom levels, they are almost the same as for the pristine NTs tructure. N dopants, however, induce empty states inside the band gap.

Photocatalytic suitability of N_O+S_O co-doped TiO_2 (101) NTs was found to be markedly higher than S and N mono-doped ones. Indeed, in the latter case, there are only four non-equivalent dopant positions (Figure 7b). Once one dopant is introduced, a number of options for different co-dopant sites appear. Due to limited computational resources, S dopant was put in its most preferable position, *S*1, while N dopants were inserted in different surrounding positions (as typed at the bottom of Figure 8).

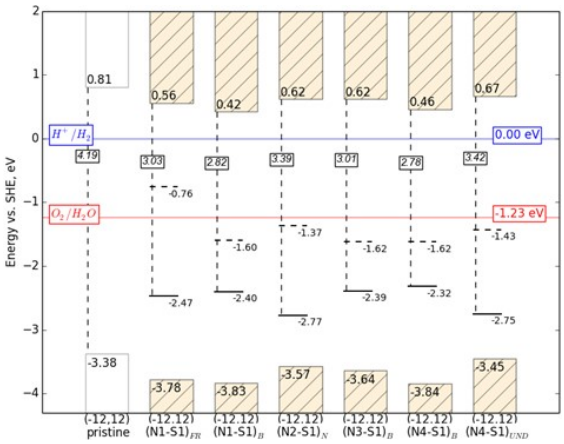

Figure 8. Schematic of the band edges and mid-gap states of pristine and N+S codoped 6-layered (-12,12) TiO_2(101) NTs (for 2.8% dopant concentration). Red and blue horizontal lines describe oxidation and reduction electrochemical potentials, respectively.

PHOTOCATALYTIC SUITABILITY OF Ag-, C- AND N-DOPED WURTZITE-STRUCTURED [0001]-ORIENTED PRISMATIC ZnO NANOWIRES: *AB INITIO* EVALUATION

Yu.F. Zhukovskii, S. Piskunov, O. Lisovski

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Wurtzite-structured zinc oxide (ZnO) is considered in general as a promising photoelectrode for solar water splitting at the corresponding surface immersed in aqueous electrolyte. However, ZnO bulk samples, due to wide enough band gap (3.4 eV), can be considered as active for photocatalytic applications only under ultraviolet (UV) irradiation, where they possess ~1% efficiency of sunlight energy conversion. Although pristine zinc oxide prismatic nanowires (NWs) possess noticeably narrower band gaps than the corresponding bulk, the tendency of their reduction with increasing NW diameter was found to be still insufficient, thus, further structural modification is required to achieve photocatalytic suitability of ZnO NWs. To fill this gap, a series of *ab initio* calculations were performed on prismatic [0001]-oriented ZnO nanowires of different diameters, monodoped by metal (Ag) or non-metal atoms (C, N) with varied concentration (~3 *vs.* ~6%) and arrangement around nanowires (Figure 9).

In order to reproduce qualitatively the energies of one-electron states of doped ZnO nanowires, the hybrid DFT-HF Hamiltonian was used for large-scale first principles calculations based on the PBE0 exchange-correlation functional. Changes in the electronic structure induced in a few defect composition scenarios clearly show that, for specific concentrations and locations of the dopants, the optical absorption peak of doped ZnO can be shifted to the visible light range with promising efficiency. In agreement with experimental observation, the most significant results have been achieved for C-doped ZnO nanowires. They possess the highest photocatalytic suitability, since the band gap was reduced in this case down to 2.1–2.2 eV (for nanowire diameters of 2.9–3.5 nm), which corresponds to optimal 15–17% efficiency of solar energy conversion.

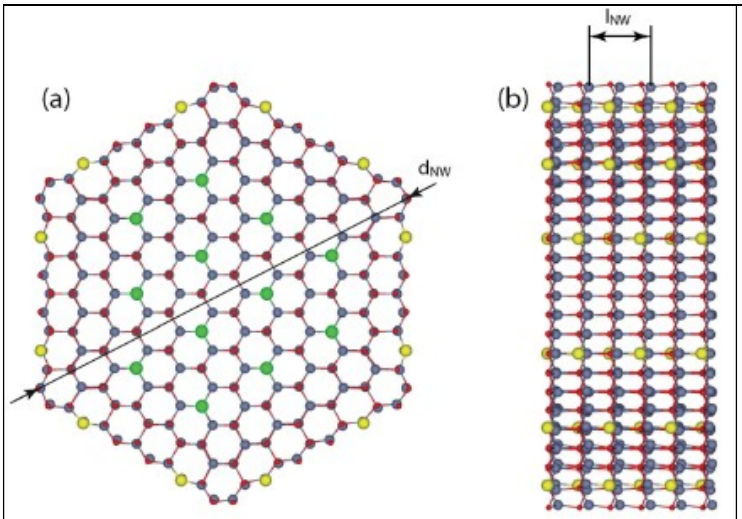

Figure 9. Cross-sectional (a) and lateral (b) images of the doped wurtzite-based hexagonal-shaped ZnO nanowire extended by 6×6 atomic shells around the hollow-centered [0001]-oriented axis, containing 216 formula units (or $432=12\times6^2$ atoms) *per* NW unit cell. The diameter and period of a nanowire are shown by the double arrows d_{NW} (a) and l_{NW} (b), respectively. An example of defect distribution at 3% concentration in a ZnO NW unit cell is given. Zn and O atoms are shown as small red and middle blue-grey balls, respectively. Outer (yellow) or inner (green) balls correspond to arrangement of Ag, C and N mono-dopants or O vacancies.

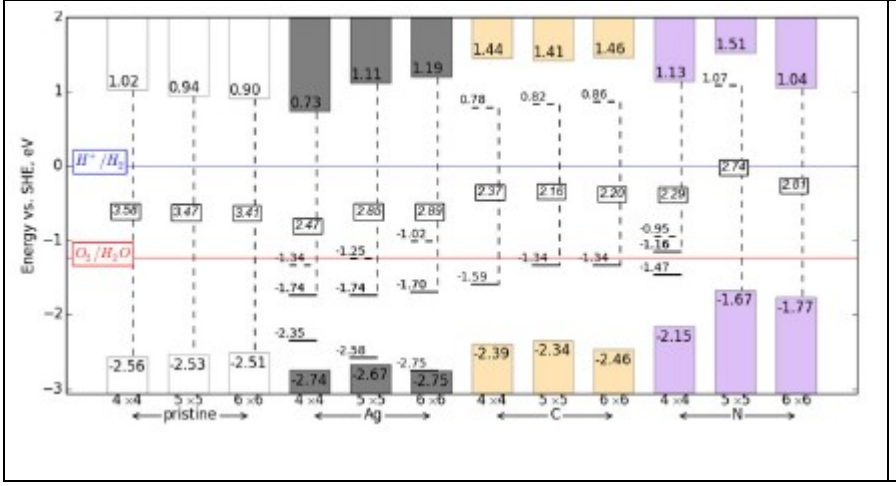

Figure 10. Energy diagram for pristine and doped ZnO NWs with ~6% defect concentration depending on d_{NW}. The red and blue horizontal lines correspond to the redox ε_{O_2/H_2O} and ε_{H^+/H_2} potentials, respectively. The zero of the energy scale corresponds to the standard hydrogen electrode (SHE) level. Solid and dashed horizontal lines describe the induced ε_{HOIL} and ε_{LUIL} levels, respectively.

The energy diagram shown in Figure 10 for different d_{NW} diameters and 6% defect concentration clearly demonstrates the highest photocatalytic suitability of C-doped nanowires with 5×5 and 6×6 thicknesses (their reduced band gaps correspond to 2.18 and 2.20 eV, respectively) as compared to pristine as well as Ag- and N-doped ones.

EPITAXIAL GROWTH OF $WS_2(0001)$ MONOLAYERS ON $\{1\bar{1}00\}$ FACETS OF WURTZITE-STRUCTURED ZnO NANOWIRES: EXPERIMENTAL STUDY AND THEORETICAL SIMULATION

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Core–shell nanowires (NWs) are perspective radially heterostructured nanomaterials which epitaxial growth can be realized even at noticeable core–shell lattice mismatch. Hexagonally shaped shell consisting of WS_2 nanolayers was grown on $\{1\bar{1}00\}$ facets of

prismatic wurtzite-structured [0001]-oriented ZnO NWs (Figure 11). The morphology and phase composition of synthesized ZnO/WS_2 core−shell NWs were confirmed by scanning and transmission electron microscopy, micro-Raman, and photoluminescence spectroscopy.

Epitaxial growth of a few WS_2(0001) monolayers on the $\{1\bar{1}00\}$ NW facets is unexpected due to incompatibility of their symmetry and structure. In order to relax this incoherence, a model of WS_2-containing bridging groups inside core-shell ZnO/WS_2 NW interface was proposed to perform large-scale *ab initio* simulations and to support its feasibility.

