Institute of Solid State Physics
University of Latvia

ANNUAL REPORT

2012

Riga 2013

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Riga, Institute of Solid State Physics, University of Latvia, 2013, p.155

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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.

The International Supervisory Board of ISSP was established in 1999 and it consists now of 11 members (Table 3). The first International evaluation of ISSP was perfomed in 2002. The second Meeting of International Supervisory board took place at April 3, 2007. Below is a short excerpt citation from the evaluation report: "… the overall development of ISSP has been good with excellent quality of research as evidenced by publications, active participation in international projects etc…"

Table 1

ORGANIZATIONAL STUCTURE OF THE ISSP IN 2012

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. Külis*

- 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. Krūmiņš*
- Scientific Secretary — *L. Grīnberga*
- Accounting Department — *A. Jozepa*

DOMESTIC SERVICES

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

The interdisciplinary approach of research at the ISSP is reflected by its **highly qualified staff.** At present there are 176 employees working at the Institute, 26 of 103 members of the research staff hold Dr.habil.degrees, 66 hold Dr. or PhD. At the end of 2012 there were 21 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. Kaiva Lūse, 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.

Table 3

International Advisory Board of the Institute

1. Prof. Dr.J.Banys, University of Vilnius, Lithuania
2. Prof. Dr. Gunnar Borstel, University of Osnabruck, Germany
3. Prof. Niels E.Christensen (chairman), University of Aarhus, Denmark
4. Prof. Dr.R.Evarestov, St.Petersburg University, Russia
5. Prof. Claes – Goran Granqvist, Uppsala University, Sweden
6. Dr. Dag Høvik, The Research Council of Norway, Norway
7. Prof. Dr.M.Kirm, University of Tartu, Estonia
8. Prof. Wolfgang Kleemann, Universität Duisburg-Essen, Germany
9. Prof. Paolo Nanni, University of Genoa, Italy
10. Prof. Ergo Nommiste, University of Tartu, Estonia
11. Prof. Tashio Ogawa, Shizuoka Institute of Science and Technology, Japan
12. Prof. Jiri Kulda, Institu Laue-Langevin, France
13. Prof. Andrejs Silins, Latvian Academy of Sciences, Latvia
14. Prof. George W.Taylor, Princeton Resouces Inc., USA
15. Prof. Sergei Tuituinnikov, Joint Institute for Nuclear Research, Dubna, Russia
16. Prof. Juris Upatnieks, Applied Optics, USA
17. Prof. M. Van de Voorde, Max – Planck – Institute, Stuttgart, Germany
18. Prof. Harald W.Weber, Atomic Institute of Austrian Universities, Vienna, Austria

The annual report summarizes the research activities of the ISSP in 2012. The staff of the Institute has succeed in 5 **national science grants** and in **two national cooperation projects** with the total financing 159.4 thous. Ls (ca. 223.2 thous. EUR).

In 2005 a the new Law of Science was passed by Parliament of Latvia. According to this law the state **budgetary financing in Latvia** for science has to **increase yearly per 0.15% from GDP** up to reaching a 1% value. The budgetary increase 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 266.8 thous. Ls budget in 2012. The infrastructure financing for ISSP in 2012 was 467.1 thous. Ls. and it was partly used also for the salaries of the scientific and maintenance staff of the Institute. (Table 4).

Main awards, received at 2012:

No	Author	Award
1.	Dr.phys. M.Kirm	The International Member of Latvian Academy of Science
2.	Dr.phys. A.Luschik	The International Member of Latvian Academy of Science
3.	Dr.habil.phys. P.Stradins	The International Member of Latvian Academy of Science
4.	Dr.habil.phys. J.Timoshenko	Author of the best scientific achiewment (from Latvian Academy of Science)
5.	I.Smeltere	The L'OREAL-UNESCO sholarship „For Women in science 2011"
6.	Dr.habil.phys. L.Skuja	Award of Latvian Cabinet of Ministrs
7.	Ms.phys. G.Kuchinskis	Siemens Prize

At the end of 2012, more than 50 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 2012 **four international conferences** have been organised at the Institute:

1. International Young Scientist Conference "Developments in Optics and Communications 2012", April 12 – 14, 2012, Riga, Latvia;
2. The International Workshop "Oxygen Related Optical Properties of Nano Zirconia", April 6 – 7, 2012, Riga, Latvia;
3. Annual International conference "Functional materials and nanotechnologies", April 16 -17, Riga, Latvia;
4. The First Baltic School on Application of Neutron and Synchrotron Radiation in Solid State and Materials Science, October 1 – 4, 2012, Riga, Latvia;
5. The International Workshop "Hydrogen and Fuel Cells in Research and Applications", October 4 – 5, 2012, Riga, Latvia.

Table 4

INCOME OF ISSP, THOUSAND Ls, FROM 2006 - 2011

Year	Total financing	Grants and programmes from budget	Other financing from budget	Contracts, market oriented research	Internat. funds	Structural funds from EU
2006	**1586,1**	**466,9**	**403,4 + 169)***	**152,4**	**135,6**	**249,2**
2007	**3 236,5**	**721,9**	**1110,2**	**98,7**	**92,6**	**1201,7**
2008	**4 261,3**	**1 024,4**	**1 088,8**	**155,9**	**291,8**	**1 691,1**
2009	**1717,4**	**631,6**	**578,1**	**64,2**	**162,4**	**281,1**
2010	**2135,6**	**446,2**	**675,4**	**83,3**	**118,8**	**814,7**
2011	**2719,1**	**448,0**	**515,5**	**104,6**	**121,1**	**1530,0**
2012	**3462,0**	**462,3**	**552,1**	**120,0**	**41,5**	**2322,1**

*) – investment for building reconstruction

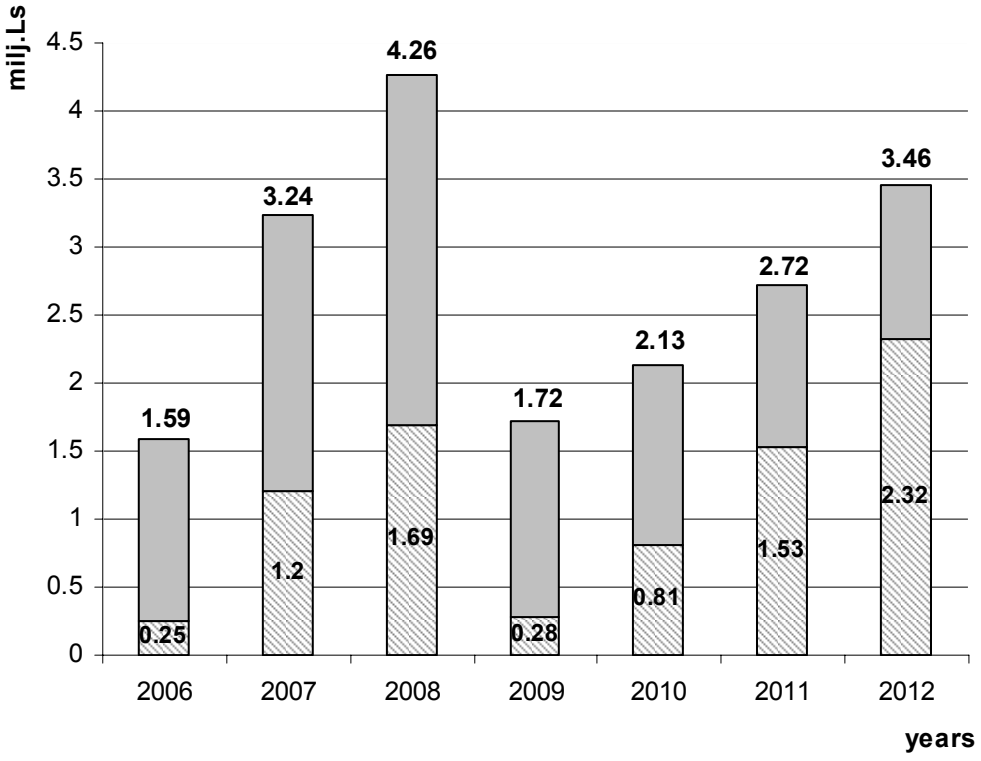


Fig.1. Total financing of the ISSP milj. LVL from 2006 to 2012

▨ - *financing from EU Structural funds*

The main source for **international funding** were three EC 7th Framework Programme contracts:
- 3 EURATOM projects – 25.6 thous. EUR
- 2 Taiwan – Lithuania – Latvia projects – 12.5 thous. USD
- International conference FMNT - 2012 – 15.4 thous. EUR

Main achievments in 2012:

1. 152 SCI papers published by the staff of Institute;
2. 2 patent applicatiosn;
3. 17 B.sc. thesis and 9 M.Sc. thesis in physics, optometry and chemistry were defended under the supervision of our scientists;
4. D.Bocharovs, A.Kalinko, V.Karitans, V.Korsaks and A.Vembris were acquired degree of doctor of physics (PhD);
5. The formation of "National Research Centre for nanostructures and multifunctional materials, constructions and technologies" by the ISSP .

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 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 OPTICAL SPECTROSCOPY

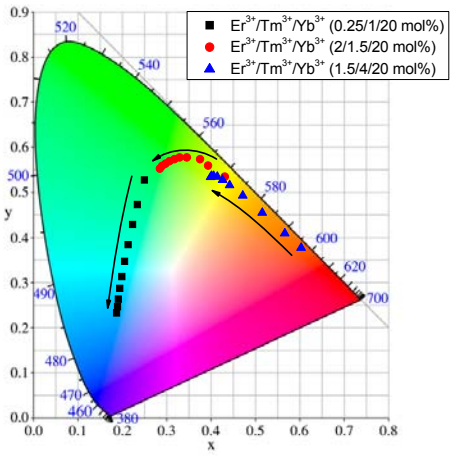
Head of Laboratory Dr.habil.phys. M.Springis

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. 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. Possible applications involve efficient transformation of the infrared radiation into visible (visualization of infrared radiation, enhancement of Solar cells efficiency) and generation of different light colors (light sources).

The staff of the laboratory is taking part in the preparation and supervision of practical works in spectroscopy of solid state physics courses for Master students at the University of Latvia (Dr. hab. phys. M. Springis, M. Sc. J. Grube). Dr.phys. A. Sarakovskis is a

lector 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
M. Voss

Scientific visits abroad

G. Doke (1 week Germany)
J. Grube (1 week Germany)

Cooperation

Latvia
Riga Technical University (Prof. A. Medvid).
RTU Institute of Nonorganical Chemistry (Dr. J. Grabis, Dr. D. Jankovica).

Main results

SYNTHESIS AND LUMINISCENCE STUDIES OF Eu^{3+} DOPED $NaLaF_4$

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

Great attention has been paid for searching of perspective luminescence materials which could be used in various areas, for example, plasma panels or fluorescent lamps. Rare-earth (including europium) doped materials have been found to be perspective candidates for such uses thereby further investigation of their properties is required. In this work LaF_3 and NaF mixtures with different EuF_3 concentrations (0.05, 0.1, 0.5, 1 and 2mol%) were annealed at different temperatures (450, 500, 550, 600, 650^{O}C) to obtain $NaLaF_4:Eu^{3+}$. For the obtained samples luminescence and excitation spectra as well as luminescence decay kinetics were measured. Based on the experimental results peculiarities of the sample composition, quality and luminescence properties and their dependence on the annealing temperature are discussed.

CONCENTRATION IMPACT ON Er^{3+} GREEN LUMINESCENCE DECAY KINETICS IN $NaLaF_4$

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

For the materials doped with Er^{3+} ions intensive luminescence bands are often observed in wide spectral region (500 – 1000nm). Our previous studies have showed that $NaLaF_4$ could be promising host material for practical application due to low phonon energy [1]. In this work Er^{3+} doped $NaLaF_4$ at different Er^{3+} ion concentrations (0.2 – 10mol%) were synthesized. Intensive green luminescence band (origin from 4S3/2 to 4I15/2 transition) was observed for all Er^{3+} content. Studies of Er^{3+} green luminescence decay kinetics at different Er^{3+} ion concentration, which could not be fitted by a simple exponent, reveals that energy transfer process appears. Several energy transfer processes, like direct relaxation, fast migration and migrationlimited relaxation, have been proposed to describe luminescence decay kinetics. Based on the experimental results peculiarities of energy transfer processes in $NaLaF_4$ and their variation at different Er^{3+} content are discussed.

PHOTOLUMINESCENCE AND ENERGY TRANSFER IN Nd^{3+} AND Er^{3+} DOPED $NaLaF_4$ MATERIAL

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

Due to very promising optical applications rare-earth doped fluorides have been intensively studied for several decades. In past few years as one of the best host material for rare-earth ions $NaLaF_4$ is mentioned [1]. In this work $NaLaF_4$:Er^{3+}, $NaLaF_4$:Nd^{3+} and $NaLaF_4$:Er^{3+},Nd^{3+} at different Er^{3+} and Nd^{3+} concentrations were synthesized. For these samples photoluminescence and excitation spectra as well as photoluminescence kinetics were measured. From the analysis of the experimental data it is concluded that there are energy transfer from Nd^{3+} to Er^{3+} (Fig. 1). The most likely transfers are 2H11/2 (Nd^{3+}) → 4F9/2 (Er^{3+}) and 4G7/2 (Nd^{3+}) → 2H11/2; 4S3/2 (Er^{3+}) followed by 4S3/2 (Er^{3+}) → 4F9/2 (Er^{3+}). Electronic transition within Er^{3+} from 2H11/2, 4S3/2 and 4F9/2 to ground state 4I15/2 results in emission of “green” (540 nm, 520 nm) and “red” (660 nm) luminescence.

UP-CONVERSION LUMINESCENCE IN ERBIUM DOPED CUBIC AND HEXAGONAL $NaYF_4$

A. Sarakovskis, M. Voss, G. Doke, D. Jankovica, J. Grube, M. Springis

Up-conversion luminescence process, which is related to absorption of several light photons (usually infrared) followed by emission of light in the visible or even ultraviolet spectral regions, has attracted interest of scientists due to its potential practical use in various applications including biolabels, temperature sensors, light sources etc. Although observable in d- and f-ions doped materials, the highest efficiency of up-conversion luminescence is usually attained in lanthanides doped hosts. Among huge variety of materials suitable as up-conversion hosts the most prominent is considered to be $NaYF_4$, both due to its low phonon energy and multisite nature of the crystalline lattice. In the present report erbium doped $NaYF_4$ nanomaterial has been synthesized by molten salt method. Depending on the synthesis temperature the structure of the material varied from solely cubic to exclusively hexagonal. Up-conversion luminescence spectra and luminescence kinetics for

the samples having different phase compositions have been measured. It was found that the shapes of the up-conversion luminescence spectra related to the cubic and the hexagonal phase were almost independent of the structure while the overall efficiency of the up-conversion process in hexagonal phase was at least order of magnitude higher compared to the cubic.

Scientific publications

1. **A.Sarakovskis, M. Voss, G. Doke**, D. Jankovica and **J. Grube**, Synthesis of cubic and hexagonal $NaYF_4:Er^{3+}$, IOP Conf.Series:Materials Science and Engineering **38** (2012), doi:10.1088/1757-899X/38/1/012038.
2. Berzins, Dz., Fedotovs, A., Kiselova, O., **Sarakovskis, A**.,EPR spectra of the Mn2+ ion in the oxyfluoride glass ceramics containing BaF2 nanocrystalline phase,IOP Conference, Series: Materials Science and Engineering, **38** (2012) (1), art. no. 012046.
3. Fedotovs, A., Berzins, Dz., Kiselova, O., **Sarakovskis, A**. Characteristics of the Mn2+ EPR spectra in the oxyfluoride glass ceramics containing SrF2 nanocrystals. IOP Conference Series: Materials Science and Engineering, **38** (2012) (1), art. no. 012047.
4. Rogulis, U., Elsts, E., Jansons, J., **Sarakovskis, A., Doke,** G., Stunda, A., Kundzins, K.,Rare earth activated oxyfluoride glasses and glass-ceramics for scintillation applications, IEEE Transactions on Nuclear Science, 59 (5 PART 2), (2012) art. no. 6316153, pp. 2201-2206.
5. Grigorjeva, L., Millers, D., Smits, K., **Sarakovskis, A**., Lojkowski, W., Swiderska-Sroda, A., Strek, W., Gluchowski, P. The time-resolved luminescence characteristics of Ce and Ce/Pr doped YAG ceramics obtained by high pressure technique. Optical Materials, 34 (6), (2012), pp. 986-989.

Lectures on Conferences

28th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2012, February 8-10.

1. G.Doke, M.Voss, J.Grube, A.Sarakovskis, M.Springis, Photoluminescence of Nd^{3+} and Er3+ doped $NaLaF_4$ material, Abstracts of the 28th Scientific Conference ISSP LU, 2012, p. 31.
2. J.Grube, G.Doke, M.Voss, A.Sarakovskis, M.Springis**,** Er^{3+} green liminescence decay kinetics analysis in $NaLaF_4$, Abstracts of the 28th Scientific Conference ISSP LU, 2012, p. 32.
3. M.Voss, G.Doke, J.Grube, A.Sarakovskis, M.Springis, Synthesis and luminescence studies of Eu^{3+} doped $NaLaF_4$, Abstracts of the 28th Scientific Conference ISSP LU, 2012, p. 58.

International conference "Functional materials and nanotechnologies" FM&NT, Riga, 2012, April 17-20.

4. A.Sarakovskis, M. Voss, G. Doke, D. Jankovica, J. Grube, M. Springis, Up-conversion luminescence in erbium doped cubic and hexagonal $NaYF_4$", FM&NT 2012, Book of abstracts, ISSP LU, Riga, April 17 - 20, p. 205.
5. G. Doke, M. Voss, J. Grube, A. Sarakovskis, M.Springis, Photoluminescence and Energy Transfer in Nd^{3+} and Er^{3+} Doped $NaLaF_4$ Material, FM&NT 2012, Book of abstracts, ISSP LU, Riga, April 17 - 20, p. 204.

6. J. Grube, G.Doke, M. Voss, A. Sarakovskis, M. Springis, Concentration Impact on Er^{3+} Green Luminescence Decay Kinetics in $NaLaF_4$, FM&NT 2012, Book of abstracts, ISSP LU, Riga, April 17 - 20, p. 203.

8th International conference on Luminescenct detectors and Tramsformers of Ionizing Radiotion LUMDETR 2012, Halle (Saale), Germany, September 10.-14.

7. J. Grube, G. Doke, M. Voss, A. Sarakovskis and M. Springis, Photoluminescence of Er^{3+} Activated $NaLaF_4$ with Different Activator Concentration, Book of Abstracts of LUMDETR 2012, Halle (Salle) Germany, 2012, P-Tue-61.
8. G. Doke, M. Voss, J. Grube, A. Sarakovskis, and M. Springis, Photoluminescence and Energy Transfer in Nd^{3+} and Er^{3+} doped $NaLaF_4$ Material, Book of Abstracts of LUMDETR 2012, Halle (Salle) Germany, 2012, P-Tue-65.

