Institute of Solid State Physics

University of Latvia

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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). This honorary recognition with the accompanying financial support of 0,7 million 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.

The research of the ISSP includes:

- electron and ion process in wide-gap materials with different degree of ordering;
- functional organic molecules and polymers for photonics and organic electronics;
- multifunctional and hybrid materials for energy applications: light emitting diodes, photovoltaic elements and coatings for solar baterries, storage of hydrogen for fuel cell devices;

- electrodes and plasma technologies for hydrogen production, polymer membranes with ionic conduction for fuel cells and gas separations;
- inorganic single crystals, ceramics, glasses, thin films, and nano-structured surfaces for application in optics, electronics, photonics and energetics.

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

Table 1

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2014

International Supervisory Board

Council of Institute
Dr.phys. L.Trinklere

Director
Dr.habil.phys. A. Sternberg

RESEARCH DEPARTMENTS AND LABORATORIES

ADMINISTRATION AND DOMESTIC SERVICES

SCIENTIFIC UNITS

DEPARTMENT OF CRYSTAL PHYSICS AND OPTOELECTRIC MATERIALS	*P. Kūlis*
Laboratory of Optical Spectroscopy	*M. Spriņģis*
Laboratory of Magnetic Resonance Spectroscopy	*U. Rogulis*
Laboratory of Wide Band Gap Materials	*B. Bērziņa*
Laboratory of Semiconductor Optoelectronics	*B. Poļakovs*

DEPARTMENT OF PHOTONICS MATERIALS PHYSICS	*D. Millers*
Laboratory of Solid State Radiation Physics	*L. Grigorjeva*
Laboratory of Amorphous Materials Spectroscopy	*L. Skuja*
Laboratory of Optical Recording	*J. Teteris*
Laboratory of Surface Physics	*J. Maniks*
Laboratory of Organic Materials	*M. Rutkis*

DEPARTMENT OF FERROELECTRICS	*V. Dimza*
Laboratory of Physics and Application of Functional Materials	*V. Dimza*
Laboratory of Synthesis and Processing	*M. Antonova*
Laboratory of Visual Perception	*M. Ozoliņš*

DEPARTMENT OF SEMICONDUCTOR MATERIALS	*A. Lūsis*
Laboratory of Solid State Ionics	*A. Lūsis*
Laboratory of EXAFS Spectroscopy	*J. Purāns*
Laboratory of Hydrogen Energy Materials	*J. Kleperis*

DEPARTMENT OF THEORETICAL PHYSICS AND COMPUTER MODELING	*J. Kotomins*
Laboratory of Computer Modeling of Electronic Structure of Solids	*J. Žukovskis*
Laboratory of Kinetics in Self-organizing Systems	*V. Kuzovkovs*

Laboratory of Radiation Physics	*J. Bērziņš*
Laboratory of Electronic Engineering	*A. Kristiņš*

ADMINISTRATION AND DOMESTIC SERVICES

ADMINISTRATION	*A. Šternbergs*
Deputy director of Science	*M. Rutkis*
Deputy director of Studies	*A.Šarakovskis*
Scientific Secretary	*L. Grīnberga*
Accounting Department	*A. Jozepa*

	DOMESTIC SERVICES
D. Popele	Human Resources
R. Siatkovskis	Procurement Department
J. Ruhmanis	Main Power Engineer Department
L. Rihtere	Library
V. Ivanovs	Main Engineer and Mechanical Workshops

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff.** At present there are 172 employees working at the Institute, 24 of 114 members of the research staff hold Dr.habil.degrees, 68 hold Dr. or PhD. At the end of 2014 there were 19 PhD students and 46 undergraduate and graduate students in physics and optometry programmes working at the ISSP.

Table 2

The Scientific Council of the Institute

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

The annual report summarizes the research activities of the ISSP in 2014. The staff of the Institute has succeed in 5 **national science grants** and in **one national cooperation project** with the total financing 263,4 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 297,9 thous. EUR budget in

2014. The infrastructure financing for ISSP in 2014 was 707,2 thous. EUR and it was partly used also for the salaries of the scientific and maintenance staff of the Institute. (Table 3).

Main awards, received at 2014:

No	Author	Award
1.	Dr..phys. R. Eglitis	The Corresponding Member of Latvian Academy of Science
2.	Dr. habil..phys. E. Lippma (Estonia)	The International Member of Latvian Academy of Science
3.	J. Mikelsone	The L'OREAL-UNESCO sholarship „For Women in science 2014"
4.	Dr.habil.phys. V. Kuzovkovs	E. Silins award in physics of Latvian Academy of Science
5.	J.Purāns, A.Kuzmins, J.Kalinko, A. Anspoks, J. Timošenko	Authors of the best scientific achiewment (from Latvian Academy of Science)

At the end of 2014, 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. During 2006 – 2008 a teaching module "Functional material and nanotechnologies" was introduced in bachelor and master physics curricula. This project was supported by European Social Fund. Many co-workers of the Institute were involved in preparation of lecture courses.

In 2014 **four international conferences** have been organised:

1. International Young Scientist Conference "Developments in Optics and Communications 2014", April 9 – 12, 2014, Riga, Latvia;
2. Saules kauss 2014, May 17, Riga, Latvia.
3. International Joint event of 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International Conference on Functional Materials and Nanotechnologies (RCBJSF-2014-FM&NT) , September 29 – October 2, 2014 Riga, Latvia
4. Workshop of FP-7 project "Waste Heat to Electrical Energy via Sustainable Organic Thermoelectric Devices" 8.09. – 10.09. Rīga, Latvia

Table 3

INCOME OF ISSP, THOUSAND EUR, FROM 2007 -2014

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Structural funds from EU
2007	4 605.12	1 027.17	1 579.67	140.44	131.76	1 709.87
2008	6 063.28	1 457.59	1 549.22	221.83	415.19	2 406.22
2009	2 443.64	898.69	822.56	91.35	231.07	399.97
2010	3 038.68	634.89	961.01	118.53	169.04	1 159.21
2011	3 868.93	637.45	733.49	148.83	172.31	2 176.99
2012	4 925.98	606.57	785.57	170.74	59.05	3 304.05
2013	3 518.90	345.92	787.27	232.21	393.42	1 405.66
2014	3 029.00	562.30	891.00	361.20	178.70	1 035.80

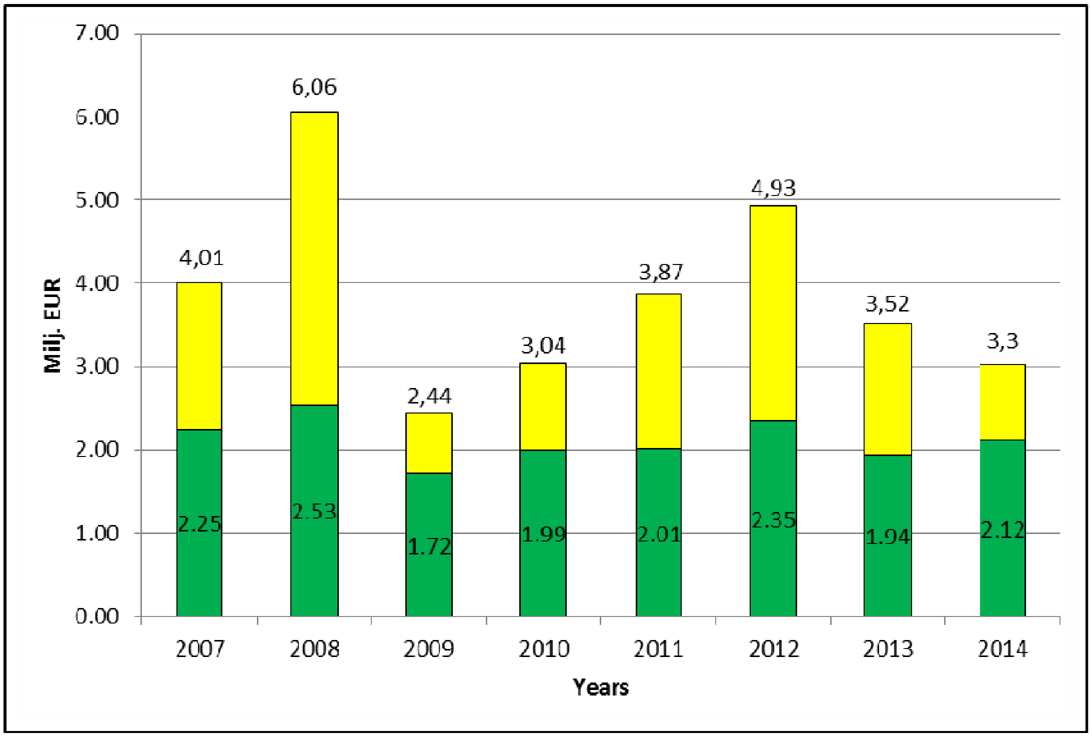


Fig.1. Total financing of the ISSP milj. EUR from 2007 to 2014

🟩- *salaries*

The main source for **international funding** were two EC 7th Framework Programme (H2020) contracts:

- 3 EURATOM projects – 155,3 thous. EUR;
- Latvian – Belarus project – 22,8 thous. EUR;

Main achievments in 2014:

1. 91 SCI papers published by the staff of Institute;
2. 4 patent applications;
3. 15 B.sc. thesis and 13 M.Sc. thesis in physics, optometry and chemistry were defended under the supervision of our scientists;
4. A. Anspoks, A. Voitkans and M. Dunce were acquired degree of doctor of physics (PhD);
5. The development of “National Research Centre for nanostructures and multifunctional materials, constructions and technologies” by the ISSP (ERDF project).

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

Prof. Dr. A.Krumins

DEPARTMENT OF CRYSTALS PHYSICS AND OPTOELECTRONIC MATERIALS

Head of Department Dr. phys. P. Kulis

LABORATORY OF MAGNETIC RESONANCE SPECTROSCOPY

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

RESEARCH TOPICS

Research of defect structure, luminescence centres and mechanisms using magnetic resonance spectroscopy techniques (EPR, ODMR).

Research of intrinsic and activator-related defects in oxyfluoride composites, fluoride micro- and nano-crystals in glass matrixes.

Investigations of luminescence properties of oxyfluoride glass and glass-ceramics, as well as application possibilities of these materials.

LABORATORY EQUIPMENT

ODMR spectrometer: Oxford Instruments Magneto-optical cryostat with magnetic fields up to 7 T at temperatures 1.5-4.2 K, spectral range 200-800 nm and microwave frequencies 36 and 45 GHz.

EPR spectrometer: X-Band (9.3 GHz), magnetic fields up to 0.7 T, temperature range 6-300 K.

SCIENTIFIC STAFF

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

PhD students	**Students**
1. A. Antuzevičs	1. M. Kemere
2. Dz. Bērziņš	2. J. Sperga
3. O. Kiseļova	3. A. Cvetkova

SCIENTIFIC VISITS ABROAD

U. Rogulis (1 month, Germany)
E. Elsts (1 week, Spain)

COOPERATION

Latvia

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

Germany

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

Romania

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

MAIN RESULTS

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

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

Terbium, cerium and europium activated oxyfluoride glasses and glass ceramics have been studied by thermally stimulated luminescence (TSL) and optical absorption techniques after the X-ray irradiation. A creation of colour centres in oxyfluoride glass matrix and TSL peaks depending on the activator type were observed. LaF3 and rare earth activators were analysed by SEM–EDS.

ADVANCES IN OXYFLUORIDE GLASS-CERAMICS

U. Rogulis, A. Sarakovskis, E. Elsts, A. Fedotovs, I. Brice

Besides being a good medium for up-conversion displays, oxyfluoride glass-ceramics have shown several new prospective application directions. For investigations of the up-conversion mechanisms, the comparison of the optical spectra of the glass-ceramics and corresponding fluoride macrocrystals has been fruitful. We compared cathodoluminescence decay times for terbium-, cerium- and europium-doped oxyfluoride glass-ceramics and obtained that cerium-doped glass-ceramics have shortest decay times. Formation of fluoride crystallites in the oxyfluoride glass-ceramics could be tracked by the EPR hyperfine structure of impurity ions. Activator ions in the oxyfluoride glass-ceramics could be embedded in the oxide glass as well as in the fluoride crystal parts of the ceramics, revealing new possibilities of the construction of the spectral shape for solid state lighting.

SCIENTIFIC PUBLICATIONS

1. **E. Elsts, E. Rogulis**, K. Bulindzs, K. Smits, A. Zolotarjovs, L. Trinklere, K. Kundzins, Studies of radiation defects in cerium, europium and terbium activated oxyfluoride

glasses and glass ceramics, Optical Materials, 2015, vol. 41, pp. 90-93; DOI 10.1016/j.optmat.2014.10.042

2. **A. Antuzevics, U. Rogulis, A. Fedotovs, Dz. Berzins** and J. Purans, Electron paramagnetic resonance study of point defects in ScF$_3$, Digest of the International Conference on Global Research and Education, Inter-Academia 2014, Riga, Latvia, p. 94-95.

LECTURES ON CONFERENCES

1. E. Elsts, U. Rogulis, K. Bulindzs, K. Smits, A. Zolotarjovs, L.Trinkere, K. Kundzins, Studies of radiation defects in Ce, Eu, Tb doped oxyfluoride glasses and glass ceramics, Abstracts of 5th International Workshop on Photoluminescence in Rare Earths PRE´14, 2014, San Sebastián, Spain, O113.
2. U. Rogulis, I. Brice, E. Elsts, J. Grube, D. Millers, Luminescence of Eu ions in oxyfluoride glasses and glass-ceramics, 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International conference on Functional Materials and Nanotechnologies – RCBJSF–2014-FM&NT, 2014, Riga, Latvia, p. 382.
3. A. Antuzevics, U. Rogulis, J. Purans, A. Fedotovs, Dz. Berzins, EPR Spectra of ScF$_3$, 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International conference on Functional Materials and Nanotechnologies – RCBJSF–2014-FM&NT, 2014, Riga, Latvia, p. 353.
4. A. Fedotovs, Dz. Berzins, U. Rogulis, K. Smits, G. Doke, A. Medvids, P. Onufrijevs, Angular Dependence of Recombination Luminescence Detected EPR in ZnO Crystal, 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International conference on Functional Materials and Nanotechnologies – RCBJSF–2014-FM&NT, 2014, Riga, Latvia, p. 352
5. E. Elsts, G. Krieke, U. Rogulis, K. Smits, R. Ignatans, A. Sarakovskis, Luminescence of terbium activated NaLaF$_4$ in oxyfluoride ceramics,12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International conference on Functional Materials and Nanotechnologies – RCBJSF–2014-FM&NT, 2014, Riga, Latvia, p. 387
6. E. Elsts, E. Rogulis, K. Bulindžs, K. Šmits, A. Zolotarjovs, L. Trinklere, K. Kundziņš, Radiācijas defektu pētījumi ar Ce, Eu, Tb aktivētos oksifluorīdu stiklos un stikla keramikās, LU CFI 30. zinātniskās konferences tēzes, 2014, 7. lpp.

7. U. Rogulis, I. Brice, E. Elsts, J. Grūbe, Eu un Ce luminiscences joslu novietojums oksifluorīdu stikla keramikās, LU CFI 30. zinātniskās konferences tēzes, 2014, 13. lpp.

8. A. Fedotovs, U. Rogulis, Dz. Bērziņš, K. Šmits, G. Doķe, A. Medvids, P. Onufrijevs, Magnētiskās rezonanses spektri un rekombinatīvā luminiscence ZnO, LU CFI 30. zinātniskās konferences tēzes, 2014, 14. lpp.

9. A. Antuzevičs, U. Rogulis, J. Purāns, A. Fedotovs, Dz. Bērziņš, ScF_3 EPR spektri, LU CFI 30. zinātniskās konferences tēzes, 2014, 15. lpp.

10. O. Kiseļova, A. Cvetkovs, U. Rogulis, V.Serga, R. Ignatāns, Zn_xCd_{1-x} plāno kārtiņu pētījumi, LU CFI 30. zinātniskās konferences tēzes, 2014, 90. lpp.

MASTER THESIS

Andris Antuzevičs, "Skandija fluorīda elektronu paramagnētiskās rezonanses spektri", maģistra darbs, Rīga, LU, 2014.

BACHELOR THESIS

Ingmārs Felcis, "LED moduļu spektru pētījumi", bakalaura darbs, Rīga, LU, 2014.

LABORATORY OF OPTICAL SPECTROSCOPY

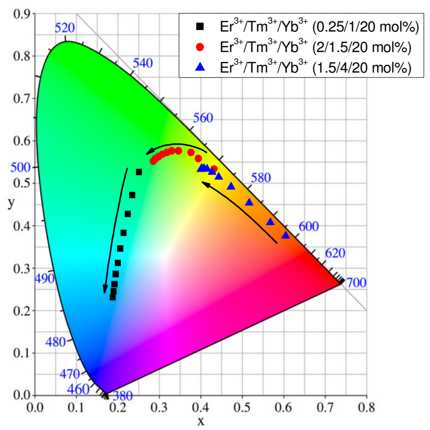
Head of Laboratory Dr.habil.phys. M.Springis

RESEARCH TOPICS

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

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

SiO_2 based glasses and nanostructured glass ceramics with RE doped (Er^{3+}, Yb^{3+}, Tm^{3+}) LaF_3 nanocrystals were synthesized. Mechanisms of the up-conversion luminescence in these materials were studied at different temperatures. It was found that in silicate glass ceramics with LaF_3:Er^{3+} the main mechanism responsible for the up-conversion luminescence at room temperature is excited state absorption while at lower temperatures energy transfer up-conversion prevails.



Up-conversion luminescence color calculated according to CIE chromaticity diagram in $NaLaF_4$:Er^{3+}, Tm^{3+}, Er^{3+} materials excited by laser diode at 980 nm. Black arrows indicate trends of the color when the excitation power density is increased

A synthesis procedure of $NaLaF_4$:RE^{3+} was elaborated and systematic studies of the material were performed. $NaLaF_4$ doped with

$Er^{3+}$of different concentrations reveals characteristic Er^{3+} luminescence bands. The green luminescence is the most intensive one in the luminescence spectrum. As the concentration of the activator is increasing, the intensity of all luminescence bands changes significantly due to the cross- relaxation process between the activator ions.

It was concluded, that $NaLaF_4:RE^{3+}$ is a perspective material for efficient up-conversion luminescence solutions due to its particularly low phonon energy.

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

PhD Students

M.Sc. Jurgis Grube
M.Sc. Guna Doke

Students

K. Strals
G. Krieķe
A. Ansbergs
G. Zageris

SCIENTIFIC VISITS ABROAD

J. Grube (1 week Poland)

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

$NaLaF_4$ MATRIX MULTI SITE NATURE IMPACT ON Er^{3+} LUMINESCENCE

J. Grube, G. Doke, A. Sarakovskis, and M. Springis

Different kinds of materials doped with rare-earth (RE) elements often serve as up-conversion (UC) luminescence sources. One of the requirements for the high UC luminescence efficiency is low material phonon energy, other – existence of sites where RE ions can freely incorporate within the lattice. Previous studies have shown that $NaLaF_4$ meet these requirements [1]. In this work we will show $NaLaF_4$ matrix multi site nature impact on Er^{3+} luminescence.

Spectroscopic measurements at low temperature (10K) were done for the $NaLaF_4$ doped with Er^{3+} (2mol%). Characteristic Er^{3+} luminescence bands were observed. Combined excitation-emission spectroscopy (CEES) for the dominant green luminescence band shows different luminescence spectra which proves the multi site nature of crystalline lattice where Er^{3+} can incorporate. Excitation spectra show sharp peaks caused by transition between energy levels multiplet from ground state to one of the excitated state. In addition to each of this sharp peaks broad excitation band at the shorter wavelength side of sharp peaks appears. For some of the luminescence peaks luminescence decay kinetics shows not only a decaying part but also a rising part suggesting an energy transfer processes between Er^{3+}.

Based on the experimental results the impact of the multi site nature of $NaLaF_4$ on Er^{3+} luminescence is discussed.

IMPACT OF Er^{3+} CONCENTRATION ON LUMINESCENCE IN $NaLaF_4$

J. Grube, A. Sarakovskis, G. Doke, M. Springis

NaLaF4 doped with Er3+ of different concentrations was synthesized. The luminescence spectrum for NaLaF4:Er3+ (0.2 mol%) at 489nm excitation reveals characteristic Er3+ luminescence bands in the green (540 nm), red (660 nm) and infrared (980 nm) spectral regions. The green luminescence band originated from the 4S3/2 → 4I15/2 transition is the most intensive one in the luminescence spectrum. As the concentration of the activator is increasing, the intensity of all luminescence bands changes significantly. The super-linear increase of the infrared luminescence intensity with increasing Er3+ concentration as well as the quenching of green luminescence at the concentrations exceeding 2 mol% can be attributed to the cross-relaxation process between the activator ions.

EXAMINING TEMPERATURE INFLUENCE ON Er^{3+} LUMINESCENCE IN $NaLaF_4$ MATRIX

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

Different kinds of materials doped with rare-earth (RE) elements often serve as upconversion (UC) luminescence sources where photons with lower energy (usually IR) are converted into higher energy photons (VIS, and UV). One of the requirements for the high UC luminescence efficiency is low material phonon energy, other – existence of sites where RE ions can freely incorporate within the lattice. Previous studies have shown that $NaLaF_4$ meets these requirements [1]. Different green luminescence spectra under various excitation wavelength are observed at low temperature (15K) clearly indicating multisite nature of $NaLaF_4$. At room temperature (300K) such significant differences in luminescence spectra are not observed. Therfore in this work we will show temperature influence on $NaLaF_4:Er^{3+}$ luminescence. In this report spectroscopic measurements at different temperatures (15K-300K) for $NaLaF_4$ doped with Er^{3+} (0.1 and 2 mol%) will be shown. Variations of the shape of the green luminescence (origin from $^4S_{3/2}$ to $^4I_{15/2}$ transition) were observed when temperature was increased. In addition, variation in green luminescence decay kinetics at different temperatures depends on Er^{3+} concentration. For the low Er^{3+} concentration (0.1 mol%) green luminescence decay kinetics remains nearly unchanged at different temperatures (15K-300K), but at higher Er^{3+} concentration (2 mol%) significant variations in the kinetics of the green luminescence decay are observed. Based on the experimental results temperature impact on Er^{3+} spectroscopic properties in $NaLaF_4$ will be discussed.

INFLUENCE OF DIFFERENT CRYSTAL FIELD ENVIRONMENTS ON THE LUMINESCENCE OF $NaLaF_4:Er^{3+}$

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

Low phonon energy of the matrices and multisite nature of the crystalline lattice make complex fluoride materials attractive for the upconversion luminescence. The aim of this work has been to study multisite formation in $NaLaF4:Er^{3+}$ and the influence of the multisite structure on the luminescence processes in the material. The results of low-temperature site-selective spectroscopy measurements in hexagonal $NaLaF4:Er^{3+}$ will be shown. Three distinct luminescence spectra in the green spectral region associated with $^4S_{3/2}\rightarrow{}^4I1_{5/2}$ electronic transition could be extracted under the photoexcitation at different positions corresponding to the excitation of $^4F_{7/2}$ level of $Er^{3+.}$ It was possible to model the experimentally obtained luminescence spectra at any excitation wavelength by a linear combination of the extracted spectra with a tolerance better than 5%. The results of the site-selective spectroscopy suggest the presence of three different crystalline field environments where Er^{3+} ions incorporate. The analysis of the structure of the material and time-resolved luminescence have been used to differentiate between cationic sites with C_3 and C_{3h} symmetries in the structure of $NaLaF_4$ available for Er^{3+} incorporation. Site-selective excitation of Er^{3+} located at a specific site induced energy transfer to erbium ions located at other sites has been observed in both the upconversion and traditional luminescence processes. The enhanced energy transfer between the different sites in $NaLaF4:Er^{3+}$ signifies the importance of multisite nature of the structure, which is a key factor for an efficient upconversion luminescence.

NaLaF4 MATRIX MULTI SITE NATURE IMPACT ON Er^{3+} LUMINESCENCE

J. Grube, G. Doke, A. Sarakovskis, M. Springis

Different kinds of materials doped with rare-earth elements often serve as upconversion luminescence sources. One of the requirements for the high up-conversion luminescence efficiency is low material phonon energy, other – existence of sites where rare-earth ions can freely incorporate within the lattice. Previous studies have shown that NaLaF4 meet these requirements [1]. In this work we will show NaLaF4 matrix multi site nature impact on Er3+ luminescence.

Spectroscopic measurements at low temperature (10K) were done for the NaLaF4 doped with Er3+ (2mol%). Characteristic Er3+ luminescence bands were observed. Combined excitation-emission spectroscopy for the dominant green luminescence band shows different luminescence spectra which proves the multi site nature of crystalline lattice where Er3+ can incorporate. Excitation spectra show sharp peaks caused by transition between energy levels multiplet from ground state to one of the excitated state. In addition to each of this sharp peaks broad excitation band at the shorter wavelength side of sharp peaks appears. Based on the experimental results the impact of the multi site nature of NaLaF4 on Er3+ luminescence is discussed.

Eu AND Ce LUMINESCENCE BAND POSITIONS IN OXYFLUORIDE GLASS-CERAMICS

U. Rogulis, I. Brice, E. Elsts, J. Grūbe

Cerium Ce3+ and europium Eu2+ activator ions in the oxyfluoride glasses and glass-ceramics show broad luminescence bands with their maxima in the blue spectral region. Eu3+ luminescence lines could be observed in the red region. The luminescence intensity of several oxyfluoride compositions is comparable with the intensity of commercial white LED phosphors [1].

Eu and Ce luminescence band positions in the oxyfluoride glass-ceramics are determined by the composition of the oxide glass matrix, as well as by the fluoride crystallites. The concentration and size of the fluoride crystallites could be varied by appropriate temperature procedures. By varying the annealing temperatures, also the relative intensities of the Eu2+ and Eu3+ luminescence bands can be changed. These possibilities of the luminescence band position variations will be discussed, concerning the improvement of the spectrum of the oxyfluoride glass-ceramics to adjust it to one of the white light standards.

MAGNETIC RESONANCE SPECTRA AND RECOMBINATION LUMINESCENCE IN ZnO

A. Fedotovs, U. Rogulis, Dz. Bērziņš, K. Šmits, G. Doķe,
A. Medvids, P. Onufrijevs

Zinc oxide is known as a promising material for production of opto-electronic semiconducting devices. It is possible to obtain structural changes in these samples using laser-treatment which could be detected in the recombination luminescence (RL) spectra. It has been observed that in the laser-treated ZnO sample RL consists of two bands (630nm and 740nm) with different decay times. All bands detected in the RL-EPR belong to the RL band with slower decay time. Using modulation of microwaves (PL-EPR), it is possible to observe one donor band which does not appear in the RL-EPR spectra. The detected RL-EPR spectrum has a pronounced angular dependence. The EPR measurements show presence of some transition elements in the investigated samples. The mechanisms of the RL in the laser-treated samples will be discussed.

SCIENTIFIC PUBLICATIONS

J. Grube, A. Sarakovskis, G. Doke, M. Springis. Impact of Er3+ Concentration on Luminescence in NaLaF4. Latvian Journal of Physics and Technical Sciences, 2014, N3, pp. 42-50.

POPULAR SCIENCE PUBLICATIONS

A.Šarakovskis: New luminescent materials are syntesized.Illustrated Science, 2014, Nr.103, p.10.

LECTURES ON CONFERENCES

30th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2014, February 19-21.

1. J. Grube, G. Doke, A. Sarakovskis, and M. Springis. NaLaF4 Matrix Multisite Nature Impact on Er3+ Luminescence. Abstracts, p.9.
2. U. Rogulis, I. Brice, E. Elsts, J. Grūbe. Eu and Ce Luminescence Band Positions in Oxyfluoride Glass-Ceramics. Abstracts, p.13.
3. A. Fedotovs, Dz. Berzins, U. Rogulis, K. Smits, G. Doke, A. Medvids, P. Onufrijevs.Magnetic Resonance Spectra and Recombination Luminescence in ZnO. Abstracts, p.14.

International conference "Functional materials and nanotechnologies" FM&NT, Riga, Latvia, 2014, September 29 – October 2.

4. J. Grube, G. Doke, G. Krieke, A. Sarakovskis, M. Springis. Examining Temperature Influence on Er3+ Luminescence in NaLaF4 Matrix. Book of Abstracts, p. 37

5. A. Sarakovskis, G. Krieke, G. Doke, J. Grube, L. Grinberga and M. Springis. Influence of Different Crystal Field Environments on the Luminescence of NaLaF4:Er^{3+}. Book of Abstracts, p. 376.

International conference on Luminescence, Wroclaw, Poland, 2014, July 13-18.

6. J. Grube, G. Doke, A. Sarakovskis, and M. Springis. NaLaF4 Matrix Multisite Nature Impact on Er3+ Luminescence.

BACHELOR THESIS

Martins Osis. „Up-conversion Luminescence of Er^{3+} doped Oxyfluoride Glass and Glass-Ceramics", supervisor Anatolijs Sarakovskis.

Jēkabs Narvaišs. "Influence of Synthesis Atmosphere on the Up-conversion Luminescence in $NaLaF_4$:Er^{3+} Material", supervisor Guna Doķe.

Krišjānis Kirilovs.„Multiphoton excited Luminescence of Yb^{3+} and Tm^{3+} doped $NaLaF_4$ Matrix", supervisor Jurgis Grube.

LABORATORY OF WIDE BAND GAP MATERIALS

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

RESEARCH AREA AND POSSIBILITIES

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

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

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., researcher.

Students - Technicians:

1. Paula Jankovska, student,

2. Ivo Megnis, 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,

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Center for Physical Sciences and technology, Optoelectronics department, Vilnius (Drs R.Nedzinskas, S.Tumenas)

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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)

Romania

"Raluca Ripan" Institute for Research in Chemistry, Babeş Bolyai University, Cluj-Napoca, Romania (Dr. L. E. Muresan)

MAIN INVESTIGATIONS AND RESULTS

SPECTRAL CHARACTERIZATION OF AlN NANOPWDER

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

Spectral characteristics of AlN nanopowder synthesized in Institute of Inorganic Chemistry, Riga Technical University were studied in order to examine the sensing properties of the material for oxygen gas. Luminescence spectra (PL) of material under excitation with light from the ultraviolet region at different temperatures were studied. Besides the well-known luminescence at 380 nm – 400 nm caused by oxygen- related defects, luminescence at 420 nm was also observed, which possible could be related to defects based on nitrogen vacancies. It was found that the intensity of 420 nm luminescence is maximal, when the sample is in vacuum, but this intensity considerably decreases, when sample is surrounded with oxygen gas or oxygen containing gases, demonstrating oxygen sensing properties of aluminum nitride nanopowder.

These studies were performed within a support of European project ERDF 2014/0047/2DP/2.1.1.1.0/14/APIA/VIAA/007.

SPECTRAL CHARACTERIZATION OF HEXAGONAL BORON NITRIDE

B. Berzina, L.Trinkler, V.Korsaks

Spectral characteristics of hBN powder were studied including photoluminescence (PL) and its excitation (PLE) spectra within a wide spectral region and temperature range (8K – 300K). From the complex luminescence spectra observed a special interest was dedicated to the native defect-induced blue luminescence (BL) at 380 nm forming some phonon assisted sub-bands due to its sensitivity to presence of oxygen gas surrounding the material. The BL kinetics and material absorption within the infrared spectral region were also studied. The results obtained allowed to propose the BL mechanisms in hBN. There are possible two mechanisms coexisting and originating the BL. One of them is intra-center luminescence mechanism realized under direct excitation of the luminescent defect, when optical absorption/excitation and the following emission occur within one and the same luminescent defect. The second one is the recombination mechanism, when at least two different defects are involved in luminescence formation and the luminescence process can be characterized with interaction of the donor-acceptor center pairs (DAP). The nitrogen vacancies and F centers are considered as possible candidates originating the BL.