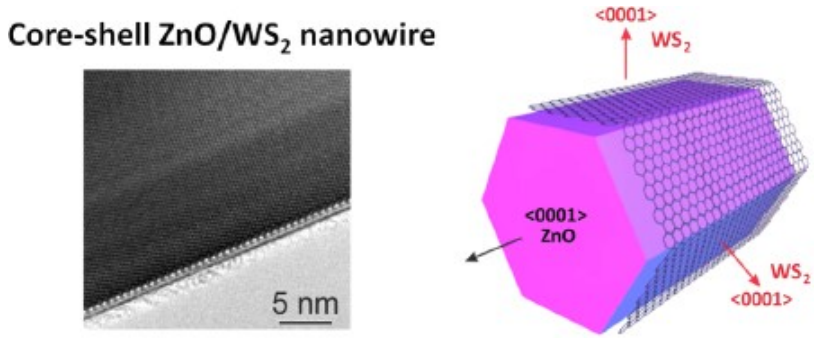

Figure 11. Transmission electron microscopy (TEM) image (left) and structural model of newly synthesized hexagonal-prism-shaped, wurtzite-structured and [0001]-oriented ZnO nanowire covered by epitaxially grown WS_2 monolayers.

Regular hexagonal prismatic shape of wurtzite-structured ZnO NWs can be formed if the NW axes are oriented along [0001] crystallographic directions being hollow-centered. Otherwise their symmetry described by $P6_3mc$ rod group will be reduced while stability (when NW is terminated by lateral facets possessing the smallest surface energy among any wurtzite faces) is lowered. This requirement is fulfilled for the family of six identical $\{1\bar{1}00\}$, $\{\bar{1}100\}$, $\{10\bar{1}0\}$, $\{\bar{1}010\}$, $\{01\bar{1}0\}$, and $\{0\bar{1}10\}$ ZnO facets (Figure 11). Alternative $\{11\bar{2}0\}$ faceting of [0001]-oriented ZnO NW was found to be energetically less favorable (by ~0.2 eV).

Large enough diameters (>50 nm) of ZnO NWs synthesized using the CVD method allowed us to assume that the key role in epitaxial WS_2 layer adhesion to nanowire is played by a family of $(1\bar{1}00)$ planes but not by tiny areas around ZnO NW ribs. This is why the 2D ZnO$(1\bar{1}00)$/WS_2 interface was selected for comparison with the experimental data for ZnO/WS_2 core-shell NWs. Since the latter cannot be atomistically simulated in principle when using the first-principle theory (due to a complexity of their morphology and essentially reduced symmetry) a 20-layer ZnO$(1\bar{1}00)$ slab model.was chosen for simulations of zinc oxide substrate (Figure 12b,c), thickness of which corresponds to [0001]-oriented NW possessing diameter of ~3.5 nm.

Both relaxed 3D models of ZnO and WS_2 lattices as well as 2D ZnO$(1\bar{1}00)$/WS_2 interfaces were calculated using the periodic hybrid DFT−HF Hamiltonian (exchange-correlation functional PBE0) as implemented in CRYSTAL code.

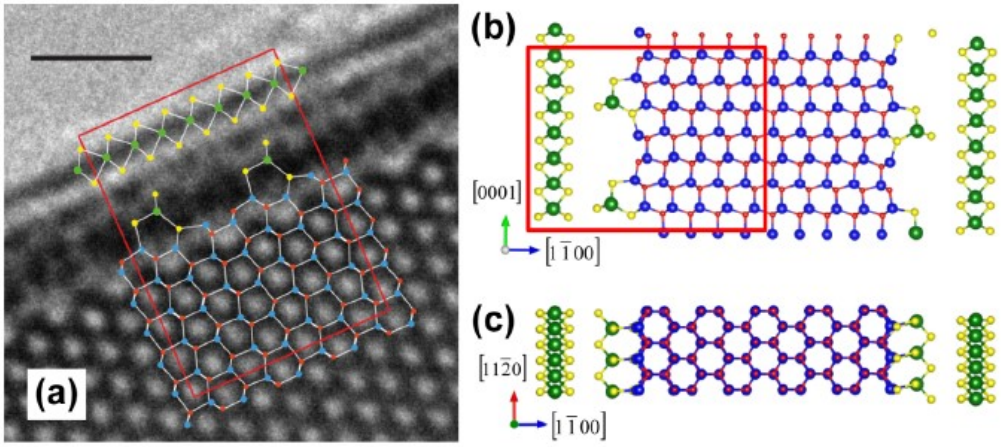

Figure 12. Imposition of optimized atomistic model of ZnO($1\bar{1}00$)/striped 0.5 ML WS_2($1\bar{1}00$)/WS_2(0001) interface on top of the TEM image of ZnO/WS_2 core-shell NW (scale bar is 1 nm) and sections of the same interface across (b) ($11\bar{2}0$) and (c) (0001) planes. All three atomistic models contain WS_3 bridging groups.

NEUTRAL AND CHARGED OXYGEN ATOM INTERSTITIALS IN CORUNDUM CRYSTAL: FIRST PRINCIPLES SIMULATIONS

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Combining a 2×2×1 supercell corundum model (consisting of 72 oxygen anions and 48 aluminium cations in their regular lattice sites) and hybrid B3PW exchange-correlation functional, large-scale *ab initio* LCAO calculations on both quasi-stable dumbbell configuration of interstitial neutral O_i^0 atom and charged O_i^- ion configuration in α-Al_2O_3 (corundum) crystal and possible migration trajectories have been modelled. Lattice distortion around quasi-metastable and migrating oxygen interstitials were optimized including determination of the relaxed interatomic distances. The effective atomic charges and redistributions of the electronic density in O impurity-containing corundum were estimated too. Unlike the neutral O_i^0 interstitial atom forming dumbbell O_i^0 – O_{reg}^{q-} configurations along migration trajectories (Figure 13), the charged O_i^- interstitial does not form dumbbells with the nearest regular O_{reg}^{q-} anion (Figure 14), due to the stronger repulsion between them and Coulomb attraction to the ne Al_{reg}^{q+} cations. Thus, three types of oxygens can be considered in α-Al_2O_3 lattice in absence or presence of interstitial impurity (Figure 15).

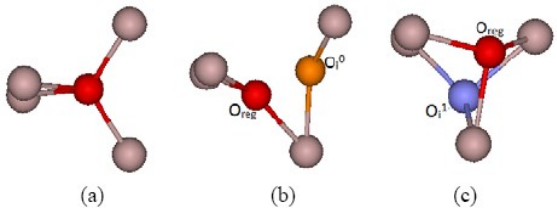

Figure 15. Reference oxygen sites in (a) perfect corundum crystal, (b) that containing neutral oxygen interstitial leading to the dumbbell formation O_i^0 – O_{reg}^{q-} ($d_{O_i\text{-}O_{reg}}$ = 1.40 Å), (c) that containing charged oxygen interstitial ($d_{O_i^- - O_{reg}}$ = 1.87 Å). All views are shown across the vertical z-axis (Al ions oriented along them).

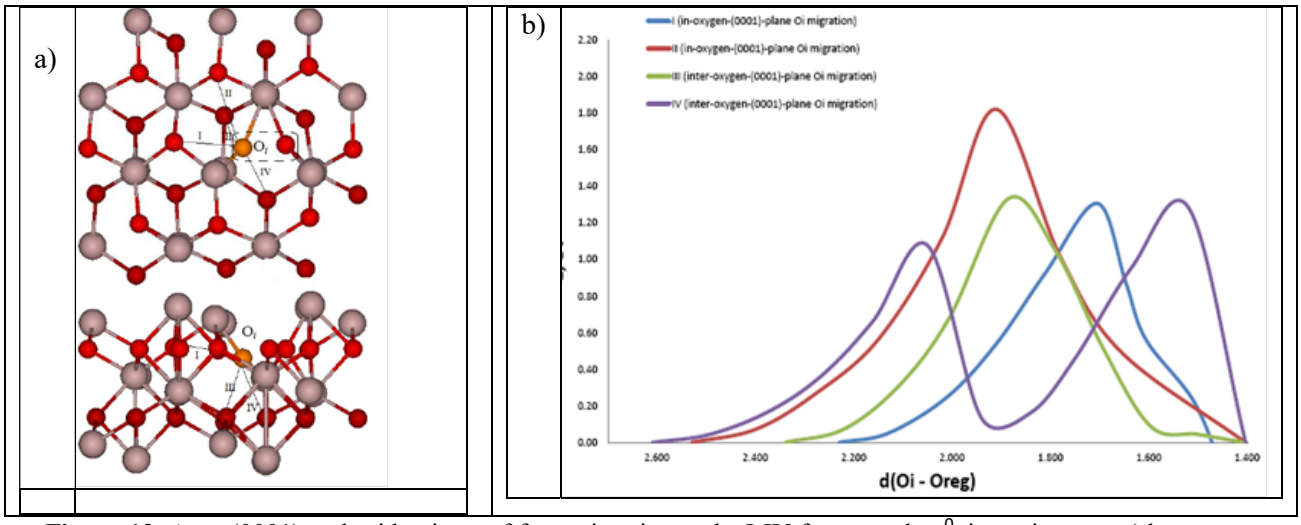

Figure 13. Atop (0001) and aside views of four migration paths I-IV for neutral O_i^0 impurity atom (shown as an orange ball) in α-Al_2O_3 lattice (a). Small red and large brown-gray balls correspond to O and Al atoms, respectively. Dumbbell (O_i-O_{reg}) pair is shown by a dotted rectangle. The energy curves for four migration paths I, II, III and IV of interstitial O_i^0 atom in corundum (b) and estimated energy barriers (transition states).