Master thesis

G.Doke. Photoluminescence in Nd^{3+} and Er^{3+} doped $NaLaF_4$ Material.

Bachelor thesis

M. Voss. Synthesis and photoluminescence of Eu^{3+} doped $NaLaF_4$.

LABORATORY OF MAGNETIC RESONANCE SPECTROSCOPY

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

Research Areas
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,
Luminescence investigations in oxyfluoride glass and glass-ceramics and application of these materials.

Scientific Staff
1. Prof., Dr. habil. phys. U. Rogulis
2. Dr. phys. A. Fedotovs
3. Dr. phys E. Elsts
4. Dr. phys. J. Trokšs

PhD Students
1. Dz. Bērziņš
2. O. Kiseļova

Students
1. I. Brice
2. A. Antuzēvičs
3. A. Cvetkovs
4. K. Bulindžs
5. U. Balmaks

Scientific visits abroad

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

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. University of Paderborn (Dr. habil. phys. S. Schweizer, Dr. habil. phys. S. Greulich-Weber)

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

Main results

RARE EARTH ACTIVATED OXYFLUORIDE GLASSES AND GLASS-CERAMICS FOR SCINTILLATION APPLICATIONS

U. Rogulis, E. Elsts, J. Jansons, A. Sarakovskis, G. Doke, A. Stunda, K. Kundzins

Oxyfluoride glasses $49SiO_2 \cdot 6Al_2O_3 \cdot 24Li_2O \cdot 20LaF_3$ activated with Tb, Ce, Eu have been synthesized and studied. After heating at 580^0C and 750^0C crystalline phases were obtained. The samples were studied by DTA (Differential thermal analyzer), CL (cathodoluminescence), XRD (X – ray diffraction), SEM (scanning electron microscope), EDS (energy dispersive x-ray spectroscopy) methods. We found out that presence of crystalline phase enhances the CL of Tb activated samples significantly; whereas, the shortest decay time of 0.29 μs has been observed for less intense Ce doped glass sample.

PHOTOLUMINESCENCE OF Eu AND Ce ACTIVATED OXYFLUORIDE GLASS AND GLASS CERAMICS

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

The photoluminescence of SiO_2-Al_2O_3-LiO_2-LaF_3 oxyfluoride glass and glass ceramic samples doped with Ce^{3+}, Eu^{2+} and Ce^{3+}/Eu^{2+} is investigated. The spectra and fluorescence intensities are compared. The luminescence of samples activated by Eu ions is found to be of greater intensity than that of the samples doped with Ce or Ce/Eu. The luminescence of glass ceramics is higher than that of the corresponding glass, which indicates that a proportion of the activator ions is embedded in the fluoride crystallites.

EPR SPECTRUM ANGULAR DEPENDENCES IN $LiYF_4$ CRYSTAL

A. Antuzevičs, A. Fedotovs, U. Rogulis

Electron paramagnetic resonance (EPR) measurements have been made for two perpendicular planes in a $LiYF_4$ crystal before and after x-ray irradiation at room temperature. Analysis of the EPR spectrum angular dependence shows the presence of two defects – an impurity ion, which was embedded during the crystal growth process, and an x-ray induced defect with the g-factor of approx. 2.0. Parameters of the spectra and possible defect models are discussed.

EPR HYPERFINE STRUCTURE OF RADIATION DEFECT IN OXYFLUORIDE GLASS CERAMICS

Dz. Berzins, A. Fedotovs, U. Rogulis

We have investigated the samples of thermally treated oxyfluoride glass ceramics $50SiO_2 – 25LiO_2 – 20YF_3 – 3ErF_3 – 2YbF_2$ by means of electron paramagnetic resonance (EPR) techniques. After irradiation of the samples with X-rays, in the EPR spectra a hyperfine structure characteristic of F-centres could be observed in different fluoride crystals. The structure of F-centre in the oxyfluoride glass ceramics containing $LiYF_4$ crystallites is discussed.

Scientific publications

1. **U. Rogulis, E. Elsts, J. Jansons, A. Sarakovskis, G. Doke,** A. Stunda, **K. Kundzins**, Rare earth activated oxyfluoride glasses and glass-ceramics for scintillation applications, IEEE Transactions on Nuclear Science, 2012, Volume: 59 , Issue: 5, Page(s): 2201 – 2206, Doi: 10.1109/ TNS.2012.2212724.
2. **I. Brice, U. Rogulis, E. Elsts, J. Grūbe***,* Photoluminescence of Eu and Ce activated oxyfluoride glass and glass ceramics. Latvian Journal of Physics and Technical Sciences, 2012, Nr. 6(I), p. 44.
3. **A. Antuzevičs, A. Fedotovs, U. Rogulis**, EPR spectrum angular dependences in $LiYF_4$ crystal, Journal of Physics and Technical Sciences, 2012, Nr. 6(i), p. 49.
4. **Dz. Berzins, A. Fedotovs, U. Rogulis**, EPR hyperfine structure of radiation defect in oxyfluoride glass ceramics, Latvian Journal of Physics and Technical Sciences, 2012, Nr. 6(I), p. 55.

Lectures on Conferences

1. U. Rogulis, E. Elsts, J. Jansons, A. Sarakovskis, G. Doke, A. Stunda, K. Kundzins, Cathodoluminescence of oxyfluoride glass-ceramics, Abstracts International Conference LUMDETR'2012, Halle, Germany, 2012, P-Tue-2168.
2. E. Elsts, J. Jansons, U. Rogulis, A. Sarakovskis, G. Doke, A. Stunda, K. Smits, Rare earth activated oxyfluoride glass-ceramics for scintillation applications, Abstracts International Conference LUMDETR'2012, Halle, Germany, 2012, P-Tue-2169.
3. E.Elsts, J.Jansons, U.Rogulis, A.Šarakovskis, G.Doķe, A.Stunda, K.Kundziņš, Oksifluorīdu stikla keramikas katodluminiscence, LU CFI 28. zinātniskās konferences tēzes, 2012, 30. lpp.
4. I.Brice, U.Rogulis, E.Elsts, J.Grūbe, L.Skuja, Eu un Ce jonu luminiscence oksifluorīdu stikla keramikā, LU CFI 28. zinātniskās konferences tēzes, 2012, 75. lpp.
5. A.Antuzevičs, A.Fedotovs, U.Rogulis, EPR spektru leņķisko atkarību modelēšana $LiYF_4$ kristālā, LU CFI 28. zinātniskās konferences tēzes, 2012, 78. lpp.

Master thesis:

1. Olga Kiseļova, "CaF_2 , BaF_2 un SrF_2 nanokristālu struktūru pētījumi oksifluorīdu stikla keramikās ar EPR paramagnētisko zonžu metodi", vad. A. Fedotovs

Bachelor thesis:

1. Andris Antuzevičs, "EPR spektru leņķisko atkarību modelēšana $LiYF_4$ kristālā", vad. U. Rogulis
2. Ludmila Jefimova, "Oksifluorīdu stikla keramiku punktveida defektu pētījumi", vad. U. Rogulis

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 in order to reveal:

- defect-induced luminescence mechanisms as well as with 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 white light emitters with defined properties.

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

Scientific Staff

1. Dr.habil.phys. Baiba Berzina
2. Dr.phys. Laima Trinkler
3. Dr.phys.Valdis Korsaks

Students – Technicians

1. Jana Grigorjeva
2.. Roberts Kirsteins

Collaborations

Latvia

Laboratories and departments of ISSP University of Latvia (Drs. J.Maniks, L.Skuja, K.Kundzins, L.Grigorjeva, Y. Zhukovskii, S. Piskunov),
Institute of Inorganic Chemistry, Riga Technical University (Prof. J. Grabis),
Institute of Technical Physics, Riga Technical University (Profs. A.Medvid, M.Knite).

Lithuania

Institute of Applied Research, Department of Semiconductor Optoelectronics, Vilnius University (Dr. K. Jarasiunas)

Taiwan

National Taiwan University, Taipei (Profs. Li-Chyong Chen, Kuei_Hsien Chen)

Main investigations and results

ALUMINUM OXYDE Al_2O_3

L.Trinkler, B.Berzina

Photoluminescence studies were fulfilled for nominally pure Al_2O_3 nanopowder samples with different grain size and different lattice structure phases synthesized in RTU Institute of Inorganic Chemistry. It was found that luminescent properties of this material are determined primarily by a phase of crystal lattice and uncontrolled impurities, which are present in very small concentrations. Phase transition from δ to α structure is followed with drastic changes in luminescence spectra – wide diffuse bands in 600-900 nm range are replaced by narrow lines. This phenomenon is explained by switching of active luminescence centers due to transformation of crystal field symmetry as a result of phase transition. It was found that wide diffuse luminescence bands typical for samples with δ phase occur due to emission titanium, iron and chromium ions (at 750 nm, 700-900 nm and 690-710 nm, correspondingly), while narrow lines in photoluminescence of samples with α phase arise due to emission of chromium and manganese ions. The results obtained allow evaluate the Al_2O_3 being useful for red light emitters.

These studies were performed within a support of European project ERDF 2010/0253/2DP / 2.1.1.1.0/10/APIA/VIAA/079.

HEXAGONAL BORON NITRIDE hBN

V.Korsak, B. Berzina, L.Trinkler

Spectral characterization of hBN consisting of macro-size grains or nanotubes was performed. Photoluminescence spectra of materials were studied within a wide temperature range between 8 K and 300 K [1]. It was found that in all materials studied there are two main phonon-assisted luminescence bands at ~300 nm and ~400 nm caused by native defects of hBN appearing independently on a particle size and material origin. The 300 nm luminescence is related to the intracenter processes of a single defect, characterized with the phonon-assisted luminescence/exitation spectra presenting a common zero-phonon line (Fig.4). It was found that the 400 nm luminescence is caused by recombination of a donor-acceptor pair, which is located at or near material surface. It was also found that the intensity of the 400 nm luminescence in hBN depends on oxygen content in ambient atmosphere surrounding the sample. This feature allows propose hBN as a material applicable for oxygen sensors.

On basis of investigations mentioned above Valdis Korsaks has defended his PhD Thesis.

These studies were performed within a support of European project ERDF 2010/0253/2DP / 2.1.1.1.0/10/APIA/VIAA/079.

ALUMINUM NITRIDE AlN

L.Trinkler, B. Berzina, V.Korsaks, R.Kirsteins

The native defect-induced photoluminescence of AlN of different structures (ceramics, macro-size powder, nanopowder, nanorods, nanotips) was studied using the spectral methods mentioned above. It was found that there are two main luminescence bands at ~400 nm (UV band) and 480 nm (blue band), which are observable in all AlN structures with varied ratio of their intensities. It allows conclusion that the same defect

types responsible for the UV and blue luminescence are characteristic for AlN crystalline lattice irrespective to material size and structure. The oxygen-related defects together with the host material vacancies from the bulk AlN are the more probable candidates for the UV luminescence centers, whereas the blue luminescence could be related to the defects situated near or at the material surface. The recombination mechanism of UV luminescence was confirmed using the 263 nm laser excitation of AlN ceramics with varied intensity in 10-300 K temperature range. It was found that increase of excitation density causes blue shift of the band maximum, typical for recombination luminescence in semiconductors. Results of the study of the photoluminescence under varied laser intensity as well as that of afterglow allow elucidating of donor-acceptor pair distribution and recombination processes in AlN ceramics.

Photoluminescence of doped AlN with Mn and other elements also was studied. It allows evaluate AlN as prospective material for visible and white light emitters.

These studies were performed within a support of European project ERDF 2010/0253/2DP / 2.1.1.1.0/10/APIA/VIAA/079.

COMPOUND MATERIALS $Al_XGa_{1-X}N$

B.Berzina, L.Trinkler, J.Grigorjeva, V.Korsaks

Compound materials $Al_xGa_{1-x}N$ in form of nanorods or thin layers are synthesized in National Taiwan University (Dr. Li-Chyong Chen). The band gap of the material depends on parameter x which varies between 3% and 12%. The photoluminiscence spectra of $Al_xGa_{1-x}N$ were studied within a temperature range between 8 K and 300 K. The exciton-induced luminescence demonstrating the band gap variations is observed in UV spectral region and its properties are studied.

These studies were performed within a support of collaboration project between Taiwan-Lithuania-Latvia.

Scientific Publications

1. T.Glaskova, M.Zarelli, A.Anishkevich, M.Giordano, **L.Trinkler, B.Berzina**, *„Quantitative optical analysis of filler dispersion degree in MWCNT-epoxy nanocomposite”*. Composites Science and Technology, 72 (2012) 477-481; http://www.sciencedirect.com/science/article/pii/S0266353811004210
2. **V. Korsaks, B. Berziņa, L. Trinklere**, “*Influence of air, oxygen, nitrogen and argon gases on 400 nm luminescence in hexagonal boron nitride”*. Latvian journal of physics and technical science 49 (2012) 57-62.
3. **L. Trinkler, B. Berzina, Z. Jevsjutina**, J. Grabis, I. Steins and C. J. Baily, “*Photoluminescence of Al_2O_3 nanopowders of different phases”*. Optical Materials 34 (2012) 1553–1557; http://dx.doi.org/10.1016/j.optmat.2012.03.029
4. **V. Skvortsova, N. Mironova-Ulmane, L. Trinkler, D. Riekstina**, *”Impurity defects in wide gap inorganic materials”*. Proceeding of the 5th WSEAS International Conference on Materials Science (MATERIALS '12), Sliema, Malta, 7-9 September 2012, In book: “Advances in Data Networks, Communications, Computers and Materials”. Editors V. M. Marques and A. Dmitriev, Published by WSEAS Press, Sliema, Malta, 2012, pp.233-238.

Lectures on Conferences

28th LU Scientific Conference of Institute of Solid State Physics, University of Latvia, February 8 - 10, 2012, Riga, Latvia

1. V.Korsaks, B.Berziņa, L.Trinklere, *"Native defect luminescence in different structured hBN",* Book of Abstracts, 2012, p. 59.

2. J.Grigorjeva, B.Berzina, L.Trinklere, A.Sarakovskis, *"Luminescence of ternary nanostructure AlGaN"*, Book of Abstracts, 2012, p.33.

International Conference FM&NT; Functional materials and nanotechnologies 2012; Institute of Solid State Physics University of Latvia April 17 – 20, Riga

3. R.Aleksiejunas, S.Nargelas, S. Miadojedovas, P. Scajev, K. Jarasiunas, L.Trinkler, J.Grigorjeva, B.Berzina, K.H.Chen, Li-C.Chen, "*Carrier dynamics in nanostructures of ternary AlGaN with tunable bandgap"*. Book of Abstracts, 2012, p. 264.

19th International Symposium on Matestable, Amorphous and Nanostructured Materials, 18-22 June, 2012, Moscow, Russia

4. L.Trinkler, B.Berzina, J.Grabis, „*Influence of phase transition on photoluminescence of Al_2O_3 nanopowders"*, Book of Abstracts, 2012, p.89.

International Conference on Defects in Insulating Materials (ICDIM 2012), 24-29 June, 2012, Santa Fe, USA

5. V. Korsaks, B. Berzina, L. Trinklere, „*Surface defects related photoluminescence of hexagonal boron nitride dependent on surrounding gases"*, Book of Abstracts p. 53.

International Conference on Luminescence and Laser Physics, 16-22 July, 2012, Pescanka, Irkutsk, Russia

6. L.Trinkler, B.Berzina, J.Grigorjeva, *„Peculiarities of laser-induced luminescence proceses in AlN ceramics at low temperatures",* Book of Abstracts, 2012, p.15.

14th International Conference-School Advanced Materials and Technologies, 27-31 August, 2012, Palanga, Lithuania

7. V. Korsaks, R. Kirsteins, B. Berzina, L. Trinkler, *"Photoluminescence of hexagonal boron nitride macro and nano materials dependent on surrounding gases and pre-treatment"*, Book of Abstracts, 2012, p.53.

8. J. Grigorjeva, V. Korsaks, L. Trinkler, B. Berzina, *„Luminescence of ternary AlGaN nanomaterials",* Book of Abstracts, 2012, p.76.

International Conference on Diamond and Carbon Materials 2012, 2 – 6 September, 2012,Granada, Spain

9. B.Berzina, V.Korsaks, L.Trinkler, *„Carbon related hexagonal boron nitride as oxygen sensor",* Programme book, 2012, P1.60.

LABORATORY OF SEMICONDUCTOR OPTOELECTRONICS

Head of Laboratory Dr. phys. B.Polakovs

Research Area and Main Problems

1. Laser processing of amorphous hydrogenised silicon thin films for solar cell applications. Investigation of effects of pulsed laser processing on electric, structural, morphological and photoconductive properties of a-Si:H films. Development of solar cell prototypes. Scientific cooperation with semiconductor joint stock company Alfa.
2. Laser scribing and laser processing of graphite, graphene and graphene oxide, advanced methods of graphene printing on solid substrates. Optical microscopy, Atomic force microscopy and Scanning Electron microscopy investigation of printed graphene structures.
3. Synthesis of metal and semiconductor nanocrystals for photonic and solar cell applications. Investigation of optical, electrical and photoconductive properties of nanocrystals thin films. Development of nanocrystals based solar cell and hybrid nanocrystals-polymer solar cell prototypes.
4. MOCVD synthesis of group III-nitrides for photonic and electronic applications. Investigation of structure and morphology (XRD, RHEED, SEM, AFM). Investigation of electronic processes using stationary and time-resolved nano- and picosecond UV-VIS spectroscopy.
5. Controlled manipulations of 1D and 0D nanostructures inside Scanning Electron Microscope. Investigation of tribological aspects of nanostructures manipulation (adhesion, static, kinetic friction), nanoindentation experiments, mechanical characterization (Young modulus, bending strength and yield strength) of semiconducting and metallic nanowires. Scientific cooperation with Institute of Physics (University of Tartu) and Estonian Nanotechnology Competence Centre.