These studies were performed within a support of European project ERDF 2014/0047/2DP/2.1.1.1.0/14/APIA/VIAA/007

LUMINESCENCE PROPERTIES OF $ZnO/LiGaO_2$

L.Trinkler, B. Berzina, V.Korsaks

Nonpolar m-plane ZnO epilayers and ZnO/ $Zn_{1-x}Mg_xO$ multiple quantum wells grown on $LiGaO_2$ substrate by plasma-assisted molecular beam epitaxy were studied by means of photoluminescence and polarized luminescence in the 10-300 K thermal range. It was found that PL spectra of all studied ZnO/LGO samples contain two major bands – one of them in the region 400-900 nm (3-1.5 eV), called "green" band and ascribed to defects present in ZnO, such as basic stacking faults and others, and another – around 370 nm (3.25 eV), called "blue" band and ascribed to exciton emission. Contrary to epilayer samples characterised with exciton band position at 3.2-3.25 eV, the sample with 5-period ZnO (1.1 nm)/$Zn_{0.55}Mg_{0.45}O$ (0.6 nm) multiple quantum wells exhibits a strong emission at 3.65 eV (at 10K), resulting from the positive quantum confinement effects and the absence of internal polarization fields. PL of all samples is polarized in the whole studied spectral range (1-4 eV), the most interesting being the region of the exciton band. Polarization rate and sign varies from sample to sample, depending on its structural orientation and decreases with temperature rise.

These studies were performed within a support of the Latvian-Lithuanian-Taiwan project "Nonpolar ZnO thin films: growth-related structural and optical properties". No. LV-LT-TW/2015/3.

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1. L.Trinkler, B.Berzina, Localised transitions in luminescence of AlN ceramics. (2014) Radiation measurements, 71, pp. 232-236.

2. L.Trinkler, B.Berzina, Recombination luminescence in aluminum nitride ceramics (2014) Physica Status Solidi (B) Basic Research, 251 (3), pp. 542-548.

3. A.Šutka, R.Pärna, J.Kleperis, T.Käämbre, I.Pavlovska, **V.Korsaks,** K.Malnieks, L.Grinberga, V.Kisand, Photocatalytic activity of non-stoichiometric ZnFe2O4 under visible light irradiation. Phys. Scr. 89 (2014) 044011 (8pp)
Volume 89, Issue 4, April 2014, Article number 044011

4. L.Trinkler, B.Berzina, E.Palcevskis**,** AlN Ceramics from nanosized plazma processed powder, its properties and application. Chapter in Book: Nitride ceramics. Combustion synthesis, properties and applications. Ed. by A.Gromov and L. Chukhlomina, Wiley-VCH, 2014, pp.265-293.

LECTURES ON CONFERENCES

30th Scientific Conference of Institute of solid State Physics, University of Latvia, February 19-21, 2014, Riga, Latvia

1. **L.Trinkler, B.Berzina**. Localised transitions in luminescence of AlN ceramics. Book of Abstracts, p.16.

2. E.Elsts, U.Rogulis, K.Bulidžs, K.Smits, A.Zolotarjovs**, L.Trinklere**, K.Kundziņš. Studies of radiation defects in Ce, Eu,Tb doped oxyfluoride glasses and glass ceramics. Book of Abstracts, p.7.

3.V.Skvotsova, N.Mironova-Ulmane, **L.Trinkler**, V.Merkulov. Chromium and iron ions optical properties of topaz and beryl crystals. Book of Abstracts, p.8

Joint 12 Russia/CIS/ Baltic/Japan Symposium on Ferroelectricity and 9th International Conference Functional Materials and Nanotechnologies, Riga, September 29-October 2, 2014.

4. T.Yan, C.Y.J.Lu, **L.Trinkler, B.Berzina, V.Korsaks,** L.Chang, M.M.C.Chou, K.H.Ploog, Nonpolar ZnO epilayers and ZnO/$Zn_{1-x}Mg_xO$ multiple quantum well grown on $LiGaO_2$ by Molecular beam epitaxy. Book of Abstracts, p. 240.

5. P.Ščajev, R.Nedzinskas, S.Tumenas, **L.Trinkler, B.Berzina, V.Korsaks,** M.M.C. Chou, L.W.Chang, L.C.Chen and K.H.Chen, Electronic properties of polar and nonpolar ZnO films on $LiGaO_2$. Book of Abstracts, p.369.

6. R.Nedzinskas, A.Rimkus, A.Balčiunas, S.Tumenas, P.Ščajev, **L.Trinkler, B.Berzina, V.Korsaks,** M.M.C.Chou, L.W.Chang, L.C.Chen and K.H.Chen, Optical properties of polar and nonpolar ZnO films on $LiGaO_2$. Book of Abstracts, p.365.

7.V. Skvortsova, N. Mironova-Ulmane, **L. Trinkler,** V. Merkulov. Optical Properties of Natural and Synthetic Beryl Crystals. Book of Abstracts, p.373.

8. **B. Berzina, V. Korsaks, L. Trinkler, R. Kirsteins**, M. Knite, and J. Grabis. AlN Based Composite – White Light Emitter. Book of Abstracts, p.389.

LABORATORY OF SEMICONDUCTOR OPTOELECTRONICS

Head of Laboratory Dr.phys. B. Polyakov

RESEARCH AREA AND MAIN PROBLEMS

1. Engineering, synthesis, and functional processing of advanced 0D and 1D hybrid nanostructures. Scanning probe and electron microscopy characterization of nanomaterials.
2. Development of nanomechanical tests for 1D nanostructures and simulations of their mechanical properties, prototyping of nanodevices.
3. Synthesis of inorganic nanocrystals, nanotubes, and nanowires for photonics, electronics and biomedicine. Investigation of their structural, optical, and other properties.
4. Spectrochemical characterisation and depth profiling of plasma-facing components of the thermonuclear fusion reactors by means of laser-induced breakdown spectroscopy (LIBS).

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. G. Marcins

Students

B. Sc. E. Butanovs
B. Sc. J. Zideluns

COOPERATION

Latvia

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

Germany

University of Rostock, Rostock

Company “Aixtron”, Aachen

Max Plank Institute of Plasma Physics, Garching

Estonia

Institute of Physics, University of Tartu

Estonian Nanotechnology Competence Centre, Tartu

MAIN RESULTS

HYBRID AG-SIO$_2$ CORE-SHELL NANOWIRES

S.Vlassov, B. Polyakov, L.M. Dorogin, M.Vahtrus, M.Antsov, R. Lohmus

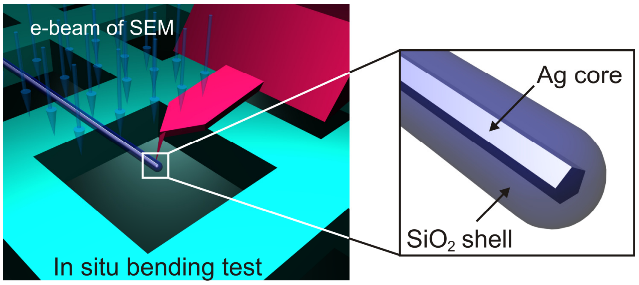

Fig. 1. In situ bending tests of Ag-SiO2 core-shell nanowire

The combination of two different materials in a single composite core–shell heterostructure can lead to improved or even completely novel properties. In this work we demonstrate the enhancement of the mechanical properties of silver (Ag) nanowires (NW) achieved by coating them with a silica (SiO2) shell using sol-gel method. Ag NWs can serve as waveguides for plasmon propagation in nanophotonics. In nanophotonics, a significant degree of bending is often required in order to guide the light in the desired direction, which may cause crack formation in Ag NW, and strongly disturb plasmons propagation. In situ scanning electron microscope (SEM) nanomechanical tests of Ag–SiO2 core–shell nanowires reveal an improved fracture resistance and an electron-beam induced shape restoration effect. Shape restoration was shown to be a phenomenon exclusively inherent to core–shell heterostructures, and absent for pure Ag NWs or SiO2 shells separately. Shape restoration was explained as e-beam induced structural relaxation of the SiO2 shell governed by elastic forces generated by the deformed Ag core. Test conditions were simulated using FEM (finite element modelling), and the average value of e-beam induced viscosity of the shell $\eta = 7 \times 10^{11}$ Pa·s was extracted by fitting simulated relaxation curves with experimental data. The stresses in the core of core–shell NWs in bending experiments can reach to 15 GPa without visible fracture, in contrast to uncoated Ag NWs, which start to fracture at a stress of 8.5 GPa. According to FEM simulations, the shell can dampen the mechanical stresses in the core in the vicinity of the contact with a stiff substrate and mitigate the plastic yield in the core.

MECHANICAL PROPERTIES OF SOL–GEL DERIVED SIO_2 NANOTUBES

B. Polyakov, S. Vlassov, R. Zabels, L. M. Dorogin, M. Antsov, R. Lohmus

The mechanical properties of thick-walled SiO2 nanotubes (NTs) prepared by a sol–gel method while using Ag nanowires (NWs) as templates were measured by using different methods. It is important to measure mechanical properties of nanostructures by set of different method to possible exclude errors specific for every measurement technique. In this work we measured the Young's modulus of SiO2 nanotubes by using three different methods. Half-suspended bending tests were carried out inside a SEM by using a nanomanipulator equipped with force sensor. The average value of the Young modulus was found to be 24.5 ± 11.1 GPa. Unexpectedly, significant plasticity of SiO2 nanotubes was observed for inside SEM in situ measurements. AFM nanoindentation and three-point bending tests were performed on the same set of NTs under ambient conditions, resulting in values of 20.1 ± 7.5 GPa and 41.3 ± 5.8 GPa, respectively. Finite element method simulations were used to extract Young's modulus values from the nanoindentation data. Half-suspended and three-point bending tests were processed in the framework of linear elasticity theory. Three-point bending tests were found to be the most appropriate method for measuring the Young's modulus of sol–gel synthesized SiO2 NTs.

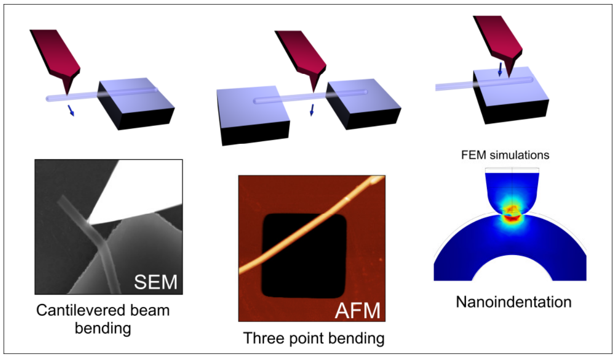

Fig. 2. Nanomechanical tests of sol-gel derived SiO2 nanotubes: AFM 3-point bending test, AFM nanoindentation, bending of half-suspended nanotube inside SEM [2].

SYNTHESIS OF NANOCRYSTALS, NANOTUBES AND NANOWIRES FOR PHOTONIC AND BIO APPLICATIONS

B. Polyakov, A. Kuzmin, R. Zabels, K. Smits, J. Butikova, P. Kulis

Metal nanoparticles and nanowires are novel and perspective nanomaterials having wide range of possible applications. These materials can be synthesized using simple wet chemical methods. Metal nanoparticles, nanotubes and nanowires (Ag and Au) can be used in photonics and plasmonics, for single or double photon luminescence yield enhancement, photon absorption enhancement in solar cells, etc.

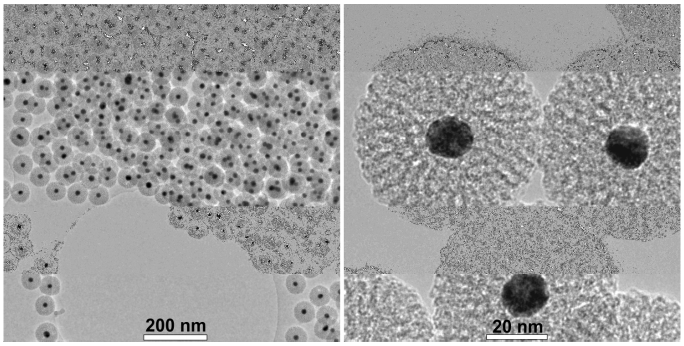

Fig. 3. TEM images of Au – mesoporous SiO2 nanoparticles synthesized by wet chemical method

We synthesized semiconducting nanocrystals (CdS, PbS, Bi_2S_3) and metal nanoparticles (Au, Ag, Pd), nanotubes (Au-Ag) and nanowires (Au, Ag, Cu) as well as hybrid core-shell (Au / mesoporous SiO_2 nanoparticles), investigated their morphology by SEM and internal structure using TEM microscopy. Currently we are working on doping by rare earth elements silica shell in core-shell nanostructures system for biomedical applications and nanophotonics. Magnetron sputtering technique was applied to prepare ZnO-WO_3 and CuO-WO_3 core-shell hybrid nanowires. Subsequent thermal treatment used to induce interdiffusion and solid state chemical reactions, where copper or zinc tungstates are produced.

PREPARATION OF EFFICIENT PFC OPERATION FOR ITER AND DEMO: POST-MORTEM ANALYSIS AND MATERIAL MIGRATION. QUALIFICATION OF LASER-INDUCED BREAKDOWN SPECTROSCOPY

J. Butikova, A. Voitkans, P. Kulis, I. Tale

The studies of material modification under plasma exposure generate basic expertise with regard to plasma-facing component (PFC)-related questions in future fusion reactors. Laser-Induced Breakdown Spectroscopy (LIBS) is an analytical method of obtaining the surface distribution of elements. This powerful tool for spectrochemical analysis provides both the elemental depth profiling and the content layer-by-layer imaging.

We have developed a 2D scanning LIBS set-up in order to visualise a spatial distribution of the elements on the round robin and plasma-exposed samples. Currently, it is possible to analyse an area of 1 × 8 mm^2 of the surface, with the diameter of ablation crater of ~ 250 μm so that the ablation rate remains below 100 nm per pulse. The energy of used 1064 nm laser pulse is ~ 10 mJ. Comparing to the standard LIBS, the 2D scanning method has allowed improving the sensitivity significantly. The future plans include developing the procedures for deuterium spectroscopy, as well as performing the double-pulse LIBS experiments.

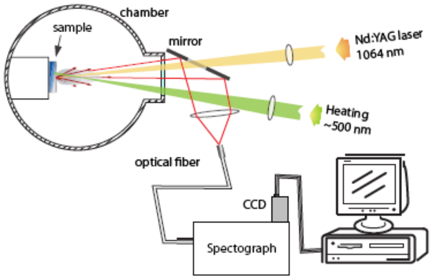

Fig. 4. Set-up for double-pulse LIBS experiments

SCIENTIFIC ARTICLES

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2. **B.Polyakov**, M.Antsov, S.Vlassov, L.Dorogin, M.Vahtrus, R.Zabels, S.Lange, R. Lõhmus. Mechanical properties of sol-gel derived SiO_2 nanotubes. *Beilstein Journal of Nanotechnology*, 2014, 5, 1808-1814.
3. **S.Vlassov, B.Polyakov**, L.Dorogin, M.Antsov, M.Mets, M.Umalas, R.Saar, R.Lõhmus, I.Kink. Elasticity and yield strength of pentagonal silver nanowires: in situ bending tests, *Materials Chemistry and Physics*. 143, 1026–1031, 2014.
4. **B.Polyakov, S.Vlassov**, L.Dorogin, N.Novoselska, **J.Butikova**, M.Antsov, S.Oras, I.Kink, R.Lõhmus. Some aspects of formation and tribological properties of silver nanodumbbells, *Nanoscale Research Letters* 9, 186, 2014.
5. **B.Polyakov, S.Vlassov**, L.Dorogin, **J.Butikova**, M.Antsov, S.Oras, I.Kink, R.Lõhmus. Manipulation of nanoparticles of different shapes inside a scanning electron microscope, *Beilstein Journal of Nanotechnology* 5, 133–140, 2014.

6. M.Antsov, L.Dorogin, **S.Vlassov, B.Polyakov**, K. Mougin, I.Kink, R. Lõhmus. Analysis of elastic and static friction forces in a nanowire bent on a flat surface: a comparative study, *Tribology International*. 72, 31–34, 2014.

PRESENTATIONS ON CONFERENCES

International conference "Functional materials and nanotechnologies" FM&NT, Riga, September 29 – October 2, 2014

1. B. Polyakov, S. Vlassov, L.M. Dorogin, J. Butikova, M. Antsov, S. Oras, R. Saar, I. Kink, R. Lõhmus. *Manipulation of Nanoparticles with Different Morphology Inside a Scanning Electron Microscope.*
2. B. Polyakov, S. Vlassov, L. Dorogin, M. Antsov, R. Zabels, J. Butikova, K. Smits, R. Lõhmus. *Silver and Gold Nanodumbbells for Tribological Experiments.*
3. S. Vlassov, B. Polyakov, L.M Dorogin, M. Vahtrus, M. Antsov, M. Mets, R. Saar, R. Lõhmus. *Shape Restoration Effect and Enhanced Fracture Resistance of Ag/SiO2 Core-Shell Nanowires.*
4. B. Polyakov, R. Zabels, A. Sarakovskis, S. Vlassov, A. Kuzmin. *Plasmonic Photoluminescence Enhancement by Silver Nanowires.*
5. E. Butanovs, J. Butikova, B. Polyakov, G. Marcins, R. Zabels, I. Tale. *HOPG Patterning Methods for Graphene Transferring Onto the Substrate.*

The First European Workshop on Understanding and Controlling Nano and Mesoscale Friction, May 26-29, 2014, Can Picafort, Majorca (Spain)

6. B. Polyakov, S. Vlassov, L. Dorogin, N. Novoselska, J. Butikova, M. Antsov, S. Oras, R. Zabels, I. Kink, R.Lõhmus.

Some aspects of formation and tribological properties of silver nanodumbbells.

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 AND MAIN RESEARCH TOPICS

The time-resolved luminescence and absorption methods were used for electronic properties studies of single crystals, ceramics, nanostructured materials.

Excitation sources: a pulsed electron beam accelerator (10 ns, 270 keV, 10^{12} electrons/pulse), YAG:Nd and nitrogen lasers (266 nm and 532 nm, 2 ns; 337 nm, 10ns); for steady state luminescence spectra and radiation defect creation X-ray source and 980 nm laser diode were used. TSL methods were developed.

Steady state and time resolved absorption spectroscopy. VIS-UV absorption spectrometer LABOMED for measurements in 190-1100 nm range. FTIR absorption spectroscopy: EQUINOX 55 (10000-400 cm^{-1} and 22000-7000 cm^{-1} spectral regions) developed also for dispersed materials in wide temperature range.

Luminescence measurements. The luminescence was measured through monochromator MDR-3 with HAMAMATSU H8259 photon counting head and photon counting board FastComTech module P7887 with 500 channels. The minimal time bins is 250 ps. The laser frequency and time bins can be adjusted. The luminescence spectra were recorded using the Andor Shamrock B-303i spectrograph equipped with CCD camera (ANDOR DU-401A-BV). The luminescence measurements will be carried at temperature regions 8-300K and 300K-500K.

TSL and FGT methods. The temperature regimes are easy realized by using special programs. The activation energies was calculated by Hoogenstraaten and fraction glow methods.

SCIENTIFIC STAFF

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

Students

M.Vanks,
A.Zolotarjovs

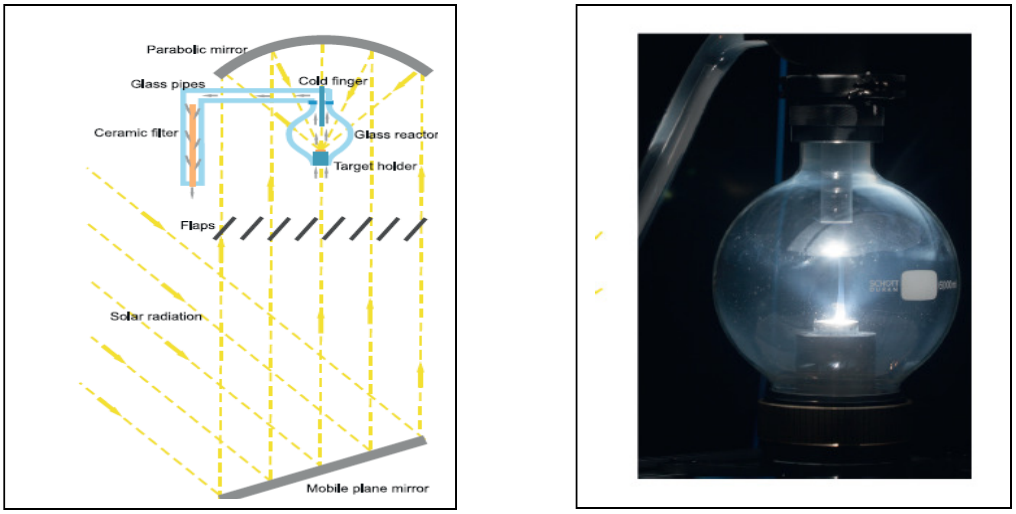
MAIN RESULTS

LUMINESCENCE PROPERTIES OF ZIRCONIA NANOCRYSTALS PREPARED BY SOLAR PHYSICAL VAPOR DEPOSITION

K.Smits, L.Grigorjeva, D.Millers, K.Kundzins, R.Ignatans, J.Grabis, C.Monty.

Zirconia nanocrystals have attracted considerable interest as biolabels, which can be used as probes for medical imaging and biosensor applications. However, zirconia particle agglomeration forms a major limitation to its use for biolabeling. In this backdrop, for the first time, well-separated zirconia nanocrystals were obtained in a Heliotron reactor (PROMES CNRS, France) via the solar physical vapor deposition (SPVD) method. As the raw material target for solar evaporation, zirconia nanopowders obtained via the sol–gel process were used. The luminescence and upconversion luminescence properties of the Sol Gel nanopowders were compared with those of the SPVD nanocrystals. Erbium was chosen as the luminescence center with ytterbium as the sensitizer, and along with these two dopants, niobium was also used. Niobium acts as a charge compensator to compensate for depletion in the charge due to the introduction of trivalent erbium and ytterbium at tetravalent zirconium sites. Consequently, the oxygen-vacancy concentration is reduced, and this results in a significant increase in the upconversion luminescence.

The SPVD-prepared samples showed less agglomeration and a fine crystal structure as well as high luminescence, and thus, such samples can be of great interest for biolabeling applications.



Schematic of Heliotron reactor (left panel) and its photograph (right panel).

THE ROLE OF Nb IN INTENSITY INCREASE OF Er ION UPCONVERSION LUMINESCENCE IN ZIRCONIA

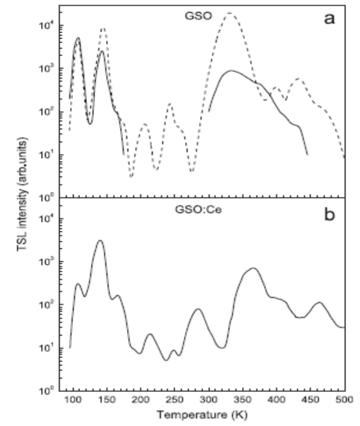
K. Smits, A. Sarakovskis, L. Grigorjeva, D. Millers and J. Grabis

It is found that Nb co-doping increases the luminescence and upconversion luminescence intensity in rare earth doped zirconia. Er and Yb-doped nanocrystalline samples with or without Nb co-doping were prepared by sol-gel method and thermally annealed to check for the impact of phase transition on luminescence properties. Phase composition and grain sizes were examined by X-ray diffraction; the morphology was checked by scanning- and high-resolution transmission electron microscopes. Both steady-state and time-resolved luminescence were studied. Comparison of samples with different oxygen vacancy concentrations and different Nb concentrations confirmed the known assumption that oxygen vacancies are the main agents for tetragonal or cubic phase stabilization. The oxygen vacancies quench the upconversion luminescence; however, they also prevent agglomeration of rare-earth ions and/or displacement of rare-earth ions to grain surfaces. It is found that co-doping with Nb ions significantly (>20 times) increases upconversion luminescence intensity. Hence, ZrO2:Er:Yb:Nb nanocrystals may show promise for upconversion applications.

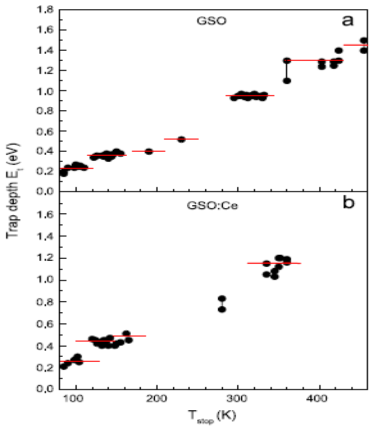
THERMALLY STIMULATED LUMINESCENCE OF UNDOPED AND Ce^{3+}-DOPED Gd_2SiO_5 AND $(Lu,Gd)_2SiO_5$ SINGLE CRYSTALS

V. Bondar, L. Grigorjeva, T. Kärner, O. Sidletskiy, K. Smits, S. Zazubovich, A. Zolotarjovs.

Thermally stimulated luminescence (TSL) characteristics (TSL glow curves and TSL spectra) are investigated in the 4–520 K temperature range for the single crystals of gadolinium and lutetium–gadolinium oxyorthosilicates X-ray irradiated at 4 K, 8 K, or 80 K. The nominally undoped Gd_2SiO_5 and $(Lu,Gd)_2SiO_5$ crystals, containing traces of Ce^{3+}, Tb^{3+}, and Eu^{3+} ions, and Ce^{3+}-doped Gd_2SiO_5 and $(Lu,Gd)_2SiO_5$ crystals are studied. For the first time, the TSL glow curves of these materials are measured separately for the electron (intrinsic, Ce^{3+}- or Tb^{3+}-related) and hole (Eu^{3+}-related) recombination luminescence, and the TSL glow curve peaks, arising from thermal decay of various electron and hole centers, are identified. Thermal stability parameters of the electron and hole traps are calculated.



TSL after irradiaion at 80K for 3.1 eV emission solid lines and 1.85 eV ($Eu^{3+)}$ – dashed line.



Dependence of Ea on the temperature obtained from TSL glow curves foe Eu^{3+} (a) and for the Ce^{3+} emission (b).

SCIENTIFIC VISITS ABROAD

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

5. Dr.L.Grigorjeva, France, PROMES, 2 weeks.
6. A.Zolotarjovs, Wroclaw, Poland

COOPERATION

Latvia

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

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

Estonia

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

Russia

GIREDMET, Moscow (Pr. I.S Lisitskii)

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

Poland

Institute of High Pressure Physics, PAN, Warszawa, Poland (Prof.W.Lojkowski,)

France

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

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

SCIENTIFIC PUBLICATIONS

1. **K.Smits, L.Grigorjeva, D.Millers**, K.Kundzins, R.Ignatans, J.Grabis, C.Monty. Luminescence properties of zirconia nanocrystals prepared by solar physical vapor deposition.2014, Opt.Mat. V.37, 256-261. DOI: 10.1016/ j.opt.mat.2014.06.003.
2. **K. Smits,** A. Sarakovskis, **L. Grigorjeva, D. Millers** and J. Grabis. The role of Nb in intensity increase of Er ion upconversion luminescence in zirconia J. Appl. Phys. 115, 213520 (2014). DOI: 10.1063/1.4882262.
3. V. Bondar, **L. Grigorjeva**, T. Kärner, O. Sidletskiy, **K. Smits**, S. Zazubovich, **A. Zolotarjovs.** Thermally stimulated luminescence of undoped and Ce^{3+}-doped Gd_2SiO_5 and

$(Lu,Gd)_2SiO_5$ single crystals. Journal of Luminescence, v. 159, 2014, 229–237. DOI: 10.1016/j.jum.2014.11, 034.

4. A.N. Trukhin, **K. Smits**, G. Chikvaidze, T.I. Dyuzheva, L.M. Lityagina. Luminescence of rutile structured crystalline silicon dioxide (stishovite). Solid State Communications, v. 189, 2014,10–14. DOI: 0.1016/j.ssc.2014.03.010.
5. J. Maniks**, L. Grigorjeva**, R. Zabels**, D. Millers**, I. Bochkov, J. Zicans, T. Ivanova, J. Grabis. Swift heavy ion induced modifications of luminescence and mechanical properties of polypropylene/ZnO nanocomposites. Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms. 2014, v.326, 154–157. DOI:10.1016/j.nimb.2013.10.090

LECTURES IN CONFERENCES

International Conference "Functional materials and nanotechnologies 2014 (FM&NT)", (29.Sept.-02.Okt), Rīga, Latvia.

1. Donats Millers, Larisa Grigorjeva, Igor S.Lisitskij, Mikhail S.Kouznetsov, Ksenia Zaramenskikh. The radioluminescence and cathotodoluminescence of TlCl:Bi crystals. F-123.
2. Larisa Grigorjeva, Krishjanis Šmits, Donats Millers, Dz.Jankoviča. Luminescence of Er/Yb doped HAp-FAp nanocrystals and ceramics. F-118.
3. V. Bondar , L. Grigorjeva , T. Kärner , O. Sidletskiy , K. Smits, S. Zazubovich, A. Zolotarjovs. Thermally stimulated luminescence of undoped and Ce^{3+}-doped Gd_2SiO_5 and $(LuGd)_2SiO_5$ single crystals . F113.
4. F.Mukepavela, L.Grigorjeva, E.Gorohova, et al. Structure, nanohardness and photoluminescence og ZnO ceramics based on nanopowders. F-47.
5. K.Smits, A.Zolotarjovs et al., Comparative studies of alumina prepared with electrochemical and plazma electrolytic oxidation routs. F-60.

LU CFI 30th Scientific Conference, 2014, 19-21. Febr. Riga, Latvia

6. V.Liepiņa, D.Millers, K.Šmits. Luminiscences mehamisma pētījumi $SrAl_2O_4$:Eu,Dy materiālā. Abstracts, 10 lpp.

7. L.Puķina, L.Grigorjeva, D.Millers, K.Šmits. Hidroksilapatītu un fluorapatītu luminiscence. 88 lpp.
8. E.Elsts, U.Rogulis, K.Bulindžs, K.Šmits, A.Zolotarjevs, L.Trinklere, K.Kundziņš. Radiācijas defektu pētījumi ar Ce, Eu, Tb aktivētos oksifluorīdu stiklos un stikla keramīkās. 7 lpp.
9. E.Elsts, U.Rogulis, K.Bulindžs, K.Šmits, A.Zolotarjevs, L.Trinklere, K.Kundziņš. Radiācijas defektu pētījumi ar Ce, Eu, Tb aktivētos oksifluorīdu stiklos un stikla keramīkās. 7 lpp
10. A.Zolotarjevs, K.Šmits, D.Millers. Termostimulētās luminiscences pētījumi oksīdu materiālos. 11 lpp.
11. K.Smits, K.Kundzins. Transmisijas elektronu mikroskops FEI: tehniskās iespējas un pielietojumi, 44 lpp.
12. A.Fedotovs, U.Rogulis, Dz.Bērziņš, K.Smits, G.Doķe. Magnētiskās rezonanses spektri un rekombinatīvā luminiscence ZnO. 14 lpp.

17th International Conference on luminescence and optical spectroscopy of Condenced Matter, 2014, 13-18 July, Wroclaw, Poland.

13. A.Zolotarjevs, K.Smits, D.Millers, C.Monty, L.Grigorjeva. Thermal activation energies of defect states in ZnO single crystals, ceramics and nanostructues. Book of Abstracts, , P.171.

MASTER THESIS

Virgīnija Liepiņa „ Studies of luminescence mechanisms on $SrAl_2O_4$:Eu,Dy”
Univerisity of Latvia. Riga, 2014.

BACHELOR THESIS

Aleksejs Zolotarjovs „TSL and fractional glow methods used for defects states investigations on oxide materiāls”, Univerisity of Latvia, Rīga, 2014.