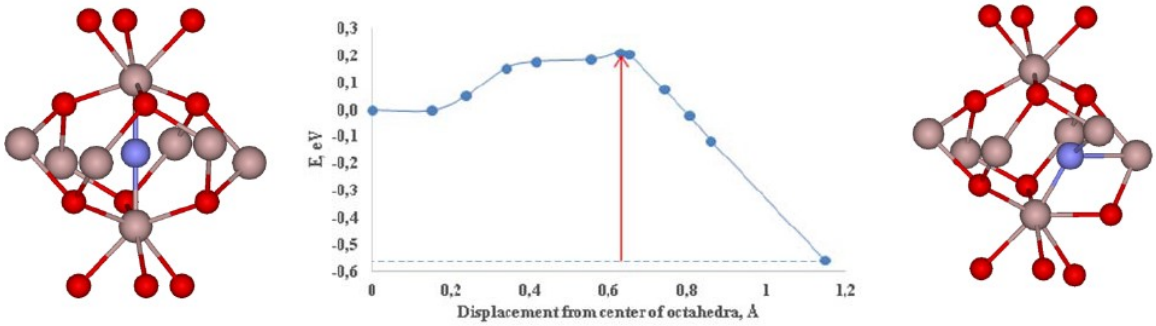

Figure 14. The potential energy curve for migration of interstitial O_i^- ion (shown as a blue ball) in corundum lattice. Zero point corresponds to its initial position in a centre of octahedron formed by six nearest O_{reg}^{q-} anions (left image), while the distance is counted from this centre to a final position (right image). The total height of the energy barrier for O_i^- ion is 0.76 eV being essentially smaller in comparison with the corresponding energy barrier of interstitial O_i^0 atom in α-Al_2O_3 lattice (~1.3 eV).

LARGE-SCALE PLANE-WAVE DFT CALCULATIONS NECESSARY FOR MODELING OF Y–O PRECIPITATE FORMATION IN γ-Fe LATTICE

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Numerous experiments and theoretical studies clearly show that after high-temperature (>1000 C) mechanical alloying of steel and yttria a significant part of Y and

O atoms is distributed in γ-Fe matrix with concentration above their equilibrium solubility. This might mean that nucleation and growth of Y_2O_3 clusters occurs already during the hipping stage in *fcc*-Fe phase.

Ab initio calculations of Y and O impurity atoms as well as V_{Fe} vacancies in the γ-Fe lattice were performed in order to describe the interactions between these defects, which are important for understanding of nanoparticles' formation within the oxide dispersed strengthened (ODS) steels. Large scale DFT calculations performed using plane-wave approach (as realised in VASP computer code) show that V_{Fe} vacancies considerably influence the binding between the impurity atoms. The results of performed calculations provide the detailed information about the binding energies between the defects, the changes of their effective charges and displacements of the substitute atoms relatively the host atom positions. The energy barriers necessary for the migration trajectories of impurity atoms in the γ-Fe lattice were found by performing the large-scale DFT calculations within the nudge-elastic band (NEB) method.

There is a strong repulsion between oversized yttrium solute atoms (at least their diameters essentially exceed those of iron atoms), which unavoidably leads to appearance of V_{Fe} vacancies close to newly-formed Y_{Fe} substitutes. Moreover, the latter willingly collect these vacancies in order to reduce the elastic relaxations of the lattice in their neighbourhood while the former can be occupied later by oxygen atoms (O_{Fe} substitutes) captured there from adjacent octahedral and tetrahedral interstitial sites in *fcc*-lattice. Due to lower energy barriers, O atom migrates much faster than Y, which is a limiting factor of Y–O precipitate growth inside iron matrix. In any case, adjacent O_{Fe} and Y_{Fe} substitutes can create in *fcc*-lattice different types of Y–O bonds (Figure 15).

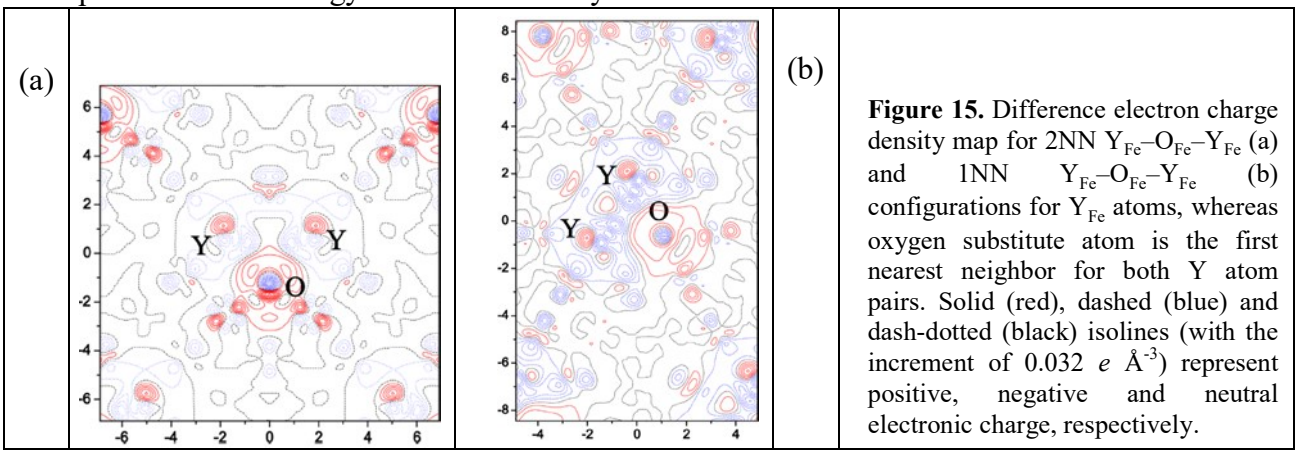

Figure 15. Difference electron charge density map for 2NN Y_{Fe}–O_{Fe}–Y_{Fe} (a) and 1NN Y_{Fe}–O_{Fe}–Y_{Fe} (b) configurations for Y_{Fe} atoms, whereas oxygen substitute atom is the first nearest neighbor for both Y atom pairs. Solid (red), dashed (blue) and dash-dotted (black) isolines (with the increment of 0.032 e Å^{-3}) represent positive, negative and neutral electronic charge, respectively.

QUANTUM CHEMICAL AND MOLECULAR DYNAMICAL CALCULATIONS ON THE ELECTRONIC STRUCTURE AND LATTICE DYNAMICS OF ScF_3

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Scandium fluoride ScF_3 is a perovskite-type crystal which possesses a simple cubic structure (Figure 16) and attracts enhanced attention due to its large negative thermal expansion (NTE) over a wide range of temperatures (0-1100 K).

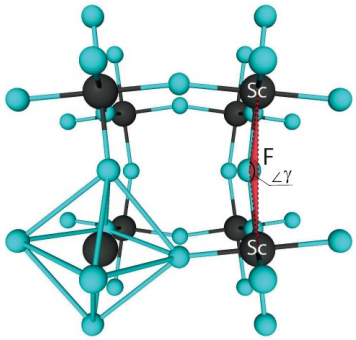

Figure 16. Prospective image of cubic ScF_3 lattice unit cell with parameter a_o equalled to the shortest Sc-Sc distance. Angle γ corresponds to the deviation of joint Sc-F bonds from the vertical direction. ScF_6 octahedron around the left bottom Sc atom corresponds to the primitive unit cell.

The electronic structure, lattice dynamics, and phonon anharmonicity of ScF_3 crystal were studied within the framework of quantum chemistry approaches (LCAO, hybrid HF-DFT) using Crystal09 and VASP computer codes. *Ab initio* hybrid electronic structure calculations were found to be able to reproduce qualitatively well the experimental values of lattice parameter (a_0 = 4.0257 Å at T = 0 K). The width of band gap (ε_{gap} > 8.9 eV) also confirms available experimental data. Calculated partial density of electron states (PDOS) is also in good agreement with valence-band photoelectron as well as the F 1*s* X-ray absorption spectra available in literature. The total density of phonon states determined within quasi-harmonic approximation from phonon dispersion curves and calculated along the high-symmetry directions Γ-X-M-R-Γ of the Brillouin zone, agrees reasonably well too.