Scientific Staff
Prof., Dr. habil. phys. I. Tale
Dr. phys. J. Butikova
Dr. phys. L. Dimitrocenko
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Cooperation

Latvia
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G. Liberts Innovative Microscopy Center, University of Daugavpils
Joint stock company “Alfa”

Germany
University of Rostock, Rostock
Company “Aixtron”, Achen
Max Plank Institute of Plasma Physics, Garching

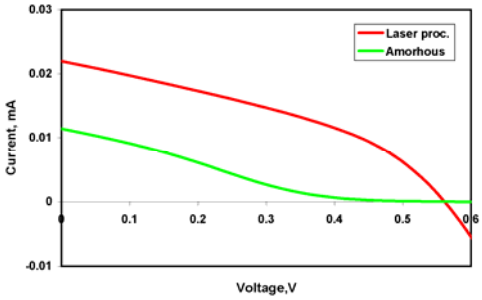
Estonia
Institute of Physics, University of Tartu
Estonian Nanotechnology Competence Centre, Tartu

Main Results

LASER CRYSTALLIZATION OF a-Si:H FOR SOLAR CELL APPLICATIONS

G. Marcins, J. Butikova, J. Pervenecka, B. Polyakov, A. Muhin, I. Tale

Manufacturing of thin film amorphous silicon solar cells has perspectives with a condition of improving solar cell efficiency and reducing production costs. Efficiency of amorphous silicon solar cells decreases with time due to formation of metastable light-induced defects. Laser crystallization helps to prevent this effect. We apply visible laser wavelength for laser crystallization in contrast to widely used exciton laser crystallization, which able to process only ~100 nm thick a-silicon layer. Primary effects of laser crystallization of a-silicon are dopants activation, and increase of charge carrier mobility due to higher crystallinity of processed silicon. Additional effect is texturing of initially smooth surface, which decreases back reflection of incident light and increases efficiency of a solar cell.



I-V curves of amorphous and laser processed a-Si:H solar cells.

Amorphous silicon crystallization by laser beam of visible wavelength opens additional possibilities to process the whole p-i-n structure of thin film solar cell simultaneously. A-Si:H p-i-n thin film solar cell was grown by PECVD on ITO-coated glass substrates. Laser crystallization was successfully applied for processing the whole p-i-n structure of total thickness around 300 nm. A significant improvement of solar cell output parameters in comparison to a non-processed cell was achieved.

GRAPHENE STAMP PRINTING

J. Butikova, B. Polyakov, E. Butanovs, L. Dimitrocenko, I. Tale

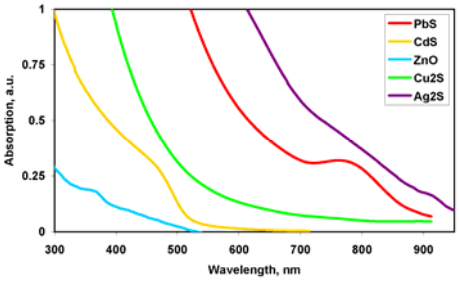
Graphene as a single monolayer of covalently bonded carbon atoms is an intriguing material for both fundamental and applied science. Due to its outstanding electronic and thermal properties (high charge carrier mobility, high heat conductance, etc.) graphene raised huge interest in the last decade, and became a real candidate as a successor of silicon in future microelectronics. There is plenty of graphene synthesis methods, however, the best electric properties were demonstrated by graphene mechanically cleaved from HOPG. Cleaved HOPG graphene sheets, nevertheless, are usually irregular in shape and thickness, and therefore are not suitable for integration in microelectronics devices.

Highly oriented pyrolytic graphite (HOPG) was scribed by the pulsed laser beam to produce square patterns. Patterning of HOPG surface facilitates the detachment of graphene layers during contact printing. Direct HOPG-to-substrate and glue-assisted stamp printing of a few-layers graphene was compared. Printed graphene sheets were visualized by optical and scanning electron microscopy. The number of graphene layers was measured by atomic force microscopy. Glue-assisted stamp printing allows printing relatively large graphene sheets (40×40 μm) onto a silicon wafer. The presented method is easier to implement and is more flexible than the majority of existing ways of placing graphene sheets onto a substrate.

NANOCRYSTALS SYNTHESIS FOR SOLAR CELL APPLICATIONS

P. Kulis, J. Butikova, B. Polyakov, I. Tale

Solution-processed nanocrystals quantum dot solar cells is a novel field in photovoltaics. Semiconducting nanocrystals possess many fascinating properties which are not present in the corresponding bulk materials. The most famous property is quantum confinement effect: band gap widens in nanocrystals having diameter smaller than exciton bohr radius. The ability to obtain nanocrystals of different band gap simply varying their size is highly important for the effective utilization of solar spectrum and engineering of tandem solar cell architectures. The main advantage of nanocrystals for solar cell manufacturing is the possibility of solution-based deposition of nanocrystals thin films, which is many times less expensive in comparison to monocrystal silicon technology and even chemical vapor deposition technology.



Optical absorption spectra of colloidal nanocrystals.

We employed methods of colloidal chemistry to synthesize semiconducting nanocrystals, which are perspective for solar cell applications. Colloidal suspensions of CdS, PbS, Cu_2S, Ag_2S and ZnO nanocrystals were prepared in presence of organic capping ligands. The formation of nanocrystals was studied using UV-visible absorption spectroscopy. Shottky type solar cell based on PbS nanocrystals was demonstrated.

ELECTRON PROCESSES IN InGaN HIGH INDIUM CONTENT NANOSTRUCTURES

A. Voitkans, L. Dimitrocenko, J. Jansons, I. Tale

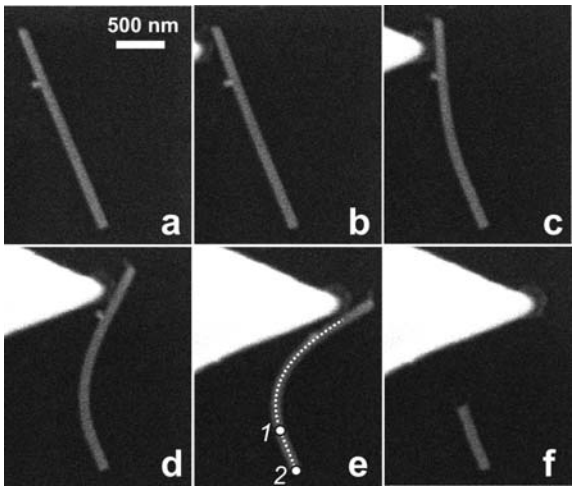
Group III-nitrides have been considered a promising system for semiconductor devices applications, especially for the development of blue- and UV-light emitting diodes (LEDs), and high power and high frequency transistors. InGaN LEDs has high internal quantum efficiency, and are suitable for white light emission devices. Structures based on AlGaN compound could be used for as light source (such as Laser Diodes or Light Emitting Diodes) of UV or VUV light wavelength region and high electron mobility transistors (HEMTs).

The aim of this study is to obtain and investigate a nanostructured InGaN compound with high indium concentration for solid state lighting (SSL) applications. The formation of InGaN QDs on GaN surfaces has been known as a result of Stranski-Krastanov (S-K) growth mode at indium concentrations above 13%. The indium incorporation rate for MOCVD was found to increase significantly as the growth temperature decreased, and at temperatures below 700°C it became saturated close to the input gas-phase ratio of TMIn to TMGa, and indium concentrations can be risen above 70%. Further more, a significant increase in indium content of InGaN QDs is expected by QD layer reconstruction with a pulsed UV photon beam of an additionally deposited amorphous low-temperature InN thin film. Structural investigations are performed using – SEM, AFM, RHEED and XRD. For structure modification, FIB and ps-laser will be exploited. Electronic processes are investigated by stationary and time-resolved nano- and picosecond UV-VIS spectroscopy.

CONTROLLED MANIPULATION AND MECHANICAL CHARACTERIZATION OF NANOWIRES

B. Polyakov, P. Kulis, S. Vlassov, L. Dorogin, I. Kink, R. Lohmus

One-dimensional solids such as nanowires (NWs) and nanotubes (NTs) exhibit many unique optical, electrical, mechanical, and other properties that make them candidates for numerous future nanoscale devices. In many applications NWs are subjected to mechanical stresses and deformations. In flexible electrodes, as well as various nanoelectromechanical systems (NEMS) like, e.g., nanorelays, nanoswithces and nanoresonators, NWs are required to withstand numerous repetitive deformations. The investigation of NWs mechanical characteristics is of a great importance for performance of the named systems.



Gradual bending and fracture of a ZnO NW during controlled loading by AFM tip inside SEM (a-f). Calculated the "most bent state" laid over the SEM image was used to estimate static friction and strength of NW (e).

The manipulation of NWs or NTs is frequently employed to position and assemble prototype nanodevices. Depending on the magnitude of its static friction and its ultimate strength, a NW may be displaced or broken as a result of manipulation. Static friction of NW on flat substrates is strong enough to maintain even highly deformed NWs in a bent state, which produces high strain and is especially important for piezoelectric materials such as zinc oxide.

Young's modulus, bending strength or yield strength of copper oxide (CuO), zinc oxide (ZnO) and silver (Ag) NWs were measured in situ using nanomanipulation techniques inside a scanning electron microscope (SEM). Young's modulus was measured by bending half-suspended NWs and simultaneously measuring the force using a sensor based on a quartz tuning fork. Bending strength was measured for the NWs on a flat surface by bending them from one end with an AFM tip until the NW breaks or plastically deforms. The profile of the elastically deformed NW and the average value of Young's modulus were used to calculate the bending strength or yield strength of the NWs.

Scientific Articles

1. **P. Kulis, J. Butikova, B. Polyakov, G. Marcins**, J. Pervenecka, **K. Pudzs, I. Tale**. Work function of colloidal semiconducting nanocrystals measured by Kelvin probe, *IOP Conf. Ser.: Materials Science and Engineering*, 38, 012048, 2012.
2. **J. Butikova, G. Marcins, B. Polyakov**, A. Muhins, **A. Voitkans, I. Tale**. Processing of amorphous Si by pulsed laser irradiation at different wavelengths, *IOP Conf. Ser.: Materials Science and Engineering*, 38, 012009, 2012.
3. **B. Polyakov**, L. Dorogin, S. Vlassov, M. Antsov, **P. Kulis**, I. Kink, R. Lohmus. In situ measurements of ultimate bending strength of CuO and ZnO nanowires, *European Physical Journal B*, 85, 366, 2012.
4. **B. Polyakov**, S. Vlassov, L. Dorogin, **P. Kulis**, I. Kink, R. Lohmus. The effect of substrate roughness on the static friction of CuO nanowires, *Surface Science*. 606, 1393-1399, 2012.

5. **B. Polyakov**, L. Dorogin, S. Vlassov, I. Kink, A. Romanov, R. Lohmus. Simultaneous measurement of static and kinetic friction of ZnO nanowires in situ with a scanning electron microscope, *Micron*. 43, 1140–1146, 2012.
6. **B. Polyakov**, L. Dorogin, A. Lohmus, A. Romanov, R. Lohmus. In situ measurement of the kinetic friction of ZnO nanowires inside a scanning electron microscope, *Applied Surface Science*. 258, 3227-3231, 2012.
7. L. Dorogin, **B. Polyakov, A. Petruhins**, S. Vlassov, R. Lohmus, I. Kink, A. Romanov. Modeling of kinetic and static friction between an elastically bent nanowire and a flat surface, *Journal of Material Research*. 27, 580-585, 2012.

Popular Science Articles

1. J. Jansons. Fizikas profesoram Jurim Zaķim – 75. – „Zvaigžņotā Debess" 2012. g. vasara (216), 27. – 35. lpp.
2. J. Jansons. Fizikas docents Jānis Kariss (22.06.1927. – 22.09.2011.). –„Zvaigžņotā Debess'' 2012. g. rudens (217), 31. – 33. lpp.

Lectures on Conferences

International conference "Functional materials and nanotechnologies" FM&NT, Riga, 2012, April 17-20

1. I.Tale, J. Butikova, G. Marcins, A. Muhins, B. Polyakov, A. Voitkans, Processing of amorphous Si by pulsed laser irradiation at different wavelengths.
2. P. Kulis, J. Butikova, B. Polyakov, I. Tale, Nanocrystals for solar cell applications.
3. M. Antsov, L. Dorogin, B. Polyakov, S. Vlassov, R. Lohmus, Measurement of static friction force of complex shaped ZnO nanowires on a flat surface.
4. Anspoks, A. Kalinko, P. Kulis, A. Kuzmin, B. Polyakov, J. Timoshenko, X-ray absorption spectroscopy of the local atomic structure in PbS quantum dots.

E - MRS 2012, Strasbourg, 2012, May 14-18

5. G. Marcins, J. Butikova, I. Tale, B. Polyakov, A. Muhin, A. Voitkans, Polycrystalline Si grain size dependence of film temperature during laser crystallization process.

3rd European Nanomanipulation Workshop, IMDEA Nanoscience, Madrid, Spain, 2012, April 25-27

6. B. Polyakov, L. Dorogin, S. Vlassov, A. Lohmus, A. Romanov, M. Antsov, I. Kink, R. Lohmus, In situ measurements of static friction of CuO nanowires and influence of the substrate roughness on static friction.

28th Scientific Conference of the Institute of Solid State Physics, University of Latvia, Riga, 2012, February 8-10

7. J.Jansons, Profesors Juris Zaķis – 75

DEPARTMENT OF FERROELECTRICS

Head of Department, Dr.phys. V.Dimza

LABORATORY OF PHYSICS AND APPLICATION OF FUNCTIONAL MATERIALS

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

LABORATORY OF SYNTESIS AND PROCESSING

Head of Laboratory M.chem. M.Antonova

Reaearch areas

Methods:
1) Production of new ferroelectric materials by modification of known ferroelectric compounds by doping with monoxides, developing binary or multicomponent solid solutions:
– complex lead-containing perovskite family with general chemical formulas $PbB'_{1/2}B''_{1/2}O_3$ (where B'=Sc^{+3}, Lu^{+3}, Yb^{+3}, Tm^{+3} etc.; B''= Nb^{+5}, Ta^{+5}) and $PbB'_{1/3}B''_{2/3}O_3$, (where B'=Mg^{+2}, Zn^{+2}, Ni^{+2}, Cd^{+2} etc., B"- Nb^{+5}, $Ta^{+5}$and etc);
– modified (Pb,La)(Zr,Ti)O_3 (PLZT);
– lead-free perovskite ceramics based on $(K_{0.5}Na_{0.5})NbO_3$, $(Na_{0.5}Bi_{0.5})NbO_3$, or $BaTiO_3$;
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), magnetic properties, electronic structure**;**

Materials: Large variety of ferroelectric compositions, thin films, multiferroic materials, inorganic functional and nanomaterials;

Problems: Phase transitions (including field-induced ferroelectric phase transitions) and ordering effects in "ordinary" ferroelectrics and ferroelectric *relaxors* along with new compositions (including 3d elements doping of ABO3 perovskites); replacement of lead-containing materials in various applications

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6. Dagestan State University (Prof. S.A. Sadikov).
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8. Russia, Tver State University, Prof. O. Malyshkina.

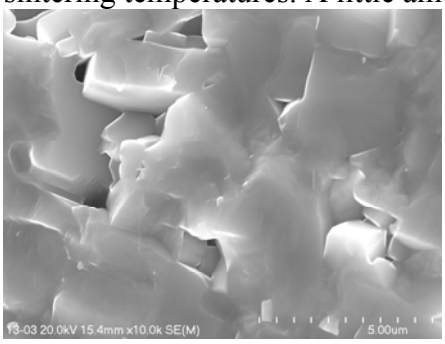
MAIN RESULTS

SYNTHESIS AND CHARACTERIZATION OF MODIFIED $(K_{0.5}Na_{0.5})NbO_3$ LEAD-FREE PIEZOELECTRIC CERAMICS

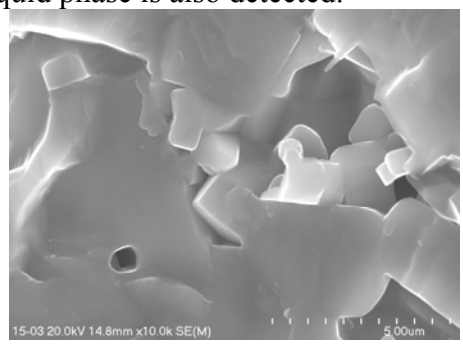
I.Smeltere, M.Antonova, A.Kalvane, M.Livinsh

In the present work solid solutions with chemical formula $(1-x)(K_{0.5}Na_{0.5})Nb_{1-y}Sb_yO_3$-$xBaTiO_3$ (x=0.01; 0.015; 0.02; 0.04; y=0.04; 0.07) (KNNSy%-xBT) were made by conventional solid state sintering. Phase structure changes from monoclinic to tetragonal with increasing x in NS4. Density measurements detected by Archimedes method showed that $BaTiO_3$ addition to the original composition increased the density of the ceramic sample reaching 4.51g/cm^3 (99% from theoretical density) for KNNS4-1BT. X-ray diffraction analysis confirmed single phase perovskite structure with monoclinic or tetragonal cell depending on x.

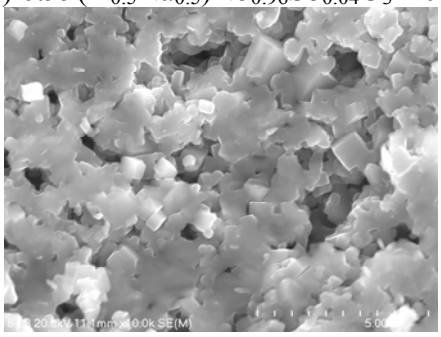
Solid solutions with increasing $BaTiO_3$ addition have smaller average grain sizes; the shape of grains is a little rounded. MnO_2 addition suppresses the grain growth even more and the microstructure is more homogenous which could be the result of lower sintering temperatures. A little amount of liquid phase is also detected.



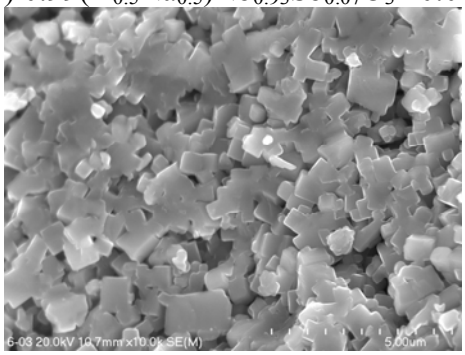
a) $0.99(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3 - 0.01BT$



b) $0.99(K_{0.5}Na_{0.5})Nb_{0.93}Sb_{0.07}O_3$ - 0.01BT



c) $0.96(K_{0.5}Na_{0.5})Nb_{0.96}Sb_{0.04}O_3$-0.04BT



d) $0.96(K_{0.5}Na_{0.5})Nb_{0.93}Sb_{0.07}O_3$-0.04BT

Figure 1. SEM microstructure for $(1-y)(K_{0.5}Na_{0.5})Nb_{1-x}Sb_xO_3$-$yBaTiO_3$+ 0.5wt%$MnO_2$

Material constants: the Young′s modulus *E*, the shear modulus *G* and the Poisson′s ratio *v* were measured by an ultrasonic method. The highest velocity of the longitudinal waves was observed for sample KNNS4-1.5BT (V_L = 4720.5 m/s). The transverse wave velocity for this sample is higher then for other samples (V_T = 2699.6 m/s). The values of both Young′s modulus E and the shear modulus G are relatively high taking into account modest densities of the samples (E = 64.96 GPa, G = 25.86 GPa).