OPTICAL RECORDING

Head of Laboratory Dr. J.Teteris

RESEARCH AREA AND MAIN PROBLEMS

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

SCIENTIFIC STAFF

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

PhD Students

1. J.Aleksejeva
2. U.Gertners

Students

1. E. Potanina
2. K. Klismeta
3. M. Jirgensons

COOPERATION

Latvia

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

USA

3. Boise State University (Dr. M. Mitkova).

Czech Republic

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

FOREIGN SCIENTIST VISITS IN LABORATORY

1. Mg.Sc. Tyler Nichol, USA, Boise State University, 25.05.2014- 18.08.2014.
2. Dr. Sc. Luidmila Loghina, Czech Republic, Uniuversity of Pardubice, 04.08.2014-01.11.2014.

MAIN RESULTS

SUBWAVELENGTH STRUCTURES IN AMORPHOUS CHALCOGENIDE THIN FILMS

Mara Reinfelde and Janis Teteris

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

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

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

OPTICAL RECORDING IN AMORPHOUS CHALCOGENIDE THIN FILMS

Janis Teteris

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

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

HOLOGRAPHIC LITHOGRAPHY IN AMORPHOUS CHALCOGENIDE THIN FILMS

J.Teteris, J.Aleksejeva and M.Reinfelde

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

SURFACE RELIEF FORMATION DURING HOLOGRAPHIC RECORDING

U.Gertners and J.Teteris

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

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

OPTICAL RECORDING IN AZOBENZENE CONTAINING POLYMER FILMS

A. Gerbreders and J. Teteris.

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

The transmission spectra of composites were measured before and after illumination by laser beams with different wavelengths. Transmission of composite film of merocianine form was measured by laser beam wavelength 532 nm in dependence on beam intensity.

The holographic recording of diffraction gratings was performed by different laser lines (325, 532 nm). During recording the diffraction efficiency was measured in transmission mode. The profiles of the gratings area were analyzed by AFM microscope.

SCIENTIFIC PUBLICATIONS

1**. A.Gerbreders**, A.Bulanovs, E.Sledevskis, Vj. Gerbreders, **J. Teteris**, Optical properties of composite films based on copper chloride in PMMA matrix*, Key Engineering Materials*, **605** (2014) 445-448.

2. **J.Aleksejeva, M.Reinfelde, J.Teteris**, Direct surface relief patterning of azo-polymers films via holographic recording, *Can. J.Phys.,* 92 (2014) 842-844.

3. **M.Reinfelde, J.Teteris, E.Potanina**, Surface relief grating formation in amorphous $As_{40}S_{15}Se_{45}$ and As_2S_3 films under 0.532 μm wavelength illumination, *Can. J. Phys.,* 92 (2014) 659-662.

4. **J.Aleksejeva, A Gerbreders, J.Teteris**, A.Vembris, E.Zarins, V.Kokars, Photoinduced surface patterning in low molecular organic glasses; 5th International Conference Radiation Interaction with Materials: Fundamentals and Applications 2014;Book Series Title: Radiation Interaction with Materials and Its Use in Technologies Pages: 73-76

5. **U.Gertners, J.Teteris**, Z.Gertnere, **E.Potanina**, Investigation of several techniques for light induced surface patterning, 5th International Conference Radiation Interaction with Materials: Fundamentals and Applications 2014;Book Series Title: Radiation Interaction with Materials and Its Use in Technologies Pages: 79-82

LECTURES ON CONFERENCES

30th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Rīga, Latvia, February 19-21, 2014.:

1. J.Aleksejeva, J.Teteris, A.Vembris, Virsmas reljefa veidošanās azo-savienojumos (Surface relief formation in azo-compounds), Book of Abstracts, p.101.
2. K.Klismeta, J.Teteris, Fotoinducētās masas pārbīde un dubultlaušana azo savienojumā W-75 (The photoinduced mass transport and birefringence in azo compound W-75), Book of Abstracts, p.58.
3. E.Potaņina, J.Teteris, Ierosinošā starojuma viļņa garuma ietekme uz virsmas reljefa veidošanos As_2S_3 plānajās kārtiņās (Recording light source wavelenght influence on surface formation process in As_2S_3 thin films), Book of Abstracts, p.59.
4. M.Jirgensons, J.Teteris, Foto-inducētā dubultlaušana As_2S_3 plānajās kārtiņās (Photoinduced birtefringence in As_2S_3 thin films), Book of Abstracts, p.103.
5. M.Reinfelde, J/Teteris, Parauga biezuma ietekme uz virsmas reljefa veidošanās procesu amorfajos halkogenīdos (Influence of sample thickness on formation of surface relief in amorphous chalcogenides), Book of Abstracts, p.101.

57th Scientific Conference for Students of Physics and Natural Sciences; March 19-21, Vilnius.

6. U.Gertners, J.Teteris, Z.Gertnere, E.Potaņina, Direct light-induced patterning in a-As_2S_3 thin films,

International Young Scientist Conference "Developments in Optics and Communications 2014", Riga, Latvia, April 9-12, 2014:

7. K.Klismeta, J.Teteris, The photoinduced birefringence and recording of surface relief gratings in azo compound W-75, Book of abstracts, p. 28.
8. E.Potaņina, J.Teteris, Light wavelength influence on surface relief recording process in As_2S_3 thin films, Book of abstracts, p. 29.

5th International Conference Radiation Interaction with Materials:Fundamentals and Applications 2014, Kaunas, Lithuania, May 12-15, 2014

9. J.Aleksejeva, A.Gerbreders, J.Teteris, A.Vembris, E.Zarins, V.Kokars, Photoinduced surface patterning in low molecular organic glasses, P1-1, p.73-76.
10. U.Gertners, J.Teteris, Z.Gertnere, E.Potaņina, Investigation of several techniques for light induced surface patterning, P1-3, p.79-82.

6th International Conference on Optical, Optoelectronic and Photonic Materials and Applications, Leeds, UK, July 27 – August 1, 2014

11. K.Klismeta, J.Teteris, The photoinduced birefringence and mass transport in azo compound K-D-2, 00141, p. 93
12. A.Gerbreders, Optical properties of the low-molecular amorphous azochromophores and their application in holography, 00046, p. 113.
13. J.Teteris, Optical Field-induced Surface Patterning of Amorphous Chalcogenide and Low Molecular Organic Glass Films, 00147, p. 201.
14. A. Ogurcovs, Vj. Gerbreders, E. Tamanis, A. Gerbreders, Characterization of screen-printed ZnO/CuInSe2 p-n junction before and after laser ablation, 00185, p. 245.
15. M. Reinfelde, J.Teteris, Influence of Film Thickness on Photoinduced Formation of Surface Relief Gratings in Amorphous Chalcogenides, 00079, p. 76.

19th International Symposium on Non-Oxide and New Optical Glasses *ISNOG2014), Jeju.Republic of Korea, August 24-28, 2014

16. J.Teteris, Photoinduced mass transport in amorphous chalcogenide films, Abstract book, p. 102.
17. M.Reinfelde, J.Teteris, Spectral dependence of photoinduced formation of surface relief gratings in amorphous chalcogenides. Abstract book, p. 102.

8th International Conference on Advanced Optical Materials and Devices, Riga, Latvia, August 25-27, 2014

18. K.Klismeta, J.Teteris, Photoinduced mass transport and birefringence in azobenzene containing low molecular weight organic glasses, ,

International Conference FM&NT2014 (Functional materials and nanotechnologies 2014) Riga, Latvia, September 29 – October 2, 2014:

19. K.Klismeta, J.Teteris, Recording of Surface Relief in Azobenzene Containing Low Molecular Weight Organic Glasses Book of abstracts,. PO-122.
20. A.Gerbreders, Optical Properties of the Low-Molecular Amorphous Azochromophores, F-65.
21. M.Reinfelde, Kinetics of Diffraction Efficiency During the Holographic Recording of Surface Relief Gratings, F-66.

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.

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, energy-dispersive X-ray microanalysis, thermal desorption mass-spectrometry.

Several of these experimental techniques are available by 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) or CCD-based spectrometers (Andor/Shamrock 303-i) and Hamamatsu TM-UV/VIS C10082CAH portable spectrograph. Configurations for NIR-VIS-UV measurements of attenuation in optical fibers are available (using OceanOptics DH-2000-S-TTL D_2-halogen light source).

Luminescence spectroscopy. Luminescence excitation by the following sources is available : YAG:Nd laser (266 nm, 532 nm), nitrogen laser (337 nm), excimer lasers (248, 193 and 157 nm), semiconductor lasers (650, 765 nm), deuterium and xenon lamps. 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..vacuumUv range is developed.

Raman spectroscopy: Andor Shamrock303i spectrometer with Newton DU971N electron multiplying cooled CCD, NIR to UV spectral range.

Energy-dispersive X-ray fluorescence microanalysis (EDAX Eagle III spectrometer, Rhodium X-ray source with micro-capillary focusing lens, detected elements from Na to U, spatial resolution ~50 µm).

Mass spectrometry: Dycor LCD-300 quadrupole mass-spectrometer, 1-300 a.m.u. with oil-free vacuum station.

MAIN RESULTS

LUMINESCENCE OF RUTILE STRUCTURED CRYSTALLINE SILICON DIOXIDE (STISHOVITE)

A. N.Trukhin, K.Smits, G. Chikvaidze, T. I. Dyzheva, L. M.Lityagina

Luminescence spectrum of synthetic mono-crystalline stishovite comprises a slow blue band at ~ 400 nm(~3.1 eV) and a fast UV band at ~260 nm (~4.7 eV), as well as some bands in near-infrared range of spectra. The NIR luminescence of stishovite crystal, excited with lasers 532 nm, 248 nm and 193 nm as well as x-ray, possesses several sharp lines. A zero phonon line is situated at 787 nm (1.57 eV) and grows with cooling. An anti-Stokes line is located at 771 nm (1.68 eV). This line disappears with cooling. In a powder sample of stishovite created by shock waves generated by the impact of a 50-m-diameter meteorite in Arizona 50,000 years ago, the PL broad blue band is situated at 425 nm (2.9 eV), the UV band at ~260 nm (~4.7 eV), and the sharp lines, seen only under 193 nm laser, at 689 nm (1.789 eV), 694 nm (1.785 eV) and 706 nm (1.754 eV).We ascribe the fast UV luminescence to singlet–singlet transitions and the slow blue band to triplet–singlet transitions of the same intrinsic defect of stishovite in both types of samples. The blue band in stishovite crystal exhibits delayed luminescence of recombination nature, whereas the blue band of Arizona's powder sample does not exhibit such effect. This difference is explained by different surroundings of luminescence center in those samples. NIR luminescence of mono-crystalline stishovite is ascribed to carbon impurity penetrated in the sample from graphite heater. NIR luminescence of powder from Arizona has not yet found an explanation.

DIFFUSION AND REACTIONS OF PHOTOINDUCED INTERSTITIAL OXYGEN ATOMS IN AMORPHOUS SiO_2 IMPREGNATED WITH ^{18}O -LABELED INTERSTITIAL OXYGEN MOLECULES

Koichi Kajihara, Linards Skuja, and Hideo Hosono

Both diffusion and reactions of interstitial oxygen atoms (O^0) in amorphous SiO_2 (*a*-SiO_2) were examined using oxygen-excess *a*-SiO_2 containing ^{18}O-labeled interstitial oxygen molecules (O_2) and exposed to F_2 laser light ($h\nu$ = 7.9 eV). Both the F_2 laser photolysis of interstitial O_2 at 77K and subsequent heat treatment at $\gtrsim$200°C give rise to oxygen exchange between residual interstitial O_2 and oxygen atoms in the *a*-SiO_2 network, and these temperatures are far lower than the temperature at which conventional thermal network-interstitial oxygen exchange in unirradiated *a*-SiO_2 occurs ($\gtrsim$700°C). However, at the initial stage of the low-temperature F_2 laser photolysis, an efficient formation of interstitial ozone molecules (quantum yield $\gtrsim$0.06) via nearly exchange-free diffusion of photogenerated interstitial O^0 is observed and this reaction predominates over the network-interstitial oxygen exchange.

LUMINESCENCE OF PHOSPHORUS CONTAINING OXIDE MATERIALS: CRYSTALLINE SiO_2-P AND $3P_2O_5 \bullet 7SiO_2$; $CAO \bullet P_2O_5$; $SRO \bullet P_2O_5$ GLASSES

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

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

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

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

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

LUMINESCENCE OF SILICON DIOXIDE DIFFERENT POLYMORPH MODIFICATION: SILICA GLASS, α -QUARTZ, STISHOVITE, COESITE

A. N.Trukhin

Abstract. Stishovite, coesite, oxygen deficient silica glass as well as irradiated α-quartz, exhibit two luminescence bands: a blue one and an UV one both excitable in the range within optical gap. There are similarities in spectral position and in luminescence decay kinetics among centers in these materials. The interpretation was done on the model of Oxygen Deficient Centers (ODC) . The ODC(II) or twofold coordinated silicon and ODC(I) are distinguished. ODC(I) is object of controversial interpretation. The Si-Si oxygen vacancy and complex defect including latent twofold coordinated silicon are proposed. Remarkably, this luminescence center does not exist in as grown crystalline α-quartz. However, destructive irradiation of α-quartz crystals with fast neutrons, γ rays, or dense electron beams creates ODC(I) like defect. In tetrahedron structured coesite the self trapped exciton (STE) luminescence observed with high energetic yield (~30%) like in α-quartz crystals. STE in coesite coexists with oxygen deficient-like center. In octahedron structured stishovite STE was not found and only ODC exists.

INHOMOGENEOUS BROADENING AND PEAK SHIFT OF THE 7.6 EV OPTICAL ABSORPTION BAND OF OXYGEN VACANCIES IN SiO_2

K.Kajihara, L.Skuja, H. Hosono

The peak parameters of radiation-induced 7.6 eV optical absorption band of oxygen vacancies (Si–Si bonds) were examined for synthetic high-purity α-quartz and amorphous SiO_2 (a-SiO_2) exposed to ^{60}Co γ-rays. The peak shape is asymmetric with the steeper edge at the lower energy side both in α -quartz and a-SiO_2, and the peak energy is larger for α-quartz than that for a-SiO_2. The full width at half maximum for a-SiO_2 is larger by ~40-60% than that for α -quartz, and it increases with an increase in the disorder of the a-SiO_2 network, which is enhanced by raising the temperature of preannealing before irradiation, i.e., fictive temperature. These data are interpreted from the viewpoint of the site-to-site distribution of the Si–Si bond length in a-SiO_2.

LUMINESCENCE OF NON-BRIDGING OXYGEN HOLE CENTERS IN CRYSTALLINE SiO_2

L. Skuja, K. Kajihara, J.Grube, H. Hosono

Oxygen dangling bonds (nonbridging oxygen hole centers, NBOHCs), which are characteristic to amorphous SiO_2, were studied in amorphized regions of neutron-irradiated α-quartz crystal and on their boundaries by time-resolved site-selective photoluminescence (PL) at 20K. Along with the usual disorder-broadened PL band of NBOHCs, sharp, "crystal-like" zero-phonon lines (ZPLs), whose positions do not shift with the excitation wavelength, are observed. In addition to the previously reported NBOHCs with ZPL at 1.933 eV, a second sub-type of NBOHCs with ZPL at 1.883 eV is confirmed by observation of its vibrational sideband due to Si-(dangling O) stretching mode (897cm^{-1}) under resonance 1.883eV excitation. A third sub-type of NBOHCs with an excitation energy at 1.879 eV, distinguished by a strong coupling to low-energy (66 cm^{-1}) vibrational mode is found. This mode is weakly coupled also to the other two sub-types of NBOHCs.

SCIENTIFIC VISITS ABROAD

1. Anatoly Trukhin, X International Symposium "SiO_2: Advanced Dielectrics and Related Devices", June 14-16 Cagliari, Italy.
2. Linards Skuja X International Symposium "SiO_2: Advanced Dielectrics and Related Devices", June 14-16 Cagliari, Italy.

COOPERATION

Latvia

Institute of Atomic Physics and Spectroscopy, University of Latvia (Prof. J.Spigulis, Dr. A.Skudra)

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 Of Saint-Etienne (France) (Prof. Y Ouerdane, Prof. A. Boukenter).

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. K.Kajihara, **L.Skuja**, H. Hosono, Diffusion and reactions of photoinduced interstitial oxygen atoms in amorphous SiO_2 impregnated with ^{18}O-labeled interstitial oxygen molecules. J. Phys. Chem. C v. 118, pp.4282 – 4286 (2014).
2. **A. N.Trukhin**, K.Smits, G. Chikvaidze, T. I. Dyuzheva, L. M.Lityagina, Luminescence of rutile structured crystalline silicon dioxide (stishovite), Solid State Communication 189 pp.10-14(2014).
3. **A. N. Trukhin**, K. Smits, J. Jansons, D. Berzins, G. Chikvaidze, and D. L. Griscom Luminescence of Phosphorus Containing Oxide Materials: Crystalline SiO_2-P and $3P2O_5 \bullet 7SiO_2$; $CaO \bullet P_2O_5$; $SrO \bullet P_2O_5$ Glasses, AIP Conference Proceedings 1624, 154 (2014); doi: 10.1063/1.4900472.
4. **A. N. Trukhin**, Luminescence of silicon dioxide different polymorph modification: Silica glass, α-quartz, stishovite, coesite, AIP Conference Proceedings 1624, 167 (2014); doi: 10.1063/1.4900473.

5. **L. Skuja**, K. Kajihara, J.Grube, H. Hosono, Luminescence of Non-bridging Oxygen Hole Centers in Crystalline SiO_2, AIP Conference Proceedings, v.1624, p.130-134 (2014). doi: 10.1063/1.4900468

6.. K.Kajihara**,** **L.Skuja**, H. Hosono, Inhomogeneous broadening and peak shift of the 7.6 eV optical absorption band of oxygen vacancies in SiO_2, AIP Conference Proceedings, v.1624 p.58-63 (2014), doi: 10.1063/1.4900457

LECTURES IN CONFERENCES

X International Symposium "SiO_2: Advanced Dielectrics and Related Devices", June 14-16 Cagliari, Italy:

1. A.N.Trukhin, K. Smits, J. Jansons, D. Berzins, G. Chikvaidze, and D. L. Griscom Luminescence of Phosphorus Containing Oxide Materials: Crystalline SiO_2-P and $3P2O_5$•$7SiO_2$; CaO•P_2O_5; SrO•P_2O_5 Glasses,
2. A. N. Trukhin, Luminescence of silicon dioxide different polymorph modification: Silica glass, α-quartz, stishovite, coesite.
3. L.Skuja, K. Kajihara, J.Grube, H. Hosono Luminescence of Non-bridging Oxygen Hole Centers in Crystalline SiO_2.
4. K.Kajihara, L.Skuja, H. Hosono, Inhomogeneous broadening and peak shift of the 7.6 eV optical absorption band of oxygen vacancies in SiO_2.

30th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Rīga, Latvia, February 19-21, 2014:

5. K.Kajihara, L.Skuja, H.Hosono Exchange between interstitial and structural oxygen in excimer laser-irradiated SiO_2 glass. Abstracts, p.6
6. L.Skuja, K.Kajihara, A.Siliņš Luminescence kinetics of molecular oxygen in silicon dioxide. Abstracts, 93.lpp.
7. A.Trukhin, K.Šmits, J.Jansons, Dz.Bērziņš, G.Čikvaidze, D.L.Griscom Luminescence of phosphate-containing materials: crystalline SiO_2:P and glassy $3P_2O_5 \cdot 7SiO_2$; $CaO \cdot P_2O_5$; $SrO \cdot P_2O_5$, Abstracts, p.12
8. Dz. Briljonoks, A. Trukhin ArF lase-induced luminescence of sodium silicate glasses, Abstracts, p.92.

LABORATORY OF SURFACE PHYSICS

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

RESEARCH AREA AND MAIN PROBLEMS

The research interests are focused on problems related to structure, micromechanical and optical properties of surfaces, interfaces and thin films of advanced materials for micro/nanotechnologies (e.g. oxides, halides, metals, alloys, and composite systems). The area of research also includes a development of methods for the modification of surfaces of functional materials and studies of surface and interface effects on properties. The research is mainly based on methods of micro- and nanoindentation, AFM, SEM and XRD.

Main research topics in 2014 were

- Micro- and nano-mechanical characterization of surface layers, thin films and interfaces of advanced materials;
- Modification of surfaces of functional materials (wide band-gap oxides, alkali halides) by irradiation with high energy (MeV-GeV) ions;
- Interaction processes (adhesion, wetting and corrosion) on contact surfaces, including interaction processes with liquid metals.

SCIENTIFIC STAFF

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

PhD Students

M.sc.phys. R.Zabels

Students

B.sc.R.Grants

Technical Staff

A.Petersons

VISITORS FROM ABROAD

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

COOPERATION

Latvia

Daugavpils University, Innovative Microscopy Centre;

Institute of Physics, University of Latvia (Dr.A.Shisko);

NACO Technologies.

Germany

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

Kazakhstan

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

Russia

Institute of Solid State Physics RAN, Chernogolovka (Prof.B.Straumal, Dr.V.Sursajeva)

MAIN RESULTS

DISLOCATION FORMATION IN LiF CRYSTALS IRRADIATED WITH SWIFT IONS

R. Zabels, I. Manika, J. Maniks, R. Grants

Swift- ion-induced formation of radiation defects and their aggregates at high irradiation doses are of importance for ion-induced nanostructuring and radiation resistance studies in materials for nuclear and related applications. Formation of dislocations in LiF irradiated to high-dose with MeV-GeV ^{36}S and ^{238}U ions has been investigated by AFM and chemical etching. The chosen ions form tracks with different morphology. It has been established that in individual tracks of ^{238}U ions, exhibiting track core damage, tiny dislocation loops and their nuclei are created. Increasing fluence till overlapping of tracks leads to pronounced rows of dislocation loops in ion trajectory. Their size reaches 600-1000 nm. The light sulphur ions also cause formation of dislocations. The size of dislocation loops varies along the ion trajectory reaching maximum in the region were calculated energy loss of ions displays a maximum. At moderate fluences (absorbed dose 1.75 MGy) the density of dislocations created by U ions was 1.7×10^{10} cm^{-2} while for S ions - 9×10^{7} cm^{-2}. It confirms that the efficiency of dislocation production is substantially higher in the case of irradiation with heavy ions. Estimates show that a substantial part of radiation defects is included in the system of dislocations.

SCIENTIFIC PUBLICATIONS

SCI publications

1. **R.Zabels, I.Manika**, K.Schwartz**, J.Maniks, R.Grants**. MeV-GeV ion induced dislocation loops in LiF crystals. Nuclear. Inst. and Methods B 326 (2014) 318-321.
2. **J.Maniks**, L.Grigorjeva, **R.Zabels**, D.Millers, I. Bochkov, J. Zicans, T. Ivanova, J. Grabis. Swift heavy ion induced modifications of luminescence and mechanical properties of polypropylene/ZnO nanocomposites, Nuclear. Inst. and Methods B 326 (2014) 154-157
3. V. Sursaeva, A. Gornakova, **F. Muktepavela**, Grain Boundary ridges slow down grain boundary motion: In-situ observation, Materials Letters, 124 (2014) 24-27
4. A. Shishko, **F. Muktepavela,** A. Klukin, **E. Platacis** and A. Sobolev. The effect of the divertor poloidal magnetic field on liquid metal thin film flow. Magnetohydrodynamics, 50(2) (2014) 207-2016

Other publications

5. **E. Platacis**, A. Sobolev, A. Shishko, **F. Muktepavela** . Experimental studies of liquid lithium film flow in magnetic field. Proceedings of Pamir International conference: Fundamental and Applied MHD Vol 2, p.16-19.

Lectures at Conferences

International Conference on Functional Materials and Nanotechnologies FM&NT 29.09.-02.10. 2014, Riga, Latvia.

1. K. Schwartz, J. Maniks, I. Manika. Irradiation Induced Nanostructures in LiF Crystals and Possible Applications. Abstracts p.91.

2. F. Muktepavela, L. Grigorjeva, K. Chernenko, E. Gorokhova, P. Rodnyi.Structure, Nanohardness and Photoluminiscence of Zn N Ceramics Based on Nanopowders. Abstracts p.312.
3. R. Zabels, I. Manika, K. Schwartz, J. Maniks, M. Sorokin, A. Dauletbekova, M. Zdorovets. Depth Profiles of Indentation Hardness and Dislocat ion Mobility in MgO Single Crystals Irradiated with Swift Kr and N Ions. Abstracts p.343.
4. R. Grants, V. Sursaeva, F. Muktepavela. Kinetic Properties of Grain Boundary with Ridges in Zn bicrystal. Abstracts p.362.

Pamir International Conference Fundamental and Applied MHD.
June 16 - 20, 2014 Riga, Latvia

5. E. Platacis, A. Sobolev, A. Shishko, F. Muktepavela. Experimental studies of liquid lithium film flow in magnetic field.

30th Scientific Conference, ISSP, University of Latvia February 19 – 21, 2014, Riga, Latvia

6. R. Zabels, I. Manika, J. Maniks, R. Grants. Mechanisms of Dislocation Formation in LiF Crystals Irradiated with Swift Ions. Abstracts p.47.
7. A. Shishko, E. Platacis, A. Sobolevs, A.Klukins, F.Muktepavela, A. Ziks, S. Ivanovs, F. M. Gryaznevich, L. Zakharov. MHD effects and wetting problems during lithium gravitational flow in the divertor zone of “low-power”(spherical) TOKAMAK. Abstracts p.107.

LABORATORY OF ORGANIC MATERIALS

Head of laboratory Dr. phys. M.Rutkis

SCIENTIFIC STAFF:

Mārtiņš Rutkis	Dr.phys.
Lilita Gerca	Dr.chem.
Oskars Vilītis	Dr.phys.
Aivars Vembris	Dr.phys.
Andrejs Tokmakovs	MSc.
Andrejs Jurģis	
Jānis Busenbergs	

Students:

Mārtiņš Narels BSc
Igors Mihailovs BSc
Jūlija Perveņecka BSc
Arturs Bundulis BSc
Elza Līna Linina

PhD students:

Elīna Laizāne	MSc.
Jānis Latvels	MSc.
Edgars Nitišs	MSc.
Kaspars Pudžs	MSc
Raitis Gržibovskis	MSc

RESEARCH AIM:

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

Research topics:

- Quantum chemical investigation of structure and properties of chromophores;
- Design of thin films;
- Energy structure of thin films;
- Electrical and photoelectrical properties;
- Nonlinear optical phenomena;
- Stimulated emission;
- Thermoelectrical properties;
- 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 Materials Science and Information Technologies IMIS (2010-2014):

Project No.1 “Multifunctional materials for high-tech applications in conversion of radiation energy, information recording, storage, transfer and processing”
Project No.6 “Graphene, modified graphene and graphene containing composites for surface coatings, nanodevices, sensors and energy conversion.”

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

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

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

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

International projects:

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

COLLABORATION:

Latvia:

- Riga Technical University;
- Institute of Organic Synthesis;

- Institute of Physical Energetics;
- Daugavpils University.

Lithuania:

- Vilnius University (Prof. S. Jursenas);
- Kauņas universitāte (Prof. J. V. Grazulevicius);
- Center for Physical Sciences and Technology (Prof. L. Valkunas un Prof. V. Gulbinas).

Taiwan:

National Sun Yat-sen Universty (Dr. Li-Yin Chen).

France:

Institut des Nanosciences de Paris (Prof. N. Witkowski).

England:

Nottingham University (Prof. S. Woodward).

Germany:

Julius-Maximilians Universitaet Wuerzburg (Prof. J. Pflaum).

Bulgaria:

Institute of Organic Chemistry, Bulgarian Academy of Sciences (Prof. V. Dimitrov).

Moldova:

Universitatea Tehnica a Moldovei (Prof. A. Casian).

MAIN RESULTS

ENERGY STRUCTURE AND ELECTRO-OPTICAL PROPERTIES OF ORGANIC LAYERS WITH CARBAZOLE DERIVATIVE

K. Pudzs, A. Vembris, I.Muzikante, R. Grzibovskis, B. Turovska, J. Simokaitiene,
S. Grigalevicius, J.V. Grazulevicius

Phosphorescent organic light emitting diodes are perspective in lighting technologies due to high efficient electroluminescence. Not only phosphorescent dyes but also host materials are important aspect to be considered in the deviceswhere they are a problemfor blue light emitting phosphorescentmolecules. Carbazole derivative 3,6- di(9-carbazolyl)-9-(2-ethylhexyl)carbazole (TCz1) is a good candidate and has shown excellent results in thermally evaporated films. This paper presents the studies of electrical properties and energy structure in thin films of spin-coated TCz1 and thermally evaporated tris[2-(2,4-difluorophenyl)pyridine]iridium(III) (Ir(Fppy)3). The 0.46 eV difference of electron conduction level between TCz1 and Ir(Fppy)3 compounds was obtained from the cyclic voltammetry and photoconductivitymeasurements. Temperaturemodulated space charge limited current (TM-SCLC)method is used tomeasure the local trapping states for charge carrier in the energy gap. The TMSCLC measurements for the system TCz1 + 8 wt.% Ir(Fppy)3 show a trapping state with the value of 0.4 eV which is comparable to the conduction level difference of these materials. It allows to conclude that Ir(Fppy)$_3$ molecules act as electron traps in the TCz1 matrix and the TM-SCLC method is applicable to investigate dopants as trapping states. To show the trap effect, an organic light emitting diode was made where the electroluminescent layer was a spin-coated host-guest system of TCz1 with incorporated 8 wt.% Ir(Fppy)$_3$.

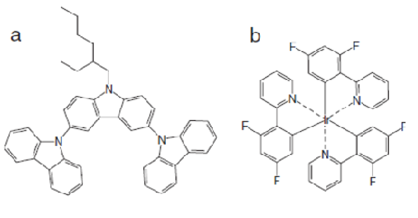


Fig. 1. Chemical structure of (a) the carbazole derivatives TCz1 and (b) the electro phosphorescent compound Ir(Fppy)3.

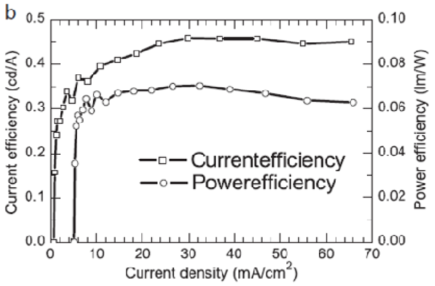


Fig. 2. Dependence of current and power efficiency on the current density of the ITO/PEDOT:PSS/TCz1 + Ir(Fppy)3/LiF/Al device.

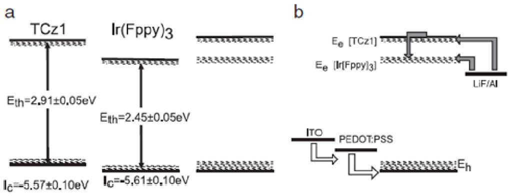


Fig. 3. (a) Energy diagramof the TCz1 compound and the Ir(Fppy)3 compound in solid state. (b) Energy diagrams of the device ITO/PEDOT:PSS/TCz1 + 8 wt.% Ir(Fppy)3/LiF/Al. Gray filled arrows show injection of the electrons and unfilled arrows — injection of holes. Ee and Eh are the conduction levels of electrons and holes respectively.

The values of the ionization energy characterizing the hole conducting energy level are similar for TCz1 and Ir(Fppy)3 - 5.57 and 5.61 eV respectively. The difference of the electron affinity energy of the TCz1 and Ir(Fppy)3 was obtained from the ionization energy and the threshold energy of photoconductivity. The value of this difference is 0.46 ± 0.10 eV and it is close to the estimated electron local trap state 0.40 ± 0.04 eV. One can conclude that this energy level corresponds to the Ir(Fppy)3 molecules as the electron trap in the TCz1 matrix. The charge carrier trap concentration is several orders of magnitude lower than the concentration of Ir(Fppy)3 molecules. There could be two explanations: not all molecules work as traps or there could be aggregates formed by Ir(Fppy)3 molecules where each of them is working as only one electron trap object. This local trapping state is very important in electroluminescence because it corresponds to the electron affinity level in the electroluminescence material— Ir(Fppy)3. Electrons fromthe electron conductivity level of TCz1 are caught in these traps thereby increasing electron density on the electron affinity level of Ir(Fppy)3 molecules thus providing electrons for electroluminescence.