At the same time, the temperature dependence of the experimentally measured infra-red (IR) absorption spectra, consisting of two bands at 220 and 520 cm^{-1} cannot be explained within the quasi-harmonic approach, which predicts shifts of these bands in an opposite direction relatively to that experimentally observed. To resolve this issue, a simple model was developed based on the symmetry analysis of phonon modes and use of the temperature-dependent experimental results of diffraction and EXAFS studies. Suggested model allows us to reproduce the unexpected experimental behavior observed for two bands in the IR absorption spectrum of ScF_3 and can be also applied for the interpretation of its other spectroscopic properties.

Calculations on ScF_3 bulk performed using CP2K code package demonstrated efficiency of the MD-EXAFS approach in combination with *ab initio* molecular dynamics for theory validation and description of temperature-dependent structural properties for ScF_3. Within this approach configuration-averaged Sc *K*-edge EXAFS spectra were reproduced using molecular dynamics with NVT ensemble for three different temperatures (T = 300 K, 600 K and 1000 K) as well as compared with the experimental data suggesting a good qualitative agreement. It was found that upon temperature increase the ScF_6 octahedra do not behave as rigid units: the strong rotation of ScF_6 octahedra is accompanied by their expansion caused by the anharmonic Sc-F bonding, despite of a negative thermal expansion of ScF_3 crystalline lattice.

INTERPRETATION OF THE U *L*3-EDGE EXAFS IN UO_2 USING MOLECULAR DINAMICS AND PLANE-WAVE DENSITY FUNCTIONAL THEORY CALCULATIONS

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The experimental U *L*3-edge EXAFS spectra of uranium dioxide were interpreted up to 6 Å in *R*-space using the results of both classical and *ab initio* molecular dynamics simulations (CMD and AIMD, respectively) as well as taking into account the multiple scattering effects.

The accuracy of CMD method relies on the used force-field model; therefore EXAFS spectra can be employed for its further validation. Nine different force-field models of uranium dioxide differ mainly in description of the U-O vibrational amplitudes. Thus, the EXAFS data provide valuable information in order to evaluate the quality of the force-field modeling. The importance of the multiple-scattering contributions for the EXAFS analysis was also estimated. The obtained results suggest that they are not sufficiently large for UO_2 but remain still important in the range of the second (U2) and third (O3) coordination shells around uranium.

The advantage of the AIMD method is the absence of the adjustable parameters, except for the choice of the functional model. The exchange-correlation functional PBE employed in plane-wave DFT calculations on uranium dioxide predicts too rigid interactions.

The Cr *K*-edge XANES was simulated within the full-multiple-scattering formalism considering a substitutional model (Cr at U site). The analysis of the Cr K-edge XANES spectrum of Cr-doped UO_2 suggests that the substitutional model (Cr at U site) differs fromthe experimental data, even when structure relaxation is taken into account. Therefore, further investigations are required to shed light on the accommodation of Cr atoms and precipitates within the UO_2 host lattice.

B. Kinetics of processes with self-organization

THEORETICAL ANALYSIS OF DEFECT RECOMBINATION KINETICS IN INSULATORS

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As is well known, irradiation of insulating crystals results in formation of the primary complementary Frenkel defects – vacancies and interstitials (called in alkali halides as *F* and *H* centers) – which become mobile above some critical temperatures, and then either recombine or aggregate. Despite numerous experimental studies of the kinetics of primary defect annealing upon temperature increase obtained by a number of optical, magnetic methods, very little *quantitative* information is available on the defect migration energies and their pre-exponential

factors. These parameters are necessary for the prediction of possible secondary reaction kinetics and, in general, material radiation stability.

The experimental kinetics of the low-temperature diffusion-controlled *F* amd *H* center recombination was carefully analyzed in a series of irradiated alkali halides and oxides. As a result, the migration energies and pre-exponential parameters for the hole centers (called the color *H* center in alkali halides, and interstitial oxygen ions in aluminum oxides), were extracted.

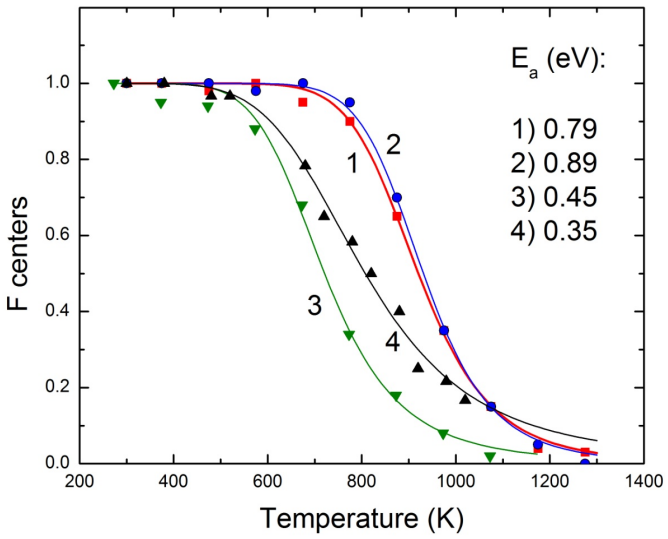

Figure 17. The experimental kinetics of *F* –type centers annealing in four different neutron irradiated Al_2O_3 samples. The full lines are drawn based on theory. The effective migration energies are shown in the legend.

In particular, a comparison of the calculated and experimental annealing kinetics for the *F* centers in both neutron irradiated and thermochemically reduced Al_2O_3 samples (Figure 17) allowed us to estimate the migration energy of interstitial oxygen ions and that for the *F* centers as ~0.8 eV and ~4.5 eV. The former energy was checked with that estimated by means of atomistic defect calculations (Section A) - a qualitative agreement was observed.

Kinetics of metal colloid formation in thermochemically reduced and heavily irradiated ionic solids

V.N. Kuzovkov, E.A. Kotomin, A.I. Popov

It is known that mobile *F* centers in alkali halides produce complex defects containing the dimer (*M* centers), trimer (*R*), tetramer (*N*) *F*-aggregates and finally, metal colloids. In particular, such kinetics was studied in hevily electron-irradiated NaCl crystals. It was shown that the *F* center concentration decay above 400 K is accompanied by a simultaneous growth of the *colloid* X-absorption band. In this case, the main mechanism of colloid formation is the mutual encounter of mobile *F* centers and their aggregation caused by an elastic attraction, which can be characterized by the interaction energy ε for the nearest neighbor defects. We developed the relevant theory and computer code.

Fig. 18 depicts the calculated annealing kinetics of *F* centers for different values of migration energy E_a and simultaneous temperature-induced growth of the

concentration of colloids consisting of different number of defects (N_0) in a NaCl crystal. The best agreement with experimental data (filled squares) is achieved for $E_a = 1.13$ eV which is close to the previous estimates. It is commonly accepted that the peak energy and halfwidth of the X-absorption band of metal colloids depend strongly on colloid size: very small colloids possess broad structureless bands, whereas the well-pronounced experimental optical band presented in Fig. 18 definitely corresponds to large-size colloids. We assume here the Poisson distribution of colloids in size. Fig. 18 shows that the best agreement with experimental data is achieved assuming that each colloid contains at least $N_0 = 20$ defects.

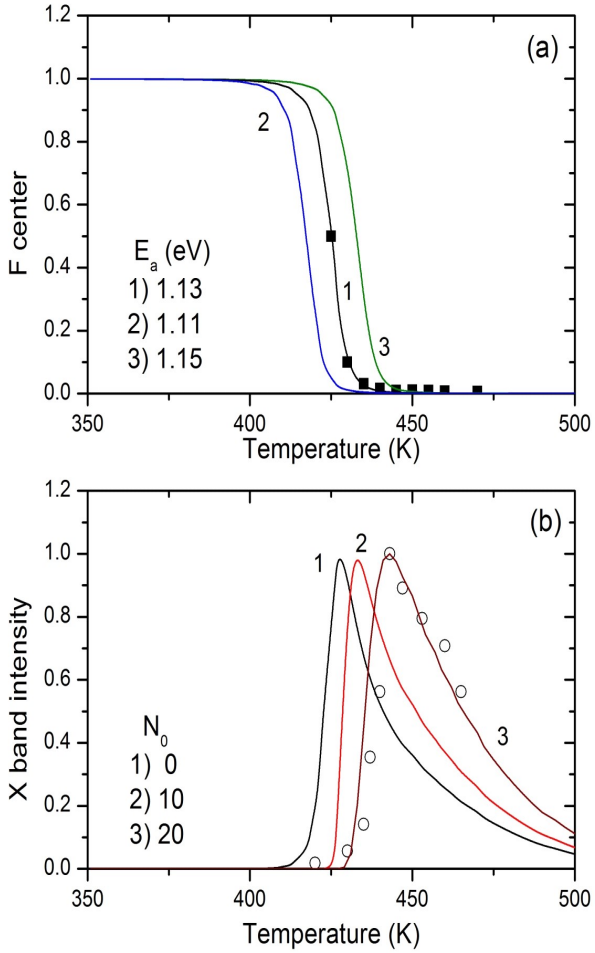

Figure 18. The calculated annealing kinetics (solid lines) of the F center concentration in NaCl for different values of migration energies E_a (a) as well as the growth of the colloid concentration with the certain defect number N_0 (b). The experimental points are shown by filled squares (a) and open circles (b).