The addition of 1 mol% of BT increases the value of dielectric permittivity ε and decreases T_C. In the same time BT decreases dielectric losses. Phase transition becomes more diffuse while increasing x. Table 1 summarizes the results of dielectric properties.

Table 1

Density and dielectric properties for different compositions

Composition	*Density g/cm^3*	*Dielectric permittivity ε (room T)*	*Dielectric loss tanδ (room T)*	*T_{max} (C°)*	*γ*
S4-1BT	4.51	1400	0.043	305	1.34
S4-2BT	4.44	1240	0.652	270	1.45
S4-4BT	4.34	1380	0.727	178	1.73
S7-1BT	4.31	1800	0.100	245	1.39
S7-2BT	4.34	940	0.490	211	1.57
S7-4BT	4.43	1400	0.549	129	1.76

PHASE TRANSITIONS AND PHYSICAL PROPERTIES IN $Na_{1/2}Bi_{1/2}TiO_3$-$BaTiO_3$ SOLID SOLUTIONS

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

$Na_{1/2}B_{1/2}TiO_3$ and its solid solutions attract interest mostly as an alternative for nowadays widely used lead-containing ferroelectric, use of which is gradually limited due to ecological considerations.

$Na_{1/2}B_{1/2}TiO_3$ solid solutions with $BaTiO_3$ or (1-x)NBT-xBT show good piezoelectric properties. Most of the studies of (1-x)NBT-xBT are focused on the region around the morphotropic phase boundary, which is observed at BT concentration $0.05 \leq x \leq 0.07$. There is very little information about the compositions with higher BT content.

In this work dielectric properties, polarization and x-ray diffraction are studied for NBT-BT solid solutions in a concentration range above the morphotropic phase boundary. Parameters, characterizing crystallographic structure and phase transition, are determined depending on the ratio of components of the solid solution. The results show that that all the studied compositions have tetragonal structure with maximal tetragonality slightly above the morphotropic phase boundary. In a wide concentration range ferroelectric relaxor properties are observed with a spontaneous transition to ferroelectric state at a temperature below the maximum of dielectric permittivity. Stability of the relaxor state decreases with increasing $BaTiO_3$ concentration, but only for compositions with low $Na_{1/2}Bi_{1/2}TiO_3$ content the normal ferroelectric-paraelectric phase transition, which is characteristic to pure $BaTiO_3$, occurs. The change of diffuseness of the temperature dependence of dielectric permittivity is studied, using the power law. Attention is paid also to the concentration dependence of the thermal hysteresis. Mechanisms, which influence the change of the phase transition character and promote the appearance of the relaxor state, are discussed. The phase diagram of (1-x)$Na_{1/2}Bi_{1/2}TiO_3$-x$BaTiO_3$ is revised.

Special attention is paid to the phase coexistence region in the tetragonal side from the morphotropic phase boundary. The x-ray diffraction results show that the 1st order ferroelectric phase transition, determined from a jump at temperature dependence of dielectric permittivity, is located inside the coexistence region of cubic and tetragonal phases and is below the temperature, where tetragonality disappears. At low $BaTiO_3$ concentrations phase transition into ferroelectric state at cooling is slowly approached in time and is smeared over large temperature range. Rietveld method, applied for more precise evaluation of phase content, reveals large local deformations inside the ferroelectric phase.

PHASE TRANSITIONS IN Li, K AND Ag MODIFIED $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ SOLID SOLUTIONS

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

$Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$ is a well-known relaxor ferroelectric. The transfer from relaxor to normal ferroelectric state, passing various intermediate states, characteristic for relaxor ferroelectrics, was found in $Na_{1/2}Bi_{1/2}TiO_3$-$SrTiO_3$-$PbTiO_3$ solid solutions, if Pb content is increased. Particularly for $0.4Na_{1/2}Bi_{1/2}TiO_3$-$0.4SrTiO_3$-$0.2PbTiO_3$ the spontaneous transfer between relaxor and ferroelectric state at temperature T_t is approaching the relaxing maximum of temperature dependence of dielectric permittivity at temperature T_m. As a result the relaxing state almost disappears.

In the present work the influence of monovalent metals (Me^{1+}: Li, K, Ag) on the properties of $0.4(Na_{1-x}Me^{1+}_x)_{1/2}Bi_{1/2}TiO_3$-$0.4SrTiO_3$-$0.2PbTiO_3$ solid solutions is studied in the concentration range till x=0.25. The x-ray diffraction results show that all obtained compositions are single-phase solid solutions with tetragonal symmetry. The concentration dependences of the unit cell parameters indicate that Me^{1+} ions in all cases substitute Na^{1+} ions in the A-site of the perovskite structure. The obtained compositions can be characterized by phase transition and dielectric properties, qualitatively similar to those of $0.4Na_{1/2}Bi_{1/2}TiO_3$-$0.4SrTiO_3$-$0.2PbTiO_3$. However their concentration dependences are mostly not monotonous. Substitution by Li increases, while substitution by K and Ag decreases tetragonality of unit cell. Li increases, Ag decreases while K weakly influences phase transition temperature. The characteristic for the parent phase relaxor state with phase transitions temperature T_t approaching temperature of dielectric permittivity maximum T_m in case of substitution by K and Li transfers into diffused phase transition without T_m dependence on frequency and extended region of thermal hysteresis.

STRUCTURE OF TANTALUM AND NIOBIUM PENTOXIDE CERAMICS TREATED BY CONCENTRATED LIGHT FLOW*

K. Bormanis, M. Palatnikov, O. Shcherbina, and N. Sidorov

Ceramic Nb_2O_5 and Ta_2O_5 refractory oxides obtained by conventional techniques have a macro-crystalline structure, are particularly brittle of feeble plasticity and weak crack resistance limiting practical applications. Mechanical characteristics of the ceramics can be improved to obtain material of the smallest (micro- and nano-meter scale) structure by employing advanced treatment techniques. Atomic force microscopy (AFM) and Raman studies of the effect of concentrated light flow (CLF) on nano-, micro- and macro-structures, and disordering of the structural units in ceramic tantalum and niobium pentoxides are reported.

High-energy concentrated light transforms the structure of Nb_2O_5 and Ta_2O_5 ceramics at different scales starting from fractal macro-, micro- and nano-structures and ending by altering of the character of chemical bonding and the degree of coordination in the structural polyhedrons. The complex transformations radically change the physical characteristics of Nb_2O_5 and Ta_2O_5 including mechanical properties and thermal expansion. The differences in reaction of Nb_2O_5 and Ta_2O_5 ceramics to CLF (a larger proportion of the nano-meter structures in Ta_2O_5 ceramics, chemical bonding, and coordination of structural polyhedrons) can be accounted for by different melting temperature of the oxides and the difference in covalent bonding of Nb-O and Ta-O.

* In cooperation with Institute of Chemistry, Kola Science Centre RAS, Apatity, Russia.

CONCENTRATION AND THERMAL PHASE TRANSITIONS IN PEROVSKITE SOLID SOLUTIONS*

K. Bormanis, N. Sidorov, M. Palatnikov, N. Teplyakova, and E. Obryadina

Solid solutions (SS) of $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$ are of interest as ceramic materials of lithium super-ionic (SI) conductivity. Ordering of Li^+ and Na^+ cations and deformations of oxygen octahedrons in the SS structure at the ratio of Na : Li = 7 : 1 provide specific channels of conductivity formed of Na^+ cation vacancies. Position and broadening of the transition to the SI state vary over a wide temperature range (~ 670 ÷ 730 K) depending on the degree of ordering of the structural units in the niobium and tantalum sub-lattices. The change of the geometry of the oxygen octahedrons and the type of dipole ordering in the $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$ SS is accompanied by a variety compositional phase transitions (PT).

Phase transitions and structural disordering of the $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$, SS preceding transition to the SI state is studied by Raman spectroscopy. A series of compositional phase transitions and structural reordering in $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$ SS is observed at y ≈0.25; 0.6; 0.8. At the ferroelectric to antiferroelectric PT occurring in the $Li_{0.12}Na_{0.88}Ta_yNb_{1-y}O_3$ SS at 570÷620 K, the Raman band corresponding to stretch of the oxygen bridge disappears. Thermal disordering caused by highly mobile lithium ions, proceeds gradually and relatively uniformly. The increase of translational mobility of the light lithium ions is facilitated by disorientation of the oxygen octahedrons BO_6 on the whole and by considerable deformation significantly altering the octahedron symmetry. Static disordering in the Nb^{5+} and Ta^{5+} sub-lattice occurring under varied tantalum content decreases the temperature of the ferroelectric to antiferroelectric PT promoting transition to the SI state. However, our data suggest that transition to the SI state is spread over a broad range of temperatures and does not show up as a stepwise change in the Raman spectrum.

* In cooperation with Institute of Chemistry, Kola Science Centre RAS, Apatity, Russia.

CONDUCTIVITY PROCESSES IN $CoFe_2O_4$ AND $NiFe_2O_4$ CERAMICS INVESTIGATED BY DIELECTRIC SPECTROSCOPY*

M. Kinka, K. Bormanis, V. Samulionis, and A. Kalvane

Recently, special interest has been paid to the possible use of spinel ferrites as magnetic components in the design of artificial multiferroic heterostructures and composite materials [1]. Furthermore, they have been shown to exhibit interesting magnetic properties in the nanocrystalline form compared with those of the micrometre-size grains [2]. Despite the growing number of publications addressing the properties of small size $CoFe_2O_4$ and $NiFe_2O_4$ structures (thin films, nanoparticles, etc.), few reports are available in the literature on the electrical conductivity and dielectric properties of bulk $CoFe_2O_4$ and $NiFe_2O_4$. The dielectric properties of these ferrites are dependent on several factors, such as the method of preparation, sintering temperature, sintering time and chemical composition.

We have investigated $CoFe_2O_4$ and $NiFe_2O_4$ ceramics prepared by conventional ceramic technology. Powders of $CoFe_2O_4$ and $NiFe_2O_4$ were synthesized from the corresponding oxides by solid phase thermal chemical reactions. Dielectric properties were measured in the 20 Hz – 1 MHz frequency range starting from 120 K and reaching temperatures above magnetic phase transitions. Dielectric responses of characteristic shape, caused by electrical conductivity, common for both investigated materials were

obtained. Two conductivity processes were distinguished with Arrhenius behaviors of σ_{DC} and possible underlying mechanisms of charge transport are discussed.

[1]. J. Ryu, S. Priya, K. Uchino and H. Kim, Journal of Electroceramics, **8**, 107 (2002)

[2]. I. P. Suzdalev, Russian Chemical Reviews **78** (3), 249 - 282 (2009)

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DIELECTRIC NONLINEARITY AND MAGNETIC PROPERTIES OF $Pb(Fe_{1/2}Ta_{1/2})O_3$ CERAMICS AT LOW TEMPERATURES*

K. Bormanis, A. Kalvane, A.I. Burkhanov, M. Maiorov,
S.V. Trukhanov, and O. Malyshkina

Lead ferrotantalate $PbFe_{1/2}Ta_{1/2}O_3$ (PFT) is known as ferroelectric in which anti-ferromagnetic ordering arises at low temperatures [1]. Studies of dielectric and magnetic properties of PFT ceramics at low temperatures are reported. Dielectric nonlinearity at low- and infra-low-frequencies over a wide range of temperature under applied bias field was measured. The features of dielectric nonlinearity deduced from behaviour of reversive $\varepsilon'(E_=)$ curves at different temperature including regions of ferroelectric phase transition and vicinity of the Neel point are examined. The $PbFe_{1/2}Ta_{1/2}O_3$ ceramics was obtained by conventional ceramic technology. Powders lead ferrotantalate were synthesized from the corresponding oxides by solid phase thermal chemical reactions.
Behaviour of $\varepsilon'(E_=)$ at $T>T_{room}$ ($T_m \approx -40^0$C) is illustrated in Figure 1. The room temperature T_{room} = 20 ^{0}C corresponds to the paraelectric phase in PFT. Behaviour of $\varepsilon'(E_=)$ at temperature below the Neel point ($T_N \approx$ -140 ^{0}C) is illustrated in Figure 2.

Figure 1

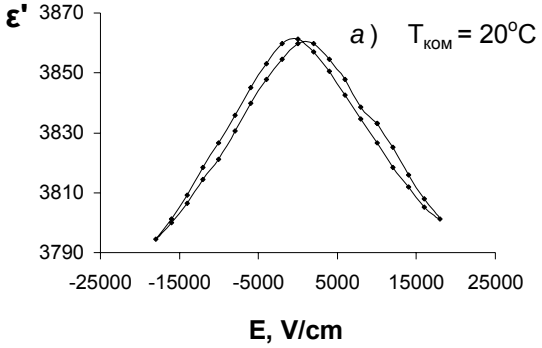
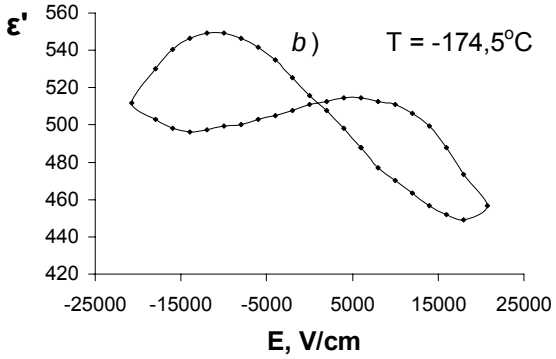


Figure 2



Obtained results show that, despite of the temperature considerably exceeding T_m, a weak hysteresis of $\varepsilon'(E_=)$ is observed in agreement with other data [2] indicating substantial broadening of the ferroelectric phase transition. Reversive $\varepsilon'(E_=)$ curves at T=-174.5 ^{0}C of the PFT ceramics comply with polarisation switching in a material in the ferroelectric state. It should be noticed though that unipolarity is considerably pronounced at polarisation switching. The results are discussed with respect to co-existing polar and non-polar phases over a wide range of temperature and effects of ferromagnetic – anti-ferromagnetic ordering in relaxor materials of such a kind.

[1] Venevtsev YuN, Gagulin VV, and Ljubimov VN: Ferroelectrics-magnetics. Moscow: Science; 1982.

[2] R. Martínez V, Ashok Kumar, Dilsom A. Sanchez, R. Palai, and R. S. Katiyar. Journal of Applied Physics, 108, 084105 (2010).

* In cooperation with Volgograd State Architectural and Engineering University, Volgograd, Russia; Institute of Physics, University of Latvia, Salaspils, Miera 31,

Latvia; SSPA ”Scientific-Practical Materials Research Centre of NAS of Belarus”, Minsk, P.Brovka 19, Belarus; and Tver State University, Russia.

THE EFFECT OF LIGHT ON LOW FREQUENCY RELAXATION OF POLARISATION IN FERROELECTRIC BARIUM-STRONTIUM CERAMICS*

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

The action of light on features of the low-frequency dielectric response in the $Sr_{0.75}Ba_{0.25}Nb_2O_6$ (SBN-75) is studied under electric field.

The measurements with the SBN-75 ceramics specific of a broad phase transition ($T_m \approx 110\ ^0C$) [1] were made under illumination of 0.15 mW white LED radiation and bias fields up to 15 kV/cm in the 0.1 Hz — 10 Hz frequency range.

The low-frequency hysteresis loops of polarisation are studied as functions of the temperature and illumination. The contribution of processes related to the relatively high conductivity of the ceramics into polarisation (“rounded” loops, Fig.1.) at temperatures of the relaxor phase (close to T_m) is found to be substantially suppressed by illumination (Fig.2, T=45 ^{0}C). At the same time, at lower temperatures (T=25 ^{0}C), parameter describing the relative change of polarisation $\Delta P = (P_{ill} - P_{dark})/P_{max}$ increases with illumination up to some E, then decreases. At the 10 Hz frequency ΔP increases with illumination regardless to E, which is consistent with earlier data [2]. Results on photocurrents measured in shortcut SBN-75 ceramic samples are investigated.

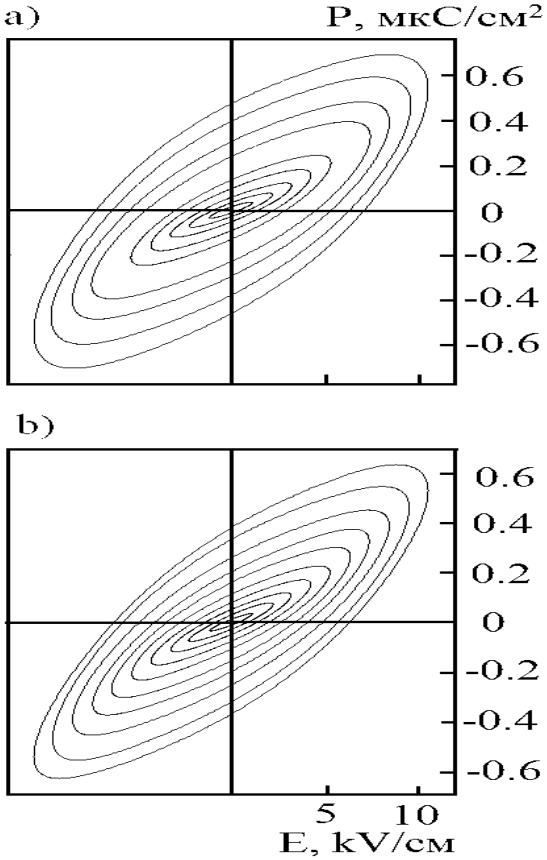


Fig. 1. Polarisation loops at 45 ^{0}C and 1 Hz frequency of dark (a) and illuminated (b) SBN-75 ceramics.

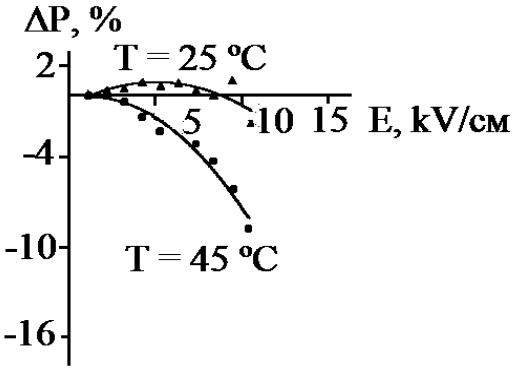


Fig. 2. Change of polarisation ΔP as a function of the applied field intensity E.

[1]. K. Bormanis, A.I. Burkhanov, S.V. Mednikov, Luu Thi Nhan, A. Kalvane, and M. Antonova. Ferroelectrics, **417**, 01, 58–62 (2011).

[2]. A.I. Burkhanov, K.P. Guzhakovskaya, L.I. Ivleva, Izvestiya RAS, ser. Phys. **75**, 10, 1484-1487 (2011, in Russian).