HYBRID SOI/POLYMER ELECTRO OPTICAL INTENSITY MODULATOR OPERATING AT 780 nm

E. Nitiss, J. Busenbergs, M. Rutkis

Broadband electro optical (EO) modulators are among the key elements for the future development of the communication technology. In order to satisfy the ever growing need for an increase in data transfer rate, there is a demand for a high speed, low loss and low production cost EO modulator. Several directions of EO modulator technology development have been advanced in the last decade. It has been shown that a further increase in data transfer speeds of modulators based on inorganic EO components may be achieved by optimizing the structure and introducing new concepts and materials with enhanced nonlinear properties. Nevertheless the main disadvantages such as high fabrication costs and dielectric losses would still remain. Furthermore, the high dielectric constants of inorganic non-linear optical (NLO) materials set limits to the maximal bandwidth obtainable in a travelling wave modulator design. Due to the low EO coefficients of the inorganic materials, the light and the electric field interaction length should be long in order to achieve low driving voltages thus causing the light wave and the microwave propagation velocity to mismatch. Thus a considerable attention has been devoted to new EO active organic materials due to their multiple advantageous properties such as a low cost, an easy processability, low dielectric constants and a high nonlinearity. Devices based on highly nonlinear organic EO materials with EO coefficients up to 300 pm/V could satisfy the future bandwidth and chip scale requirements.

In this contribution we have proposed a design for a new type of hybrid silicon-on-insulator (SOI)/polymer waveguide EO modulator that could operate both in the visible and the infrared wavelength range. The preparation steps of the modulator waveguide are shown in Fig. 1. The MZI modulator design is shown in Fig. 2. The design was optimized for highest bandwidth, lowest optical loss including the light splitting loss (see Fig. 3.) and other parameters. By optimizing the travelling wave modulator structure parameters using a rough modulator bandwidth estimation model, we have shown that it is theoretically possible to achieve a halfwave voltage-interaction length of 1.56 V·cm and a bandwidth of 1.9 Ghz for MZI modulator with 0.5 cm long arms and an EO coefficient of 100 pm/V. The advantages of the proposed modulator structure that should emphasized are the simplicity of preparation, low drive voltages values and the expected low light propagation loss. Unfortunately, such design also possesses an important drawback. The operational bandwidth of the MZI type EO modulator on SOI platform would not exceed a couple of GHz. Thus we doubt that it could be

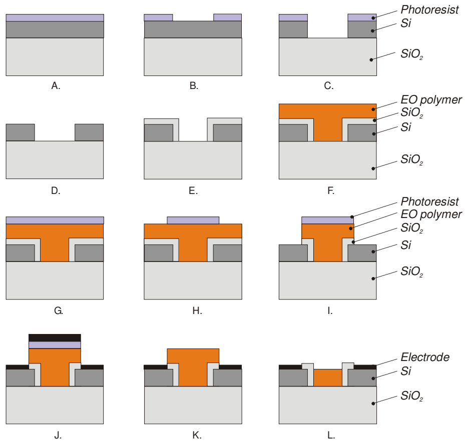


Fig. 1. Preparation steps of SOI/polymer waveguide: A photoresist masking layer is applied on the SOI wafer (A). Si layer is patterned using conventional lithography steps (B-D) thus yielding a trench for further waveguide formation. The SiO$_2$ cladding layer is obtained by thermal oxidation of Si (E) for a fixed period of time to obtain the required thickness of SiO$_2$. Afterwards, a ridge waveguide core is created in the formed trench by the spin coating or a blade casting of EO polymer (F). Additional photolithography steps are applied (G-I) in order to remove the polymer and SiO$_2$ layers where contact metal electrodes will be applied (J). The photoresist layer is removed (K) and, if necessary, the EO polymer thickness is reduced via etching (L). The step (L) is optional and could be applied in order to obtain a waveguide core with desired parameters.

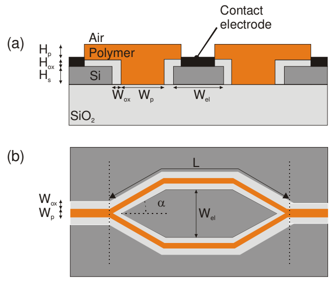


Fig. 2. (a) The Cross-section and (b) the top view of the MZI SOI/polymer waveguide intensity modulator: W_p – polymer waveguide width, W_{el} – central Si electrode width, H_s – Si electrode height, W_{ox}=H_{ox} – SiO$_2$ cladding thickness, H_p – EO polymer thickness above the trench, L – length of the MZI modulator arm.

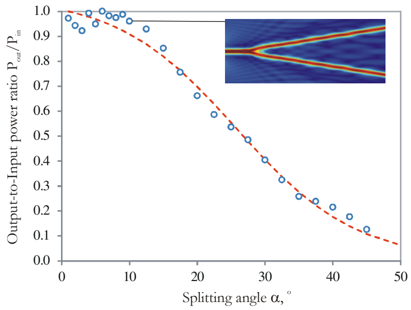


Fig. 3. The 2D numerically simulated output to input power ratio P_{out}/P_{in} as a function of splitting angle α, n_p=1.67.

used for an ultra-high speed light modulation. Despite this we believe that such active waveguide structure and preparation technology could find its applications for making light switches, array waveguides for dense wavelength division multiplexing etc.

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REAEARCH AREAS

Materials

1. Production of new modified ferroelectric ceramics by doping with monoxides, developing binary or multicomponent solid solutions:

– complex lead-containing perovskite family with general chemical formulas
PbB'1/2B''1/2O3 (where B'=Sc+3, Lu+3, Yb+3, Tm+3 etc.; B''= Nb+5, Ta+5) and
PbB'1/3B"2/3O3, (where B'=Mg+2, Zn+2, Ni+2, Cd+2 etc., B"- Nb+5, Ta+5 and etc);
– modified (Pb,La)(Zr,Ti)O3 (PLZT);
– lead-free perovskite ceramics based on $(K_{0.5}Na_{0.5})NbO_3$, $(Na_{0.5}Bi_{0.5})NbO_3$, or $BaTiO_3$;
- $BiFeO_3$, $Bi(Fe_{0.5}Cr_{0.5})O_3$,$SrMnO_3$,

2. Thin films, multiferroic materials, inorganic functional and nanomaterials

Methods

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

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

Problems

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

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MAIN RESULTS

PREPARATION AND ELECTRIC PROPERTIES OF BARIUM ZIRCONIUM TITANATE CERAMIC

B.Garbarz-Glos, W.Bąk, M.Antonova, A.Budziak, K.Bormanis, C.Kajtoch

Barium titanate is a well-known, intensively studied and technologically important ferroelectric material with a perovskite structure. The doped $BaTiO_3$ systems - barium zirconium titanate - has attracted considerable attention in both bulk and thin film, due to its potential applications for various device in particular as piezoelectric transducers, tunable filters, phase shifters, terrestrial and satellite communications (operating in the microwave frequency range), the GPS system and radiolocation. Substitution of Ti^{4+} with Zr^{4+} in $BaTiO_3$ exhibits an interesting behavior in the dielectric study. All the three phase transitions correspond to pure $BaTiO_3$ are merged or pinched into single phase transition depending on the content of zirconium. Therefore, in this study the structure and dielectric properties of pure barium titanate and barium zirconate titanate ceramics (for selected compositions) were investigated. These ceramics were prepared by solid-phase reaction from simple oxides and carbonates using the conventional method. The structure and morphology of sintered samples were characterised by X-ray diffraction (XRD) and scanning electron microscopy (SEM). The dielectric measurements, in the frequency range between 20 Hz and 1 MHz, were performed by means of QUATRO KRIO 4.0 temperature system together with precise LCR Agilent 4284A meter, BDS 1100 cryostat and WINData 5.62 Novocontrol software. The heating and cooling agent used was nitrogen. The data were taken at stabilized temperature points within the range from 500 K to 140 K with 5 K step. The application of dielectric spectroscopy made possible to determine independently both real and imaginary parts of the response function of various excitations related to polarization in solids in particular the study of quantitatively ferroelectric dispersion.

ELECTRICAL CHARACTERIZATION OF FE DOPED BT CERAMIC BY IMPEDANCE SPECTROSCOPY

D.Sitko, W.Bąk, B.Garbarz-Glos, M.Livinsh, I.Smeltere, C.Kajtoch

The ABO_3-type compounds with perovskite structure are one of the most interesting group of materials. Among them, the titanates are of great interest from the point of view of fundamental research as well as regarding their possible applications. Barium titanate ($BaTiO_3$, BT) was the first developed piezoelectric ceramic and even now due to its excellent ferroelectric properties and the high electric permittivity at room temperature it is still widely used as capacitors, thermistors, chemical sensors, and piezoelectric devices.

The electric behavior of the of Fe-doped and undoped $BaTiO_3$ were investigated as a function of frequency and temperature. These ceramics were prepared by solid state reaction using the conventional method. The microstructures were observed on the surface of the polycrystalline specimens, with use of a scanning electron microscopy Model Hitachi S4700 with a field emission and a Noran Vantage EDS system .The performed EDS investigations revealed that the all investigated samples were perfectly sintered. They contained a little glassy phase and their grains were well shaped. The impedance measurements were carried out in the temperature from 150K to 600K, and in the frequency range from 0.1Hz to 10MHz. All the electric measurements of the samples were performed with use of an Alfa - AN modular measurement system with a temperature control system Quatro Krio 4.0 range from 0.1Hz to 1-MHz. Based on these parameters the electrical properties of the grains and grains boundaries were described. The grain and grain boundaries relaxation frequencies were shifted to higher frequency with increasing temperature. Bulk resistance of ceramics and the thermal activation energies were determined.

THERMAL PROPERTIES OF RELAXOR $PbNi_{1/3}Nb_{2/3}O_3$ SOLID SOLUTION CERAMICS *)

K. Bormanis, S.N. Kallaev, Z.M. Omarov, A.R. Bilalov,
S.A. Sadykov, and R.G. Mitarov

Ceramic ferroelectric relaxors of specific crystal structure and unique physical properties make a promising class of functional ferroelectric materials the multicomponent perovskite solid solutions of mixed oxides, such as $PbNi_{1/3}Nb_{2/3}O_3$, being special interest. The studies of the behavior of heat capacity and dielectric permittivity of $PbNi_{1/3}Nb_{2/3}O_3$-$PbTiO_3$ (PNN-PT) solid solutions over a wide temperature range from 150 to 800 K are reported.

The temperatures characterizing the anomalies of dielectric permittivity ε(T) and of heat capacity $C_p(T)$ are found for the (1-x)PNN-xPT system at x = 0.3, 0.4, 0.5, the temperatures T_m of the maximums of dielectric permittivity of which are around 315, 385, and 455 K, respectively. The 0.7PNN-0.3PT composition has a noticeable frequency-dependence of the broad phase transition peak of dielectric permittivity not being observed in compositions of x = 0.4 and 0.5. The extended shape of the anomaly of heat capacity at $T_m \approx 315$ K in the 0.7PNN-0.3PT composition is typical to ferroelectric relaxors.

The temperature dependence of the heat capacity $C_p(T)$ of the 0.7PNN-0.3PT ceramics has an λ anomaly at T≈225 K another anomaly being discovered extending from 250 to 650 K around T≈520 K. A quantitative analysis of the temperature dependence of heat capacity and separation of the anomalous contribution from phonon contribution, as in most cases, is made by estimating the phonon heat capacity of the compounds as the sum of the Debye and Einstein functions the anomalous component being found as the difference between the measured and calculated phonon heat capacities $\Delta C = C_p - C_p^o$. Local distortions of the structure revealed in the Brillouin scattering spectra are found in two regions of the ΔC(T) anomaly: 250-450 K coinciding with the ε(T) and within 450-650 K. The temperature dependence on temperature of the ΔC anomaly separated from the phonon contribution is described by expression for the Schottky heat capacity of two-level states separated by an energy barrier.

*) In cooperation with Institute of Physics, Dagestan Science Centre, RAS, Makhachkala, Russia and Dagestan State Technical University, Makhachkala, Russia.

ELECTROLUMINESCENCE OF $(\mathbf{Pb_{0.91}La_{0.09}})(\mathbf{Zr_{0.65}Ti_{0.35}})\mathbf{O_3}$ RELAXOR CERAMICS *)

K. Bormanis, S.A. Sadykov, S.N. Kallaev, S.M. Alieva, A.Sh. Agalarov,
M. Livinsh, and M. Antonova

Lanthanum doped lead zirconate titanate (PLZT) relaxor ceramics with $(Pb_{0.91}La_{0.09})(Zr_{0.65}Ti_{0.35})O_3$ composition exhibits a repolarization induced by electroluminescence with a pronounced discrete character of emission. It is established that this behavior is related to the reorientation of nanodimensional polar regions in a strong pulsed electric field in the vicinity of a smeared phase transition [1,2].

The time and temperature dependences of the electroluminescence are studied; the intensity of luminescence at switching polarization in PLZT ceramics as a function of temperature over the wide range including the maximum point of dielectric permittivity under condition of fast rise (0.1 kV/cm per μs) of a strong applied field is presented.

There is a critical (dynamic coercive) field E_c at which the domain reorientation starts (decreasing with rising the temperature), which is similar to ferroelectrics and indicates to decreasing internal bias fields. The temperature being higher the polarised state (determined from the duration of electroluminescence) at switching the strong applied field within ~50 μs is achieved faster – formation and evolution of the relevant domain structure is intensified by temperature.

The discrete character of electroluminescence from PLZT within the entire range of temperatures studied is supposed to be related to temperature-induced variation in dimensions and the number of nano-polar regions increasing the number of charged phase boundaries when polar domains are split as the temperature increases. Under a rapidly growing applied field the microscopic regions of individual critical field intensities E_c are successively involved in formation of the domain structure and further rearrangement the distribution of the internal and coercive fields determining the scatter of separate emission peaks in time.

*) In cooperation with Institute of Physics, Dagestan Science Centre, RAS, Makhachkala, Russia and Dagestan State Technical University, Makhachkala, Russia.

INTERPRETATION OF THE ELECTROCALORIC EFFECT IN NBT-ST-PT SOLID SOLUTIONS

Marija Dunce, Eriks Birks, Jani Peräntie, Juha Hagberg, Maija Antonova, Andris Sternberg

There is a lot of attempts to create $Na_{1/2}Bi_{1/2}TiO_3$ (NBT) -based compositions with improved properties for different applications. The aim of the present study is to analyze the relationship between polarization and electrocaloric effect (ECE) in 0.4NBT-(0.6-x)$SrTiO_3$-x$PbTiO_3$ (0.4NBT-(0.6-x)ST-xPT) solid solutions. Earlier a wide stability range of the relaxor state depending on $PbTiO_3$ concentration was found in these solid solutions. The pronounced electrocaloric effect at high concentrations of $PbTiO_3$, as well as extremely low values of the electrocaloric effect at low concentrations of $PbTiO_3$ were observed, which does not correspond to the variation of polarization depending on $PbTiO_3$ concentration. The measured values of the electrocaloric effect do not correspond also to the values, calculated from frequently used thermodynamic equations.

It is shown that behaviour of ECE in compositions where FE state can not be induced even by electric field, corresponds to compositions where FE state exists in temperature region far above T_t. $\Delta T(P)$ dependence in the region of electric field-induced phase transition corresponds to change of volume of FE phase. Evaluation of polarization from ECE in FE phase allows us to conclude that polarization hysteresis loops are not always reliable measurement of polarization.

DIELECTRIC AND ELECTROMECHANICAL PROPERTIES IN NBT-BT SOLID SOLUTIONS WITH Na AND K NIOBATES

M. Dunce, E. Birks, M. Antonova, and A. Sternberg

The wide attention is paid to ternary solid solutions $Na_{0.5}Bi_{0.5}TiO_3$ with $BaTiO_3$ and $K_{0.5}Na_{0.5}NbO_3$ in the concentration range of the morphotropic phase boundary, with

K0.5Na0.5NbO3 (KNN) added. 2 mol% of KNN is sufficient to shift the depolarization temperature below room temperature. As a result, a large deformation can be achieved at the electric field-induced phase transition between relaxor and ferroelectric states. In spite of the large number of studies, the choice of KNN in this solid solution, instead of pure NaNbO3 (NN) or KNbO3 (KN), is still not clear. In this work addition of NN, KNN or KN to NBT-BT solid solution is compared. It is shown that role of $K_{0.5}Na_{0.5}NbO_3$, $NaNbO_3$ or $KNbO_3$ reduces mainly in suppressing of ferroelectric properties like in other perovskite ferroelectrics where Ti is replaced by Nb, and development of relaxor state. Besides frequency dependent dielectric permittivity relaxor state is characterised by dependence of critical fields, corresponding to phase tradition between relaxor and ferroelectric state, on temperature, reflecting metastability of ferroelectric phase. Na/K plays only marginally role in change of physical properties and phase diagram of those ternary solid solutions. Comparing considered $K_xNa_{1-x}NbO_3$ compositions, $NaNbO_3$ is preferred because in this case field induced phase transitions are less smeared due to more homogeneous composition with less atomic species involved. The influence of Nb is compared with compositions outside morphotropic phase boundary, by study of solid solutions $(0.80Na_{0.5}Bi_{0.5}TiO_3 – 0.20BaTiO_3)_{1-y}$- $(K_xNa_{1-x}NbO_3\ )_y$.

X-RAY DIFFRACTION AND RAMAN SPECTROSCOPY STUDIES IN $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ SOLID SOLUTIONS

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

$Na_{1/2}Bi_{1/2}TiO_3$ (NBT) and its solid solutions attract a lot of interest as an alternative for nowadays widely used lead-containing ferroelectric materials, use of which is gradually limited due to environmental considerations. Besides, understanding and characterisation of phase transitions in pure or modified NBT are challenging topics of studies in the physics of ferroelectrics.

Previously a transfer from relaxor to ferroelectric state, passing different stages of relaxor behaviour, was established in triple solid solutions $0.4Na_{1/2}Bi_{1/2}TiO_3$-$(0.6\text{-}x)SrTiO_3$-$xPbTiO_3$ (0.4NBT-(0.6-x)ST-xPT) by studying their dielectric properties. In this study, 0.4NBT-(0.6-x)ST-xPT solid solutions were investigated by x-ray diffraction and Raman spectroscopy. Although compositions with low concentration of PT exhibit pure relaxor behaviour even without electric field-induced phase transition to ferroelectric state, some traces of tetragonal phase were observed in x-ray diffraction patterns. An amount of tetragonal phase and a degree of tetragonality upon temperature variation were determined for several compositions with different content of PT, using the Rietveld method.

From the x-ray diffraction measurements we found that the tetragonal phase in 0.4NBT-(0.6-x)ST-xPT solid solutions is present at the long range order at low temperatures for all PT concentrations, including compositions, which remain in a relaxor state even in the presence of electric field. The fraction of the tetragonal phase and tetragonality increase with increasing of PT concentration. An influence of local inhomogeneous lattice strains on the broadening of x-ray diffraction maxima and concentrations of tetragonal and cubic phases was studied. It was detected that Raman spectrum, representing local tetragonal symmetry, is almost concentration-independent at room temperature. Upon temperature increase the spectrum becomes featureless for all studied compositions. Approaching of cubic structure at elevated temperatures is observed either at the long or short range order.

AGING AND MEMORY EFFECTS IN ELECTRO-OPTICAL PLZT 8/65/35 CERAMICS MODIFIED WITH 3D TRANSITION-METAL IONS

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The temperature and frequency dependencies of the dielectric susceptibility in relaxor electro-optical PLZT 8/65/35 (La8) modified with 3d transition-metal ions (Mn, Fe, Co, Ni) ions measured to study the aging and memory (AM) effects are reported. The studies of aging at room temperature show that 3d admixtures (Me) in La8 ceramics at small to medium concentration range (Me < 1.0 wt.%) changes the depth of dispersion, the aging amplitude and the temperature range of the memory effect. At Me concentrations exceeding 1.0 wt.% the aging and memory effect are significantly reduced (or eliminated) at Me → 1.0 wt.%.

The obtained results suggest that the changes of the aging effects are determined by two substantial acceptor effects of the introduced 3d ions: 1) formation of Me^{2+} - V_O type dipoles (V_O - oxygen vacancy); 2) Jahn-Teller (JT) effect.

THE EFFECT OF CU ADMIXTURE ON RELAXOR PROPERTIES OF THE ELECTROOPTICAL PLZT 8/65/35 CERAMICS

Vilnis Dimza, Lelde Kundzina, Maris Kundzins, Karlis Kundzins, Maris Livins, Maija Antonova and Aina Plaude

Behaviour of the complex dielectric permeability ε* = ε′ – iε″ and polarisation in relaxor electro-optical PLZT 8/65/35 ceramics modified by admixture of Cu studied within the 20 – 400oC range of temperatures at frequencies from 130 Hz to 1 MHz is reported. Admixture of Cu is found 1) to shift the maximums of ε′(T) and ε″(T) curves to a higher temperature, 2) to increase polarisation, 3) to affect essentially the dielectric relaxation behaviour of PLZT as a result of a combined effect of relaxor dispersion and Debye-like dispersion; 4) to produce dispersion of the 1/ωn type ($\omega = 2\pi f$ is the angular frequency; $0<n<1$) at high temperatures. Involvement of different dispersion mechanisms at increasing Cu concentration is explained by diversity of the mechanisms compensating the effects of Cu acceptors possible implications of the Maxwell-Wagner dispersion being discussed. The shift of the ε′(T) maximum and the increase of polarisation are explained by the Jahn-Teller effect (the axial Cu2+ being Jahn-Teller ions).

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<u>MASTER THESIS</u>

Lelde Kundzina, INVESTIGATION OF AGEING AND MEMORY EFFECTS IN MN DOPED PLZT 8/65/35 ELECTROOPTICAL CERAMIC, RTU, 2014

LABORATORY OF VISUAL PERCEPTION

Head of Laboratory Prof. M.Ozolinsh

Human vision is a complex phenomenon. Its optical part is essential, however optical image stays only at the very beginning of the visual pathway and information processing in the cortex. We see with our brains, and as a result in some provocative cases it is very hard for us to accept the final outcome. Laboratory is a joint between colleagues in institute and Department of Optometry and vision science of the University. Most of Department's Master thesis have been accomplished due to collaboration between units. In 2012 more than 20 Bachelor's and 10 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;
- studies of binocular and stereovision, suppression and rivalry mechanisms of binocular vision, evaluation of suppression strength and depth effect on quality of vision binocular functions;
- fast eye kinematics studies for children and adults without and with several disorders of visual perceptions, eye kinematics studies in sport vision.
- evaluation of accommodation/convergence mechanisms reading print materials and for regular computer users;
- digital visual stimuli image processing determinant for analyse of the human visual response;
- multispectral material surface reflectance and emission analysis in visible and near IR and UV range, and its visual recognition by humans with normal and colour deficient vision;
- providing illumination and material visual appearance testing expertise and quality of products correspondence according to standards.

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SCIENTIFIC PROJECTS

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

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MAIN RESULTS

MODELLING THE APPEARANCE OF CHROMATIC ENVIRONMENT USING HYPERSPECTRAL IMAGING.

Ausma Gutmane, Kaiva Jurashevska and Sergejs Fomins

Color vision test called KAMS was created to determine color resolution threshold for each individual with red-green color vision defects. The aim of the study is to determine how long the test will be useful for it’s purpose?

Purpose: Analyse changes over time of isochromatic color pair’s physical parameters and changes in color perception of participants with color vision defects.

Method: Take 2 different physical measurements once in a month for both printed copies of obtained isochromatic color pairs:

1. The chromaticity coordinates (x, y) and brightness (Y) by Konica Minolta CS - 100A colorimeter at standard light source D65 (T = 6500K) in the Super Daylight GT - 100W1 light box.
2. The color values with the multispectral camera CRI Nuance Vis 07 with Nikon AF Micro-Nikon 60mm F2.8D objective at standart light source D65 in the Super Daylight GT - 100W1 light box in a range of wavelength from 420 to 720 nm (with a step of 10 nm).

And secondly, to perform psychophysical measurments on people with color vision deficiency.

Results: Color samples were measured 9 times (from the May 2013 to January 2014). Changes in ΔE of isochromatic color pairs were insignificant during these 9 months. For example, for one individual green - gray color plate that was held in daylight ΔE value for the light sample pair measured in May is 27 units, but when measured in January it is 23 units. From so far analysed data we can observe tendency that the green colored samples might be fading faster than red colored samples.

POSITIVE AND NEGATIVE CHROMOSTEREOPSIS USING LED DISPLAYS

Maris Ozolinsh, Kristine Muizniece and Gunta Krumina

Illusory depth sense observing colour planar image such as images presented on computer screen is determined and analyzed. The colour difference threshold needed to induce the depth sense is determined. The induced effect polarity reversal – the source image red plane in front of blue plane is observed by partial covering of eye pupils nassaly or temporary. It is explain by the changes of eye point spread function taking into account coloured ray source and longitudinal chromatic eye aberrations. Illumination conditions affect the inducing of colour stereopsis due to changes of pupil size.

VISION SCIENCE AND PSYCHOLOGY APPROACH TO ADAPTATION PROCESSES

M. Ozolinsh, D. Lauva and O. Danilenko

We have experimentally studied visual adaptation processes and compared results in various visual perception tasks. Adaptation stimuli were demonstrated on computer screen and differed each from other by their luminance, colour, duration and dynamics related to the excited retinal and consequently the cortex neural cells and corresponding visual areas. Depth and characteristic times of adaptation processes depend on visual perception task. The slowest characteristic times (in range up to 10 sec and more) from studied processes are for adaptation to size of moving targets exciting retinal cells by equiluminant and isochrome stimuli, that are processed along parvocellular and magnocellular visual pathways. We assume that neural cell physiology lays on the base of this kind of size adaptation. Another kind of size adaptation where retinal cell excitation is static realizes in Ebbinghaus illusion. Here parallel to ongoing adaptation process brain uses also previously acquired knowledge to make shift in decision about stimuli size, and physiological effects dominate over psychological effects in perception of such stimuli. Over- or underestimating sizes in Ebbinghaus illusion with non-moving stimuli realizes much faster, and the degree of perception errors practically does not depend whether margnocellular or parvocellular visual pathway are activated – contrary to adaptation to dynamic moving targets.

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

Varis Karitans, Liene Jansone, Maris Ozolinsh and Gunta Krumina

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

PUBLICATIONS

1. Trukša R., **Fomins S.**, Krūmiņa G., Dzenis J. „Picture segmentation applications in optometry and vision science" *Laboratorine medicina*, Vol.**16**, Nr.1(61), p.38-42, ISSN 1392-6470 (2014) .
2. **Ozolinsh M.**, Muizniece K., Krumina G. „Distortion of color images on flat computer screen due to chromostereopsis" . *European Scientific Journal*, Vol.**10**(SE1), p.533-538, ISSN 1857-7881 (2014).
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4. **Ozolinsh M.**, Paulins P. "Multicolour LEDs in educational demonstrations of physics and optometry". *Proc SPIE.* Vol.**9289**, 92891D, (2014), doi:10.1117/12.2070522.

5. **Karitans V**., Jansone L., **Ozolinsa M**. and Krumina G. “Validation of a method for measuring the retinal thickness with Shack–Hartmann aberrometry in an artificial eye.” *Journal of Modern Optics* Vol.**62**, p.1-14 (2015), doi: 10.1080/09500340.2014.1003253.
6. **Ozolinsh M**., Muizniece K. “Color Difference Threshold of Chromostereopsis Induced by Flat Display Emission”. *Frontiers in Psychology* Vol.**6**, p.1-8, article 00337, ISSN 1664-1078; doi:10.3389/fpsyg.2015.00337.

PATENTS.

EP13193137.0 S.Fomins, M.Ozoliņš, MULTISPECTRALLY TESTED, PRINTED COLOUR VISION TEST FOR THE FINE EVALUATION OF THE DEGREE OF DEFICIENCY.

PARTICIPANCE IN INT. CONFERENCES

1. DOC-2014. Riga, April 2014.
2. FMNT-2014, Riga, October 2014.
3. VPO-2014,Wroclaw, August 2014.

1st Global Multidisciplinary Academic Meeting, GAM 2014, CaboVerde, April, 2014

DEPARTMENT OF SEMICONDUCTOR MATERIALS

Head of Department Dr.phys. A.Lusis

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.

• Functional fibers (glas and hemp) and textiles for technical application.

• Material characterization by spectroscopic methods (Raman scattering, Furrier IR, optical and Xray absorption, EXAFS), electrical and electrochemical impedances, Mott-Schottky plott, photoelectrochemical, SEM, AFM, TGA/DTA, etc

• Solid state ionics:
  - electro-, photo-, thermo-, chemo- or gaso-chromic phenomena in transition metal oxides
  - structural changes due to ion intercalation
  - lattice dynamics and structural and electronic phase transitions
  - solid state reactions at interfaces electrode – solid electrolyte
  - gases and ions sensing phenomena and detection technologies

• Hydrogen absorption phenomena in metals, semiconductors and insulators

• Development of hydrogen generation equipment and new nano structured materials for hydrogen storage

• Renewable energy technologies (solar, static electricity, water, microbial fuel cells);

• Development of cathode materials for Lithium and Sodium thin film batteries;

• Odour removal with low temperature plasma discharge technologies.

• Kinetic of gas medium reaction with solid surface, glas fiber reactions with the environmental gas.

RESEARCH TOPICS

- Ion transfer in solids, over two phase interfaces and composites as well as structural changes due to ion intercalation, lattice dynamics and structural and electronic phase transitions.
- Ion transfer problems related to electro-, photo-, chemo-, thermo-chromic phenomena in transition metal oxides as well as to solid state reactions at interfaces electrode – solid electrolyte and electrode water.
- Application of electrical and electrochemical impedances for characterization of ionic systems, nanostructured and porous materials, composites.
- Development of nanostructuring methods and coating technologies for functionalization of plate glass and fiber glass surfaces as well investigation influence of ultrasound on leaching processes, pores structure and ion exchange of glass fibers.
- Application of thermal analyses (TGA/DTA) and sorptometry for investigation of porous materials and absorbing capacity of functional species.
- Investigation of stability of materials for electrochemical multi layer systems and electrochromic coatings as well as intergrain activity in solid electrolyte layers based on polymer composites.
- Development methods and techniques for functilization
- Thin films preparation by magnetron sputtering techniques.
- Servicing of common research facilities: thin film vacuum coating machines, TGA/DTA equipment and powerful ultrasound bath-reactor.
- Membranes and membrane/electrode systems for fuel cells and gas seperation.
- The technologies for hydrogen production, storage, transportation, applications in transport and stationary applications; for energy storage and electricity/heat generation; synthesis and research of new materials for hydrogen technologies (electrodes in electrolysers and microbial fuel cells, structured nanomaterials for photoelectrolysis, hydrogen storage media, polymer membranes and membrane-electrode assemblies for fuel cells);
- Lithium intercalation materials and their application for thin film rechargeable battery; the technologies for electricity generation from renewables (solar, static electricity, water, algae and microorganisms);
- Odour removal with adsorbents and corona discharge technologies;

- X-ray Absorption Spectroscopy of functional materials and development of advanced EXAFS data analysis methodologies, based on Molecular Dynamics and Reverse Monte Carlo methods.
- Confocal laser spectromicroscopy.
- The use of high performance computing for functional materials simulations.
- The magnetic ions exchange interaction in the antiferromagnetic oxides MeO-MgO solid solutions were studied using of optical absorption, luminescence, EPR and Raman spectroscopies: exchange interaction between radiation defects and transition metals ions in the dielectric crystals doped with the transition metals ions
- EPR , FTIR, Raman and optical spectroscopies study of human blood after irradiation
- The use of high performance computing for functional materials first principles and Molecular Dynamics simulations.
- Investigations of tritium release properties of neutron multiplier beryllium materials for fusion reactor development. Analysis of tritium distribution in plasma-facing carbon-based components.