We performed also calculations for Al colloids in corundum which arise in thermochemically reduced corundum during annealing above 1700 K. The Al colloids are predicted here to be quite small, 10-20 Å, in agreement with the available experiments.

STABILIZATION OF PRIMARY MOBILE RADIATION DEFECTS IN MgF_2 CRYSTALS

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Non-radiative decay of the electronic excitations (excitons) into point defects (*F-H* pairs of Frenkel defects) is main radiation damage mechanism in many ionic (halide) solids. Typical time scale of the relaxation of the electronic excitation into a primary, short-lived defect pair is about 1–50 ps with the quantum yield up to 0.2-0.8. However, only a small fraction of these primary defects are spatially separated and survive after transformation into stable, long-lived defects.

The survival probability (or stable defect accumulation effeciency) can differ by orders of magnitude, dependent on the material type; *e.g.*, ~10% in alkali halides with *fcc* or *bcc* structure, 0.1% in rutile MgF_2 and <0.001% in fluorides MeF_2 (Me: Ca, Sr, Ba). The key factor determining accumulation of stable radiation defects is stabilization of primary defects, first of all, highly mobile hole *H* centers, through their transformation into more complex immobile defects.

Theoretical calculations of the migration energies for *F* and *H* centers were perofrmed in poorely studied MgF_2 crystals with a focus on the *H* center stabilization in the form of the interstitial F_2 molecules (Figure 19) which is supported by presented experimental data. Formation of these very stable and optically inactive molecules (unlike X_3^- complex hole *H* centers in alkali halides) explains peculiarities of the radiation stability of MgF_2 crystals.

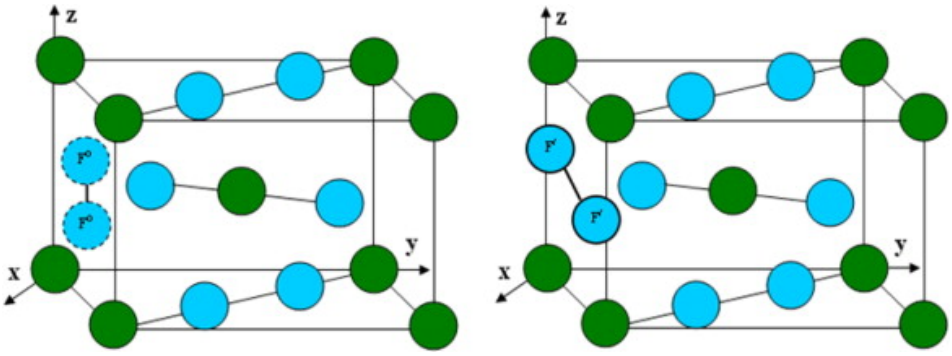

Figure 19. The initial (left) and optimized (right) configurations of interstitial F_2 molecule in a rutile MgF_2 structure.

VOID LATTICE FORMATION IN ELECTRON-IRRADIATED CaF_2: STATISTICAL ANALYSIS OF EXPERIMENTAL DATA AND CELULLAR AUTOMATA SIMULATIONS

G. Zvejnieks, V.N. Kuzovkov, E.A. Kotomin, P. Merzlyakov

Calcium fluorite (CaF_2) is an important optical material widely used in both microlithography and deep ultraviolet (UV) windows. It is well known that under certain conditions the electron beam irradiation can create therein a super-lattice consisting of vacancy clusters (called a *void lattice*). The goal of this study is the two-fold.

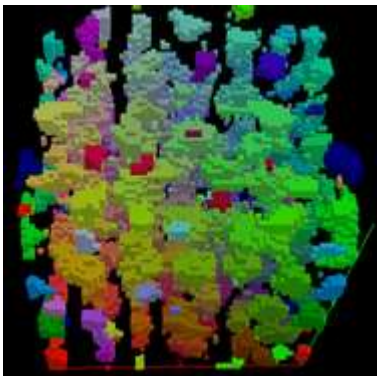

Figure 20. Snapshot of the cellular automata modelling of the *F, H* center formation in CaF_2 (voids are red, interstitials green).

Firstly, to perform a quantitative analysis of experimental TEM images demonstrating void lattice formation, we developed two distinct image filters. As a result, we can easily calculate vacancy concentration, vacancy cluster distribution function as well as average distances between defect clusters. The results for two suggested filters are similar and demonstrate that experimental void cluster growth is accompanied by a slight increase of the void lattice constant.

Secondly, we proposed a microscopic model that allows us to reproduce a macroscopic void ordering, in agreement with experimental data, and to resolve existing theoretical and experimental contradictions (Figure 20). Our computer simulations demonstrate that macroscopic void lattice self-organization can occur only in a narrow parameter range. Moreover, we studied the kinetics of a void lattice *ordering*, starting from an initial disordered stage, in a good agreement with the TEM experimental data.

A NOVEL QUANTUM FIELD APPROACH TO PHOTOEXCITED INSULATORS

E. Klotinsh

In order to predict optical properties of insulating materials under intensive laser excitation, methods of quantum electrodynamics were generalized, which allowed us to simulate excitation of electrons and holes, interacting with each other and acoustic phonons.

The prototypical model considers a two-band dielectric material which is characterized by the dispersion relations for the electron and hole states. Universal description of the excited electrons, holes and acoustic phonons was developed within the formalism of a joint quantum kinetics.

Illustrative solutions for the quasiparticle birth-annihilation operators, applicable at short laser pulses at 0 K, were obtained by the transition from the macroscopic description to the quantum field formalism.

C. Plasma Physics

SELF-CONSISTENT NON-STATIONARY THEORY OF GYROTRONS

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For a long time, the gyrotron theory was developed assuming that the transit time of electrons through the interaction space is much shorter than the cavity fill time. Correspondingly, it was assumed that during this transit time the amplitude of microwave oscillations remains constant. A recent interest to such additional effects as the after-cavity interaction between electrons and the outgoing wave in the output waveguide had stimulated some studies of the beam-wave interaction processes over much longer distances than a regular part of the waveguide which serves as a cavity in gyrotrons. Correspondingly, it turned out that the gyrotron theory free from the assumption about constant amplitude of microwave oscillations during the electron transit time should be developed. The present study presents some results obtained in the framework of such theory.

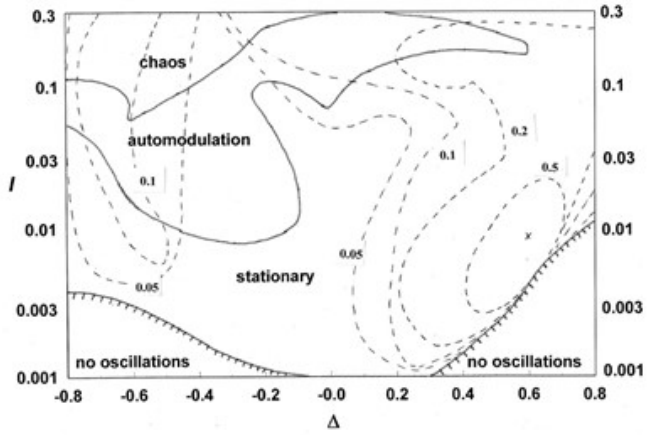

Figure 21. Zones of different kinds of oscillations are separated by solid lines. The normalized interaction length μ = 15 allows realizing the maximum orbital efficiency. The contours of constant orbital efficiencies are shown by dashed lines. The point of the maximum orbital efficiency 0.7 is marked by the cross.

The main attention is paid to modification of the boundary between the regions of oscillations with constant amplitude and auto-modulation in the plane of normalized parameters characterizing the external magnetic field and the beam current (Figure 21). It is shown that the theory free from the assumption about the frozen wave amplitude during the electron transit time predicts some widening of the region of auto-modulation.

HYSTERESIS AND FREQUENCY TUNABILITY OF GYROTRONS

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We presented the first devoted theoretical and experimental study of hysteresis phenomenon in relation to frequency tunability of gyrotrons. In addition, we generalized theory describing electron tuning of frequency in gyrotrons developed earlier, to arbitrary harmonics. It is found that theoretical magnetic and voltage hysteresis loops are about twice larger than experimental loops. In gyrotrons whose cavities have high quality factors hysteresis allows one only little to broaden the frequency tunability range.