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

HEAT CAPACITY AND DIELECTRIC PROPERTIES OF THE PNN-PT FERROELECTRIC CERAMICS*

K. Bormanis, S.N. Kallaev, Z.V. Omarov, A.R. Bilalov, and A. Kalvane

The multi-component mixed perovskites of extraordinary crystal structure and unique properties, an enormous dielectric permeability, strong piezoelectricity and electrostriction in particular, for decades have been of increasing interest. The (1-x)$PbNi_{1/3}Nb_{2/3}O_3$ – $xPbTiO_3$ ((1-x)PNN-xPT) solid solution system is one of mixed ferroelectric relaxors.

The presented study is focused on heat capacity and dielectric permittivity of the (1-x)PNN-xPT (x = 0.5, 0.4, and 0.3) ferroelectric ceramics within the 150 – 750 K range of temperature. The PNN-PT samples were obtained by conventional ceramics technology.

Results of dielectric measurements reveal decreasing of the temperature T_m of the maximum of dielectric permittivity ε of the (1-x)PNN-xPT system with the increase of the PNN component while the maximum value of the dielectric permittivity increases and the region of phase transition broadens. Dispersion of the dielectric permittivity peak value ε_m specific to ferroelectric relaxors is observed in case of the $0.7PbNi_{1/3}Nb_{2/3}O_3$–$0.3PbTiO_3$ compound.

Two thermal anomalies on the heat capacity c_p curve characteristic to phase transitions are observed in compounds of x = 0.5 and x = 0.4, four – in case of x = 0.3. The high-temperature anomaly around 520 k on the $c_p(T)$ curves of all the compounds has never before been observed. In the latter case a broad irregularity of heat capacity $c_p(T)$ characteristic to relaxors is observed in the 250 – 450 k range. The anomalous component of heat capacity in the range of phase transition was found as the difference between the measured value and calculated phonon heat capacity.

According to the obtained data of the (1-x)pnn-xpt measurements the "temperature-composition" phase diagram is linear indicating to regular thermodynamic type of solid solutions. The experimental results are discussed with respect to the structure of the ceramics.

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THE CHANGES OF RELAXOR BEHAVIOUR OF PLZT8/65/35 CERAMICS AT DOPING WITH 3D ELEMENTS

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M. Antonova, V. Dimza

A study of the effects of the 3d dopants Mn, Fe, Co, Ni, and Cu on relaxor behavior and other properties of the ferroelectric PLZT8/65/35(La8) ceramic compound by X-ray diffraction, electron microscopy and other techniques is reported. The complex dielectric permittivity ε*=ε'-iε'' is measured in the 20-400 ^oC range of temperature at frequencies within the range of 10^2 – 10^6 Hz.

The admixture of Mn and Co causes a low-frequency dispersion: a monotonous decrease of ε'' at frequencies 100Hz – 125 kHz (ε" ~ $1/\omega^n$ with n<1). .
The quantitive change of dielectric parameters follows the sequencies:

- ε_{max} at frequency 100Hz: Co>Fe>Ni>Cu>pureL8>Mn
- ε_{max} at frequency 1MHz: Fe>Co>~Ni>Cu>L8>Mn

- $\Delta T_{\varepsilon max}$: Mn>Co>Fe>Cu~Ni
- Depth of dispersion: -for $\Delta T_{\varepsilon max}$: Ni>~Co>pure L8>Fe>Cu>Mn
  -for $\Delta\varepsilon/\varepsilon_{max}$: Co>Cu>Fe~Ni>Mn>pure L8

Summing up 3 types of effects of the 3d dopants at 1% wt. on the relaxor behavior can be distinguished: 1) Mn – depression of ferroelectric and relaxor properties; 2) Ni - enhancement of relaxor properties; 3) Fe, Co, Cu – partial enhancement of relaxor behavior.

The change of P(E) at 20°C caused by dopants is illustrated. The values of remnant polarization (P_r) raise in the case of 1% wt. Fe, Co, Ni, Cu (Fig.3.a), but in the case of Mn the rise of P_r, is observed only up to 0.3 % wt. while being reduced at 1% wt..

The XRD results shows:

1) decreasing of unit cell volume;
2) increasing of ratio of diffraction maxima I_{210}/I_{211};
3) appearance of likely monoclinic distortion.

According to our studies, the magnitude of most of the dopant-induced effects follows the sequence Mn>Fe>~Co or Co>~Fe>Mn.

Conclusions:

1. Addition of Mn, Fe, Co, Ni, and Cu to PLZT8/65/35 ceramics essentially change the structure and the mechanism of polarization.
2. Admixtures may ameliorate as well as restrain relaxor characteristics.
3. Mn, Fe, Co, Ni, and Cu dopants are related to several competing factors affecting polarization:
   1) JTE – causing an increase of T_m, ε, and the remnant polarization (P_r) in the case of Fe, Co, Ni, and Cu;
   2) change of the concentration and orientation of polar nano-regions;
   3) the Maxwell-Wagner polarization;
   4) change of the concentration of vacancies in A and/or O sub-lattices manifested as acceptor effects.

VIBRATIONAL PROPERTIES OF LaPO4 NANOPARTICLES IN MID- AND FAR-INFRARED DOMAIN

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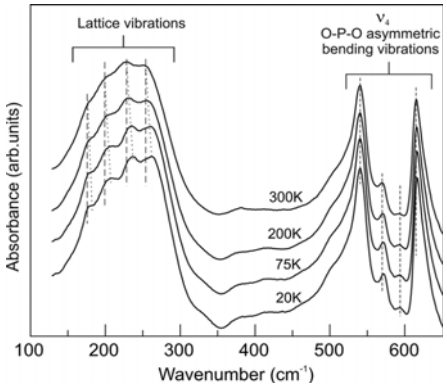
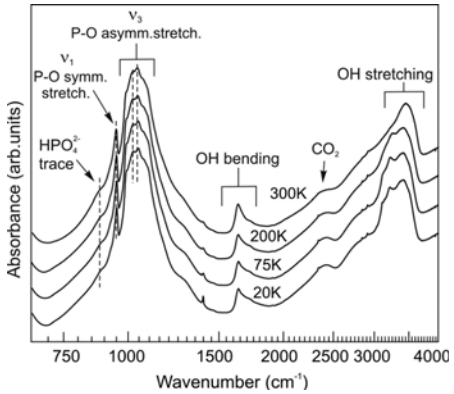
Nanopowders of LaPO4 have been grown by sedimentation-micellar method. As-prepared LaPO4 nanoparticles with the average grain size of about 8 nm have a single-phase hydrated hexagonal structure. After thermal annealing at 600 and 800 _C, the average size of nanoparticles increases up to 35 and 50 nm, respectively, and the structure transforms into single-phase monoclinic. IR spectra of LaPO4 nanoparticles of





different size were investigated in the wide range of wavenumbers from 130 to 5000 cm^{-1} in the 20–300 K temperature region. Differences between IR spectra of the bulk material and nanoparticles as well as the temperature behavior of the vibrational properties are demonstrated.

Fig. 1. Far infrared (left) and mid infrared (right) spectra of hydrated hexagonal LaPO4 nanoparticles with average size of about 8 nm at different temperatures.

SYNCHROTRON RADIATION STUDIES ON LUMINESCENCE OF Eu^{2+}-DOPED $LACL_3$ MICROCRYSTALS EMBEDDED IN A NaCl MATRIX

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$LaCl_3$:Eu^{2+} microcrystals dispersed in the NaCl matrix have been obtained in the NaCl–$LaCl_3$ (1 mol.%)– $EuCl_3$(0.1 mol.%) crystalline system. The low-temperature luminescent properties of these microcrystals have been studied upon the VUV and UV excitation by the synchrotron radiation. The spectroscopic parameters as well as decay time constants of Eu^{2+}-doped $LaCl_3$ host have been established. The excitation mechanism of divalent europium centers through energy transfer and reabsorption have been proposed.

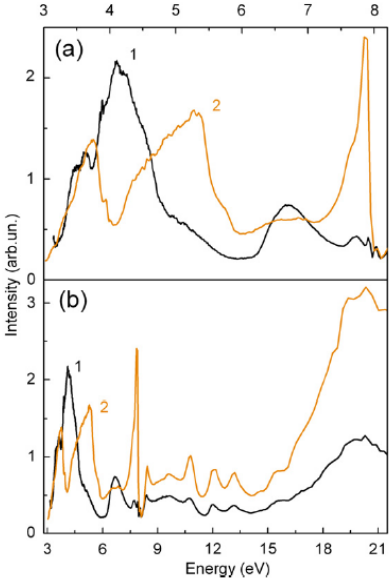

Fig. 2. Luminescence excitation spectra of Eu^{2+} single centers in the NaCl–$LaCl_3$(1 mol.%)–$EuCl_3$(0.1 mol.%) crystal (kem = 405 nm, curve 1) and the NaCl–$EuCl_3$(0.01 mol.%) crystal (kem = 428 nm, curve 2) within (a) Eu^{2+} ions andLaCl3 absorption range, (b) the whole measured range. T = 10 K.

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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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Cooperation

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

Main results

PRESENCE OF SPHERICAL ABERRATION IN THE REFERENCE AS A POSSIBLE SOURCE OF VARIATIONS IN MAGNITUDE OF MEASURED OCULAR ABERRATIONS

V. Karitans, M. Ozolinsh, K. Luse, and L. Ekimane

Different aberrometry methods exist and the magnitude of measured wavefront aberrations may differ depending on the method used. Even several Shack–Hartmann wavefront sensors may demonstrate clinically significant differences between ocular aberrations measured. In this study, we tested a hypothesis that a possible source of systematic error in Shack–Hartmann aberrometry may be the presence of spherical aberration in the wavefront used for calibrating the Shack–Hartmann wavefront sensor. Six subjects participated in the study. The Shack–Hartmann wavefront sensor was calibrated by using a spherical and an aspheric lens. Statistically significant changes in wavefront aberrations were observed when comparing both references. Clinically significant changes in magnitude of spherical aberration were also observed. We conclude that for precise measurement of aberrations the use of an aspheric lens for wavefront sensor calibration is essential and different sphericity of the wavefront used for calibration purposes may give rise to variability between wavefront data measured by different Shack–Hartmann wavefront sensors.

PSEUDOISOCHROMATIC TEST PLATE DEPENDENCE ON PRINTING TECHNOLOGY

K. Luse, S. Fomins, and M. Ozolinsh

The aim of the study is to determine best printing technology for creation of colour vision deficiency tests. Valid tests for protanopia and deuteranopia were created from perceived colour matching experiments from printed colour samples by colour deficient individuals. Calibrated *EpsonStylus Pro 7800* printer for ink prints and *Noritsu HD 3701* digital printer for photographic prints were used. Multispectral imagery (by tunable liquid crystal filters system *CRI Nuance Vis 07*) data analysis show that in case of ink prints, the measured pixel colour coordinate dispersion (in the *CIExy* colour diagram) of similar colour arrays is smaller than in case of photographic printing. The print quality

in terms of colour coordinate dispersion for printing methods used is much higher than in case of commercially available colour vision deficiency tests.

RAYLEIGH EQUATION ANOMALOSCOPE FROM COMMERCIALLY AVAILABLE LEDs

R. Trukša, S. Fomins, and M. Ozolinsh

Most precise classification of CVD (color vision deficits) can be provided by using anomaloscope. Today anomaloscopes are available, which can evaluate red-green (Rayleigh) and blue-green (Moreland) color defects. Our aim is to create and calibrate commercially available LEDs based anomaloscope for diagnosis of red-green color vision defects. Other field of use of anomaloscope is a seasonal and overall variation of normal color vision in Latvian population.

LED BASED DUAL WAVELENGTH HETEROCHROMATIC FLICKER METHOD FOR SEPARATE EVALUATION OF LUTEIN AND ZEAXANTHIN IN RETINA

M. Ozolinsh and P. Paulins

The decrease of density and consequentially optical density of macular pigment serves as a diagnostic mean for a number of ophthalmological pathologies, particularly as a risk factor for age related macular degeneration. Macular pigment absorbs light in short wavelength blue spectral range. Thus the optical density of macular pigment can be detected by various optical – both objective and subjective psychophysical techniques. Latter techniques use eye and brain visual pathway as spectral sensitive optical detector and decision maker, and exploit perception facility to process information flow in a unique manner to create various perception illusions. The psychophysical methods of detection of optical density of macular pigment include heterochromatic flicker photometry and minimum illusory motion photometry. We develop and employ a heterochromatic flicker photometry method where LEDs are used as visual stimuli. LED emission maximum wavelengths in blue spectrum region are chosen in range 445-460 nm, that corresponds to spectrally resolved maxima of light absorption for two types of macula pigments – lutein and zeaxanthin or in spectral range 500-510 nm, where lutein and zeaxanthin absorption have decay, that for both type of pigments have a detectable shift. Statistical dispersion of the results allows to use the difference between results of psychophysical measurements obtained for different LEDs to estimate the concentration of lutein and zeaxanthin in human retina.

APPLICABILITY OF A BINARY AMPLITUDE MASK FOR CREATING CORRECTORS OF HIGHER-ORDER OCULAR ABERRATIONS IN A PHOTORESISTIVE LAYER

V. Karitans, K. Kundzins, E. Laizane, M. Ozolinsh, and L. Ekimane

Ocular aberrations can be corrected with wavefront correctors created in a photoresist layer. The simplest type of the mask used in optical lithography is a binary amplitude mask. It is known that such a mask has a periodic hole pattern. The purpose of this research was to assess applicability of a binary amplitude mask for creating ocular wavefront correctors. The photoresist was applied to the substrate by using the dip-coating method. The photoresist layer was illuminated through a mask printed on a

transparent film by using a laser printer. The surface of the wavefront correctors was evaluated by aberrometry, scanning electron microscopy and profilometry method. The dip-coating method can be used to apply an uniform photoresist layer on the substrate. Despite rapid variations in the surface depth the required shape of the wavefronts can still be obtained. Because of strong light scattering the wavefront correctors manufactured by using a binary amplitude mask aren't suited for studying visual functions. However, the wavefront correctors manufactured by such a type of the mask may be used for calibration of aberrometers.

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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);
- stochastization of magnetic field lines in magnetized fusion plasma;
- 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)—for more details see our homepage http://www1.cfi.lu.lv/teor

Scientific Staff

Laboratory of kinetics in self-organizing systems	**Laboratory of computer modeling of electronic structure of solids**
Dr. O. Dumbrajs	J. Begens
Dr. D. Gryaznov	Dr. D. Bocharov
Dr. V. Kashcheyevs	Dr. R. Eglitis
Dr. E. Klotins	Msc. A. Gopejenko
Dr. hab. E. Kotomin	J. Kazerovskis
Dr.hab. V. Kuzovkov	Bsc. O. Lisovski
Msc. P. Merzlakovs	Dr. Yu. Mastrikov
Dr. A. Popov	Dr. S. Piskunov
Mcs. J. Sirmane	Dr. hab. Yu. Shunin
Dr. G. Zvejnieks	Bsc. A. Sorokin
	Dr. Yu. Zhukovskii

Scientific visits abroad

1. Dr. hab. E. Kotomin, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (9 months)
2. Dr. O. Dumbrajs, Max-Planck Institut für Plasmaphysik, Garching, Germany (2 month), Fukui University, Fukui (3 months)
3. Dr. D. Gryaznov, Max-Planck Institut für Festkörperforschung, Stuttgart, Germany (9 months); University College London (1,5 months)
4. Dr hab. V. Kuzovkov, Northwesten University, USA (3 months)
5. Dr. A. Popov, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (3 weeks), Laue-Langevin Institute, Grenoble, France (1 month), Electronic Materials Division, Institute of Materials Science, Darmstadt University of Technology, Darmstadt, Germany (2 months)
6. Dr. D. Bocharov, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany (1,5 weeks)
7. A. Gopejenko, Institute for Applied Materials, Karlsruhe Institute of Technology , Karlsruhe, Germany (5 weeks)
8. O. Lisovski, Uppsala University, Sweden (4 months)
9. Dr. Yu. Mastrikov, Institute of Applied Materials, Karlsruhe, Germany (6 weeks)
10. Dr. S. Piskunov, University of Duisburg-Essen, Germany (2 weeks), Laboratori Nationali di Frascati, Italy (7 weeks); Institute of General and Inorganic Chemistry, Moscow (2 weeks)
11. Dr. hab. Yu. Shunin, Laboratori Nationali di Frascati, Italy (5 weeks)
12. Dr. Yu. Zhukovskii, St. Petersburg State University, Russia (1 month), Institute of Applied Materials, Karlsruhe, Germany (1 month), Institute of General and Inorganic Chemistry, Russian Academy of Science, Moscow (2 weeks).

International Cooperation

Belarus	1. Belarusian State University (Prof. S.A. Maksimenko)
Finland	2. Helsinki University of Technology (Dr. T. Kurki-Suonio)
France	3. Laue-Langevin Institute, Grenoble (Dr. G.J. McIntyre, Dr. H. Schober)
Germany	4. Max Planck Institut für Festkörperforschung, Stuttgart (Prof. Dr. J. Maier) 5. Deutsches Elektronen-Synchrotron DESY, Hamburg (Dr. A. Kotlov) 6. EC Institute of Transuranium Elements, Karlsruhe (Dr. P. Van Uffelen). 7. Max Planck Institut für Plasmaphysik, Garching (Dr. V. Igochine, Prof. Dr. K. Lackner, Dr. R. Mayer-Spasche, Prof. Dr. H. Zohm) 8. Institut für Hochleistungsimpuls & Mikrowellentechnik (KIT), Karlsruhe (Dr. S. Kern, Dr. B. Piosczyk) 13. Institut für Angewandte Materialien, Karlsruhe (Dr. A. Möslang) 14. Department of Theoretical Chemistry, University of Duisburg-Essen, (Prof. E. Spohr)
Greece	11. School of Electrical and Computer Engineering, National Technical University of Athens, Zographou (Dr. K. Avramides)
Israel	12. Ben Gurion University, Beer Sheeva (Prof. A. Aharony, Prof. D. Fuks)
Italy	13. Laboratori Nazionali di Frascati (Dr. S. Bellucci, Dr. M. Cestelli-Guidi)
Kazakhstan	14. Gumilyov National University, Astana (Prof. A. 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, Dept of Chemistry (Dr A. Huczko)
Romania	18. University of Craiova (Dr. D. Constantinescu)
Russia	19. St. Petersburg State University (Prof. R.A. Evarestov) 20. Institute of General and Inorganic Chemistry, Russian Academy of Sciences, Moscow (Prof. P.N. Dyachkov)
UK	21. University College London (Prof. A.L. Shluger)
Ukraine	22. National University of Lviv (Prof. A. Voloshinovskii) 23. Institute for Scintillator Materials, Kharkov (Prof. A. Gektin)
USA	24. Northwestern University, Evanston, Illinois (Prof. M.Olvera de la Cruz) *25. University of Maryland, College Park (Dr. G.S. Nusinovich, Dr. M.M. Kukla)*

Main Results

A. Electronic structure calculations for advanced materials

THE INTRINSIC DEFECTS, DISORDERING AND STRUCTURAL INSTABILITY OF $Ba_xSr_{1-x}Co_yFe_{1-y}O_{3-\delta}$ PEROVSKITE SOLID SOLUTIONS

E. A. Kotomin, Yu. A. Mastrikov,
M.M. Kuklja, B. Jansang (Materials Science Dept., University of Maryland, USA)
R. Merkle, J. Maier (Max-Planck-Institute for Solid State Research, Stuttgart, Germany)

Among many novel advanced materials for ecologically clean energy, ABO_3-type cubic perovskite solid solutions, e.g. $Ba_xSr_{1-x}Co_{1-y}Fe_yO_{3-\delta}$ (BSCF), are currently considered to be one of the most promising for applications as cathodes in solid oxide fuel cells (SOFC), oxygen permeation membranes, and oxygen evolution catalysis. These perovskites exhibit good oxygen exchange performance, the highest oxygen permeation rates known for a solid oxide, and mixed ionic and electronic conductivity. The low oxygen vacancy formation energy that is characteristic in these perovskites leads to the high oxygen vacancy concentration, and the relatively low activation barrier for the vacancy diffusion causes the high ionic mobility. These factors largely define the fast oxygen reduction chemistry of these materials which makes them such good candidates for energy conversion. However, a serious disadvantage of BSCF is its slow transformation at intermediate temperatures into a mixture of several phases, including a hexagonal phase with strongly reduced performance.