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LABORATORY OF SOLID STATE IONICS

Head of laboratory Dr. phys A. Lusis

ABSORPTION OF WATER AND CARBON DIOXIDE IN CARBONATED GLASS FABRIC

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

The object of research was industrially produced fabrics of Na-Al-Si glass fibers. It is known that Na+ ions diffuse to surface of fibers [1] and due to reaction with H_2O and CO_2 from atmosphere form here the thin (about 1μm) carbonated shell [2], consisting of trona ($Na_3H(CO_3)_2 \cdot 2H_2O$) determined by thermo gravimetric analysis. The investigations showed [2], that the experimental weight uptake–time ΔM (t) curves for the beginning period up to some tenths of hour after heating of samples are well-fitted ($R^2 > 0,99$) to regression of

$$\Delta M(t) = A_0 - A_1 \exp(-t/t_1) - A_2 \exp(-t/t_2). \qquad (1)$$

A_0, A_1, A_2 in (1) are weight constants and t_1, t_2 are time constants ($t_1 \leq t_2$), $\lim \Delta M(t)=A_0$ when $t\to\infty$ and $\lim \Delta M_1(t)=A_1\exp(-t/t_1)= A_1$, and $\lim \Delta M_2(t)=A_2$, when $t\to 0$. In relation $A_0=A_1+A_2$.

The current work was devoted to explain the meanings of parameters in relation (1) and using the relation (1) to explain the weight uptake processes. The different fabric weight recovery atmospheres showed that the first component (with shorter t_1) of relation (1) is sensitive to concentration of CO_2 and second one to H_2O. The weight recovery by CO_2 is much more fast compare to H_2O ($t_1 \ll t_2$), but amplitude of weight recovery is many times less ($A_1 \ll A_2$). The time constants (t_1, t_2) and amplitudes (A_1, A_2) of both absorption processes highly increase after heating of samples at temperatures over beginning of decomposition of trona before. The reasons of observed dependences there are discussed.

The high degree of coincidence ($R^2>0.999$) of experimental points and regression function indicates to successful use of method to investigate the absorption processes in similar structures.

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[1] B. W. Veal, D. J. Lam and D. P. Karim, J.Nuclear technology. **51,** 136 (1980)

[2] E. Pentjuss, A. Lusis, G. Bajars and J. Gabrusenoks, IOP Conf. Series: Materials Science and Engineering. **49** 012044 doi:10.1088/1757-899X/49/1/012044 (2013)

FIRST TIME CHARACTERISATION HEMP FIBRES NONWOVEN TEXTILE MATERIAL

Uljana Iljina, Andrejs Lusis, Janis Balodis, Evalds Pentjuss

Hemp fiber nonwovens etched and coated with metals and oxides SEM micrograhp (Fig.1 – Fig.3) analysed moisture content by TGA. There are presented some first time overview SEM micrograph structure and coatings influence on it.

The research shows that even, relatively thin and flexible nonwovens can be obtained from double folded complex carding webs using hydroentanglement method at 20 bar pressure and speed of 2m/min. Unlike fabric samples, nonwoven samples attract similar water quantity irrespectively of surface modification. The smallest active resistance at low frequencies is typical for samples with coatings on both sides. The samples which were kept in normal climatic conditions can be characterised by reactive (capacitive) resistance, though after keeping them in moisture the resistance decreases and at low frequencies becomes active. The samples with active resistance under normal climatic conditions increase resistance under humidity influence.

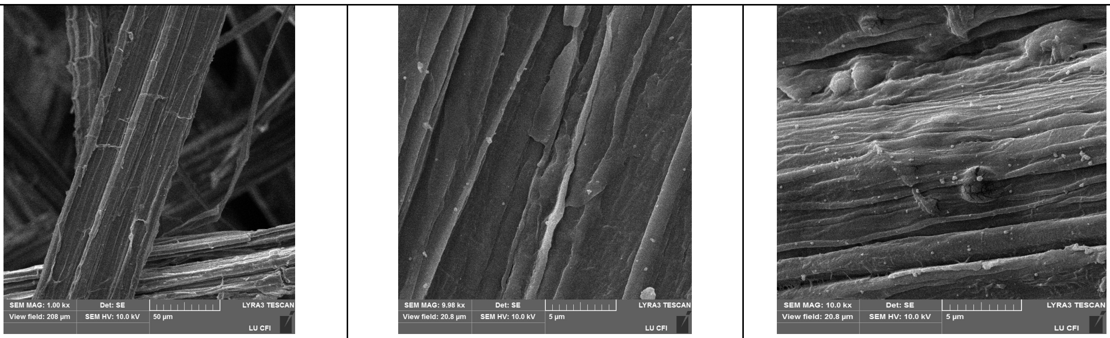

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Fig. 1. Hemp nonwoven with out coating for differant SEM scales

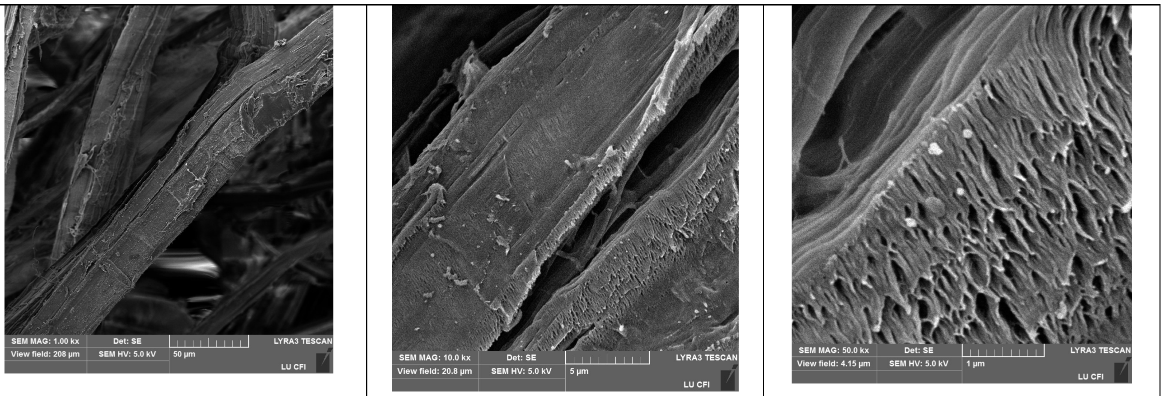

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Fig. 2. Hemp nonwoven etched with argon plasma for differant SEM scales

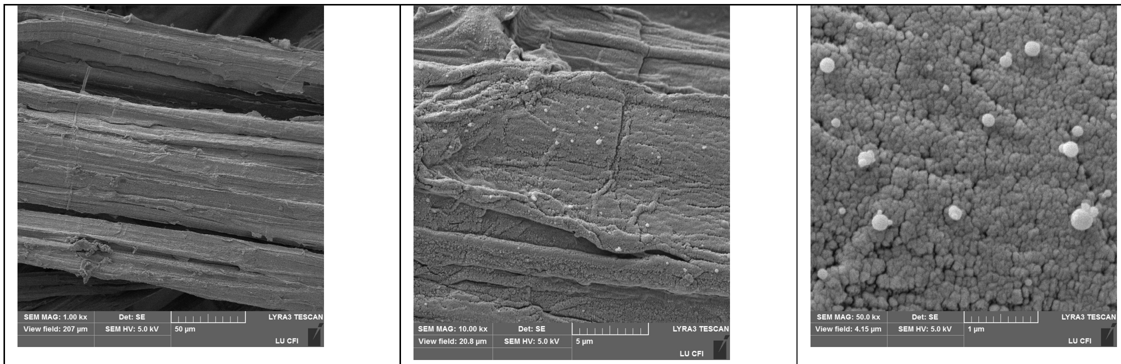

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Fig.3. Hemp nonwoven coated with CuO for differant SEM scales

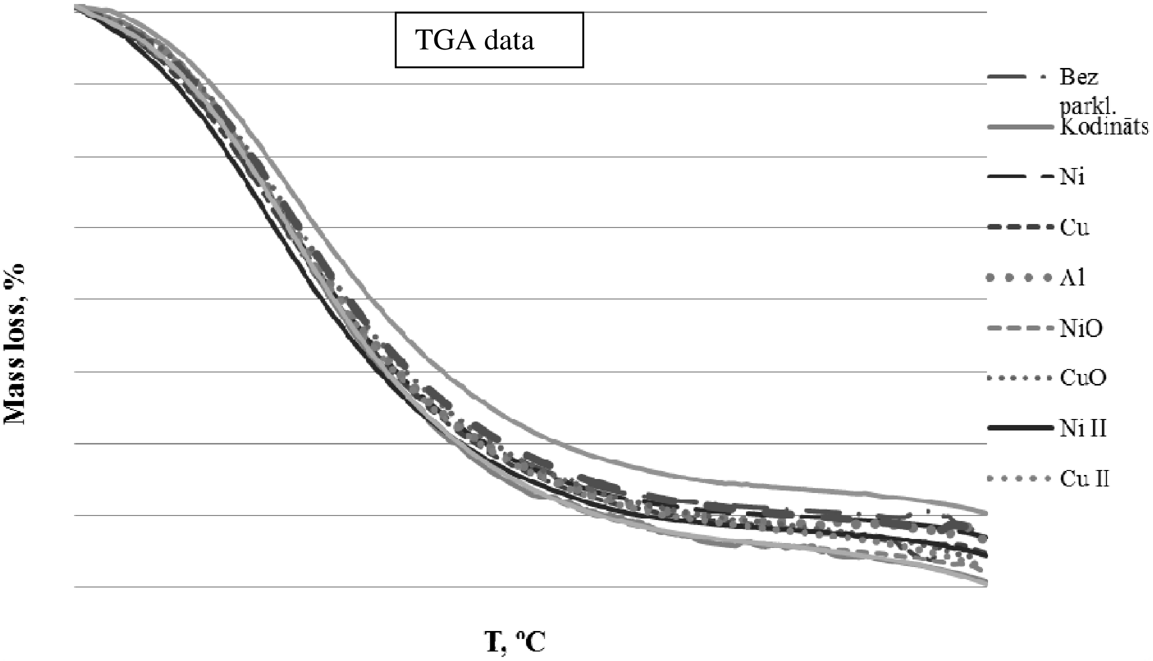

Fig. 4. Mass losses coated hemp nonwovens after keeping in room coditions

The research shows that even, relatively thin and flexible nonwovens can be obtained from double folded complex carding webs using hydroentanglement method at 20 bar pressure and speed of 2m/min. Unlike fabric samples, nonwoven samples attract similar water quantity irrespectively of surface modification (Fig.4). The SEM micrograph will be continued to deeper analyses with magnetron sputtering conditions

ELECTROPHORETICALLY DEPOSITED NANOSTRUCTURED REDUCED GRAPHENE OXIDE AS ELECTRODE MATERIAL FOR LITHIUM ION BATTERIES

Kaspars Kaprans, Gunars Bajars, Janis Kleperis, Andrejs Lusis

Recent advances in the technology of microelectronics demand micro power sources. Thin film technology offer an option of miniaturizing power sources. Most of the thin film electrode materials used in current batteries are deposited by RF or/and DC magnetron sputtering. Other methods include a variety of physical and chemical vapor deposition processes, such as aerosol spray coating and pulsed laser deposition. However above mentioned methods demand high material or energy consumption or they are relatively slow processes and require expensive equipment.

This work addresses the feasibility of an electrophoretic deposition (EPD) method for the preparation of graphene film electrode for lithium ion batteries. EPD technique has many advantages such as low deposition temperature, low consumption of energy as well as low cost and simplicity of equipment. Electrophoretic deposition (EPD) is an economical and versatile processing technique that has been applied in deposition of coatings and films, as for example phosphors for display. It has many advantages in the preparation of thin films from suspensions, such as high deposition rate and throughput, good uniformity and controlled thickness of the obtained films, noneed of binders, and simplicity of scaling up. [1]

Graphene is a new class of two dimensional carbon nanostructure owing exceptional high electric and thermal conductivity and mechanical stiffness. New electrode is made from sheets of graphene which is capable of accommodating more lithium ions and therefore delivers higher energy density than traditional carbon or graphite materials.

Graphene oxide nanosheet film was electrophoretically deposited on steel substrate from a stable water suspension with constant concentration 5 mg/ml using potenciostatic mode with the range of electric field 5-30 V/cm. Under the applied electric field, the negatively charged graphene oxide flakes migrated toward the positive electrode, and were subsequently orderly deposited onto the surface of the positive electrode. The thickness of the graphene films could be tuned ranging from several nanometers to a few micrometers. The deposition electric field was varied in order to obtain films with different thickness and density. Graphene oxide thermal treatment was performed by heating at 100 ºC in argon/hydrogen flow. Obtained graphene layers were analyzed by scanning electron microscopy, X-ray diffraction and Raman spectroscopy. These methods confirm the formation of homogeneous graphene sheet films. The application of these films as an electrode for lithium ion batteries was tested by various electrochemical methods such a voltammetry, chronopotentiometry, and electrochemical impedance spectroscopy (EIS) measurements which were performed for graphene thin films in three-electrode cell. The measurements in an open circuit state, charged and discharged states and during charging and discharging processes were carried out.

The financial support of Latvian project of scientific cooperation 666/2014 is greatly acknowledged.

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$LiFePO_4$ /C/REDUCED GRAPHENE OXIDE COMPOSITE LITHIUM ION BATTERY CATHODE WITH IMPROVED RATE CAPABILITY

Gints Kucinskis, Karina Bikova, Gunars Bajars, Janis Kleperis

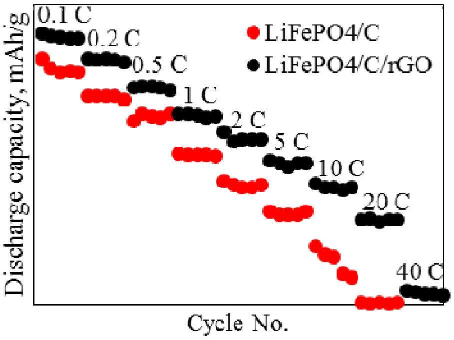


Fig.1 Rate capabilities of $LiFePO_4$/C and $LiFePO_4$/C/rGO composites

The large specific surface area of graphene along with the superior electronic conductivity suggests that graphene can be used as an additive for improving electronic conductivity in various composites, including lithium ion battery electrodes. $LiFePO_4$ is a lithium ion battery cathode material with a particularly low electronic conductivity. An increase in the overall $LiFePO_4$ cathode electronic conductivity can lead to significant improvement of its electrochemical properties. However, little is known regarding the optimal morphology and grain structure of $LiFePO_4$/reduced graphene oxide (rGO) composites.

In this research work $LiFePO_4$/C/rGO composites were synthesized by adding rGO and GO (graphene oxide) followed by thermal reduction at various steps of the $LiFePO_4$/C synthesis obtaining composites with various grain structures and morphologies. The addition of rGO and GO improved the rate capability in all cases. The superb rate capability of $LiFePO_4$/C/rGO composite can be seen in figure 1. However, it was determined that the optimum mixing of $LiFePO_4$/C and rGO can be obtained by adding GO during the initial stages of $LiFePO_4$/C synthesis. This ensured better $LiFePO_4$/C anchoring on the rGO sheets due to the hydrophilic nature of GO, therefore improving the electrical inter-particle contact and providing superior rate capability when compared to other $LiFePO_4$/C/rGO composites.

LABORATORY OF EXAFS SPECTROSCOPY

Head of laboratory Dr.habil.phys J. 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.
- Thin films and HIPIMS magnetron sputtering technologies.
- Confocal laser microscopy and Raman spectroscopy.
- The use of high performance computing for functional materials first principles and Molecular Dynamics simulations.
- Exchange interaction between radiation defects and transition metals ions in the dielectric crystals doped with the transition metals ions.

MAIN RESULTS

X-RAY ABSORPTION SPECTROSCOPY STUDIES OF LOCAL STRUCTURE AND THERMAL DISORDER IN CRYSTALLINE AND NANOCRYSTALLINE MATERIALS USING REVERCE MONTE CARLO METHOD

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

The work has been selected by Latvian Academy of Science as the BEST ACHIEVEMENT OF THE SCIENCE OF LATVIA in 2014

Material properties are determined by their chemical composition and equilibrium structure as well as by dynamics and correlation effects on the atomic scale. All this information is encoded in X-ray absorption spectrum (XAS) of a material. We have developed a new numerical simulation method, which allows one to reconstruct this information from the analysis of XAS. The method is based on the modelling of local material structure using the evolutionary algorithm - an approach that mimics genetic processes in the natural systems. The method combines the possibilities provided by modern XAS theory and available high performance computing resources and significantly expands the amount of information which can be obtained from the XAS analysis of complex crystalline and nanocrystalline materials. The method has been employed to the analysis of a number of polycrystalline Ge, ReO_3, H_xReO_3, ZnO, $SrTiO_3$ and Y_2O_3 as well as nanocrystalline $CoWO_4$, $CuWO_4$ and $Mn_{1-c}Co_cWO_4$ materials. More details can be obtained at http://www.dragon.lv/evax/.

LOCAL STRUCTURE STUDIES OF $SrTi^{16}O_3$ AND $SrTi^{18}O_3$

A. Anspoks, J. Purans

By comparing the Ti K-edge XANES of $SrTi^{16}O_3$ and $SrTi^{18}O_3$ we have identified the isotopic effect in $SrTi^{18}O_3$ which produces at $T < 100$ K a strong deviation of mean square relative displacement of Ti–O_1 bonds from the Einstein model. The corresponding amplitude of the XANES pre-peak 'B' at 4671 eV increases when temperature decreases. As in this temperature region it is unlikely that the atom oscillation amplitude increases, this is an indication of increasing off-center position of the Ti atom in the TiO_6 octahedra. This hypothesis has been supported by the optical second harmonic signal which also after sharp decrease at the ferroelectric phase transition temperature slowly decreases, having non-zero value even at 100 K.

TEMPERATURE DEPENDENCE OF THE LOCAL STRUCTURE AND LATTICE DYNAMICS OF WURTZITE-TYPE ZnO

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

Temperature-dependent (10-300 K) Zn K-edge extended X-ray absorption fine structure (EXAFS) spectra of polycrystalline wurtzitetype ZnO were analyzed using ab initio multiple-scattering theory and taking into account anisotropy of the crystallographic structure and thermal disorder. We employed two different simulation approaches: classical molecular dynamics (MD) and reverse Monte Carlo coupled with an evolutionary algorithm (RMC/EA method). The accuracy of several force-field models, which are commonly used in the MD simulations of bulk and nanostructured ZnO, was tested based on a comparison between the experimental and simulated Zn K-edge EXAFS spectra. It was found that available force-field models fail to describe accurately many-atom distribution functions. A more accurate solution was obtained with the RMC/EA method, which allowed us also to resolve the non-equivalent groups of atoms in the first two coordination shells around the absorbing Zn atom and to follow the changes of structural parameters as the temperature varied. It was found that upon increasing temperature the structure of ZnO becomes more anisotropic due to the increase of internal parameter *u* of the oxygen Wyckoff position (2b) and related Zn_0–O_2 distances.

STRUCTURAL, ELECTRICAL AND OPTICAL PROPERTIES OF ZINC-IRIDIUM OXIDE THIN FILMS DEPOSITED BY DC MAGNETRON SPUTTERING

M. Zubkins, R. Kalendarev, J. Gabrusenoks, K. Vilnis, A. Azens and J. Purans

ZnO-IrO_2 thin films were deposited on glass by DC reactive magnetron sputtering at room tem-perature. Structural, electrical and optical properties were investigated as a function of iridium atomic concentra-tion in the films. XRD data shows that ZnO-IrO_2 thin films are X-ray amorphous and Raman spectrum resembles the spectrum of IrO_2, without any distinct features of wurtzite ZnO structure. The lowest film resistivity and the highest transmittance achieved in the present study were 1.4×10^{-3} Ωcm and 33% at 550 nm, respectively. However, resistivity and transmittance are inversely related to the iridium concentration in the films.

LABORATORY OF HYDROGEN ENERGY MATERIALS

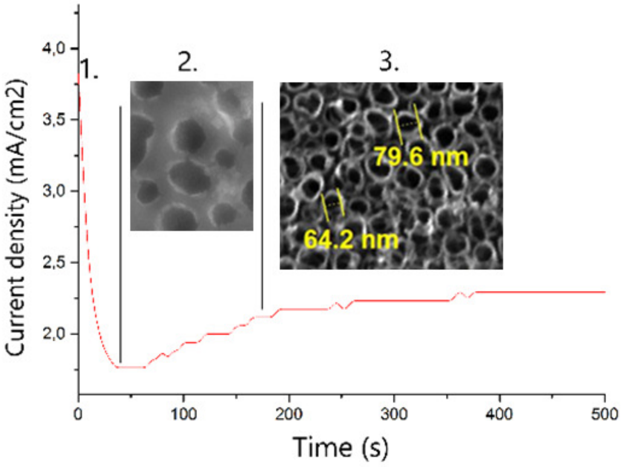
Head of laboratory J. Kleperis

RESEARCH AND DEVELOPMENT OF MATERIALS AND DEVICES FOR HYDROGEN ENERGY TECHNOLOGIES

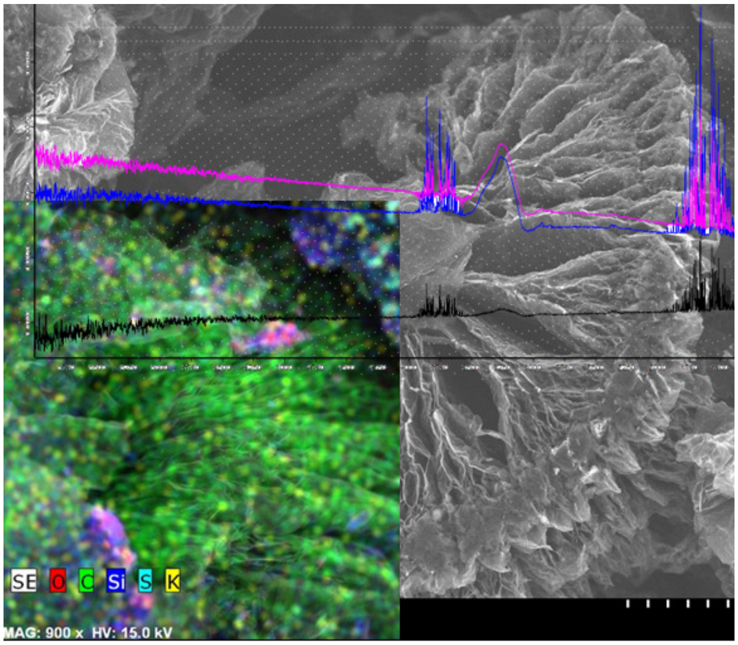
G.Bajars, J.Chikvaidze, J.Hodakovska, L.Grinberga, A.Knoks, J.Kleperis, J.Klavins, A.Lusis,
A.Sivars, J.Straumens, G.Vaivars, M.Vanags, L.Jekabsons, J.Zemitis, P.Lesnicenoks,
V.Nemcevs, I.Dimanta, S.Valucka, B.Sloka, J.Dimants

Hydrogen production studies

Photo-catalytic water splitting. Self-oriented TiO_2 nanotubes with predetermined geometrical parameters are grown and photocatalytic parameters investigated. TiO_2 nanotubes growth is based on electrochemical anodization in NaF and H_2SO_4 , H_3PO_4 solutions with different F ion concentration and Pt and Ti as electrodes. After anodization process samples are annealed at 400 ^oC to 600 ^oC in air. Morphology (SEM), structure (XRD, Raman spectroscopy) analyses are used to characterized obtained self-oriented nanostructurs (Figure). Photocatalytic activity is determined by using open circuit potential measurements with calomel reference electrode in $NaSO_4$ electrolyte and light from high pressure xenon lamp. TiO_2 nanotube growth process is separated in 3 stages (Figure) – 1) initiation and thin oxide growth, 2) selective dissolution and pore formation (Figure), and 3) dissolution/formation equilibrium, nanotube growth in length. It is found that higher voltage allows to growth nanotubes with larger diameter and with higher percentage of water in electrolyte the tubes are smoother, but best results are reported from organic solutions. Photo-catalytic activity is higher for TiO2 nanotubes with wider diameter. Another from the materials able to fulfill the requirements of efficient photo-electrode is alpha-phase ferric oxide (hematite α-Fe_2O_3). In stoichiometric mixture the hematite is an insulator, but typically it is non-stoichiometric

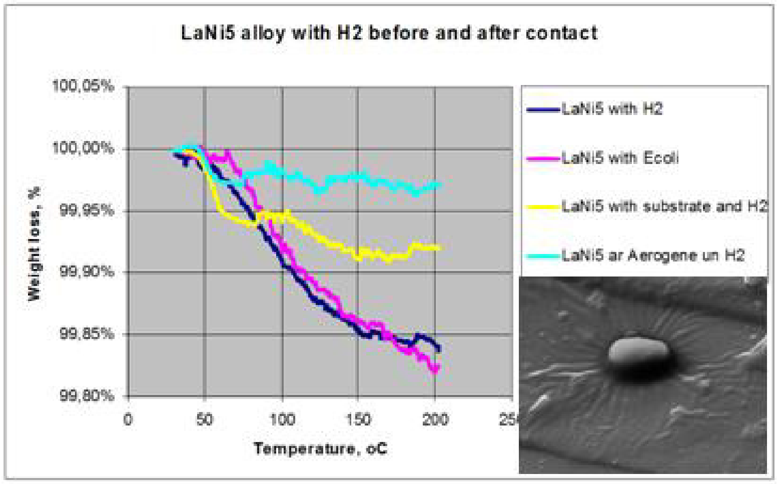


material with oxygen vacancies, as a result is the change of electrical properties from insulator to semiconductor. Hematite is a non-toxic, stable in a wide pH range, cheap and with the proper width of the forbidden gap close to the maximum of visible solar radiation. Anodic plating method was used to obtain pure hematite α-Fe_2O_3 thin films from plating solution $FeCl_2$ 0,02M at 75 °C on the FTO/glass substrate (1.3 x 2.5 cm), which served as the working electrode. The photocurrent of non-reduced thin film after light activation increase with some delay and reaches the maximal value, then is descending until a saturation value. The photocurrent of reduced thin film increases very fast after light activation, reaching defined value, and than increase slowly without saturation.



Hydrogen storage studies

Hydrogen binding with carbon nanostructures. The big challenge for carbon nanoporous materials as hydrogen storage media is to find a structure with tunable porosity and high specific surface area, where hydrogen adsorbs strongly enough on the surface as to form a thermodynamically stable arrangement but not too strongly so that reversible fast loading/unloading kinetics are possible. To obtain graphene, the electrochemical exfoliation and water-plasma methods were used, taking graphite industrial waste road as working electrode. Samples were exposed in Ar/H2 gas flow at 300°C for 3 hours and characterized by X-ray diffraction, SEM, elemental composition, FTIR. Analysis of SEM pictures show opened few layer graphite (FLG)/graphene structures



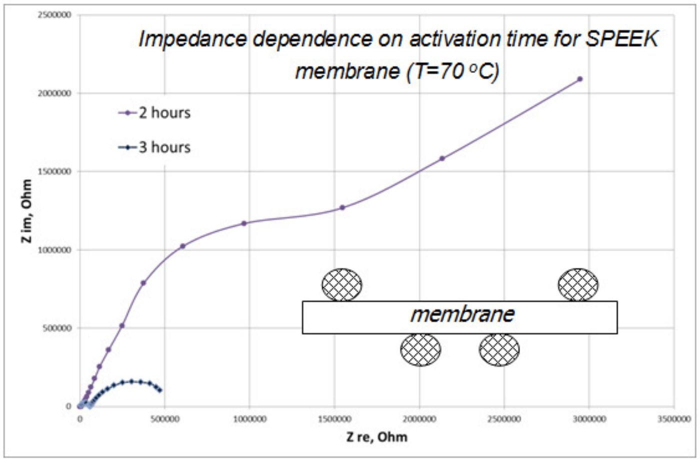
(Figure), with higher surface area than if it would be stacked together – determined by BET method - Mg FLG 0.43 m2/g and reduced FLG - 12.4 m2/g. EDAX XRF analysis shows the presence of Fe, Si and some Ti impurities in graphite substrate material and obtained FLG (Figure). Raman scattering was used to identify the presence of graphene in multistack material, and preliminary experiments were done to test hydrogen absorption capability in graphene sheet stacks, using thermal absorption/desorption methods. Two different samples were collected from both – exfoliation and plasma methods – the light fraction of material that floated on the top of solution, and heavy fraction which sank at the bottom of the solution. With graphene in FLG structures the hydrogen can interact using physisorption and chemisorption forces, poorly appearing in FTIR spectra (Figure); another possibility is to exploit intercalation of hydrogen between FLG sheet stacks (distance between sheets is important). Harvesting hydrogen from liquid phase. Usage of metal hydride to harvest hydrogen from liquid phase during dark fermentation of biomass. It was proved that hydrogen over-saturation phenomena in liquid phase during dark fermentation process occur. The task is to remove hydrogen from liquid phase. Metal hydrides forming alloy powders with mass around 10 g before usage were activated in vacuum (10-2 bars) heating them up to 130 oC and evacuated, then exposed to hydrogen (2 bars) for ½ hour and finally cooled down to room temperature simultaneously with evacuation. Argon is used to preserve activated alloys until their contact with culture medium.

Bacteria: Hydrogen producears - Enterobcater aerogenes from Microbial Strain Collection of Latvia (MSCL) and Escherichia coli BW25113 hyaB hybC hycA fdoG frdC aceE ldhA::kan (from prof. T.K. Wood, Texas A&M University, USA) were used for fermentation experiments.

Sample characterization: Differential thermogravimetric method DTG-60 (Shimadzu) was used to measure amount of adsorbed hydrogen in alloy – before and after the contact with microorganisms. The bacteria produced gas mixture from serum bottles was collected with a syringe, and subsequently injected in the mass-spectrometer RGAPro-100 (HyEnergy, Setaram, France) for calculation of amount of hydrogen gas in the gas phase. SEM-FIB Tescan Lyra microscope was used to analyze morphology of alloy grains before and after contact with microorganisms. After fermentation process for 72 hours, metal hydride alloys were measured for hydrogen storage capacity using thermogravimetric method. Three of four hydride alloys were effective and they are compared for storage properties. It is find that hydrogen starts to exit metal hydride alloy below 50°C, reaching weight loss from 0,15% to 0,4 % at 150 ^{o}C, when the weight of reference sample stabilizes but weight of alloy being in contact with Esherichia coli continues to decline. Some hydrogen uptake by in alloy is noticed also in substrate bubbled with hydrogen gas, and smallest amount of hydrogen is detected in alloy after contact with Enterobcater aerogenes (light blue curve.

Studies of proton transport in membranes

Proton transport studies is important because most important part of fuel cell is solid electrolyte: proton conductive polymer. In our research the attention is paid to sulfonated polymers poly(ether-ether-ketone) (SPEEK) and Nafion as reference. To improve characteristics of SPEEK polymer, inorganic components are added to SPEEK and reference membrane. Conductivity dependence on temperature and related parameters are measured to compare effect of dopant concentration and treatment. To measure impedance four electrode method is used - platinum electrodes were placed on membrane’s surface: outer two were connected to current surface, voltage drop was measured between inner two on the other side of membrane (Figure). In such electrode configuration surface conductivity influence is omitted. Measurements were performed in thermostatic bath and potentiostat Voltalab PGZ 301 (Radiometer Analytical). As dopant inorganic component TiO_2 was used, and activation agent was HNO_3 solution in water. The conductivity of membrane has characteristic dependence on temperature, and activation procedure has more significant influence on SPEEK membrane. Adding of TiO_2 decreased overall conductivity of all tested polymer membrane samples. Two conduction processes are observed in composite membranes, what is explained by bulk water conductivity and charge transfer along the channel borders in membrane.