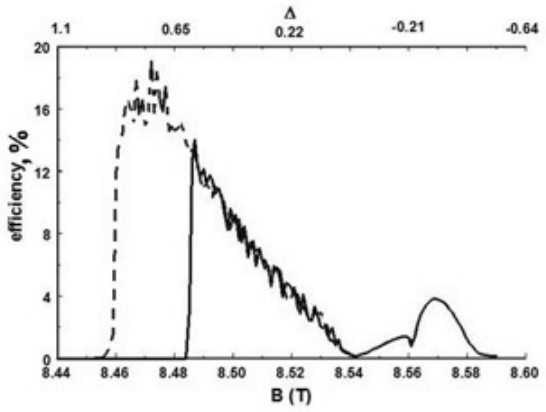

Figure 22. Efficiency as a function of magnetic field. On the upper ordinate axis frequency mismatch Δ is shown. Calculations were started at *8.44 T* and finished at *8.59 T*. Oscillation appears at *8.483 T* and disappears at *8.59 T* (solid curve). On the way back, oscillation disappears at *8.455 T* (dashed curve). Here *I=0.4 A* and *U=20 kV*. Hence, a large hysteresis region is observed between $8.455\,T$ and $8.483\,T$.

START-UP SCENARIO OF A HIGH-POWER PULSED GYROTRON FOR 300 GHz BAND COLLECTIVE THOMSON SCATTERING DIAGNOSTICS IN A LARGE HELICAL DEVICE

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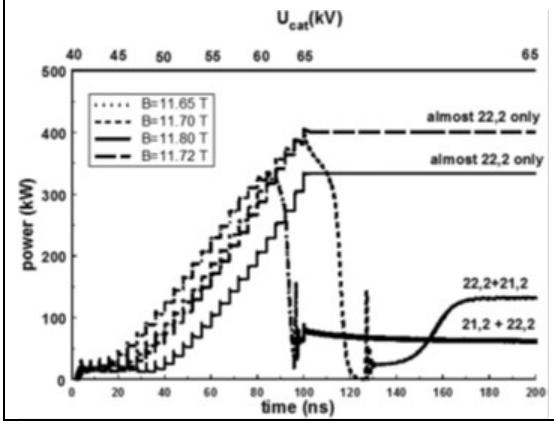
We presented results of theoretical study of mode competition during the voltage rise of a 300-kW, 300-GHz gyrotron operating in the $TE_{22,2,1}$ mode. Simulations tracking eight competing modes show that, with a proper choice of the magnetic field, stable excitation of the operating mode can be realized, despite the presence of parasitic modes in the resonator spectrum. A finite voltage rise time, 1 kV/4 ns referred to as the slow voltage rise case, is taken into account to simulate realistically the experimental condition. Simulation results with the finite voltage rise time are in good agreement with the experimental test, in which the gyrotron demonstrated reliable operation at power levels up to 300-kW. Moreover, along with voltage rise, the oscillation manner changes from backward wave oscillation to gyrotron oscillation. In the range of the magnetic field lower than the magnetic field

strength at which the $TE_{22,2}$ mode attains to the maximum power, mode competition with the $TE_{21,2}$ mode takes place although many other competing modes exist in between the two modes.



In addition to the slow voltage rise case, the fast voltage rise case, 10 kV/4 ns, and the instant voltage rise case were considered. For these cases, simulations also predict stabile oscillation of the $TE_{22,2}$ mode with the same power level with the slow voltage rise case. This indicates that stable oscillations of the $TE_{22,2}$ mode can be obtained in a wide range of the voltage rise time.

Figure 23. Output power for different magnetic fields as a function of time and voltage.

D. Experimental Studies

CATHODOLUMINESCENCE CHARACTERIAZAION OF POLYSTERENE – $BaZrO_3$ HYBRID COMPOSITES

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Both inorganic and organic nanosystems based on the semiconductor nanocrystals and either conducting or thermoplastic polymers are prospective for a number of technological applications and, thus, attract nowadays enhanced attention. $BaZrO_3$ (BZO) perovskite has found several applications, such as substrate for the synthesis of superconductors, high temperature microwave dielectrics, electrolyte for protonic fuel cells. We studied the effect of polymer matrix on the luminescent properties and the structure of hybrid composites based on suspension polystyrene (PS) and nanocrystals of BZO (d < 50 nm) have been studied using luminescent spectroscopy and XRD analysis. A strong cathodoluminescence (CL) in BZO-nanocrystals is observed in temperature range 80–293 °K. It is modified in BZO-PS composites: both the low- and a high-energy bands (near 4 eV) appear, together with a significant reduction in the CL intensity. A decrease of the lattice parameter a for BZO phase in the composite and the modification of CL spectra indicate for changes in the nanocrystalline structure induced by the polymer.

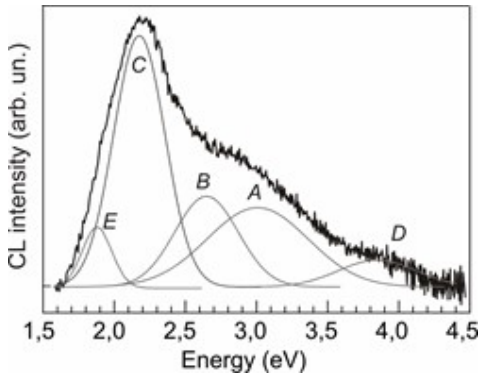

Figure 24. CL spectra of PS-BZO nanocomposite at RT.

The PS-BZO composites show the modification of the CL spectrum. The Gaussian decomposition of CL curves shows that the additional lowest energy band *E* and the highest energy band *D* (near 4 eV) arise, accompanied with a significant reduction in the CL intensity. As seen from a comparison of CL spectra of BZO–PS composites with nano-BZO (Figure 24) as well as micro-BZO, the ratio between the intensities of the lower energy CL bands and higher ones strongly depends on the BZO grain size.

PHOTOSTIMULATED LUMINESCENCE PROPERTIES OF NEUTRON IMAGE PLATES

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The luminescence properties of two commercial neutron-sensitive image-plates based on Gd_2O_3-doped BaFBr:Eu^2 storage phosphors are examined. These are white Fuji plates and blue Fuji plates (BAS-ND) with Gd_2O_3 content by weight of 34% and 50%, respectively (Figure 25). Both plates show two maxima in the photostimulation spectrum near 500 nm and 600 nm, with the ratio of the peak responses ($I_{600\ nm}/I_{500\ nm}$) 1.39 and 0.53 for the white and blue plates, respectively. The optimum wavelengths for photostimulation for the two phosphors are therefore different. The response of the blue plate is only 25% that of the white plate, if each is stimulated at its optimum wavelength. From Figure 26 we can see that the relative PSL intensity of the White NIP is 5.25 times higher than that of the Blue NIP, when the plates are stimulated with a wavelength corresponding to that of a He-Ne laser. The dye contained in the Blue NIP's will also absorb stimulating photons in the red region of the spectrum, which in turn could produce less stimulated luminescence. The better response of the White plates could also be because they contained more storage phosphor than the Blue plates and that $F(Br^-)$-centers are more efficiently created in its storage phosphor.

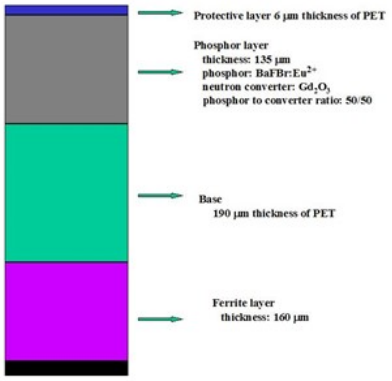

Figure 25. Structure of BAS-ND neutron image plate.

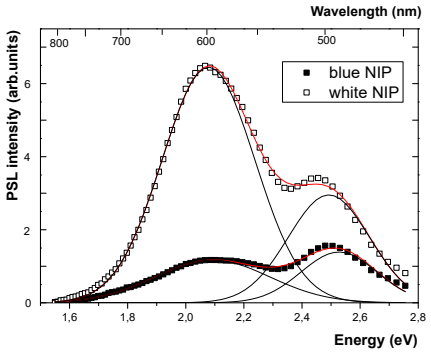

Figure 26. Stimulation spectra of X-ray irradiated Blue and White NIP's and their Gaussian deconvolution. The stimulation spectra were observed by measuring the PSL emission of Eu^{2+} at about 400 nm.

LONG-TERM EVOLUTION OF LUMINESCENT PROPERTIES IN CdI_2 CRYSTALS

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Fresh and aged melt-grown or gas-phase grown CdI_2 crystals are studied by means of low-temperature photoluminescence spectroscopy. Noticeable transformations of emission spectra are observed after long-term aging.

Time evolution of the CdI_2 emission spectra at a long-term (several years) aging in air is shown in Figure 27. Freshly grown crystals (a bottom plot in Figure 27) show an intensive band peaked at 2.48 eV (501 nm, G-band) with a weak component on the long-wavelength shoulder (2.25 eV, 551 nm, Y-band). This emission does not depend on the excitation wavelength and is related to the radiative recombination of self-trapped excitons in $[Cd^{2+}I_6^-]^{4-}$ molecular complexes.

A specific feature of 1.87 eV this narrow band is its bandwidth of $FWHM = 0.05$ eV, which is dramatically different from that for other bands. It is plausible to assume that this band is related to CdO and $Cd(OH)_2$ nanoinclusions.