The basic properties of these perovskites and their stability with respect to decomposition into several phases are governed by structural defects and disordering. Detailed information regarding defect-induced effects, even in "simple" parent ABO_3 perovskites, with the sole exception of oxygen vacancies, is largely lacking thus far because these materials are extraordinarily complex and especially difficult to tackle experimentally. Hence, our understanding of the structure-property-function relationship in BSCF and similar materials is still far from comprehensive, which significantly hampers the progress in energy research and limits prospects to enhance existing materials or design new materials to improve efficiency of energy conversion devices.

In our research, a set of point defects: all types of single vacancies, Frenkel and Schottky disorder, and cation exchange, were explored in BSCF by means of first principles density functional theory (DFT) calculations. Configurations and energies of those defects were carefully characterized and discussed in the context of available

experimental data. We focused on the defect energetics. It is confirmed that an oxygen vacancy has the lowest formation energy among all single vacancies probed. It is also established that oxygen Frenkel defects, full Schottky disorder and partial Schottky disorder accompanied by the growth of a new phase (e.g. a binary oxide) all have relatively low formation energies and are favorable. The obtained cation exchange energies are very low on both the A- and B- sublattices of the perovskite structure, which carries implications as to the stability of the materials and ultimately to the efficiency of energy conversion

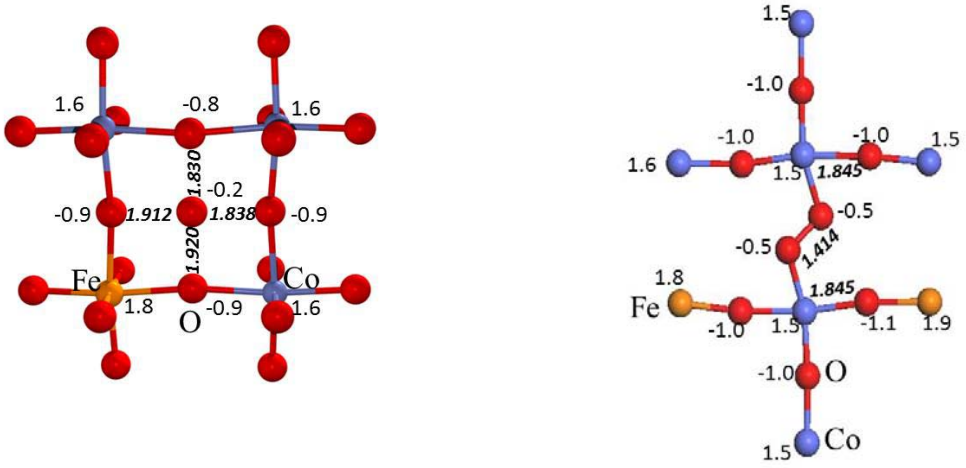

Fig. 1 Co-O-Co oxygen hollow (left) and split (right) interstitial configurations, their atomic charges, and inter-atomic distances.

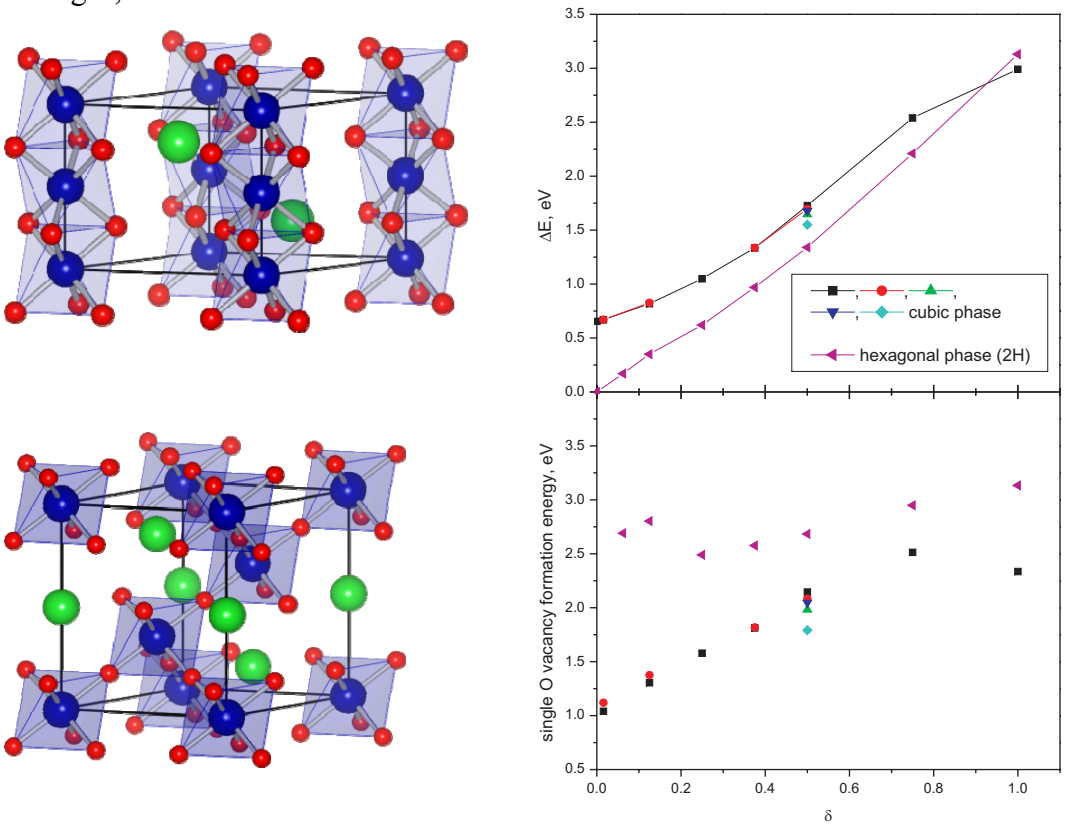

Fig.2 The cubic (left top) and the hexagonal (2H) (left bottom) BSCF structures are presented. Right- the total energy and the single vacancy formation energy of the cubic

and hexagonal phases of BSCF are shown as a function of oxygen non-stoichiometry parameter δ. The total energies are given with respect to the stoichiometric hexagonal phase BSCF unit cell, which is 0.66 eV lower than the cubic phase unit cell. Five points shown for δ=0.5 demonstrate the energy dispersion depending upon a distribution of vacancies in the crystal.

HYBRID DFT CALCULATIONS ON GRAIN BOUNDARIES IN $BaZrO_3$

D. Gryaznov,
A.L. Shluger (University College London, UK)

In cooperation with the University College London, we performed the density functional theory (DFT) calculations on the properties of grain boundaries in proton conducting $BaZrO_3$. A blocking character of grain boundaries here has been reported affecting its transport properties. Thus, the main objective of the present study was to compare the properties of grain boundaries (GB) and vacancies behaviour in cubic perovskite $BaZrO_3$ with two methods, namely standard PBE and hybrid PBE0 exchange-correlation functionals. The calculations were done on a supercomputer facility at Edinburgh University. A plane wave computer code VASP for the PBE functional and LCAO (linear combination of atomic orbitals) CRYSTAL09 code for the PBE0 functional were used. The former has been shown to be an effective tool whereas the latter code was used for the first within the present project for calculations of grain boundaries in oxides.

At the first stage, the bulk phase of $BaZrO_3$ was treated which included the calculation of density of states and oxygen vacancy formation energy using the two exchange-correlation functionals. As known for many oxides, the standard DFT (GGA/LDA) functionals underestimate their band gap. It then produces significant errors in the calculated properties. In order to solve this problem, one should go beyond the standard DFT functionals and use, for example, hybrid functionals. Also in the present study the band gap from the PBE0 functional was 4.9 eV (fig. 3) for bulk $BaZrO_3$, being well comparable to the experimental value of 5.0 eV. The band gap from the PBE functional was by 1.8 eV smaller than the experimental value.

The calculations of oxygen vacancy formation energy in the neutral supercell 2x2x2 (the concentration of oxygen vacancies 12.5%) gave 7.02 and 6.54 eV for the PBE0 and PBE functional, respectively. Note that the formation energies were calculated with respect to the energy of oxygen atom in the O_2 molecule (oxygen–rich conditions).

At the second stage, the same methods and functionals were used to calculate the properties of GBs in $BaZrO_3$ including the oxygen vacancy formation energy. In this case the calculations were at fixed (bulk) volume of the lattice but for the relaxed atomic coordinates. The GB was built in the supercell with the help of builder software on periodic models of CSL boundaries GBstudio. Supercells containing symmetric (310) [001] Σ5 tilt GBs (misorientation angle 36.86^0) were constructed and contained 120 and 360 atom. The lengths of the supercell vectors were 10, 16 (32) and 19 (28) Å for 120 (360) atoms supercells. We have observed the presence of additional electronic states (mainly due to O p-electrons) in the band gap for the GB without the translation of one grain with respect to the other one (GB1 in fig. 1) using both the functionals and independently of the supercell size. Such electronic states are at different positions in the band gap for the two functionals as they are much closer to the top of valence band for PBE in comparison with PBE0. However, we have observed that the GB1 is not most energetically favourable. Therefore, the GB with translation (0.5 Å in the direction parallel with the GB) suggested not only lower GB energy but also no additional electronic states in the band gap (GB2 in fig. 3). The analysis of the density states for the

GB1 with oxygen vacancy revealed the electronic states close to the bottom of conduction band. It was so far possible to calculate this GB for PBE only. We, thus, emphasize the importance of the choice of exchange-correlation functional and careful treatment of GB structure relaxation for the first-principle prediction of GB properties.

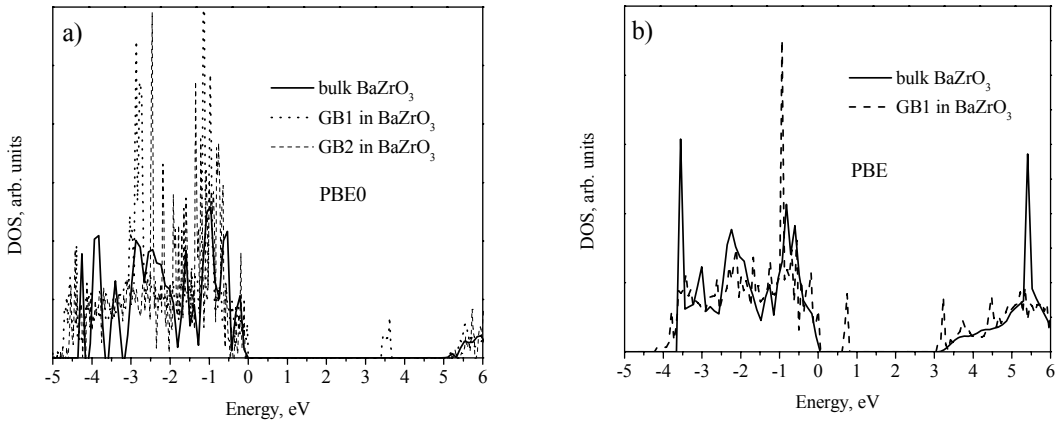

Fig. 3. The total density of states calculated for bulk and grain boundary of $BaZrO_3$ with PBE0 (CRYSTAL) and PBE (VASP) exchange-correlation functionals.

Ab initio CALCULATIONS OF DEFECTS ON MeF_2 AND $SrZrO_3$ SURFACES

R.I. Eglitis

The electronic *F*- and *R* centers in CaF_2 fluorite crystals have been studied using density functional theory (DFT) with a hybrid B3PW functional for of exchange and correlation effects. We estimated the *F*-center diffusion barrier as 1.7 eV. During the *F*-center jump, the trapped electron is more delocalized than that in the regular *F*-center case, and the gap between defect level and CB in the α-spin state decreases. The surface *F*-center investigation shows the energy preference for the *F* centers to locate near the surface. The association energy calculations of *R* centers indicate energy preference for aggregation of isolated *F* centers. During such the *F*-center aggregation, a considerable chemical bond covalency arises between two neighboring fluorine vacancies with trapped electrons. Three incompletely paired electrons trapped at the *R* center have an up-down-up spin arrangement and induce three defect levels in the gap between valence bands (VB) and conduction bands (CB) for both the α- and β-spin polarized band structures, respectively. More defect bands lead to more complex electron transitions, which were classified into two *F*- and four *M*-like transitions.

OH^- radicals in CaF_2 and BaF_2 bulk crystals and on the (111) surfaces have been studied as well. Three bulk and 20 surface OH^- configurations were investigated, and the energetically most favorable configurations detected. For the (111) CaF_2 surface atomic layers, the surface hydroxyls lead to a remarkable *XY*-translation and a dilating effect in the *Z*-direction, overcoming the surface shrinking effect in the perfect slab. The chemical bond population analysis shows a considerable covalency between the oxygen and hydrogen atoms, and the surface effect strengthens the covalency of surface OH^- impurities. There are two defect levels induced by OH^- impurities. The O 2p orbitals form two superposed occupied O bands, located above the valence bands (VBs), and the H s orbitals do the major contribution to an empty H band, located below the conduction

bands. Because of the surface effect, the O bands move downward, toward the VBs with respect to the relevant bands in the bulk case, and this leads to narrowing of the VB → O gap and widening of the O → H gap which corresponds to the first optical absorption.

We calculated also the surface relaxation and energetics for the polar (111) surface of $SrZrO_3$ with both Zr- and SrO_3-terminations. In both cases upper layer atoms are relaxed inwards. The second layer atoms, with the sole exception of Zr-terminated $SrZrO_3$ (111) surface Sr atom, relax outwards. The calculated surface relaxation energy for Zr-terminated $SrZrO_3$ (111) surface is almost 16x larger, than the surface relaxation energy for SrO_3-terminated $SrZrO_3$ (111) surface. The surface energy for Zr-terminated $SrZrO_3$ (111) surface is smaller, than that for for SrO_3-terminated one.

ELECTRONIC CHARGE REDISTRIBUTION IN $LaAlO_3$(001) THIN DEPOSITED AT $SrTiO_3$(001) SUBSTRATE: FIRST-PRINCIPLES ANALYSIS AND A ROLE OF STOICHIOMETRY

A. Sorokine, D. Bocharov, S. Piskunov, and V. Kashcheyevs

The discovery of conducting interface between two insulating materials: TiO_2-terminated (001) surface of $SrTiO_3$ (STO) substrate and $LaAlO_3$ (LAO) film deposited atop of it, has attracted colossal scientific interest during the last few years. Recently, high application potential of LAO/STO heterointerfaces has been proven *e.g.* by fabrication of highly voltage-tunable oxide diode that utilizes the advantage of the electric-field controlled interfacial metal-insulator transition of LAO/STO. Despite intense research efforts the origin of the charge carriers and the structure of the LAO/STO conducting layer are still controversially discussed. Currently, the whole picture responsible for adequate interpretation of experimental observations going in line with theoretical predictions is not yet clear. One of particular reasons for that is the fact that the major number of first principles studies carried out to describe structural and electronic properties of LAO/STO interfaces assume that the LAO films are perfectly stoichiometric. However, both pulsed laser deposition and molecular beam epitaxy vaporization processes used to facilitate transfer through the vapor LAO phase cannot preserve the target stoichiometry during LAO/STO synthesis. Taking into account that in fact La/Al ratio of nonstoichiometric LAO films may be controlled during its epitaxial growth, in our study we eliminate the above mentioned drawback by considering from first principles both n-LAO/STO and p-LAO/STO heterointerfaces having La or Al nonstoihiometry.

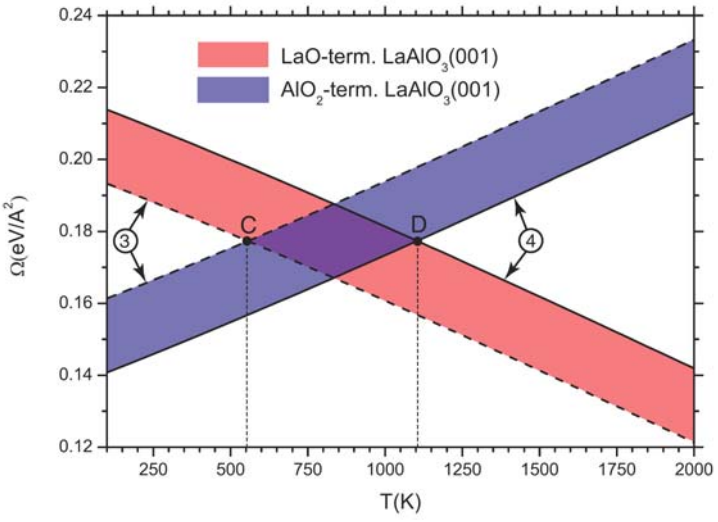

Fig. 4. The thermodynamic stability diagram calculated along the La_2O_3 and Al_2O_3 precipitation lines (numbers 3 and 4 in the circles, respectively. The dependence on the oxygen chemical potential is converted to the appropriate temperature scale at an oxygen pressure typical during LAO/STO(001) synthesis ($P = 10^{-6}$ mbar). The interval between points C and D correspond to temperature range where both LaO- and AlO_2-terminated LAO(001) surfaces are stable and may coexist.