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Andris Anspoks, „Studies of local structure relaxation in nanomaterials", University of Latvia, 2014.

LECTURES ON CONFERENCES

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1. .Ē.Pentjušs, A.Lūsis, J.Gabrusenoks, G.Bajārs (2014) Karbonizēto Na-Al-Si stikla šķiedras audumu hidratizācijas kinētika. Grām.: LU CFI 30.zin. konf. ref. tēzes. Rīga, LU Cietvielu fizikas institūts, lp.84. Ē.Pentjušs, A.Lūsis, J.Gabrusenoks, G.Bajārs (2014) Hydratation kinetics of carbonized Na-Al-Si glass fiber fabrics. University of Latvia, Institute of Solid State Physics, 30th Scientific Meeting. Abstracts, Riga, p.84.

2. G.Kucinskis, K.Bikova, G.Bajārs, J.Kleperis (2014) $LiFePO_4$/grafēns nanokompozīta sintēze un elektroķīmiskās īpašības. Grām.: LU CFI 30.zin. konf. ref. tēzes. Rīga, LU Cietvielu fizikas institūts, lp.96. G.Kucinskis, K.Bikova, G.Bajārs, J.Kleperis (2014) Synthesis and electrochemical properties of $LiFePO_4$/graphene nanocomposite. University of Latvia, Institute of Solid State Physics, University of Latvia, Institute of Solid State Physics, 30th Scientific Meeting. Abstracts, Riga, p.96.

3. K.Kaprāns, G.Bajārs, K.Bikova, J.Kleperis, A.Lūsis, Ē.Pentjušs (2014) Grafēna kārtiņu elektroforētiska uzklāšana no ūdens suspensijas. Grām.: LU CFI 30.zin. konf. ref. tēzes. Rīga, LU Cietvielu fizikas institūts, lp.98.

4. K.Kaprans, G.Bajars, K.Bikova, J.Kleperis, A.Lusis, Ē.Pentjuss (2014) Electrophoretic deposition of graphene films from water suspension. University of Latvia, Institute of Solid State Physics, 30th Scientific Meeting. Abstracts, Riga, p.98.

5. I.Liepiņa, G.Bajārs, J.Gabrusenoks, A.Lūsis (2014) Alumīnija oksīda-niķeļa kompozīta pārklājumu elektroforētiska iegūšana, sastāvs un struktūra. LU CFI 30.zin. konf. ref. tēzes. Rīga, LU Cietvielu fizikas institūts, lp.99. I.Liepina, G.Bajars, J.Gabrusenoks, A.Lusis (2014) Aluminium oxide-nickel coating electrophoretic deposition, composition and structure. University of Latvia, Institute of Solid State Physics, 30th Scientific Meeting. Abstracts, Riga, p.99.

6. A. Knoks, L. Grīnberga, J. Kleperis. Metāla oksīdu pārklājumu fotofizikālās īpašības daudzslāņu struktūrās. A.Knoks, L.Grinberga, J.Kleperis. Photophysical Properties of Metal Oxide Multilayer Films.

7. P. Lesničenoks, J. Zemītis, G. Tauriņš, J. Kleperis. Ūdeņraža adsorbcijas pētījumi ar elektroķīmisko atslāņošanas metodi iegūtā grafēnā. P. Lesnicenoks, J. Zemitis, G. Taurins, J. Kleperis. Study of Hydrogen Adsorption in Electrochemically Exfoliated Graphene.

8. A. Starikovs, J. Fricsons, B. Sloka, J. Kleperis. Ūdeņraža kā enerģijas nesēja iespēju izpēte bezizmešu transportā un enerģētikā Latvijā. A. Starikovs, J. Fricsons, B. Sloka, J. Kleperis. Studying the Latvia`s Challenges for Hydrogen as an Energy Carrier in Zero-Emission Transport and Energetics.

9. M. Gudakovska, A. Priede, J. Kleperis. Ūdeņraža tehnoloģiju ieviešana transportā Rīgas piemērā - vides ieguvumu analīze. M. Gudakovska, A. Priede, J. Kleperis. Environmental Benefit Analysis from Implementation of Hydrogen Technologies in Riga`s Public Traffic.

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11. A. Knoks, L. Kuhta, M. Milberga, L. Grīnberga, J. Kleperis. Pašsakārtotu TiO2 nanostruktūru audzēšanas īpatnības – metodika un rezultāti. A. Knoks, L. Kuhta, M. Milberga, L. Grinberga, J. Kleperis. The Features of Self-Assembling TiO2 Nanostructures Growth – Methodology and Results.

12. Hodakovska, J.Kleperis. Ar neorganiskiem savienojumiem modificētu sulfonētu poli-ēter-ēter-ketona membrānu protonu vadāmības pētījumi. J. Hodakovska, J.Kleperis. Research of

Proton Conductivity in Sulfonated Poly (Ether Ether Ketone) Membranes Modified with Inorganic Compounds.

13. M. Vanags, J. Kleperis, G. Bajārs. V-A līkņu metodes pielietošana procesu efektivitātes noteikšanai impulsu un līdzstrāvas ūdens elektrolīzē. M. Vanags, J. Kleperis, G. Bajars. V-A Curve Method for Determination the Efficiency of Water Electrolysis in Pulse and DC Processes.

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15. K.Beitāns, V. Vīgants, V. Ņemcevs, M. Vanags, J. Kleperis. Bremzēšanas enerģijas uzkrāšana elektriskā velosipēdā. K. Beitans, V. Vigants, V. Nemcevs, M. Vanags, J. Kleperis. Storage of the Braking Energy in Electric Bicycle.

European Hydrogen Energy Conference 2014, March 12th-14th, 2014 - Seville, Spain;

16.. J.Kleperis, B. Sloka, J. Dimants, I. Dimanta, A. Starikovs, M.Gudakovska, J.Fricsons. Hydrogen in Mobile Applications – the Path of Latvia to Carbon Free Economy.

15th Topical Meeting of the International Society of Electrochemistry: Interfacial Electrochemistry at Atomic, Molecular and Nanoscale. April 28-30, 2014, Niagara Falls, Canada

17. Gunars Bajars, Martins Vanags, Andris Sutka, Liga Grinberga, Janis Kleperis, Ineta Liepina. Photocatalytic Activity of Ferrite Based Nanoparticles, Their Clusters and Thin Films for Solar Water Splitting.

18. G. Vaivars, J. Kleperis and E. Sprugis. Composite SPEEK Polymer Membranes with Acidic Ionic Liquids.

Conference "International Discussion on Hydrogen Energy and Applications" Nante (France), May 11-15, 2014.

19. J. Kleperis, P. Lesnicenoks, J. Zemitis, L. Grinberga „Research of Hydrogen Bonding in Porous (Zeolite) And Layered (Graphene) Structures"

11th Internat. Symp. On Systems with Fast Ionic Transport, Gdansk, Poland, June 25-29, 2014

20. G.Bajars, J.Zemitis, P.Lesnicenoks, G.Kucinskis, J.Kleperis, G.Dobele (2014) Exfoliated graphene-like nanosheets as intercalated material for hydrogen and lithium ions.

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21. Ilze Dimanta, Zane Rutkovska, Justs Dimants, Vizma Nikolajeva, Janis Kleperis, Indrikis Muiznieks Usage of Crude Glycerol for Biological Hydrogen Production – Experiments and Analysis.

Joint 12th Russia/CIS/Baltic/Japan Symposium on Ferroelectricity and 9th International Conference Functional Materials and Nanotechnologies; Riga (Latvia), September 29-October 2, 2014

22. J. Kleperis, I. Dimanta, G. Bajars, G. Dobele, A. Dindune, G. Vaivars. Poster F-135 Research on Controlled Porosity Composite Thin Layers and Systems for Energy Storage and Conversion Applications.
23. I. Dimanta, Z. Rutkovska, J. Kleperis, V. Nikolajeva and I. Muiznieks. Poster F-136 Bacteria Produced Hydrogen Storage Possibilities in Metal Hydride Alloy.
24. G. Vaivars, J. Kleperis, E. Priede, E. Sprugis, A. Zharova, A. Zicmanis. Poster F-151 SPEEK Polymer Composites with 1-butyl-2,3-dimethyl-imidazolium dimethylphosphate Ionic Liquids for Fuel Cell Membranes.

. E-MRS 2014 Spring Meeting, Lille, France, 27.-29.05.2014.

25. "Understanding of atomic and electronic structure of $SnWO_4$" A. Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, R. Kalendarev (Oral talk).
26. "Local structure of nanosized tungstates revealed by evolutionary algorithm" J. Timoshenko, A. Anspoks, A. Kalinko, A. Kuzmin (Stenda referāts).

2. Second International Conference on Radiation and Dosimetry in Various Fields of Research (RAD 2014), May 24-30, 2014, Niš, Serbia.

27. "Analysis of the effect of radiation on human blood by EPR" M.Polakovs, N. Mironova-Ulmane, A. Pavlenko, A. Aboltinš (Poster).

3. Int. Conf. SUPERSTRIPES 2014, 25-31 July 2014, Erice, Sicily, Italy.

28. "Beyond quasiharmonic approximation: local structure of materials with negative thermal expansion" J. Purans (Invited talk).

The 17 Conference on Luminescence and Optical Spectroscopy of Condensed Matter (ICL ’14), 13-18 July 2014, Wroclav, Poland.

29. Luminescence and optical spectroscopy of charge transfer processes in solid solutions Ni_CMg_{1-C} O and $Ni_XZn_{1-X}O$. V.Sokolov,V. A Pustovarov, V. N Churmanov; N. B Gruzdev; M. A Uimin, I. V Byzov, A. V Druzhinin, N. A Mironova-Ulmane (Oral).

30. "UP-Conversion and Photoluminescence Er^{3+} Single Crystals MgAl-Spinel" N. Mironova-Ulmane, A. Sarakovskis, V. Skvortsova (Poster).

16th Int. Conf. "Advanced Materials and Technologies", 27-31 August 2014, Palanga, Lithuania.

31. "Applications of synchrotron radiation in material science" J. Purans (Invited talk).

RCBJSF-2014 -FM&NT, Riga, Latvia, 29.-02.10.2014.

32. "Beyond quasiharmonic approximation: local structure of perovskites with negative thermal expansion" J. Purans (Plenary talk).

33. „Local structure studies of Ti for $SrTi^{16}O_3$ and $SrTi^{18}O_3$ by advanced X-ray absorption spectroscopy data analysis” A. Anspoks, D. Bocharov, J. Purans, F. Rocca, A. Sarakovskis, J. Timoshenko, V. Trepakov, A. Dejneka, M. Itoh (Oral talk).

34. "High-pressure x-ray absorption spectroscopy study of tin tungstates" A. Kuzmin, A. Anspoks, A. Kalinko, J. Timoshenko, R. Kalendarev, L. Nataf, F. Baudelet, T. Irifune (Oral talk).

35. Properties of Carbonized Na-Al-Si Glass Fiber Fabrics.E. Pentjuss, A. Lusis, J. Gabrusenoks, G. Bajars

36. A Comparative Study of Natural Fiber and Glass Fiber Fabrics Properties with Metal or Oxide Coatings. A.Lusis, E. Pentjuss, G. Bajars, J. Gabrusenoks, U. Sidorovicha

37. Structure and Photocatalytic Properties of TiO2-WO3 Composites Prepared by Electrophoretic Deposition. I.Liepina1, G. Bajars1, M. Rublans2, A. Lusis1, E. Pentjuss1

38. Electrophoretic Graphene Film Electrode for Lithium Ion Battery.K. Kaprans, G. Bajars, A. Dorondo, J.Mateuss, G. Kucinskis,. Gabrusenoks, J. Kleperis, A. Lusis

39. J.Kleperis, I.Dimanta, G.Bajars, G.Dobele, A.Dindune, G.Vaivars (2014) Research on controlled porosity composite thin layers and systems for energy storage and conversion applications. Book of Abstracts: Joint symposium RCBJSF-2014-FM&NT, Riga, Latvia, p.400.

40. I.Liepina, G.Bajars, M.Rublans, A.Lusis, E.Pentjuss (2014) Structure and photocatalytic properties of TiO_2-WO_3 composites prepared by electrophoretic deposition. Book of Abstracts: Joint symposium RCBJSF-2014-FM&NT, Riga, Latvia, p.405.

41. K.Kaprans, G.Bajars, A.Dorondo, J.Mateuss, G.Kucinskis, J.Gabrusenoks, J.Kleperis, A.Lusis (2014) Electrophoretic graphene film electrode for lithium ion battery. Book of Abstracts: Joint symposium RCBJSF-2014-FM&NT, Riga, Latvia, p.410.

42. G.Kucinskis, K.Bikova, G.Bajars, A.Orliukas, K.Z.Fung, J.Kleperis (2014) Deposition and in-depth electrochemical analysis of $LiFePO_4$ thin films. Book of Abstracts: Joint symposium RCBJSF-2014-FM&NT, Riga, Latvia, p.411.

43. „Local structure of multiferroic $Mn_{1-c}Co_cWO_4$ solid solutions revealed by the evolutionary algorithm“ J. Timoshenko, A. Anspoks, A. Kalinko, I. Jonane, A. Kuzmin (Poster).

44. „Template-based synthesis of nickel oxide” N. Mironova-Ulmane, A. Kuzmin, I. Sildos (Poster).

45. "Preparation and characterization of tin tungstate thin films" A. Kuzmin, M. Zubkins, R. Kalendarev (Poster).

46. "Local structure and lattice dynamics of cubic Y_2O_3: an x-ray absorption spectroscopy study" K. Lazdins, A. Kuzmin (Poster).

47. EXAFS study of the local structure of crystalline and nanocrystalline Y_2O_3 using evolutionary algorithm method" I. Jonane, J. Timoshenko, A. Kuzmin (Poster).

48. "ODS steel raw material local structure analysis using X-ray absorption spectroscopy" A. Cintins, A. Anspoks, J. Purans, A. Kuzmin, J. Timoshenko, P.Vladimirov, T. Graning, J. Hoffmann (Poster).

49. Highly porous wood based carbon materials for supercapacitors. Aleksandrs Volperts, Galina Dobele, Aivars Zhurinsh, Daria Vervikishko, Eugeny Shkolnikov, Nina Mironova-Ulmane, Ilmo Sildos, Jurijs Ozolinsh (Poster).

50. Optical Properties of Natural and Synthetic Beryl Crystals. V. Skvortsova, N. Mironova-Ulmane, L. Trinkler, V. Merkulov (Poster).

51. Gallstones Studies by Raman, EPR and EDX Spectroscopes. D. Jakovlevs, M. Polakovs, N. Mironova-Ulmane, V. Skvortsova, L. Berzina-Cimdina, I. Sildos. (Poster).

52. Determination of methemoglobin in human blood after ionising radiation by EPR. Maksims Polakovs, Nina Mironova-Ulmane, Andreijs Pavlenko Ainars Aboltinš . (Poster).

13th Europhysical Conference on Defects in Insulating Materials EURODIM 2014, Canterbury, Kent, England, 19 July 2014.

53. Optical Properties of Irradiated Topaz Crystals V.Skvortsova, N. Mironova- Ulmane, L. Trinkler

DEPARTMENT OF THEORETICAL PHYSICS AND COMPUTER MODELLING

Head of Department Dr. hab. phys. Eugene Kotomin

RESEARCH AREA AND MAIN PROBLEMS

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

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

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

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**
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B.S. Moskina	**B.S. J. Kazerovskis**
	B.S. O. Lisovski
	M.S. A. Platonenko
	M. Sokolov

SCIENTIFIC VISITS ABROAD

1. Dr. hab. E. Kotomin, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (8 months), Eurasian National University, Astana, Kazakhstan (2 weeks), Photochemistry Center, Russian Academy of Sciences, Moscow, Russia (10 days)
2. Dr. O. Dumbrajs, Fukui University, Japan (3 months)
3. Dr. A. Popov, Laue-Langevin Institute, Grenoble, France (1 week); Institute of Materials Science, Darmstadt University of Technology, Germany (1 week); Institute of Physics, University of Tartu (2 weeks), CIEMAT, Spain (1 week)
4. Dr. D. Bocharov, University of Duisburg-Essen, Germany (1 month)
5. Dr. Yu. Mastrikov, Institute of Applied Materials, Karlsruhe, Germany (3 weeks), Eurasian National University, Astana, Kazakhstan (2 weeks)
6. Dr. S. Piskunov, University of Duisburg-Essen, Germany (6 weeks), Laboratori Nationali di Frascati, Italy (1 month); Institute of General and Inorganic Chemistry, Russia, Moscow (2 months)
7. Dr. hab. Yu. Shunin, Laboratori Nationali di Frascati, Italy (1 month); Institute of General and Inorganic Chemistry, Moscow, Russia (1 week)
8. Dr. Yu. Zhukovskii, St. Petersburg State University, Russia (3 weeks), Institute of General and Inorganic Chemistry, Moscow, Russia (2 weeks)
9. B.S. A. Chesnokov, University of Duisburg-Essen, Germany (2 weeks)
10. B.S. J. Kazerovskis, University of Ulm, Germany (10 months)
11. B.S. O. Lisovski, Uppsala University, Sweden (10 months)

INTERNATIONAL COOPERATION

Belarus	1. Institute of Nuclear Problems, Belarusian State University, Minsk (Prof. S. A. Maksimenko)
China	2. Beijing Institute of Technology, Beijing (Dr. H. Shi).
Estonia	3. Institute of Physics, University of Tartu (Prof. A. Lushchik)
Finland	4. Helsinki University of Technology, Espoo (Dr. T. Kurki-Suonio)
France	5. Laue-Langevin Institute, Grenoble, Prof. H. Schober)
Germany	6. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier)
	7. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov)
	8. Darmstadt University of Technology, Darmstadt (Prof. H von Seggern)
	9. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk)
	10. Institut für Angewandte Materialien (KIT), Karlsruhe (Dr. A. Möslang, Dr. P. Vladimirov)
	11. Dept of Theoretical Chemistry, Univ. Duisburg-Essen (Prof. E. Spohr)
Israel	12. Ben Gurion University, Beer Sheva (Prof. D. Fuks)
Italy	13. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Kazakhstan	14. Gumilyov Eurasian National University, Astana (Prof. A.T. Akilbekov)
Japan	15. FIR Center, University of Fukui (Prof. T. Idehara)
Lithuania	16. Institute of Semiconductor Physics (SPI), Vilnius (Dr. E. Tornau)
Poland	17. Warsaw University, Department of Chemistry (Prof. A. Huczko, Prof. A. Dąbrowska)
	18. Institute of Physics, Academy of Science, Warsaw (Prof. H. Szymczak)
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	21. Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (Prof. P.N. Dyachkov)
	22. Photochemistry Center, Russian Academy of Sciences, Moscow (Prof. A.A. Bagaturyants)

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UK	24. University College London (Prof. A.L. Shluger)
Ukraine	25. Ivan Franko National University, Lviv (Prof. O. I. Aksimentyeva, Prof. I. Bolesta, Dr. I. Karbovnyk)
USA	26. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)

MAIN RESULTS

A. Electronic structure calculations for advanced materials

HYBRID HARTREE-FOCK-DENSITY FUNCTIONAL THEORY CALCULATIONS OF OXYGEN VACANCY TRANSPORT IN COMPLEX PEROVSKITE OXIDES

D. Gryaznov, E.A. Kotomin, S. Baumann, R. Merkle

The hybrid HF-DFT calculations based on the PBE0 functional and the LCAO basis set were combined with the permeation measurements, in order to analyze the formation enthalpy of oxygen vacancies $V_O^{\bullet\bullet}$ in complex perovskite solid solutions, like (La,Sr)FeO$_{3-\delta}$ (LSF) with different Sr doping. The use of hybrid functionals allowed us to reproduce the bulk properties of these solid solutions and their behavior as semiconductors.

The correctness of band gap is important to calculate the formation enthalpy of $V_O^{\bullet\bullet}$ in LSF which is in agreement with previous experimental

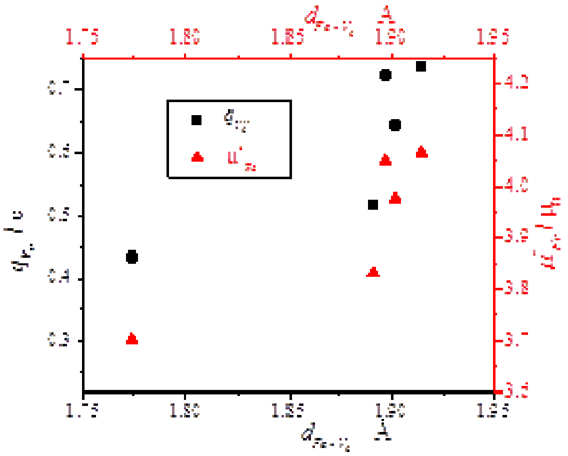

Figure 1. The Mulliken charge of $V_O^{\bullet\bullet}$ and magnetic moment on Fe depending on $d_{Fe-V_O^{\bullet\bullet}}$ for LSF with 12.5% doping (40 atom supercell with the nonstoichiometry δ = 0.125).

studies on the formation enthalpy of $V_O^{\bullet\bullet}$ in LSF. Moreover, the LCAO basis set allowed us to determine the electronic charge density within the vacancy (due to additional so-called ghost basis set at the vacancy site) and find the correlation between the charge of $V_O^{\bullet\bullet}$, the Fe-$V_O^{\bullet\bullet}$ distance and the magnetic moment on Fe. It is demonstrated that a careful comparison of the calculation results with the experiments requires the knowledge on the oxidation state of Fe under experimental conditions and thus the relation between nonstoichiometry δ and Sr doping.

We have confirmed that the formation enthalpy of $V_O^{\bullet\bullet}$ significantly decreases with the Sr doping which greatly accelerates oxygen transport through permeation membranes and SOFC cathodes and thus improves their performance.

AB INITIO THERMODYNAMICS OF OXYGEN VACANCIES AND ZINC INTERSTITIALS IN ZnO

E.A. Kotomin, T.S. Bjørheim

ZnO is an important wide band gap semiconductor with potential application in various optoelectronic devices. Recently, we have explored the thermodynamics of oxygen vacancies and zinc interstitials in ZnO based on first principles phonon calculations. While formation enthalpies are evaluated using hybrid DFT calculations, phonons are addressed using the PBE and the PBE+*U* functionals. The phonon contribution to the formation entropy of oxygen vacancies is similar for all functionals, while that of zinc interstitials is significantly

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Figure 2. Defect formation entropy from PBE and PBE+*U* of $\mathrm{Zn}_i^{\bullet\bullet}$ and $V_O^{\bullet\bullet}$.

lower with PBE+U than PBE (Fig. 2), and we suggest that the former functional is more suited for investigating vibrational properties of ZnO.

Further, the phonon contribution to the entropy is most dominant for oxygen vacancies, and their Gibbs formation energy increases when including phonons. Hence, phonons decrease the formation energy difference of oxygen vacancies and zinc interstitials and render their equilibrium concentrations more comparable at the very highest temperatures. The analysis of the phonon density of states (Fig.3) shows additional band due to oxygen vacancies which could be used for defect detection.

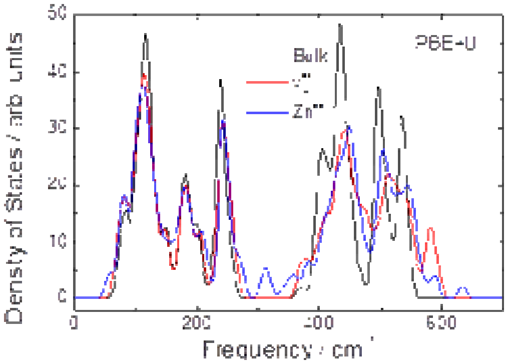

Figure 3. Phonon density of state of pure ZnO, and cells with $V_O^{\bullet\bullet}$ and $\mathbf{Zn_i^{\bullet\bullet}}$ defects, calculated at the Γ-point of the 3×3×2 supercell.

HYDROGEN-INDUCED METALLIZATION OF ZnO($1\bar{1}00$) SURFACE: FIRST PRINCIPLES STUDY

E.A. Kotomin, J. Purans, Yu.F. Zhukovskii, A. Usseinov, A.T. Akilbekov

To improve ZnO thin film production technologies, the effect of hydrogen on the structural and electronic properties of different zinc oxide surfaces have been studied. Specifically, during the growth of ZnO crystalline samples, the highest growth rates were achieved along the z-axis and most favorable facets were found to be $(1\bar{1}00)$ and $(11\bar{2}0)$ characterized by comparatively low surface energies. Meanwhile, the former has been found by us as slighly more stable. Large scale *ab initio* calculations on H/ZnO($1\bar{1}00$) system have been performed combining the basis set of linear combination of atomic orbitals (LCAO) method with the hybrid exchange-correlation Perdew–Burke–Ernzerhof (PBE0) functional as has been implemented in the *CRYSTAL2009* computer code. For simulation of hydrogen adsorption on the $(1\bar{1}00)$ surface, the slab model of finite thickness along the z axis and extended by (2×2) in the *x* and *y* directions corresponding to the periodic distribution of hydrogen adatoms has been chosen.

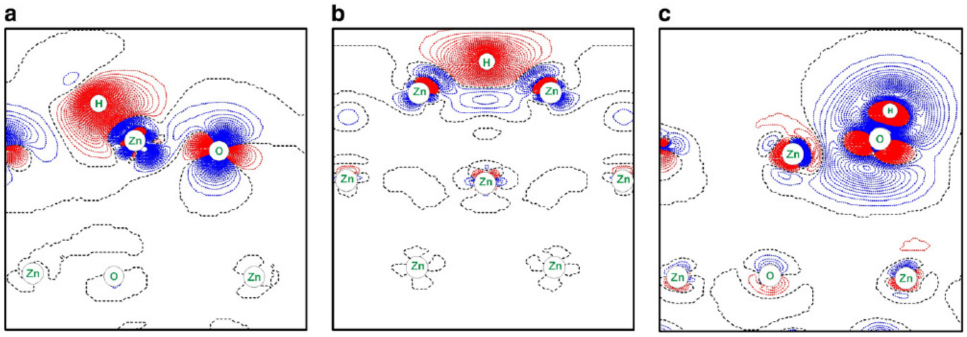

Figure 4. Differential electron density plots are drawn for the hydrogen atom upon the ZnO($1\bar{1}00$) surface positioned a) atop surface Zn ion; b) atop surface O ion; and c) atop the hollow position. The solid (red) and dotted (blue) isolines correspond to positive (excess) and negative (deficiency) electron density, respectively. Increment for isolines is 0.001 *e* within the range from −0.1 to 0.1 *e*.

We have studied adsorption of hydrogen atoms over different surface sites (Fig. 4) varying their concentration *per* unit cell. Energetically the most preferable adsorption sites have been found adatom positions atop the surface oxygen ion. Hydrogen adatoms also reduce the surface energy of ZnO($1\bar{1}00$) making it more stable (0.35 *vs.* 0.73 J/m^2) Since hydrogen atoms are mainly produced by dissociation of H_2 molecules, the adsorption energy with such the reference state are smaller by half of its binding energy (*i.e.*, 1.58 eV). Electron densiy distrbutions for H adatoms atop suface Zn (Fig. 4a), hollow (Fig. 4b) and O (Fig. 4c) sites clearly confirm results of total nergy calculations. O-H bond population on the substrate is much larger than that in the bulk (0.215 *vs.* 0.137 *e*). Electron charge redistribution cleary shows strong bonding around O sites and anti-bonding in the proximity of surface Zn ions. A comparison with ionic displacements on a perfect surface shows that both surface O and Zn ions are displaced outwards and preserve the same ordering: O ions lie higher than Zn ions. The density of states for adatom in three different positions clearly show that even at 25% coverage the adsorbed hydrogen shows the density of states in the energy range overlapping the bottom of conduction band, thus transforming ZnO thin films into a conducting state (metallization). An increase of hydrogen coverage up to 1 ML leads to a disappearance of the band gap at all.

AB INITIO MODELING OF RADIATION DAMAGE IN MgF_2 CRYSTALS

E.A. Kotomin, S. Piskunov, F.U. Abuova, A.T. Akilbekov, V.M. Lisitsyn,

MgF_2 with a rutile structure is important radiation-resistant material with numerous applications due to its transparency from vacuum ultraviolet to infrared range of photon energies. Optical devices (e.g., lenses and windows) produced from magnesium fluoride are transparent over an extremely wide range of photon energies, from vacuum ultraviolet to infrared. Another advantage of MgF_2 is high radiation stability: concentrations of stable radiation defects therein are 3–5 orders of magnitude smaller than in alkali halide crystals. Theoretical study has been based on the large scale *ab initio* DFT-LCAO calculations using hybrid B3PW exchange–correlation functional and atomic basis set.

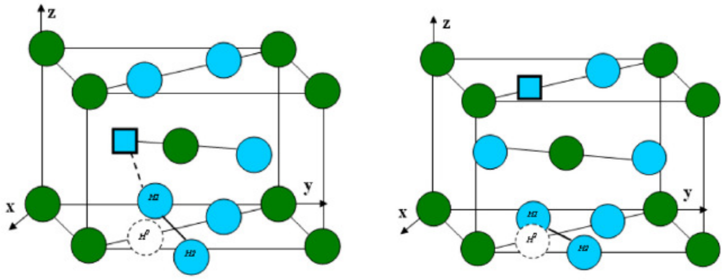

Figure 5. The nearest (left) and well separated (right) *F–H* (110) pairs in MgF_2. Blue (light) atoms are fluorine ions, green (dark) magnesium ions. Dotted circle indicates position of a regular fluorite ion before the *H* center formation. The *F* center is marked as a square while the *H* center consists of the *H*1 and *H*2 ions.

The primary radiation defects are Frenkel pairs of fluorine vacancies with trapped electrons (*F* centers) and interstitial fluorine atoms which rapidly form the diatomic F_2^- molecules (called the *H* centers) with a regular F^- ion (Fig. 5). The formation energy of the close Frenkel pair has been found to be 8.36 eV. The distance between the *F* and *H* centers is 1.85 Å only. An interatomic distance within *H* center (diatomic molecule) is 1.87 Å, considerably less than in free *H* center (1.96 Å).

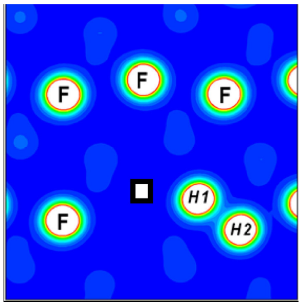

Figure 6. The total electronic charge distribution for the nearest *F–H* pair. Red colored lines correspond to 0.40 *e* while density inside dark blue area lies within interval 0.000-0.002 *e* (other details are described in Fig. 5).

The electronic density plot for a close *F–H* pair (Fig. 6) confirms a strong anisotropy of the charges in the hole center and their strong mutual perturbation.

Only ions nearest to the pair are slightly perturbed.

AB INITIO CALCULATION*S* OF SURFACE AND DEFECTS FOR ABO_3 PEROVSKITE OXIDES AND MeF_2 FLUORITES

R.I. Eglitis

We have summarized recently in the review the results of calculations on surface relaxations, energetics, and bonding properties for ABO_3 perovskite (001), (011) and (111) surfaces using mostly a hybrid description of exchange and correlation is presented. Both AO and BO_2-terminations of the nonpolar (001) surface and A, BO, and O terminations of the polar (011) surface, as well as B and AO_3-terminations of the polar (111) surface were considered. Upon the AO-terminated (001) surface, all upper-layer A atoms relax inward, while second layer atoms relax outwards. For the BO_2-terminated (001) surface, in most cases, the largest relaxations are on the second-layer metal atoms.