We have also examined the changes in the emission spectra of aged melt-grown and gas-phase-grown CdI_2 crystals (Fig. 28). In both spectra the band at 1.87 eV is clearly identified, whereas there are some noticeable differences in the short-wavelength region of the spectra.

One of the reasons for these differences is the crystal thickness: melt-grown samples are found to be 0.1 to 0.5 mm thick, whereas the thickness of single-crystalline plates of gas-phase-grown CdI_2 does not exceed 10 microns. Thin crystals possess increased ratio of the number of surface atoms (N_s) to the number of bulk (N_v) atoms. Thus, surface atoms should have the prevailing contribution to the optical properties of the crystal. Geometrical order of atom distribution in the bulk (volume) and on the surface is also different. This conclusion is confirmed by nuclear quadrupole resonance (NQR) frequency studies of ^{127}I in CdI_2 crystals.

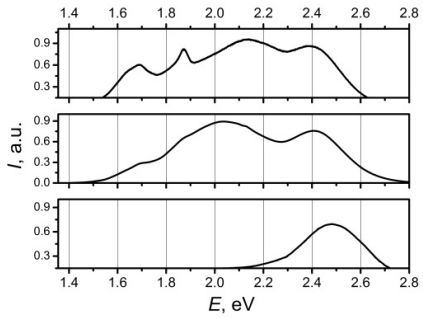

Figure 27. Photoluminescence spectra of freshly melt-grown (bottom), 2-year aged (middle) and 4-year (top) aged CdI_2 crystals. Spectra are recorded under excitation by 12.4 eV (100 nm) photons at 8 K.

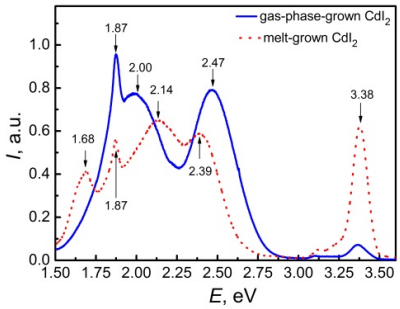

Figure 28. Luminescence spectra measured for melt-grown and gas-phase-grown CdI_2 crystals at the excitation by 12.4 eV photons at $T = 8$ K.

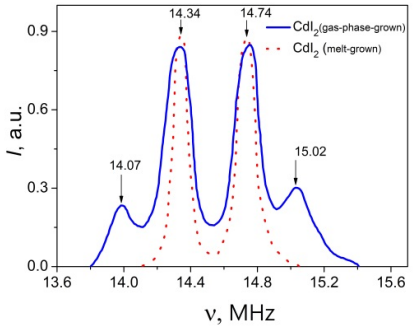

Figure 29. NQR spectra of ^{127}I isotopes in melt-grown and gas-phase-grown CdI_2 crystals.

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PRESENTATIONS AT SCIENTIFIC CONFERENCES, MEETINGS, AND WORKSHOPS

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*1. M.M. Kuklja, **E.A. Kotomin**, D. Fuks, **Yu.A. Mastrikov**, and J. Maier, "Structural (in)stability of complex perovskites for solid oxide fuel cells: first principles calculations". Abstract, p. 25.*

*2. **E.A. Kotomin**, **Yu.A. Mastrikov**, R. Merkle, M.M. Kuklja, and J. Maier, "First principles calculations of oxygen vacancies in the bulk and on the surface of complex perovskites for solid oxide fuel cell cathodes". Abstracts, p.102.*

II. 32th ISSP Conference (Riga, Latvia, February, 2016).

*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 O and V_{Fe} interaction in fcc Fe lattice". Abstract: p. 37.*

*4. V. Savchyn, O. Aksimentyeva, H. Klym, I. Karbovnyk, E. Elsts, J. Jansons, and **A.I. Popov**, "Comparative studies of cathodoluminscence properties of acceptor-doped $BaZrO_3$ and $SrTiO_3$". Abstract: p. 52.*

*5. **O. Dumbrajs**, "Present status of design, development and validation of the European gyrotron for ITER". Abstract: p. 70.*

*6. I. Jonane, J. Timoshenko, A. Kuzmin, **D. Bocharov**, and M. Krack "Temperature dependence of the local structure of scandium fluoride". Abstract: p. 76.*

7. ***D. Bocharov****, M. Krack, A. Kuzmin, J. Purans, and A. Kalinko, "Study of negative-thermal expansion in ScF_3 using first principles ab initio molecular dynamics". Abstract: p. 92.*

8. ***A. Chesnokov****,* ***D. Grjaznov****, M. Arrigoni, and R.A. Evarestov. "Calculation of pure and doped cerium dioxide properties in bulk phase". Abstract: p. 93.*

9. ***A. Platonenko****,* ***Yu.F. Zhukovskii****,* ***S. Piskunov****, and* ***E.A. Kotomin****, "First principles calculations of interstitial oxygen atom migration paths in corundum". Abstract: p. 94.*

10. ***A. Gopejenko****,* ***Yu.F. Zhukovskii****,* ***S. Piskunov****,* ***E.A. Kotomin****, "Variation of Zr and Ti concentration in PZT: first principles calculations on the electronic structure". Abstract: p. 95.*

11. ***M. Sokolov****,* ***Yu.A. Mastrikov****,* ***A. Gopejenko****,* ***Yu.F. Zhukovskii****, and* ***E.A. Kotomin****,"Ab initio modelling of Y-O complexes in α-Fe matrix". Abstract: p. 97.*

III. 50th Russian School on Condensed State Physics (St. Petersburg, Russia, March, 2016).

12. ***D. Bocharov****, M. Krack, A. Kuzmin, and J. Purans, "Interpretation of EXAFS spectra using molecular dynamics: comparison of classical and ab initio approach". Abstract: p. 213.*

13. ***D. Bocharov****,* ***Yu.F. Zhukovskii****,* ***S. Piskunov****,* ***O. Lisovski****, and* ***A. Chesnokov****, "First principles evaluation of photocatalytic suitability for TiO2-based nanotubes". Abstract: p. 214.*

IV. 14th International Conference "Information Technologies and Management", IT&M'2016 (Riga, Latvia, April, 2016).

14. ***Yu.N. Shunin****, L. Alfonta, D. Fink, A.E. Kiv, A. Mansharipova, R. Muhamediyev,* ***Yu.F. Zhukovskii****, and T. Lobanova-Shunina, "Modelling and simulation of electric response of nanocarbon nanocomposites and nanoporous polymer based structures for nanosensor devices". Abstract: p. 11-14.*

15. ***M. Sokolov****,* ***Yu.A. Mastrikov****,* ***A. Gopejenko****,* ***Yu.F. Zhukovskii****, and* ***E.A. Kotomin****, "Ab initio modelling of Y-O complexes in α-Fe matrix". Abstract: p. 18-19.*

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17. ***A. Gopejenko****,* ***Yu.F. Zhukovskii****,* ***S. Piskunov****, and* ***E.A. Kotomin****, "First principle calculations of PZT varying Zr and Ti concentrations". Abstract: p. 22.*

18. ***A. Platonenko****,* ***Yu.F. Zhukovskii****,* ***S. Piskunov****, and* ***E.A. Kotomin****, "Ab initio calculations of charged point defects in corundum". Abstract: p. 23.*

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*19. **R.I. Eglitis**, "Comparative ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ and $CaTiO_3$ (001), (011) as well as (111) surfaces". – Abstract: AA.P2.3.*

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*22. **A.I. Popov**, **E.A. Kotomin**, **V.N. Kuzovkov**, A. Lushchik, V.M. Lisitsyn, A. Akilbekov, and J. Maier, "Modelling of F center annealing kinetics in neutron- and electron-irradiated MgF_2 and MgO crystals". – Abstract: BB.8.2.*

*23. **R.I. Eglitis**, **S. Piskunov**, and **Yu.F. Zhukovskii**, "Ab initio calculations of $SrZrO_3$ bulk and surface F centers as well as $BaTiO_3/SrTiO_3$, $SrZrO_3/PbZrO_3$, and $SrTiO_3/PbTiO_3$ heterostructures". – Abstract: BB.8.3.*

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*27. **A. Platonenko**, **Yu.F. Zhukovskii**, **S. Piskunov**, and **E.A. Kotomin**, "Ab initio simulations of radiation-induced oxygen defects in corundum". – Abstract: BB.P1.8.*
*28. **Yu.A. Mastrikov**, R. Merkle, **E.A. Kotomin**, M.M. Kuklja, and J. Maier, "Effect of (La,Sr)MnO3 (001) surface terminations on oxygen reduction reaction rate". – Abstract: D.1.3.*
*29. **D. Gryaznov**, R. Merkle, **E. A. Kotomin**, and J. Maier, "First principles calculations of protonic defects in $La_{1-x}Sr_xFeO_3$-delta perovskites". – Abstract: D.3.3.*
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*31. I. Karbovnyk, I. Olenych, O. Aksimentyeva, A. Stelmashchuk, and **A.I. Popov**, "Nanotubes and nanoparticles in polymer matrices: effect of radiation on physical properties". – Abstract: J.P28.*
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*33. **R.I. Eglitis**, "Theoretical prediction of the 5 Volt rechargeable Li ion battery using $Li_2CoMn_3O_8$ as a cathode". – Abstract: U.P1.18.*
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*34. **E.A. Kotomin**, "Ab initio calculations of defects in perovskite crystals for fuel cell applications".*