In general, in collaboration with *Faculty of Computing, University of Latvia*, we have performed large-scale first-principles calculations on a number of both stoichiometric and nonstoichiometric LAO/STO(001) heterostructures. We predict that there exists a distortion in energies of band edges for stoichiometric structures which eventually leads to the appearance of the conductivity at a critical thickness in *n*-type interfaces or to the reduction of the band gap for *p*-type interfaces. Nonstoichiometric interfaces were found to be conducting independently of the LAO film thickness and possessing little or no distortion of band edges. The conductivity appears due to the nonstoichiometry of the thin film which is a conductor on its own. The degree of distortion of the band edges agree well with the estimates of the internal electric field generated by changes in the atomic charges and the geometric relaxation of the atomic structure. We confirm these factors as the ones responsible for the rise of conductivity in stoichiometric *n*-type heterostructures.
Thermodynamic analysis that we have performed for the pristine LAO(001) surface reveals that both its LaO and AlO_2 terminations may coexist at temperatures above 550 K (Fig. 4). If the LAO/STO(001) heterointerface is covered by a LaO monolayer, charge compensation mechanism of deposited polar nonstoichiometric LAO film leads to the tendency of Ti^{3+} formation at the interface. In general, we conclude that one should not disregard the stoichiometry aspect when considering ways to make the LAO/STO interfaces conducting as nonstoichiometric interfaces possess unique quasi-2D electron gas structure that gives an overall 2 times greater free charge carrier density in comparison with stoichiometric interfaces. For stoichiometric *n*-type structures, the interplay of covalent and electrostatic forces leads to a metal-insulator transition at critical film thickness but, for nonstoichiometric structures, it leads to the formation of a bilayered or monolayered quasi-2D electron gas.

Ab initio CALCULATIONS OF S-doped TiO_2-NANOTUBE FOR PHOTOCATALYTICAL WATER SPLITTING APPLICATION

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

Solar energy has the capacity to fulfill global human energy demands in an environmentally and socially responsible manner provided efficient, low-cost systems which can be developed for its capture, conversion, and storage. Toward these ends, hydrogen fuel production from sunlight using semiconductor photocatalysts is a promising route for harvesting solar energy. Conventional photocatalytic electrodes such as titanium dioxide that use sunlight to split water and produce hydrogen can operate with high efficiency under ultraviolet irradiation, but it remains a challenge of primary importance, to drive them with visible light. Engineering the electronic energy band structure of nanostructured semiconductor photoelectrodes through judicious control of their atomic composition is a promising route to increase photoresponse of visible light. A general route to obtain a visible-light-driven photocatalyst is to dope a lattice of semiconductor with a wide band gap by extraneous elements, thus creating a new optical absorption edge. In this respect, hollow nanotubes produced from semiconducting materials have some peculiar advantages, such as larger specific surface area, higher mechanical stability, integrity and unique shape with few interfacial grain boundaries,

which promote charge transport and electron-hole pair separation. Using hybrid exchange-correlation functionals within the density functional theory we have simulated in this study defective structure of TiO_2 nanotubes (fig.5).
On the basis of the performed first principles calculations, we conclude that the presence of substitutional impurities significantly affects the band structure of TiO_2 nanotubes, which must be taken into account when constructing nanoelectronic devices based on these nanotubes. Changes in nanotube's electronic structure can be observed by optical and photoelectron spectroscopy methods, as well as by measuring electrical properties of the nanotubes. According to obtained results S dopant in TiO_2 nanotube create the mid-gap states making this nanotube to be good candidate for efficient photocatalysts working under daylight irradiation.

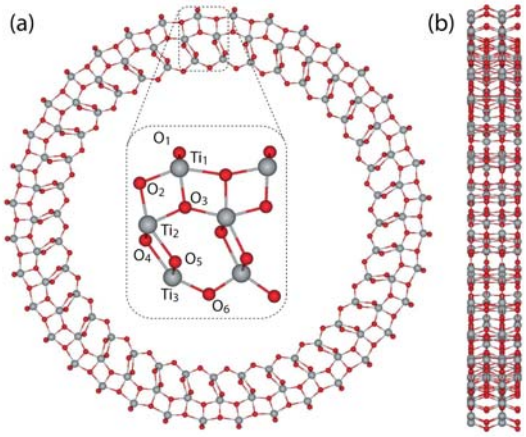

Fig. 5. Schematic representation of monoperiodically repeated unit cell of the substitutional defect containing (0,36) TiO_2 nanotube with external diameter of 4.81 nm: (a) across section view, (b) side view. Ti are shown as gray balls, while oxygen as red (light gray) ones. Inset shows the 2×2 increased "basic" unit cell of (0,36) TiO_2 nanotube repeated by 18 rototranslational symmetry operators (rotation axis of 18-th order). Numbered atoms of titans and oxygens are substituted for impurity defect atoms (A_h, where h stands for "host").

FIRST PRINCIPLES SIMULATIONS OF ELECTRONIC AND THERMODYNAMIC PROPERTIES OF DEFECTIVE ZnO

A.V. Sorokine, D. Gryaznov, Yu.F. Zhukovskii, J. Purans and E.A. Kotomin

We have performed large-scale calculations on electronic and thermodynamic properties of defective zinc oxide in its most stable phase at room temperature. Firstly, geometric and electronic bulk properties of ZnO single crystals have been considered and compared to experimental data. To improve the quality of obtained results, we have constructed new basis sets both for Zn and O. After consideration of various hybrid functionals we chose non-parametric PBE0 correlation-exchange functional for all the calculations, as it gave results both close to experimental data and stable with respect to change of computational parameters. Next, we considered intrinsic ZnO defects that are most likely to form in manufacturing processes: zinc and oxygen vacancies. Here we showed how electronic and geometric properties of defective structures change with the concentration of vacancies. For these calculations

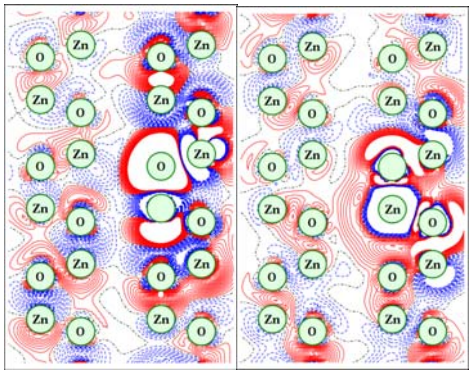

Fig. 6: Differential electronic charge density for ZnO with 6 % of vacancies of Zn (left) and O (right).

a supercell model was used, and the molar concentrations of defects were from 6 to 1.9 %, where the latter is an adequate result that can occur in experimental works. Electronic properties comprised atomic charges and differential electronic density. The latter is shown in Fig. 6.

We have also calculated defect formation Gibbs energy and its dependency on temperature and concentration of vacancies, as well as ZnO lattice vibrational phonon frequencies. Our results demonstrate how the V_O formation energy converges with the supercell size and the number of *k*-points for phonon calculations. The chemical potential of oxygen having the strongest effect for the formation energy changes its value from 4.1 eV down to 3.1 eV within a broad temperature range. Further the phonons in the solid phase produce additional effect of the order of 0.01 eV at $T = 0$ K and 0.03 eV at $T = 1000$ K. These estimations suggest that the temperature contribution to the V_O formation energy in ZnO comes from the chemical potential of oxygen.

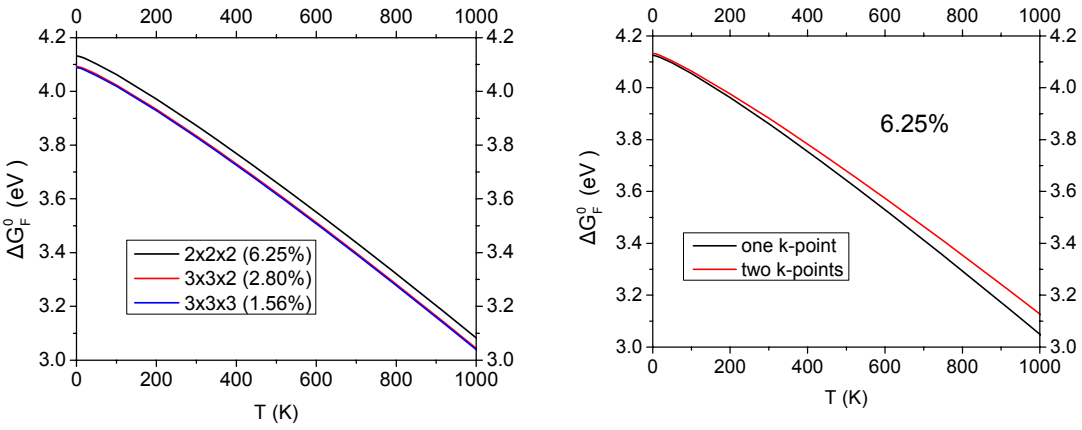

Fig. 7: Temperature effects through the chemical potential of oxygen only (left) and through the phonon contribution in solid and the chemical potential of oxygen (right).

FIRST-PRINCIPLES SIMULATIONS ON VARIOUS TYPES OF RUTILE-BASED TITANIA NANOWIRES AND THEIR STRUCTURAL ANALYSIS

Yu.F. Zhukovskii,
R.A. Evarestov (*Department of Quantum Chemistry, St. Petersburg University, Russia*),
D.B. Migas (*Belarusian University of Informatics and Radioelectronics, Minsk, Belarus)*

Within the rod group irreducible representations developed *in collaboration with Prof. R.A. Evarestov (St. Petersburg University, Russia) and Dr. D.B. Migas (Belarusian University of Informatics and Radioelectronics)* the one-periodic (1D) nanostructures have been considered for symmetry analysis of [001]- and [110]-oriented rutile-based titania nanowires of diameters terminated by either four types of related {110} facets (Fig. 8) or alternating $\{1\bar{1}0\}$ and {001} facets (Fig. 9), respectively. Symmetry of nanowires has been described using both the Ti atom-centered rotation axes as well as the hollow site-centered axes passing through the interstitial sites between the Ti and O atoms closest to the axes. For simulations on TiO_2 NWs, we have performed large-scale *ab initio* Density Functional Theory (DFT) and hybrid DFT-Hartree Fock (DFT-HF) calculations with the total geometry optimization within the Generalized Gradient Approximation (GGA) in the form of the Perdew-Becke-Ernzenhof exchange-

correlation functionals (PBE and PBE0, respectively), using the formalism of linear combination of localized atomic functions (LCAO) implemented in *CRYSTAL09* code. Both structural and electronic properties of enumerated rutile-based titania slabs and nanowires have been calculated.

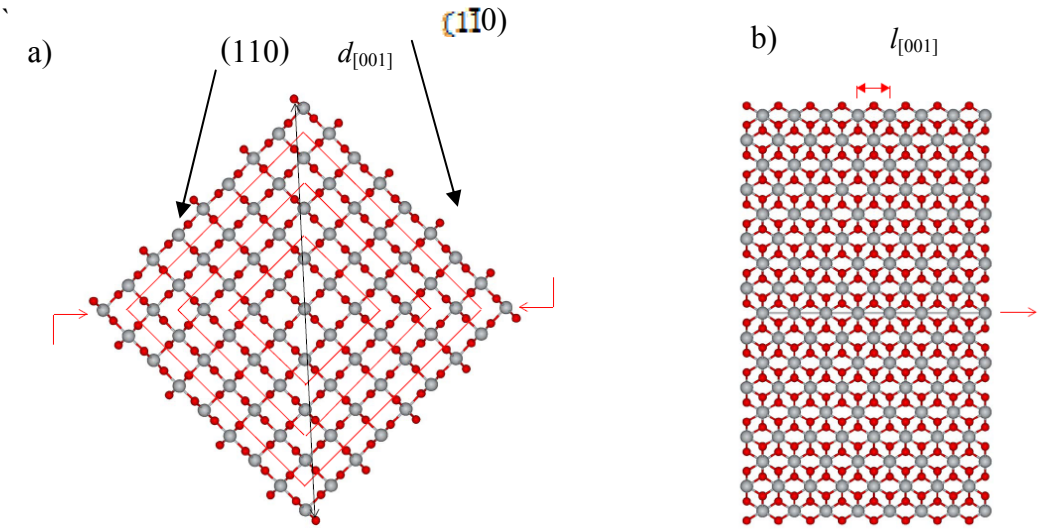

Fig. 8. Cross sectional (a) and lateral (b) images of non-optimized large rutile-based [001]-oriented Ti atom-centered nanowire possessing the D_{2h} symmetry and containing 81 formula units *per* NW unit cell with aside (110) and $(1\bar{1}0)$ facets shown in Fig. 8b. Red rhombs in Fig. 8a show borders for prism models of middle, small and smallest TiO_2 NWs (49, 25 and 9 formula units per UC, respectively). Diameter of a nanowire is shown by the twice-terminated arrow ($d_{[001]}$) while its period (length of UC) is shown in Fig. 8.b as $l_{[001]}$.

Nanowires are constructed as 1D systems cut from the 3D crystal along the direction of one of the bulk crystal symmetry axes. The translational periodicity is maintained along this direction. In the case of a rutile-based [001] TiO_2 nanowire (Fig. 8) a direction of the translation axis is orthogonal to a pair of [110] and $[1\bar{1}0]$ vectors while both titania formula units of primitive cell lie in the two cross-sectional planes. If the translational two-fold rotation axis goes through a Ti atom (Fig. 8), one can see that the reflection in the horizontal (h) plane and rotations around the two second order axes in this plane are the symmetry operations for [001]-oriented nanowires. The rod symmetry group of this system is *Pmmm* while its point symmetry group is D_{2h}.

For a rutile-based [110] nanowire (Fig. 9), the translation axis is orthogonal to [001] and $[1\bar{1}0]$ vectors while four formula units of primitive cell lie in the six cross-sectional planes. The symmetry of a rutile-based [110] nanowire coincides with the symmetry of analogous type of [001] NW if the translation axis with rotation by π goes through Ti atoms. Indeed, Fig. 9, shows that the symmetry operations for [110] NWs are reflection in the vertical (v) plane (containing the translation axis) and rotation around the 2-fold translation axis in this plane. The symmetry operations include also rotations around the 2-fold axis in the horizontal (h) plane (orthogonal to the translation axis). Thus, the rod symmetry group of the system is again *Pmmm* (the point symmetry group is D_{2h}).

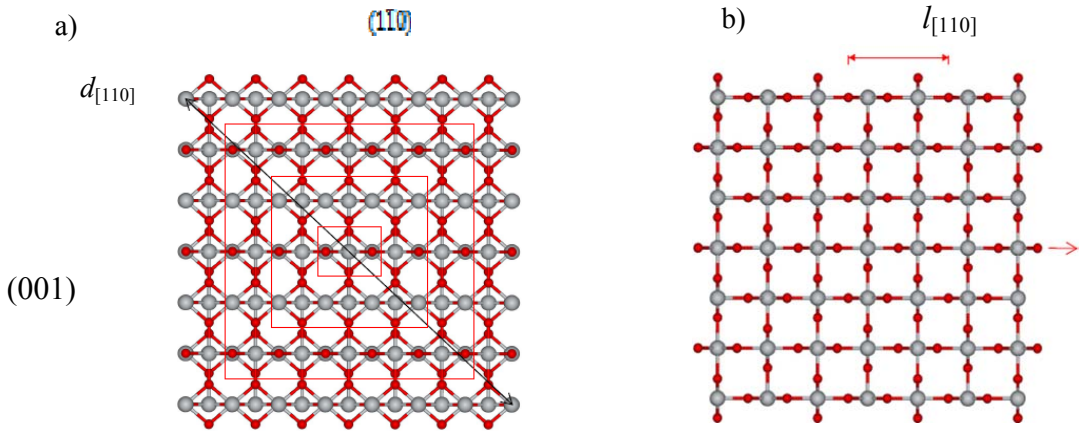

Fig. 9. Cross sectional (a) and lateral (b) images of the non-optimized large rutile-based [110]-oriented Ti atom-centered NW possessing the D_{2h} symmetry and containing 105 formula units per NW UC, with aside (001) and (1$\bar{1}$0) facets (the former is shown in Fig. 9.b). Rectangles in Fig. 9.a show borders for prism models of middle, small and smallest TiO_2 NWs (55, 21 and 3 formula units per UC, respectively). NW diameter is shown by the twice-terminated arrow ($d_{[110]}$) while its period (length of UC) is shown in Fig. 9.b as $l_{[110]}$.

The properties of titania nanowires are both the size and shape dependent. For direct comparison of relative stability of various 1D nanowires, we have performed large-scale calculations on their surface energy *per* formula unit. Values of d_{NW} slightly increase whereas l_{NW} are found to be reduced after NW geometry optimization. The larger is d_{NW}, the closer its geometry parameters as well as the band gap to those of rutile-based TiO_2 bulk and non-optimized (001) and (110) slabs whereas NW surface energy approaches to that of facets terminating the nanowire. In the case of Ti atom-centered NWs, values of $\Delta\varepsilon_g$ grow with increasing d_{NW} while in hollow site-centered NWs, these values decrease in analogous conditions, analogously to band gaps of slabs with increasing thickness.

THEORETICAL SIMULATIONS OF ELECTROMAGNTIC PROPERTIES IN CARBON NNTUBES AND GRAPHENE BASED NANOSTRUCTURES

Yu.N. Shunin, Yu.F. Zhukovskii,
S. Bellucci (*Laboratori Nazionali di Frascati, Italy*)

In collaboration with Dr. S. Bellucci (Laboratori Nazionali di Frascati, Italy), we have developed the model of *'effective bonds'* in the framework of both cluster approach based on the multiple scattering theory formalism and Landauer theory, which can allow us to predict the resistivity properties for C-Me junctions taking into account chirality effects in the interconnects of single-wall (SW) and multi-wall (MW) CNTs (Fig. 10) as well as monolayer (ML) and polylayer (PL) GNRs (Fig. 11) with the fitting metals (Me= Ni, Cu, Ag, Pd, Pt, Au) on predefined geometry of carbon nanostructure.

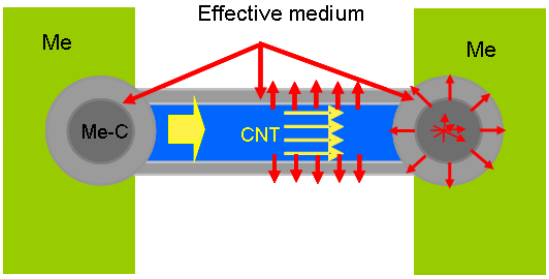

Fig. 10. Model of CNT - Me interconnect.

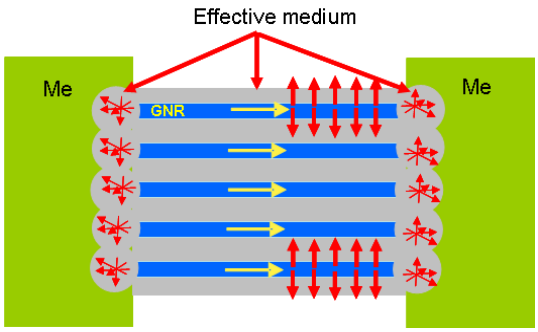

Fig. 11. GNR (polylayered) - Me interconnect.