For almost all ABO_3 perovskites, the surface rumpling is much larger for the AO-terminated than for the BO_2-terminated (001) surface, but their surface energies always are quite similar. In contrast, different terminations of the (011) ABO_3 surface lead to very different surface energies for the O-terminated, A-terminated, and BO-terminated (011) surface, respectively. A considerable increase in the Ti-O or Zr-O, respectively, chemical bond covalency near the (011) surface as compared both to the bulk and to the (001) surface in ABO_3 perovskites were predicted. According to the results of ab initio calculations for Nb doped $SrTiO_3$, Nb is a shallow donor; six nearest O ions are slightly displaced outwards from the Nb ion.

The *F* center in ABO_3 perovskites resembles the electron defects in the partially-covalent SiO_2 crystal rather than usual F centers in ionic crystals like MgO and alkali halides. The results of calculations for several perovskite $KNb_xTa_{1-x}O_3$ (KTN) solid solutions, as well as hole and electron polarons in ABO_3 perovskites are analyzed.

The *H* center, a hole trapped at an interstitial anion site, placed in the bulk and at the (111) surface of calcium fluoride CaF_2, has been studied by using DFT with B3PW hybrid exchange potentials. The *H* center is oriented in the (111) direction in the bulk case and along the (100) direction in the surface case (Fig. 7), and the hole is mainly localized on the interstitial fluorine. The surface *H* center leads to a remarkable XY-translation of the surface atoms. The hole induces an empty energy levels in the β-spin in the band gap, located 2.9 eV above the valence band (VB) top, corresponding to the first optical absorption band, and the surface effect heightens the hole level considerably.

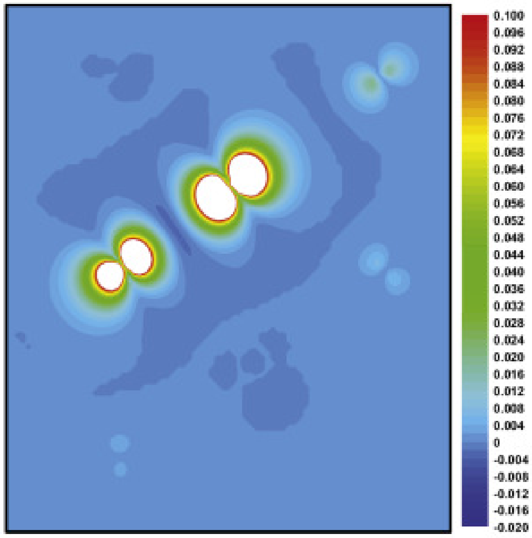

Figure 7. Electron spin density contours in CaF_2 with the *H* center in configuration *H*(111) from the (110) side view (details are explained in Figs. 5,6).

Density of states (DOS) calculations reveal that the hole band mainly consists of the *H*-center *p*-orbitals (Fig. 7), and the interstitial fluorine does the major contribution. Further study regarding the electron-hole pair, named *F*-*H* pair, in this paper, shows that the geometrical structure is similar to an *F* center and an *H* center paired together, whereas the hole localized on the *H* center in the isolated *H*-center case, moves to the fluorine vacancy (V_F) site. The electron-hole pair induces seven defect levels in the VB-CB gap, three of them located near the Fermi energy, being occupied, and four of them located above the Fermi level, forming the hole bands. The *p*-orbitals of the interstitial fluorine form the three electron bands and the four hole bands are composed of the *s*- and *p*-orbitals of the V_F.

RADIATION DEFECTS IN COMPLEX PEROVSKITE SOLID SOLUTIONS

E.A. Kotomin, Yu.A. Mastrikov, M.M. Kuklja, J. Maier

Recently, we have presented and discussed the results of first principles calculations of (Ba,Sr)(Co,Fe)O_3 known as BSCF perovskite solid solutions (Fig. 8a) containing basic point defects (cation and anion vacancies, cation exchange, and antisite defects), as well as structural and Schottky disorders have quite low formation energies and are energetically favorable. The calculated cation exchange energies are very low on both the *A*- and *B*- sublattices (Ba↔Sr and Co↔Fe) of the cubic perovskite structure; this should lead to an easy aggregation of cations with further phase separation. In contrast, antisite defects (*A*↔*B* exchange) are costly and unlikely to contribute to disorder in these materials. The oxygen interstitials form so-called dumbbell (split) configuration with a regular oxygen ions (Fig.8b). Thus, in general, complex perovskite solid solutions (for example, double perovskites) can accommodate much more expressed defect disorder than parent ABO_3 perovskites. An analysis of possible BSCF decomposition into different phases or binary oxides was also performed.

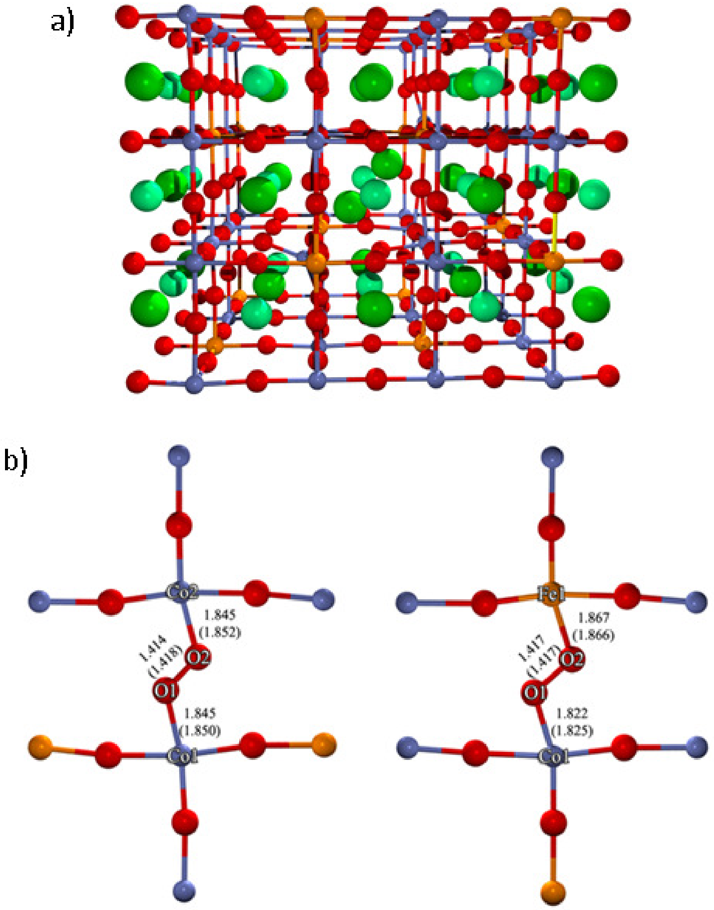

Figure 8. (a) Ba-split interstitial configuration is shown in the 320 atom model supercell of BSCF, (b) and (c) two different configurations of O split interstitial defects. The numbers indicate distances between atoms in a close Frenkel pair.

AB INITIO ***SIMULATIONS OF POINT DEFECTS (VACANCIES) AND ATOM SUBSTITUTES (O AND Y) IN*** **fcc-*Fe LATTICE***

A. Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, A. Möslang, P. Vladimirov,
V.A. Borodin

Current generation of reduced activation ferritic-martensitic steels (RAFM) strengthened by oxides permits a growth of the operating temperature for future fusion and advanced fission reactors by 100°C (up to 650°C and higher). The most frequently used oxide for the strengthening of RAFM steels is Y_2O_3, as it is one of the most stable oxides with melting temperature higher than that of the steels which might play significant role in the formation of oxide nanoparticles in oxide disperse-strengthened (ODS) steels.

The main goal of this study is to get deep insight in the formation of the ODS particles inside RAFM steel structures. To perform it, a two-step theoretical approach for atomistic simulation of this process is proposed. The *first step* includes extensive *ab initio* calculations of elementary yttrium and oxygen complexes inside the iron lattice (4×4×4 and 5×5×5 *fcc*-Fe supercell models) containing also Fe-vacancies (V_{Fe}) performed using VASP computer code. Both interaction energies between solute and matrix atoms and barriers for migration of different solute atoms are extracted from these calculations for further atomistic simulations.

Binding energies between the impurity atoms and vacancies as well as their migration barrier energies are important parameters for the LKMC modeling of the ODS particle formation (the *second step* of simulations). To perform calculations for estimating migration barriers, the nudge elastic band (NEB) method have been used (as implemented in the *VASP* computer code). The lowest calculated energy of the barrier for Y atom migration has been found to be about 1.75eV. Obviously, the increased concentration of V_{Fe} vacancies is required for interstitial Y migration and the increased size of the supercell is necessary for this aim.

AB INITIO AND ELECTROMAGNETIC SIMULATIONS OF CNT GROWTH UPON Fe-Pt NANOCLUSTERS

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

Carbon nanotubes (CNTs) of various chiralities open new wide possibilities for modern nanoelectronics as promising candidates for nanointerconnects in a high-speed electronic nanosensoring and nanomemory devices. We focus our current study on the implementation of advanced simulation models for a proper description of the fundamental electromagnetic properties (electrical resistance, capacitances and impedances) in contacts between carbon nanotubes of different morphologies and metallic substrates of different nature. We also present the model of magnetically stimulated CNT growth for a special case of Fe-Pt metallic nanoclusters (Fig. 9), which have unique magnetic properties. We have performed optimization of nanocluster shape (icosahedral or cuboctahedral), morphology (onion-like or striped) and equilibrium ratio between Fe and Pt atoms (for this aim, we have performed first principles DFT-LCAO calculations). It has been found that the energetically most preferable configuration of nanocluster is onion-type $Fe_{43}Pt_{104}$ icosahedron with external Pt shell (Fig. 9). We expect that in the presence of magnetic field, the CNTs growth will be more determined from the point of view of possible nanotube morphologies. Moreover, the creation of a CNT forest based on Pt-Fe nanoparticles (Fig. 10) provides the possibilities to consider this kind of structure as the basic fragment of nanomemory devices, where information

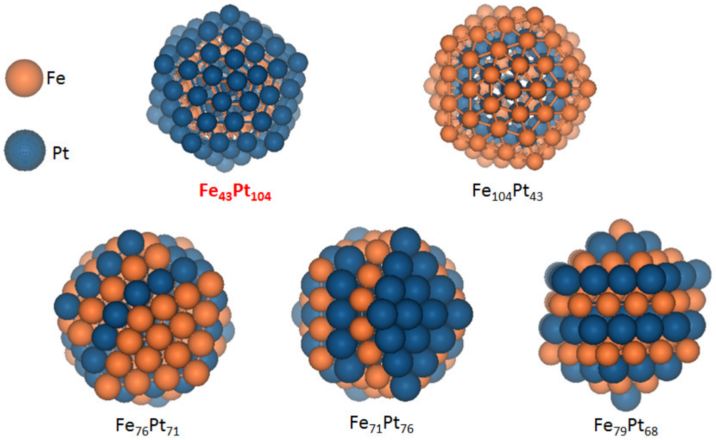

Figure 9. Equilibrium configurations of Fe-Pt nanoclusters with morphologies of onion-type (top level) and striped icosahedra.

bits are located

in nanoparticles and the CNT forest provides the necessary spin transport for reading and recording information. The parametrically controlled production of carbon nanotubes (CNTs) with predefined morphologies is a topical technological problem for modern nanoelectronics. This process can be streamlined using even minor diamagnetic properties of carbon atoms at the expense of magnetic field and strong induced ferromagnetism of the nanoparticle.

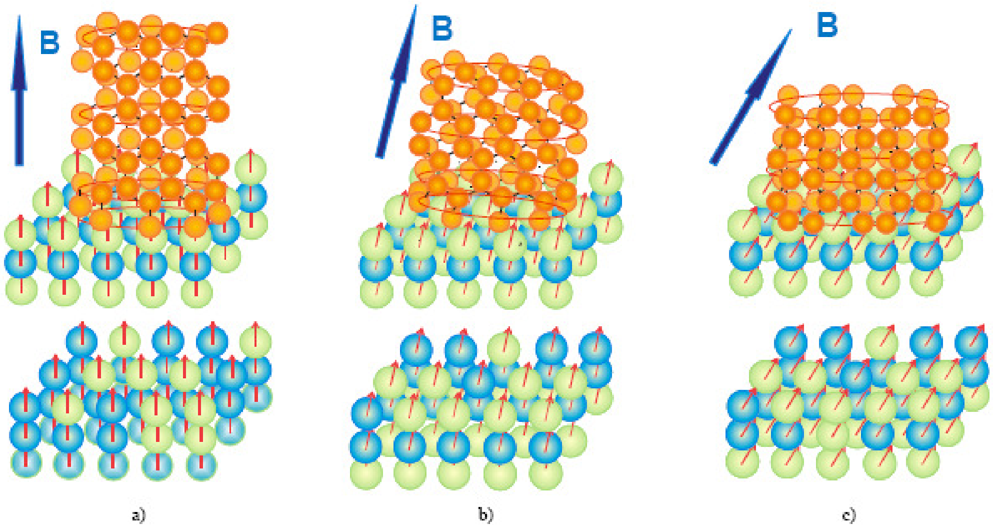

Figure 10. Magnetically stimulated orientation of magnetic moments of atoms in model interconnects during the CNTs controlled growth with the expected chiralities under the directed magnetic field with the orientation angle shown by arrows, where **B** is the magnetic induction and the chirality angle is $\phi = \Theta_B$: a) arm-chair CNT, $\phi = 0$; b) chiral CNT, $0 < \phi < 30^o$; c) zig-zag CNT, $\phi = 30^o$.

The morphology of Fe-Pt cluster and its atomic structure (including the short-range order) play a primary role in the process of CNT growth stimulated by the magnetic field. Nucleation in the process of CNT growth in cases of the ordered Fe-Pt nanoclusters hase been found to be more stable and has principal advantages relatively to the controlled CNT growth as compared to the cases of any kinds of anisotropic Fe-Pt nanocatalysts.

B. Kinetics of processes with self-organization

STATIC AND DYNAMIC SCREENING EFFECTS IN ELECTROSTATIC SELF-ASSEMBLY OF NANO-PARTICLES

V.N. Kuzovkov and E.A. Kotomin

Kinetics of processes in nanomaterials, e.g. nanoparticles in soft matter or liquid phase is of great importance for many applications. In the description of charge screening in electrostatic self-assembly of nanoparticles (molecules) embedded into a polar solvent, the *static* screening effects (a contribution associated with the rapid spatial redistribution of small and highly mobile ions of a solvent) is traditionally treated phenomenologically, using the Yukawa short-range potential for describing the interaction between these particles. However, this model has a limited range of applicability being valid only for infinitely diluted systems and high salt concentrations. During a slow self-assembling process with nanoparticle formation, very dense structural elements (aggregates) are formed, in which the distances between the nanoparticles could become comparable to the Debye radius in the Yukawa potential. For such the structural elements *dynamic* screening effects (the contribution of nanoparticles themselves into the screening potential) becomes important.

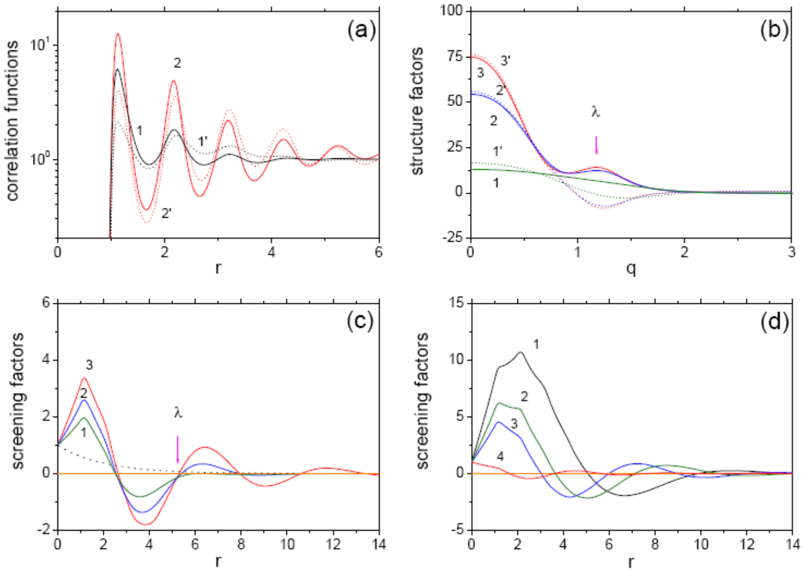

Figure 11. Ionic binary systems with Lennard-Jones and Coulomb interactions (weak static screening). (a) Joint correlation functions; (b) Structure factors; (c) Screening factors for the same times as in window (b); (d) Sreening factors at fixed time and for different values of Bjerum length.

Using a novel integrated approach (nonlinear integro-differential kinetic equations for the correlation functions of particles, Fig. 11), we have obtained the self-consistent solution in 3d case and compare roles of both static (equilibrium) and dynamic (nonequilibrium) charge screening effects in different situations. This is a continuation of our recent study)], with the polar solvent effects now taken into account.

STATISTICAL CHARACTERIZATION OF SELF-ASSEMBLED CHARGED NANOPARTICLE STRUCTURES

G. Zvejnieks, V.N. Kuzovkov and E.A. Kotomin

We proposed a novel approach for description of dynamics of nano-structure formation for a system consisting of oppositely charged particles. The combination of numerical solution of analytical Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) type equation set with reverse Monte Carlo (RMC) method allows us to overcome difficulties of standard approaches, such as kinetic Monte Carlo or Molecular Dynamics, to describe effects of long range Coulomb interactions. Moreover, this allows one to study the system dynamics on realistic time and length scales.

We applied this method to a simple short-range Lenard-Jones (LJ)-like 3d system and 2d system combining the long-range Coulomb and LJ interactions. As expected, the nanoparticle growth driven by the Ostwald ripening is observed in the former case, while long-range interaction limited self-assembled nanostructures are observed in the latter case (Fig. 12).

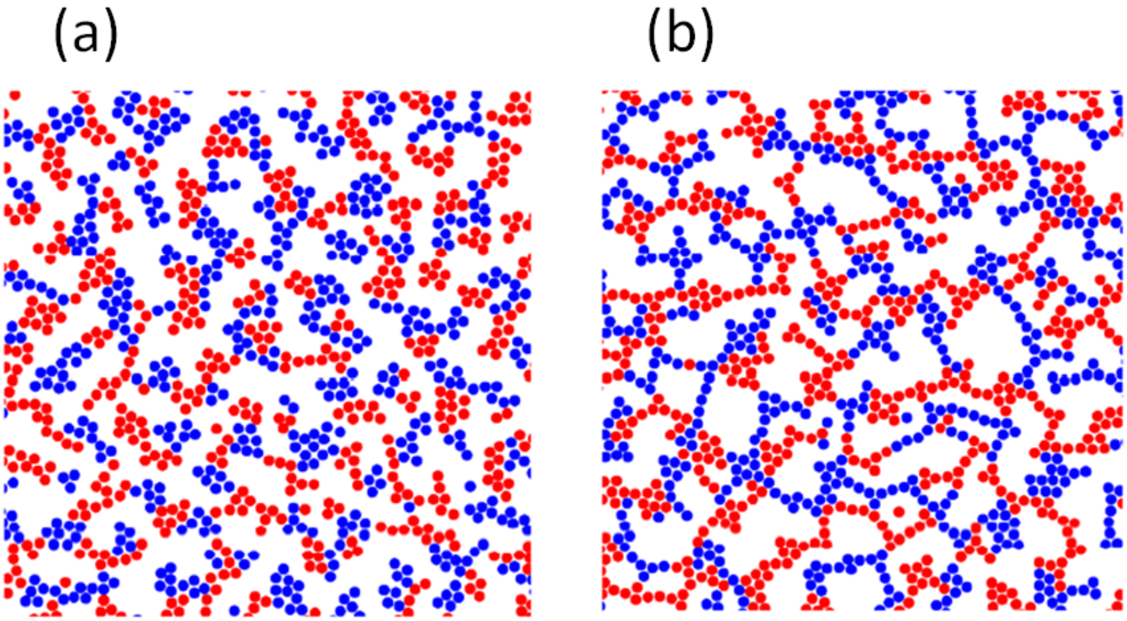

Figure 12. Aggregation in two dimensions: percolated dendritic (fractal-like) growth. Characteristic structure snapshots (small fragments) obtained using the RMC by increasing of time, (a,b).

INTERACTION OF ELECTROMAGNETIC RADIATION WITH MATTER: TIME RESOLVED APPROACH

E. Klotins

Determining the properties of electric charges excited at interaction of electromagnetic radiation is of major interest across many branches of solid state physics and advanced materials. Computational approaches to the luminescence, energy harvesting and electroconductivity rely on representing the advanced materials in terms of interacting electric charges obeying requirements of quantum mechanics, quantum field theory and relativity. Currently, there are no general efficient methods to deal with challenging problems that involves both kinetics of electrons, electron holes and their interaction with atoms constituting the material. The research is addressed to intrinsic charge transfer in dielectric materials sensitive to electromagnetic radiation within the range of visible and ultraviolet light. A special attention is paid to the time dependence of radiation field which, unlike the existing models, is arbitrary. Determining these properties relies on well-known theoretical approaches to the free particles. With application to solids distinguished by the environment of surrounding atoms these appraches become more complex and not completely understood.

What is new in the presented research is the extension of the model of noninteracting electrons and electronic holes to the back reaction of surronding atoms. This back reaction is supported by supplementary kind of particles – phonons as a challenge. In the present study, we propose a step towards this unsolved problem and derive a closed set of equations for the self-consistent treatment of electrons, the electronic holes and the back-reaction of phonons.

The key development of this work is disconnection of the electron – phonon and the electron hole – phonon interaction into purely electronic and hole parts added to the impact of electromagnetic radiation by the extra terms. Formally these extra terms contribute on equal grounds with the electromagnetic radiation with the mathematical structure of the solution maintained. Also maintained are arbitrary time dependence of radiation and full time history of the material. The necessary theory inputs are available within conventional quantum mechanics and commercial codes while the key output is the distribution function for electron – electronic hole pair determining all observables of interest.

C. Plasma Physics

DEPENDENCE OF THE GIROTRON EFFICIENCY ON ASIMUTAL INDEX OF THE NON-SYMMETRIC MODES

O. Dumbrajs, G.S. Nusinovich, T.M. Antonsen, Jr

Development of MW-class gyrotrons for future controlled fusion reactors requires careful analysis of the stability of high efficiency operation in very high-order modes. In the present paper, this problem is analyzed in the framework of the non-stationary self-consistent theory of gyrotrons.

Two approaches are used: the one based on the wave envelope representation of the resonator field and the second one based on representation of this field as a superposition of eigenmodes, whose fields are determined by a self-consistent set of equations. It is shown that at relatively low beam currents, when the maximum efficiency can be realized in the regime of soft self-excitation, the operation in the desired mode is stable even in the case of a very dense spectrum of competing modes.

At higher currents, the maximum efficiency can be realized in the regimes with hard self-excitation; here the operation in the desired mode can be unstable because of the presence of some competing modes with low start currents. Two 170 GHz European gyrotrons for the international thermonuclear experimental reactor ITER are considered as examples. In the first one, which is the 2 MW gyrotron with a coaxial resonator, the stability of operation in a chosen $TE_{34,19}$-mode in the presence of two sideband modes with almost equidistant spectrum is analyzed and the region of magnetic fields in which the oscillations of the central mode are stable is determined.

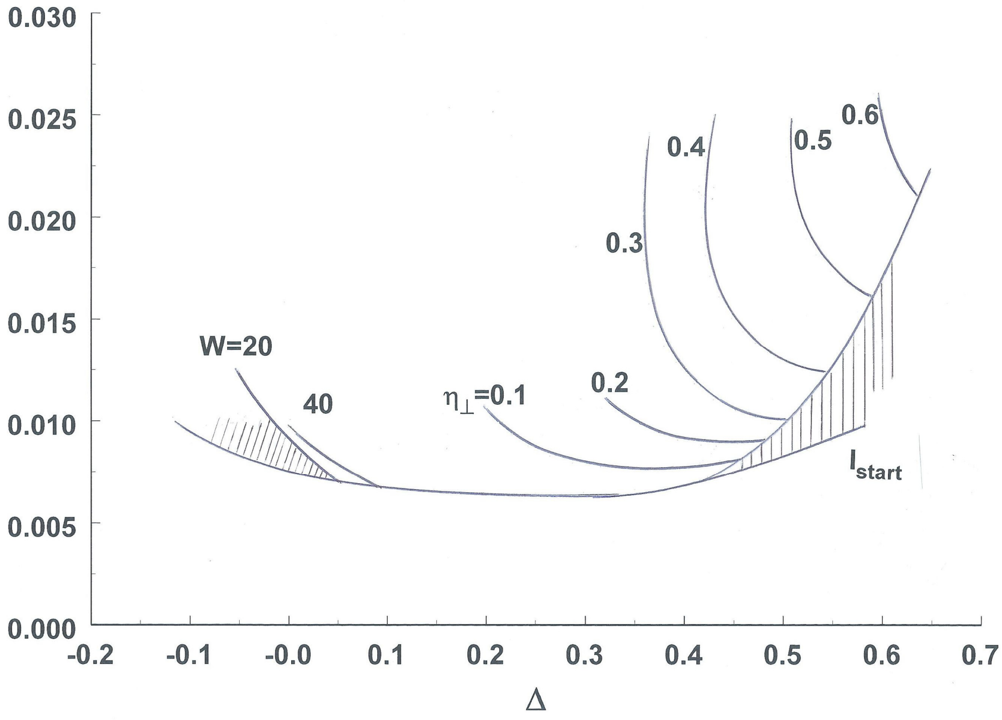

Figure 13. Region of stable operation surrounded by dashed regions in which oscillations of the operating mode are unstable. Normalized length $\varsigma_{out} = \left(\beta_{\perp 0}^2 / 2\beta_{z0}\right)\left(\omega_0 L / c\right)$ is equal to 10. Also contours of equal values of the orbital efficiency $\eta_\perp$ are shown in the region of stable operation.

The operation of the second, 1 MW gyrotron with a cylindrical cavity currently under development in Europe, is studied by using the wave envelope approach. It is shown that high efficiency operation of this gyrotron in the TE32,9-mode should be stable (Fig. 13).

ON THE DEPENDENCE OF THE EFFICIENCY 240 GHz HIGH-POWER GYROTRON ON THE DISPLACEMENT OF THE ELECTRON BEAM AND THE AZIMUTAL INDEX

O. Dumbrajs, K.A. Avramidis, J. Franck, J. Jelonnek

Two issues in the cavity design for a Megawatt-class, 240 GHz gyrotron are addressed. Those are, firstly, the effect of a misaligned electron beam on the gyrotron efficiency and, secondly, a possible azimuthal instability of the gyrotron. The aforementioned effects are important for any gyrotron operation, but could be more critical in the operation of Megawatt-class gyrotrons at the frequencies above 200 GHz, which will be the anticipated requirement of DEMO. The target is to provide some basic trends to be considered during the refinement and optimization of the design. Self-consistent calculations are the base for simulations wherever possible. However, in cases for which self-consistent models were not available, fixed-field results are presented (Fig. 14). In those cases the conservative nature of the results should be kept in mind.

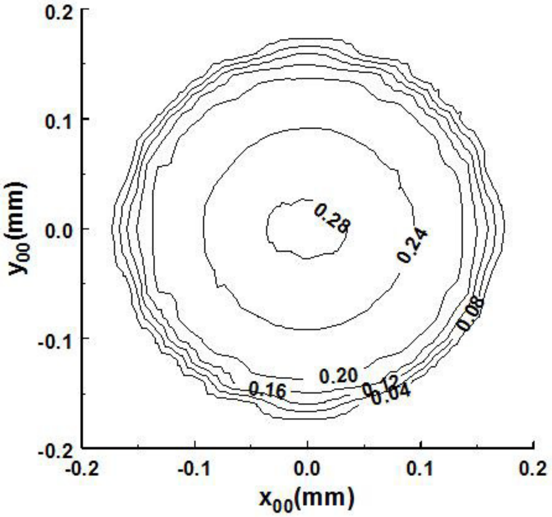

Figure 14. Fixed-field results for a parallel displacement of the electron beam (i.e. shift only, no tilt): The interaction efficiency η_{tot} is plotted as a function of the transverse coordinates. An ideal electron beam with a radius of 10 mm is assumed.

FREQUENCY TUNABILITY OF GYRO-BWO

O. Dumbrajs, G.S. Nusinovich

Gyrotron backward-wave oscillators (gyro-BWOs) are oscillators capable of producing frequency tunable, high-power radiation at millimeter and submillimeter wavelengths (Fig. 15). While in the most advanced version of gyro-devices, the gyromonotron (or simply, the gyrotron) the variation of the external magnetic field can yield a step-tunable radiation due to the gyrotron hopping from one mode to another, in gyro-BWOs the radiation frequency can be tuned continuously. In this presentation, we discuss various concepts of gyro-BWOs offering large bandwidth and give an overview of experimental results. Some new results of simulations for frequency tunable gyro-BWOs are also presented. Part of these results is obtained in the framework of the general theory of gyro-BWO, while another part is focused on the analysis of possible frequency tunability of two gyrotrons, which are currently under development at the FIR Center of the Fukui University, Japan.

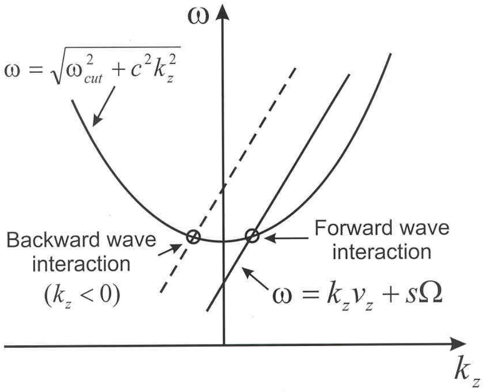

Figure 15. Dispersion diagram.

D. Experimental studies

STRUCTURE AND LUMINESCENT PROPERTIES OF BaZrO$_3$ NANOCRYSTALS IN THE POLYMER MATRIX

A.I. Popov,O.I. Aksimentyeva, V. Savchyn,

The effect of polymer environment on luminescent properties of barium zirconate nanocrystals have been studied by means of cathodoluminescence (CL) spectroscopy technique (Fig. 16). It was found that polystyrene (PS) shell around

$BaZrO_3$ nanocrystals significantly modify CL spectra. This phenomenon can be explained by a chemical interaction between PS and $BaZrO_3$ significantly changing the surface states of nanocrystals. This conclusion is confirmed by the complementary experimental studies including X-ray diffraction, FTIR spectroscopy, Energy Dispersive X-ray analysis and scanning electron spectroscopy.