VII. Functional Oxide Surfaces and Interfaces (FOXSI), (Vienna, Austria, May, 2016).

35. ***D. Gryaznov****, R. Merkle,* ***Yu.A. Mastrikov****,* ***E.A. Kotomin****, and J. Maier, "Mechanism of the oxygen reduction reaction at SOFC cathodes: combined experimental and ab-initio investigations".*

VIII. 6th International Colloids Conference (Berlin, Germany, June, 2016).

36. ***V.N. Kuzovkov****,* ***E.A. Kotomin****, A. Lushchik, and* ***A.I. Popov****, "Diffusion-controlled kinetics of metallic colloid formation in ionic crystals". Abstract: P006.*

37. ***V.N. Kuzovkov****, G. Zvejnieks,* ***E.A. Kotomin****, and P. Merzlyakov, "Modelling of metal colloid superlattice formation inirradiated wide gap insulators". Abstract: P007.*

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43. ***Yu.N. Shunin****, D. Fink, A.E. Kiv, L. Alfonta, A. Mansharipova, R. Muhamediyev,* ***Yu.F. Zhukovskii****, T. Lobanova-Shunina, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Theory and modelling of physical and bio- nanosensor systems". Abstract: p. 101.*

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45. ***A. Platonenko***, ***D. Bocharov***, ***S. Piskunov***, ***Yu.F. Zhukovskii***, *E. Spohr, and P.N. D'yachkov, "Computer modeling of 3d-metal doped fluorite-structured TiO_2 (4,4) nanotubes for efficient hydrogen synthesis from water". Abstract: D.11.2.*

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49. ***O. Dumbrajs*** *and G.S. Nusinovich, "Self-consistent non-stationary theory of gyrotrons".*

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52. ***D. Gryaznov***, *R. Merkle,* ***E.A. Kotomin***, *and J. Maier, "First-principles calculations of protonic defects in (La,Sr)FeO_3 perovskites." - Abstract: p.166.*

XV. 17th International Workshop on Nanoscience and Nanotechnology, n&n-2016 (Frascati, Italy, September, 2016).

53. ***Yu.N. Shunin***, *D. Fink, A.E. Kiv, L. Alfonta, A. Mansharipova, R. Muhamediyev,* ***Yu.F. Zhukovskii***, *T. Lobanova-Shunina, N. Burlutskaya, V.I. Gopeyenko, and S. Bellucci, "Physical and bio- nanosensors for medical applications and ecological monitoring". Abstract: p. 50-52.*

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54. ***E.A. Kotomin****, "Ab initio calculations for oxide functional materials".*

XVII. The Nuclear Materials Conference, (Montpellier, France, November, 2016).

55. ***A.I. Popov****,* ***Yu.F. Zhukovskii****,* ***E.A. Kotomin****,* ***A. Platonenko****,* ***S. Piskunov****,* ***V.N. Kuzovkov****, A. Lushchik, and R. Vila, "Computer simulations of radiation damage and defect recombination kinetics in sapphire". Abstract: P.1.72.*

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PUBLICATION 2016

1. J.Bērziņš, T.Krasta, L.Simonova, M.Balodis, V.Bondarenko, M.Jentschel, W.Urban, I.Tomandl. Levels of ^{188}Re nucleus populated in thermal neutron capture reaction. Nucl. Phys. A 947 (2016) 76-126
2.D.Riekstina, J.Berzins, T.Krasta, G.Kizane, J.Rudzitis, Impact of the former Salaspils nuclear reactor on the surrounding territory, J. of Phys. and Techn. Sciences, 2016, V. 53, Nr. 3, pp. 67-76.
3. D. Riekstina, J. Berzins, T. Krasta, O. Skrypnik, J. Alksnis, Longtime radionuclide monitoring in the vicinity of Salaspils nuclear reactor, FS fur Deutchland und die Schweiz, 25-30 September 2016, Heringsdorf, "Strahlenschutz fur Mensch und Umwelt", Publication Series: Fachverband fur Strahlenschutz e.V., 2016, pp.362-368.

LONGTIME RADIONUCLIDE MONITORING IN THE VICINITY OF SALASPILS NUCLEAR REACTOR

D. Riekstina[1], J. Berzins[1], T. Krasta[1], O.Skrypnik[2], J. Alksnis[2]
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The research nuclear reactor in Salaspils was decommissioned in 1998. Now reactor is partially dismantled and its buildings and territory are used as a temporary storage of radioactivity contaminated materials and water. Environment radioactivity monitoring for presence of artificial radionuclides in the vicinity of Salaspils nuclear reactor is carried on since 1990. Data include Cs-137 concentration in soils, tritium concentration in ground waters, as well as H-3, Cs-137, Co-60 concentration and gross beta-activity of reactors sewage and rainwater drainage. The systematic monitoring allowed to detect in

December 2014 a leakage from the special wastewater basin and so to prevent a pollution of ground waters outside reactors territory.

IMPACT OF THE FORMER SALASPILS NUCLEAR REACTOR ON THE SURROUNDING TERRITORY

Daina Riekstina[1,2], Janis Berzins[1], Tamara Krasta[1], Gunta Kizane[2], Janis Rudzitis[2]
[1]*Institute of Solid State Physics University of Latvia*
[2] *Institute of Chemical Physics University of Latvia*

This work is based on the results of long-term environment radioactivity monitoring in the vicinity of the decommissioned Salaspils Nuclear Reactor (SNR) carried out since 1990. The dynamics of artificial radionuclide concentration in soils and ground waters in the vicinity of SNR has been studied in relation with seasons, years and location. It has been found that Cs-137 concentration in the soils of SNR territory does not exceed the global Cs-137 fallout level in the rest of Latvia. The tritium concentration in the ground waters taken from wells outside SNR territory does not exceed the level allowed for drinking water. General conclusion is that the amount of radionuclides produced by SNR has little impact on the total radionuclide content in the Latvian environment.

NUCLEAR STRUCTURE STUDIES OF THE ODD-ODD RHENIUM ISOTOPES

Janis Berzins, Tamara Krasta, Lubova Simonova
Institute of Solid State Physics University of Latvia

Structure of excited levels of the odd-odd nuclei ^{186,188}Re has been studied using the experimental data of thermal neutron capture reaction measurements performed using crystall-diffraction spectrometer GAMS5 in the high-flux reactor of ILL (Grenoble). In the decay scheme of ^{188}Re, some new levels have been established below 1 MeV energy and more than 20 levels in the energy range from 1 MeV to 1.5 MeV. Proposed level scheme has been interpreted in terms of the rotor-plus-two quasiparticles model. The observed properties of ^{188}Re positive parity level decay have been explained as due to coexistence of axially-symmetric and non-axial deformed core states involving high particle momentum j orbits. The performed rotor-plus-two quasiparticles model calculations for both ^{186}Re and ^{188}Re demonstrate the utmost importance of correct choice of the residual neutron-proton interaction potential V_{np} in order to reproduce correctly the observed level energies and transition intensities. Especially important are the non-diagonal residual interaction matrix elements mostly due to space-exchange and tensor terms of the V_{np} potential.

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2. D.Riekstina, J.Berzins, T.Krasta, J.Rudzitis, O.Skrypnik, Assessment of the Salaspils nuclear reactor environmental impact, Abstract of the 32nd Scientific Conference Inst. of Solid State Physics, University of Latvia, Riga, February 17-19, 2016, p. 72.

3. D. Riekstina, J. Berzins, T. Krasta, O. Skrypnik, J. Alksnis, Longtime radionuclide monitoring in the vicinity of Salaspils nuclear reactor, Jahrestagung 2016, Fachverband fur Strahlenschutz e.V., “Strahlenschutz fur Mensch und Umwelt”, 25-30 September, 2016, Heringsdorf, Usedom, pp.44-45.

4. D.Riekstina, J.Berzins, T.Krasta, O.Skrypnik, Artifical radionuclide pollution of soils and water in the vicinity of Salaspils nuclear reactor, Abstract: 20th Int. scientific conf. “EcoBalt’2016”, Tartu, Estonia, 9th-12th October 2016, p. 84.

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.

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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
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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

32th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2016

1. Raul Land, Paul Annus, Mart Min, Alberts Kristiņš. *Interesting Rresults During Impedance Measurement. Solved.* Abstracts, p. 33.
2. I.Gvardina, A.Kristiņš, J.Melderis. *Access Control with IR Keys.* Abstracts, p. 68.