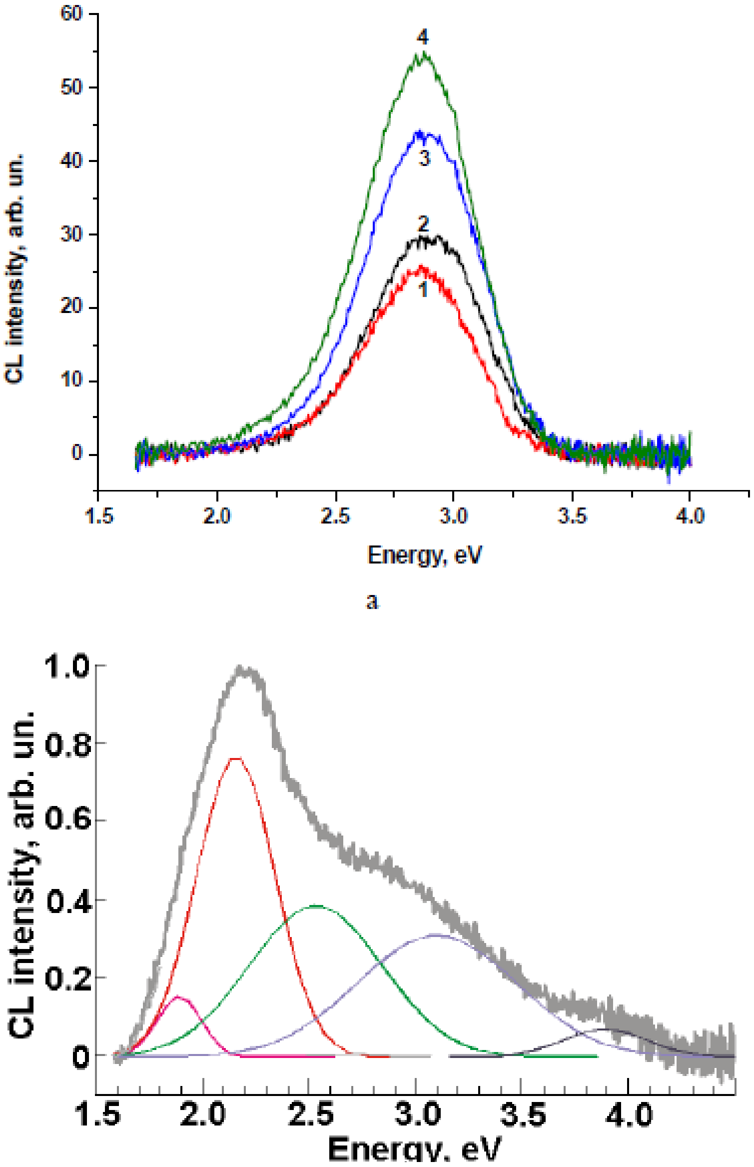

Figure 16. CL spectra of nano-$BaZrO_3$–PPA composites with a $BaZrO_3$ content of 80% (1), 90% (3) and 100% (4) and PEDOT–$BaZrO_3$ (60%) composites at T = 293 K (2); (b) CL spectrum of a PS–$BaZrO_3$ (20%) composite.

MODELING AND SYNCHROTRON DATA ANALYSIS OF MODIFIED HYDROXYAPATITE STRUCTURE

A.I. Popov, A.V. Bystrova, Yu.D. Dekhtyar, V.S. Bystrov

The obtained results are based on the first principles modeling and calculations for hydroxyapatite (HAP) nanostructures as native as well surface modified, charged and having various defects (H and OH vacancies, H internodes). HAP structures having being studied using Local Density Approximation (LDA) method with calculations of Density of States (DOS) allow us analyzing the experimental forbidden energy gap (E_g) and work function data.

Molecular modeling by HyperChem is confirmed by photoelectron monochromatic measurements up to 6 eV and photoluminescence excitation spectra (PL) data from synchrotron DESY experimental data up to 30 eV values. Brief analysis of the influence of heating, microwave radiation, hydrogenation, x-rays and synchrotron radiation on HAP surface is presented in this work. New data of the structure of modified hydroxyapatite are obtained. The determined energy levels for H internodes is $E_{\text{H-int}} \sim Ev + (1.5–2.0)$ eV, while for OH vacancy energy is in the range of $E_{\text{OH-vac}} \sim Ev + (2.9–3.4)$ eV inside the band gap E_g.

The analysis of PL emission allows us to conclude that these energies are close to observed main PL spectral line 420 nm (2.95 eV), and consequently OH vacancy could play the leading role in the surface energy levels changes and charging. But the influence of the inserted hydrogen is revealed too through excitation from most deep valence band levels due to existence of close overlapped molecular orbital with phosphorus atoms in the excited states. Both defects are observed by PL emission spectrum under synchrotron excitation energy in diapason ~8.5–14.5 eV.

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2. **D. Gryaznov**, S. Baumann, **E.A. Kotomin,** and R. Merkle, Comparison of permeation measurements and hybrid density-functional calculations on oxygen vacancy transport in complex perovskite oxides. - J. Phys. Chem. C 2014, **118**, p. 29542–29553.

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I. 30th ISSP Conference (Riga, Latvia, February, 2014).

1. D. Bocharov, S. Piskunov, P. Zhgun, J. Purans, and A. Kuzmin, “Lattice dynamics of cubic ScF_3 from first principles calculations”. Abstract: p. 32.

2. A. Platonenko, S. Piskunov, Yu.F. Zhukovskii, and D. Bocharov, “Fe-Pt nanoparticle structure: Ab initio calculations”. Abstract: p. 33.

3. J. Begens, S. Piskunov, Yu.F. Zhukovskii, and O. Lisovski, “Simulations and comparison of doped $SrTiO_3$ and TiO_2 nanotubes for application in photocatalytic water separation”. Abstract: p. 35.

4. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Möslang, “First principles calculations of the energy barriers for different trajectories of Y atom migration inside fcc-Fe lattice”. Abstract: p. 36.

II. 16th Israel Materials Engineering Conference (Haifa, Israel, February, 2014).

5. E.A. Kotomin, D. Fuks, M. Kuklja, Yu.A. Mastrikov, R. Merkle and J. Maier, "Ab initio modelling of pervoskite solid solutions for solid oxide fuel cells and permeation membranes". Abstract: p. 26.

III. The 5th International Workshop on Far-Infrared Technologies 2014 (Fukui, Japan, March, 2014).

6. O. Dumbrajs and G.S. Nusinovich, “Frequency tunability of the gyro-BWO”. Abstract: p. 5p-6.

IV. 48th Russian School on Condensed State Physics (St. Petersburg, Russia, March, 2014).

7. D. Bocharov, S. Piskunov, O. Lisovski, J. Kazerovskis, J. Begens, Yu.F. Zhukovkii, and E. Spohr, “Quantum chemical simulations of TiO_2 nanotubes for photocatalytical water splitting”. Abstract: p. 166

V. Workshop on Permeation membranes (GREEN-OTM EC Project meeting) (Valencia, Spain, March-April, 2014).

8. E.A. Kotomin and D. Gryaznov, "Ab initio modelling of a role of Sr doping in permeation membranes".

VI. Materials Research Society, MRS Spring Meeting 2014 (San Francisco, USA, April, 2014).

9. Yu.A. Mastrikov, M.M. Kuklja, R. Merkle, E.A. Kotomin, and J. Maier, "Oxygen Mobility in LSCF and BSCF Perovskites from ab Initio Modeling". Abstract: L8.02.

VII. WG4 COST Meeting, Action CM 1104 "Reducible Oxide Chemistry" (Riga, Latvia, April, 2014).

10. D. Gryaznov, J. Begens, and E.A. Kotomin, “First principles calculations on oxygen vacancy behaviour in Sr-doped complex perovskites for permeation membranes and solid oxide fuel cells”. Abstract: p. 23.

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12. A.I. Popov, A.Ch. Lushchik, Ch.B. Lushchik, and E.A. Kotomin, “Analysis of excitonic mechanism of defect formation in insulating materials: Generalization of Rabin-Klick diagram for a whole family of alkali halides”. Abstract: p. 30.

VIII. 12th International Conference "Information Technologies and Management", IT&M'2014 (Riga, Latvia, April, 2014).

13. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, “Simulation of fundamental properties in CNT- and graphene-based nanoporous materials: Electromechanics and Electromagnetics”. Abstract: p. 17-18

14. Yu.F. Zhukovskii, S. Piskunov, A. Platonenko, and E.A. Kotomin, “Simulation of radiation-induced Frenkel pairs in α-Al_2O_3: Optimization of computational procedure”. Abstract: p. 19-20.

15. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, Yu.A. Mastrikov, E.A. Kotomin,

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17. A. Chesnokov, O. Lisovski, D. Bocharov, S. Piskunov, Yu.F. Zhukovskii, M. Wessel, and E. Spohr, “Quantum-chemical study of pristine and doped TiO_2 nanotubes for water photocatalysis”. Abstract: p. 26-28.

18. P. Zhgun, D. Bocharov, S. Piskunov, J. Purans, and A. Kuzmin, “Ab initio calculations on electronic structure and phonons in cubic ScF_3”. Abstract: p. 169-170.

IX. E-MRS 2014 Spring Meeting (Lille, France, May, 2013).

19. R.I. Eglitis, „Towards a practical rechargeable 5 V Li ion battery”. – Abstract: BB.1.2.

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21. R.I. Eglitis, „Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ and $CaTiO_3$ (001), (011) and (111) surfaces”. – Abstract: C.4.7.

22. A.U. Abuova, T.M. Inerbaev, A.T. Akilbekov, Yu.A. Mastrikov, and E.A. Kotomin, „First principles modeling of Ag adsorption on the MnO_2- and LaO-terminated surfaces of $LaMnO_3$(001)”. – Abstract: C/P1.1.

23. G. Kaptagai, T.M. Inerbaev, A.T. Akilbekov, Yu.A. Mastrikov, and E.A. Kotomin, „Water interaction with fluorine-doped Co_3O_4 (100) and (111) surfaces”. – Abstract: C/P1.10.

24. Yu.A. Mastrikov, E.A. Kotomin, R. Merkle, M.M. Kuklja, and J. Maier, „First principles calculations of formation and migration of oxygen vacancies in the bulk and at the surface of complex perovskites for solid oxide fuel cell cathodes”. – Abstract: C/P1.11.

25. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, „Ab initio modeling of oxygen reduction reaction in mixed conducting perovsites for solid oxide fuel cells”. – Abstract: CC.1.6.

26. M. Arrigoni, D. Gryaznov, E.A. Kotomin, and J. Maier, „Confinement effects for ionic carriers in ABO_3 perovskite ultrathin films”. – Abstract: EO.5.3.

27. Yu.F. Zhukovskii, S. Piskunov, O. Lisovskii, J. Begens, and E. Spohr, „Doped TiO_2 and $SrTiO_3$ nanotubes for photocatalytic applications: Predictions from first principles". – Abstract: EO.8.2.

28. R.I. Eglitis, H. Shi, and R. Jia, „Ab initio calculations of the transfer and aggregation of F centers, as well as bulk and nano-surface H centers in CaF_2, BaF_2 and SrF_2". – Abstract: EP.1.9.

29. A.I. Popov, L. Shirmane, V. Pankratov, A.Ch. Lushchik, V.E. Serga, A. Kotlov, and J. Zimmermann, „Luminescence of macro- and nanocrystalline MgO excited by VUV synchrotron radiation". – Abstract: EP.2.54.

30. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, A. Gopejenko, Yu.F. Zhukovskii, E.A. Kotomin, and A. Möslang, „Ab initio simulation of the initial steps of the ODS particle formation process in bcc iron matrix". – Abstract: EP.2.73.

31. I. Karbovnyk, P. Savchyn, A. Huczko, M. Cestelli-Guidi, C Mirri, and A.I. Popov, „FTIR studies of silicon carbide nanostructures". – Abstract: G.PII.37.

32. A.I. Popov, V. Savchyn, J. Purans, A. Dabrowska, A. Huczko, B. Pathak, and D.P. Subedi, „Cathodoluminescence study of Al-doped ZnO nanofilms at 80 K and RT". – Abstract: I.P3.43.

33. O. Aksimentyeva, V. Savchyn, I. Opaynych, P. Demchenko, Yu. Horbenko, V. Pankratov, and A.I. Popov, „Effect of polymer matrix on the structure and luminescence properties of barium zirconate ($BaZrO_3$) nanocrystals". – Abstract: Q.P1.62.

34. R.I. Eglitis, H. Shi, and R. Jia, „Ab initio calculations of the self trapped hole in SrF_2, as well as bulk and surface hydroxyl impurities in CaF_2 and BaF_2". – Abstract: U.1.2.

X. International Symposium on Reactivity of Solids, (St. Petersburg, Russia, June, 2014).

35. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, "Ab initio modelling of oxygen reduction reaction in mixed conducting pervoskites for solid oxide fuell cells". Abstract: p. 99.

XI. DSL2014 conference (Paris, France, June, 2014).

36. V.N. Kuzovkov, M. Olvera de la Cruz, G. Zvejnieks, and E.A. Kotomin, "Diffusion and self-assembly of charged nanoparticles in three-dimensional condensed systems". Abstract: p. 214.

XII. Electrochemistry workshop, (Asilomar, USA, July, 2014).

37. E.A. Kotomin, Yu. Mastrikov, and M. Kuklja, "Structural instability of perovskite solid solutions".

XIII. Proceedings 9th International Workshop Strong Microwaves and Terahertz Waves: Sources and Applications, (Nizhny Novgorod, Russia, July, 2014).

38. O. Dumbrajs, G.S. Nusinovich, and T.M. Antonsen, “Stability of gyrotron operation in very high order modes”. Abstract: p. 154.

XIV. 4th International Workshop on Nanocarbon Photonics and Optoelectronics (Polvijärvi, Finland, July-August, 2014).

39. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, "Simulation of electromagnetic properties in CNT- and graphene-based nanomaterials and nanodevices". Abstract: p. 74.

XV. International conference on solid state protonic conductors (SSPC-17) (Seoul, Korea, September, 2014).

40. T. Bjørheim, E.A. Kotomin, R. Haugsrud, and J. Maier, "Defect thermodynamics of $BaZrO_3$ from first principles phonon calculations".

XVI. E-MRS 2014 Fall Meeting, (Warsaw, Poland, September, 2014).

41. D. Gryaznov, "First principles calculations on oxygen vacancy behaviour in Sr-doped complex perovskites for permeation membranes and solid oxide fuel cells". Abstract: A5.21.
42. R.I. Eglitis, "Point defects and surfaces in perovskite structured oxides". Abstract: D13.1.
43. D. Gryaznov, D. Bocharov, E.A. Kotomin, and Yu.F Zhukovskii, "Ab initio simulations of oxygen interaction with surfaces and interfaces in uranium mononitride". Abstract: G9.44.
44. R.I. Eglitis, H. Shi and R. Jia, "Ab initio calculations of F, R, bulk and surface H centers, as well as hydroxyl impurities in CaF_2, BaF_2 and SrF_2". Abstract: K2.6.
45. R.I. Eglitis, "Towards a practical rechargeable 5 V Li ion battery". Abstract: S9.1.

XVII. Joint 12th RCBJCF Symposium and 9th FMNT Conference (Riga, Latvia, September-October, 2014).

46. R. Merkle, D. Poetzsch, D. Gryaznov, E.A. Kotomin, and J. Maier, ”Mixed conducting perovskites as solid oxide fuel cell cathode materials: Insight from experiments and theory”. Abstract: p. 75.
47. E. Spohr, M. Wessel, D. Bocharov, and S. Piskunov, “Simulation of oxide nanostructures for energy conversion”. Abstract: p. 99.
48. A. Anspoks, D. Bocharov, J. Purans, F. Rocca, A. Sharakovskis, J. Timoshenko, V.A. Trepakov, A. Dejneka, and M. Itoh, “Local structure studies of Ti for $SrTi^{16}O_3$ and $SrTi^{18}O_3$ by advanced X-ray absorption spectroscopy data analysis. Abstract: p. 124.
49. Yu.F. Zhukovskii, R.A. Evarestov, and A.V. Bandura, “First principles simulations on stoichiometric $SrTiO_3$ nanowires’. Abstract: p. 160.
50. R.I. Eglitis, H. Shi, and R. Jia, “First principles calculations of the diffusion and aggregation of F centers as well as bulk and nano-surface H centers in CaF_2, BaF_2 and SrF_2”. Abstract: p. 166.
51. R.I. Eglitis, “First principles calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$ and $CaTiO_3$ (001), (011) and (111) surfaces”. Abstract: p. 167.
52. I. Bolesta, I. Karbovnyk, I. Rovetsky, S. Velgosh, I. Kityk, and A.I. Popov, “Effects of long term annealing on the nanostructures formed in CdI_2 crystals”. Abstract: p. 180.
53. V.P. Savchyn, O.I. Aksimentyeva, Yu.Yu. Horbenko, I. Karbovnyk, V. Pankratov, and A.I. Popov, “Cathodoluminescence characterization of polystyrene–$BaZrO_3$ hybrid composites”. Abstract: p. 181.
54. T.S. Bjørheim, R. Haugsrud, J. Maier, and E.A. Kotomin, “Defect thermodynamics of $BaZrO_3$ from first principles phonon calculations”. Abstract: p. 237.
55. R.I. Eglitis, “Towards a practical rechargeable 5 V Li ion battery”. Abstract: p. 242.
56. E.A. Kotomin, M.M. Kuklja, Yu.A. Mastrikov, R. Merkle, and J. Maier, “Challenges in energy applications of non-stoichiometric complex perovskites”. Abstract: p. 247.
57. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, “Electromechanics and electromagnetics of CNT- and graphene-based nanoporous materials: Interconnects and nanosensoring”. Abstracts: p. 264.
58. A.U. Abuova, T.M. Inerbaev, E.A. Kotomin, A.T. Akilbekov, and Yu.A. Mastrikov, “Ab Initio modelling of Ag adsorption on the MnO_2- and LaO-terminated LMO(001) surfaces”. Abstracts: p. 271.
59. A. Chesnokov, O. Lisovskii, D. Bocharov, S. Piskunov, Yu.F. Zhukovskii, M. Wessel, and E. Spohr, “Ab initio simulations on N and S co-doped titania nanotubes for photocatalytic applications”. Abstracts: p. 272.

60. A. Usseinov, E.A. Kotomin, Yu.F. Zhukovskii, J. Purans, A.T. Akilbekov, and A.K. Dauletbekova, “Electronic effects on hydrogen-adsorbed surfaces of ZnO: First principles study”. Abstracts: p. 275.
61. A. Platonenko, S. Piskunov, Yu.F. Zhukovskii, and E.A. Kotomin, “Ab initio simulations on Frenkel pairs of radiation defects in corundum”. Abstracts: p. 278.
62. E. Klotins, “Relativistic time-resolved approach for phonon-assisted interaction between electron and intensive radiation field”. Abstracts: p. 281.
63. A. Gopejenko, Yu.F. Zhukovskii, P.V. Vladimirov, E.A. Kotomin, Yu.A. Mastrikov, V.A. Borodin, and A. Möslang, “Ab initio calculations of interactions between Y and O impurity atoms and vacancies in bcc- and fcc-iron lattices”. Abstracts: p. 282.
64. D. Bocharov, S. Piskunov, P. Zhgun, J. Purans, and A. Kuzmin, “R and M mode softness in cubic ScF_3: Predictions from first principles”. Abstracts: p. 283.
65. V. Savchyn, C. Balasubramanian, A. Moskina, I. Karbovnyk, and A.I. Popov, “Cathodoluminescence studies of nanostructured AlN and AlN/CsI”. Abstracts: p. 313.
66. A.I. Popov, A.Ch. Lushchik, Ch.B. Lushchik, and E.A. Kotomin, “Analysis of excitonic mechanism of defect formation in insulating materials: Generalization of Rabin-Klick diagram for a whole family of alkali halides”. Abstracts: p. 333.
67. G. Kaptagay, T.M. Inerbaev, E.A. Kotomin, A.T. Akilbekov, Yu.A. Mastrikov, and F.U. Abuova, “Research of interaction fluorine-doped Co_3O_4 (100) and (111) surfaces with water”. Abstracts: p. 340.

XVIII. 15th International Workshop on Nanoscience and Nanotechnology, n&n-2014 (Frascati, Italy, October, 2014).

68. Yu.N. Shunin, S. Bellucci, Yu.F. Zhukovskii, V.I. Gopeyenko, T. Lobanova-Shunina, and N. Burlutskaya, "Nanocarbon-based Fe-Pt spintronic devices: models and simulation".

XIX. Materials Science and Technology (MS&T-14) (Pittsburgh, USA, October, 2014).

69. E.A. Kotomin, R. Merkle, Yu. Mastrikov, M.M. Kuklja, and J. Maier, "First principles calculations of oxygen transport in SOFC cathode materials". Abstracts, p.53.
70. M.M. Kuklja, E.A. Kotomin, D. Fuks, Yu. Mastrikov, and O. Sharia, "Disorder and structural stability of complex perovskites for solid oxide fuel cells: ab initio modeling". Abstracts, p. 103.
71. E.A. Kotomin, M. Arrigoni, D. Gryaznov, T. Bjørheim, and J. Maier, "Confinement

effects for ionic carriers in $BaZrO_3$ ultrathin films". Abstracts, p. 148.

XXI. Atomistic Simulations of Functional Materials (Moscow, Russia, December, 2014).

72. E.A. Kotomin, "Computer modeling of new materials from first principles".

LABORATORY OF RADIATION PHYSICS

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

RESEARCH AREA AND MAIN PROBLEMS

The following main investigations are developed in the laboratory:

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

International projects:

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

SCIENTIFIC STAFF:

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

SCIENTIFIC VISITS ABROAD

Dr. hab. J. Berzins, European Commission Euratom, Brussels, Belgium (8 days)

Dr. hab. J. Berzins, Cyclotron Workshop, Ispra, Italy 11-12 December 2014.

Dr. T. Krasta, Dr. hab. J. Berzins, Int. Symp. CGS 15, Dresden, August 25-29, 2014.

Dr. D. Riekstina, IV International Conference on Environment, Terrestrial Radioisotopes in Environment, Veszprém, Hungary, 21-23 May 2014.

COOPERATION

Latvia

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

USA

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

Germany

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

France

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

Canada

1. Memorial University of Newfoundland, Newfoundland (Dr.A.Aleksejevs)
2. Department of Physics, Acadia University, Wolfville, NS (Dr.S.Barkanova)

Czech Republik

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

Denmark

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

MAIN RESULTS

STUDY OF CORE NON-AXIALITY EFFECTS IN THE LEVELS OF ODD-ODD NUCLEI WITH A~190

T.Krasta, M.Balodis, J.Bērziņš, L.Simonova

Nuclei of the transitional A~190 region are characterized by core instability. Level spectra of these nuclei display features characteristic both to the axially-symmetric and triaxial shapes. It poses serious challenges for level scheme development, especially in the case of doubly odd nuclei. Studies of shape transitional phenomena in odd-odd nuclei are hindered, first, by the complexity of theoretical description, and, second, by the lack of experimental data related with collective core excitations.

One of the most prominent indications of triaxiality is a high level density even at relatively low excitation energies. In axially deformed odd-odd nucleus, valence proton and neutron form two configurations with parallel and antiparallel spins – the Gallagher-Moszkowski doublet. In the case of non-axial nuclear shape, orbital momentum projections Ω and K are not conserved and one observes a number of $|K\pm2|$, $|K\pm4|$,... side-bands for each two-quasiparticle configuration. These bands of collective origin are analogous to γ-vibrational bands in even-even deformed nuclei. The characteristic feature of these bands is intense decay to the levels of its parent K band, predominantly with E2, or M1+E2 transitions. However, due to high level density, one can identify these gamma-bands only for relatively weakly mixed (isolated) two-quasiparticle configurations, mostly involving high j value orbits with high Ω values.

The best established gamma bands in doubly odd nuclei with A~190 are the 351.6 keV 2^+ $|K-2|$ band of the ground state configuration $K^\pi=4^+$ (p:11/2[505]-n:3/2[512]), strongly mixed with the (p:3/2[402]-n:11/2[615]) configuration, in ^{192}Ir [1], and the 2^+ $|K-2|$ band at 518.6 keV in ^{194}Ir [2], based in the 147.1 keV 4^+ level with structure analogous to that of the 4^+ ground state in ^{192}Ir.

Using available experimental data [1-4], we propose new tentative triaxial gamma bands for rhenium and iridium nuclei: the 482.1 keV 2^+ $|K-2|$ band of the $K^\pi=0^+$ (p:9/2[514]-n:9/2[505]) two-quasiparticle configuration in ^{188}Re; the 352.9 keV 6^+ $|K+2|$ bandhead of the 4^+ ground state configuration, the 368.2 keV 4^+ $|K-2|$ bandhead of the $K^\pi=6^+$ (p:11/2[505]+n:1/2[510]) state, and the 380.4 keV 4^- $|K-2|$ bandhead of the $K^\pi=6^-$ (p:3/2[402]+n:9/2[505]) state in ^{192}Ir. Experimentally proposed structures are compared with the results of asymmetric particle-plus-rotor (PRC) model calculations.

There are indications that the uninterpreted 270.9 keV 3^+ band in ^{194}Ir [2] can be a $|K-2|$ gamma band of the $K^\pi=5^+$ (p:11/2[505]+n:1/2[510]) configuration established at 161.5 keV. The available proton and neutron orbits do not predict two-quasiparticle 3^+ band in this energy region. However, in such a case, one must consider coexistence of different non-axial shapes in ^{194}Ir since energy of the 2^+ core state is much smaller than that for the 518.6 keV 2^+ $|K-2|$ band.

Coexistence of axially-symmetric and triaxial shapes is proposed also in the case of positive parity states of ^{188}Re. Our study of the ^{188}Re level structure [4] disclosed some problems for interpretation of the level scheme above 400 keV. First, the experimentally established density of positive parity levels below 1 MeV is about three times higher than predicted by the performed PRC calculations with the axially-symmetric core deformation. Second, we have not observed population of the 1^+ bandhead of the (p:9/2[514]-n:7/2[503]) configuration predicted at about 418 keV.

Depopulation of the 482.1 keV level indicated it as a 2^+ bandhead. The associated rotational band with the 3^+ level at 575.7 keV, and the 4+ level at 703.5 keV is quite regular. In the case of $K^\pi=1^+$ (p:9/2[514]-n:7/2[503]) two quasiparticle rotational band one would expect notable staggering of odd-even spin levels due to strong Coriolis interaction with levels of the $K^\pi=0^+$ (p:9/2[514]-n:9/2[505]) band.

We have performed the PRC model calculations of the ^{188}Re positive parity levels with the non-axial core deformation. At asymmetry angle $\gamma=20^o$, the $|K+2|$ side-band bandhead is predicted at about 480 keV, and the $K^\pi=1^+$ two-quasiparticle state – about 50 keV higher. However, the results of model calculations were unsatisfactory for positive parity bands with $K\geq3$. For these levels, the axially-symmetric PRC model was preferable. Therefore, we assume that the non-axial deformation in ^{188}Re is associated only with the (p:9/2[514]-n:9/2[505]) configuration when both proton and neutron occupy high j orbits.

In general, our studies indicate that, in the case of odd-odd nuclei, phase transition from the SU(3)-symmetric shape to the gamma-unstable O(6)-symmetric shape takes place at neutron number N=113. We have observed possible non-axial states already in ^{188}Re which has been long regarded as a nucleus with strong prolate deformation. However, since the shape phase transition is strongly dependent on angular momentums of both valence particles moving in the nuclear core mean field, one observes non-axial effects for the higher-lying two-quasiparticle states of ^{188}Re and ^{190}Ir involving high j proton and neutron orbits. Unfortunately, due to strong mixing, one cannot provide a direct experimental proof of the collective nature of these states in the form of reduced B(E2) transition probability values of depopulation transitions. The gamma-bands in N=115,117 doubly-odd iridium nuclei (^{192,194}Ir), originating from the two-quasiparticle configurations involving proton orbit 11/2[505], are based on the low-lying levels and their mixing degree is relatively weak. Therefore, one can see that the doubly-odd nuclei with N>113 have non-axial deformation already in the ground state.

[1] J.Kern et al., Nucl.Phys. A534, 77 (1991).

[2] M.Balodis et al.,, Phys.Rev. C77, 064602 (2008).

[3] M.Balodis, In: Proc. CGS-9, Budapest, 1996, Vol.1, p.147.

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RADIONUCLIDES MONITORING IN THE VICINITY OF SALASPILS NUCLEAR REACTOR (1998-2013)

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

The aim of presented work was to provide an assessment of the accumulation of artificial radionuclide: cesium-137 and tritium, as well as the migration of them in the soil and ground-waters in the vicinity of the shut-down SNR.

Obtained results present dynamic of radionuclides concentration in soils and ground waters in dependence on years and locations. The results of radiation monitoring show, that amount of radionuclides, produced by SNR, have little impact of the total radionuclide content in the environment.

EVALUATION OF NATURAL RADIOACTIVITY IN BUILDING MATERIALS USED IN LATVIA

D.Riekstina, J.Berzins, T. Krasta, R.Švinka, O.Skrypnik

The obtained results have been compared with the national and EU radiation safety requirements. It has been found that:

1. Activity index for all tested building materials, except granite and fireproof bricks, is below permissible radionuclide concentration level.
2. Radionuclide concentration in Devonian period and Quaternary period clay deposits in Latvia can be differ more than two times, but radionuclide content in various clay products can differ up to five times.
3. Average concentrations of natural radionuclides and activity index values for clay and clay bricks used in Latvia are of the same level as in other North European countries, except Sweden.

PUBLICATIONS

1. M.Balodis, **T.Krasta**. Levels of two-particle and gamma bands in ^{192}Ir. Nucl. Phys. A 933 (2015) 189-211 (DOI 10.1016/j.nuclphysa.2014.11.004)

CONFERENCE PRESENTATIONS

1. J.Alksnis, J.Berzins, D.Riekstina, J.Rudzitis, Radiation monitoring in the vicinity of Salaspils nuclear reactor (1998-2013), Abstract of the 30th Scientific Conference Inst. of Solid State Physics, University of Latvia, Riga, February 19-21, 2014, p. 108.

2. D.Riekstina, J.Berzins, T. Krasta, R.Švinka, O.Skrypnik, Evaluation of natural radioactivity in building materials used in Latvia, Abstract of the IV International Conference on Environment, Terrestrial Radioisotopes in Environment, Veszprém, Hungary, 21-23 May 2014, p.17.

3.. D.Riekstina, J.Alksnis, J.Rudzitis, J.Berzins, T. Krasta, Radionuclides monitoring in the vicinity of Salaspils nuclear reactor (1998-2013), Abstract: 19th Int. scientific conf. “EcoBalt’2014”, Riga, Latvia, Oktober 8-10, 2014, p. 49.

4. T.Krasta, M.Balodis. Study of ^{192}Ir nuclear structure. LU CFI 30. zinātniskās konferences tēzes. 2014.gada 19.-21.februāris, Rīgā, p.29.

5. M.Balodis, J.Bērziņš, T.Krasta, L.Simonova. Gamma bands in doubly odd rhenium and iridium nuclei. Fifteenth International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics CGS15, Dresden, August 25-29, 2014. Book of Abstracts.

6. J.Bērziņš, T.Krasta, L.Simonova, M.Jentschel, W.Urban. Levels of ^{186}Re populated in thermal neutron capture reaction. Fifteenth International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics CGS15, Dresden, August 25-29, 2014. Book of Abstracts.

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^{TM} 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^{TM} -based electronic invoices, credit cards and so on);
   - test power units (high-voltage switches, automatic disconnecting switches, power-transformers);
   - determine a content of heavy metals (As, Cd, Co, Cu, Fe, Hg, Tl, Ni, Pb, Sn, Zn, Bi, Mn) in liquids, ground, food-stuffs;
   - check various environment parameters (temperature, lighting, humidity, radiation level);
   - control temperature and lighting at the different objects (housings, hothouses, production storehouses);
   - are used in medicine and for determining of agricultural production parameters (digestion systems, fluorimetres, fall number determinators).
   - drive and management of automatic devices.
2. Provide physical measuring and manufacturing process automation.
3. Also solve the other problems, not afore-mentioned.

SCIENTIFICAL STAFF

1. Dr. A.Kristins

Technical Staff

1. I.Gvardina
2. J.Melderis
3. J.Veinbergs
4. P.Kalinikovs

COOPERATION

Latvia

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

Estonia

1. Tallinn University of Technology
2. Competence Centre ELIKO

More information on the work of the laboratory in the last ten years, see Appendix as well as http://www1.cfi.lu.lv/radioel/RD0.htm

OUR CLIENTS

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

LECTURES ON CONFERENCES

30th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2014

1. H.Uuetoa, A.Krivoshei, J.Lamp, M.Min, T.Uuetoa, P.Annus, A.Kristiņš. *Non-invasive bio-Impedance based method for central aortic blood pressure waveform estimation*. Abstracts, p. 40.
2. I.Gvardina, A.Kristiņš, J.Melderis. *Controller for alarm sensors status monitoring* Abstracts, p. 41.
3. J.Veinbergs, V.Romaņenkovs. *Equipment of telemetry data control and transmission* Abstracts, p. 82.