We have also developed the concept of simulation of carbon based nanosensor devices. Interconnect capacitances and impedances have been evaluated in the GHz and THz regimes. Parametrical numerical simulations of conductivity have been carried out for zig-zag (*m*,0), arm-chair (*m*,*m*) and chiral (*m*,*n*) CNTs while the sensitivity of conductivity to the local electronic density of states in CNTs with local impurities (N and B atoms) has checked. CNTs, CNT-Me and GNR-Me based nanostructures are prospective nanosensor structures. Conductance and other current-voltaic parameters depend on the morphology of the nearest shells in MW CNTs and PL GNRs, which results in complications for technological synthesis. Nevertheless, the corresponding nanodevices possess the stable electrical characteristics.We have made a further step in simulations directed to nanosensor systems. In this respect, due to the sensitivity of the local electronic density of states to external influences (mechanical, chemical, electrical, magnetic, *etc*), the fundamental electromagnetic properties of CNTs, GNRs and their metal interconnects have been analyzed from the point of view of prospective nanosensor applications. We have created the database of CNT-metal and GNR-metal junction combinations taking into account a set of parameters, and namely, the angle of chirality, the CNT diameter, the number of walls or layers, the type of a metal substrate (Me), and the orientation of a metal substrate, *e.g.*, the densely-packed (100), (111) and (110) surfaces. Thus, we are able to forecast interconnect properties for various SW and MW CNT, ML and PL GNR configurations.

There are some important applications of CNT- and GNR-based interfaces with other materials for creation of novel nanosensor devices, *e.g.*, for design of prospective electron devices like FET-transistors (Fig. 12) which are very sensitive to various external influences of different nature as mentioned above.

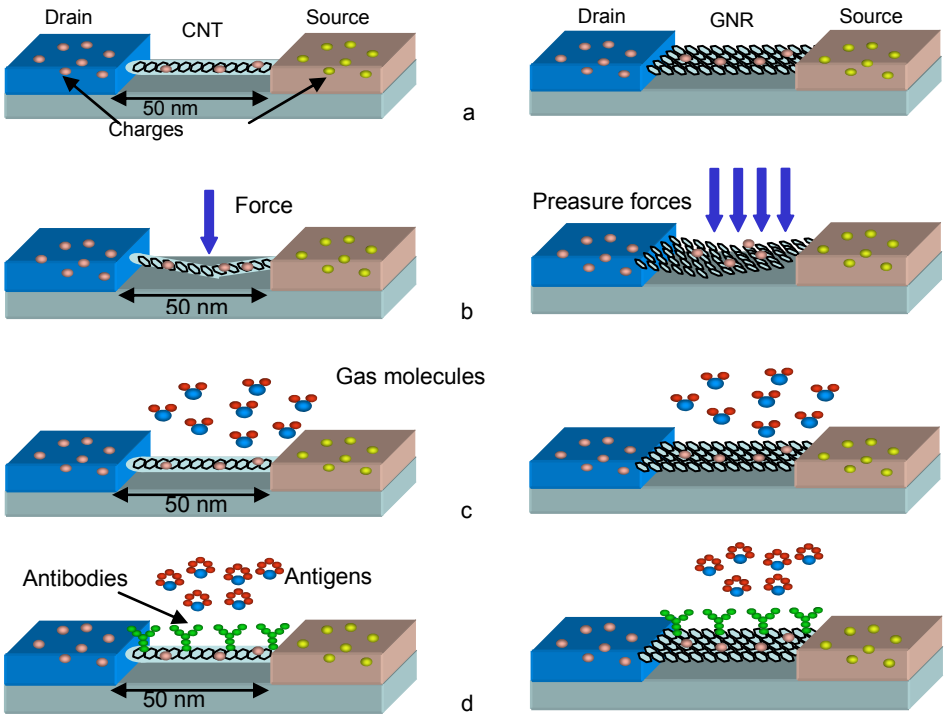

Fig.12. FET-type nanodevices as prospective nanosensor systems: a) the unperturbed field-effect transistors based on CNT and GNR are presented (CNT- or GNR- based FETs are mainly composed of the corresponding semiconducting carbon materials suspended over the two electrodes); b) physical nanosensors: a conducting threshold can be altered when the nanotube or graphene ribbon is bent; c) chemical nanosensors: this threshold can be altered when the amount of free charges on the nanotube of graphene ribbon surface is increased or decreased depending on the presence of donor or acceptor molecules of specific gases or composites; d) biological nanosensors: monitoring of biomolecular processes such as antibody/antigen interactions, DNA interactions, enzymatic interactions or cellular communication processes, *etc*.

Potential nanosensor devices based on CNTs and GNRs as well as their interconnects with various metallic electrodes are possible to design and to use for effective detection of external influences of different nature. They can change the electron transport regime and promote the current losses. At the same time, the interconnect interfaces can also be sensitive to chemical adsorbents, electrical and magnetic fields, changing the properties of interconnect potential barrier and the efficiency of conducting channels. Both these nanosensoring mechanisms can be simulated in the framework of the proposed models.

AB INITIO MODELLING OF OXYGEN INTERACTION WITH SURFACES AND INTERFACES OF URANIUM MONONITRIDE

D. Bocharov, D. Gryaznov, Yu.F Zhukovskii, E.A. Kotomin

In collaboration with *Institute for Transuranium Elements, Karlsruhe, Germany and Faculty of Computing, University of Latvia*, oxygen adsorption, migration, incorporation into the surface N vacancies on (001) and (110) surfaces as well as oxygen behaviour between UN grain boundaries have been modeled (Figs. 13 and 14) using 2D slabs of different thicknesses and supercell sizes and the GGA exchange-correlation functional PW91 as implemented in *VASP* code. The Gibbs free energies of N vacancy formation

and O atom incorporation therein at the two densely-packed surfaces and tilt grain boundaries are compared.

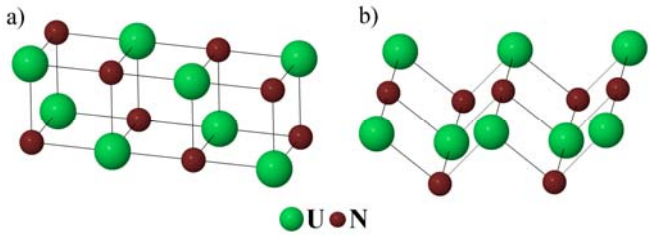

Fig. 13. The slab models for the UN (001) (a) and (110) (b) surfaces (only the two outermost layers are shown).

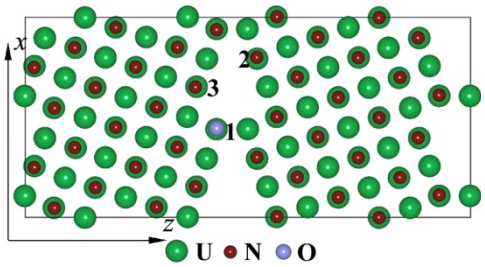

Fig. 14. The cross-section of the (310)[001](36.8°) tilt GB supercell [29] (15.40 Å × 4.87 Å × 34.13 Å with the oxygen atom incorporated into one of three possible positions.

The formation energies $E_{form}^{N\_vac}$ of N vacancy at 0 K inside the GB are equal with 3.3-3.5 eV. These values are comparable with analogous values for $E_{form}^{N\_vac}$ on UN (001) (3.6-3.7 eV) and (110) (2.9-3.1 eV) surface and are smaller than those in the bulk material (~4.4 eV) or in (001) or (110) slabs central layer (4.3-4.6 eV). It indicates a clear trend for segregation of vacancies towards the grain boundaries.

The standard *Gibbs free formation energy* as a function of temperature is plotted in fig. 15 for the two UN surfaces and grain boundary. The difference in the standard Gibbs free formation energy ΔG_F^N between the (001) and (110) surfaces is considerable, 0.7 eV (fig. 15) and, most importantly, ΔG_F^N decreases by 0.4 eV as the temperature increases from 400 to 700 K. The formation energy at the GB lies in-between that for the two surfaces. *Incorporation energy* ΔG_I^O negative values means that the reaction is exothermic and thermodynamically favorable. It *increases* with temperature by ~0.4 eV in the temperature range from 400 to 700 K but remains still negative (process energetically favorable).

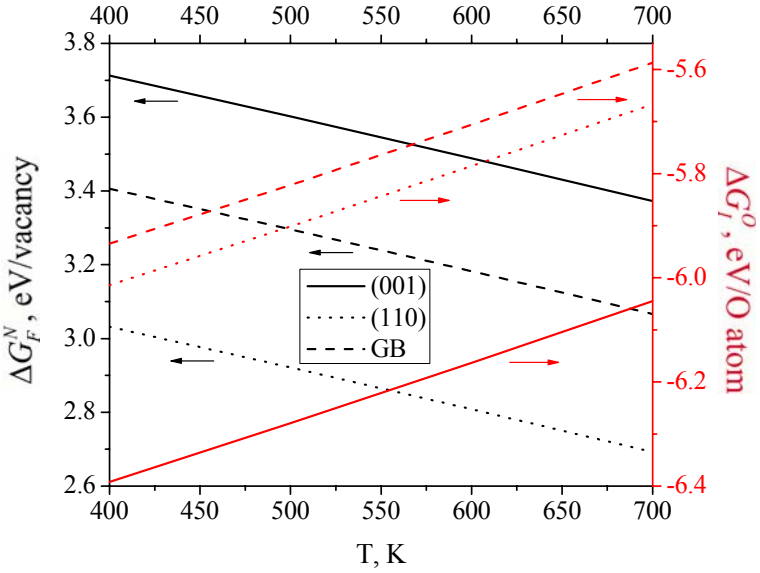

Fig. 15. *The standard Gibbs free formation energy of N vacancy (black curves) and the incorporation energy of O atom into the surface N vacancy (red curves) as a function of temperature for the (001), (110) surfaces and GB (position 2 in Fig. 14). The supercell size and slab thickness are 3×3 and 7 planes, respectively.*

The oxygen incorporation energy for the GB is smaller than for both surfaces, but remains still negative, even at 700 K. Lastly, the O solution energies (incorporating also N vacancy formation cost) in all three cases are predicted to be very close and negative (-2.5 eV), thus the oxidation process is energetically favorable at all studied temperatures that explains fast oxidation of UN on air.

FIRST PRINCPLES SIMULATIONS OF Y_2O_3 CLUSTER GROWTH IN ODS STEELS

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P.V. Vladimirov, A. Möslang (*Institut für Angewandte Chemie, KIT, Karlsruhe, Germany*)
V.A. Borodin (*Research Center Kurchatov Institute, Moscow, Russia*)

Reduced activation ferritic-martensitic steels (RAFM) strengthened by yttria precipitates are promising structure materials for future fusion and advanced fission reactors. Oxide dispersion strengthened (ODS) particles hinder dislocation motion effectively resulting in higher strength and better high-temperature creep resistance of ODS steels in comparison to basic materials. Implementation of ODS materials widen the operating temperature as compared to conventional RAFM steels as well as they are more radiation resistant. The size and spatial distribution of ODS nanoparticles significantly affect both mechanical properties and radiation resistance. Unfortunately the mechanism of the ODS particle formation is not completely understood.

In close collaboration with partners from *the Karsruhe Institute of Technology (Germany)* and from the *Kurchatov Institute, Moscow (Russia)*, we performed a computer modelling of the ODS particle formation process. Experimental studies, performed at the KIT, show that a significant part of Y and O atoms is found in the steel matrix in the concentrations exceed their equilibrium solubility after milling. Depending on Cr concentration, during the cooling process steel may or may not go through the phase transformation. Therefore, we consider the ODS particle formation process in both- *fcc* and *bcc*- phases. There is a significant lattice mismatch between the *fcc*/*bcc*-Fe and the bixbite-type Y_2O_3. At the very initial steps of the ODS particle formation process, space, necessary for creation the bixbite-type bonds within the iron matrix, could be provided by vacancies.

For the *fcc* phase, we found the most stable configuration of three vacancies and single Y atom. The lowest energy was obtained for the systems with the solute atom, located at the centre of the cluster. For the *bcc* phase we investigated the growth of vacancy cluster. The largest modelled cluster contained nine vacancies. The same process was repeated with a single Y atom. For all systems the binding energy increases with the number of vacancies, except adding the seventh vacancy. The interaction between Y atom, stabilized by divacancy with solute Y_{Fe} atom, at close distances is attractive. The largest attraction energies (1-1.1eV) are obtained for the systems with obtuse V_{Fe}-Y_i-V_{Fe}-Y_i-V_{Fe} angles. Two Y atoms, each stabilized by divacancy, attract to one another. For the first three NN spheres vacancies overlap. Without overlapping, for the nearest coordination spheres binding energy is about 1.3 eV.

The results of the calculations on both phases clearly show that Fe-vacancies play a major role in binding between defects. It was found for the *fcc* phase, that binding energy between Fe-vacancies significantly increases in the case of four vacancies in comparison to the configurations with two or three Fe vacancies. The largest binding energies were found for the configurations with a single Y atom and several vacancies. The binding energies for the configuration between two Y atoms and vacancy increase

with the increase of the distance between two Y atoms, and in the case of the 4-NN attraction was observed between two Y atoms inside the lattice. In *bcc*-Fe, vacancies segregate, creating stable clusters. The growth of the Y_i ; $6V_{Fe}$ cluster is restricted by a barrier of, at least, 1.8 eV. Y_{Fe}, surrounded by $8V_{Fe}$ may slightly oscillate along the [111] and equivalent directions. The attraction between Y_{Fe} and Y_i; $2V_{Fe}$ cluster is about 1 eV. Two Y_i; $2V_{Fe}$ complexes binding energy is 1.2-1.4 eV. Stabilization of solute Y atoms by vacancies increases the binding energy between them.

QUANTUM-CHEMICAL STUDY OF ELECTRON-PHONON INTERACTIONS IN CRYSTALS

E. Klotins and G. Zvejnieks

A fundamental problem in solid state physics is to understand what happens when electrons couples to an atomic environment of and, in particular, what is the nature of electron – phonon interaction, and what is the mathematical framework decoupling this interaction. The associated theory is still incomplete and lacks two important components: a physical picture that clarifies how electrons emerge above their ground state under electromagnetic radiation and the interaction with phonons, and a regular mathematical framework for studying these phenomena.

We investigate a minimal yet detailed model system that describes interacting electron gas moving in a charge compensating background of positive ions and interacting with external electromagnetic field.

The performed analysis suggests that for dielectrics and semiconductors modeled by effective Hamiltonians, the interaction with electromagnetic field comprises potentional energy terms additional to the conventional impact in the kinetic energy of electrons. Nevertheless, the Hamiltonian retains its second quantized form with additional terms compatible to the annihilation and creation operators, as advancement.

The electron-phonon interaction is more complex and is accounted for by a mixture of electronic and phonon birth/annihilation operators incompatible with the second quantization approach. This undesirable property is eliminated by Baker – Hausdorf transformation applicable to arbitrary electron – phonon interaction Hamiltonian and resulting in relations for the generator of this transformation and for the transformed electron-phonon interaction. This mathematical framework determines a starting point for an arbitrary effective Hamiltonian to decouple the electron-phonon interaction by transformation of a particular lattice Hamiltonian to the expected purely electronic secondary quantized two – particle interaction Hamiltonian compatible with the standard wave function and atomic orbital approaches.

VIBRATIONAL PROPERTIES OF $LaPO_4$ NANOPARTICLES IN MID- AND FAR-INFRARED DOMAIN

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P. Savchyn, V. Vistovskyy, A. Voloshinovskii, I. Karbovnyk (*I. Franko National University of Lviv, Ukraine)*
M. Cestelli, Guidi, C. Mirri (*INFN-Laboratori Nazionali di Frascati, Italy)*
O. Myahkota, A. Riabtseva, N. Mitina, A. Zaichenko *(Lviv Polytechnic National University, Ukraine)*

Lanthanum orthophosphate ($LaPO_4$), also known as monazite, has been widely used as a green phosphor, when doped with Ce and Tb in high-quality tricolour luminescent lamps. It has been used as a proton conductor, as well as in lasers, sensors, ceramic materials, catalysts, and heat resistant materials. This is due to its interesting properties,

such as high thermal stability, very low solubility in water, high index of refraction, and so on. Nanopowders of $LaPO_4$ have been grown by sedimentation-micellar method. As-prepared $LaPO_4$ nanoparticles with the average grain size of about 8 nm have a single-phase hydrated hexagonal structure. After thermal annealing at 600 and 800 C, the average size of nanoparticles increases up to 35 and 50 nm, respectively, and the structure transforms into single-phase monoclinic. IR spectra of $LaPO_4$ nanoparticles of different size were investigated in the wide range of wavenumbers from 130 to 5000 cm^{-1} in the 20–300 K temperature region. Differences between IR spectra of the bulk material and nanoparticles as well as the temperature behavior of the vibrational properties are discussed.

SYNHROTRON RADIATION STUDIES ON LUMINESCENCE OF Eu^{2+}-DOPED $LaCl_3$ MICROCRYSTALS EMBEDDED INTO NaCl MATRIX

V. Pankratov, A.I. Popov
P.V. Savchyn, V.V. Vistovskyy, A.S. Voloshinovskii (I. Franko National University of Lviv, Ukraine)
A.S. Pushak (Ukrainian Academy of Printing, Lviv, Ukraine)
A.V. Gektin (Institute for Scintillation Materials NAS of Ukraine, Kharkov, Ukraine)

The divalent europium ions Eu^{2+} are widespread activators for inorganic luminescent materials. In recent years, Eu^{2+} was considered as a promising dopant for scintillator applications due to a high light yield of doped single crystals. In this paper, we studied the luminescent properties of Eu^{2+} doped $LaCl_3$ microcrystals embedded in the NaCl matrix $LaCl_3$:Eu^{2+} microcrystals dispersed in the NaCl matrix have been obtained in the NaCl–$LaCl_3$(1 mol.%)– $EuCl_3$(0.1 mol.%) crystalline system. The low-temperature luminescent properties of these microcrystals have been studied upon the VUV and UV excitation by the synchrotron radiation. The spectroscopic parameters as well as decay time constants of Eu^{2+} doped $LaCl_3$ host have been established. The excitation mechanism of divalent europium centers through energy transfer and reabsorption is discussed.

B. Kinetics of processes with self-organization

DYNAMIC SELF-ASSEMBLY OF PHOTO-SWITCHABLE NANOPARTICLES

V.N. Kuzovkov,
Prateek K. Jha, B. Grzybowski and M. Olvera de la Cruz (*Northwestern University, Evanston, USA*)

Nanoparticles functionalized with photo-switchable ligands can be assembled into a broad range of structures by controlled light exposure. In particular, alternating light exposures provide the means to control formation of assemblies of various sizes and symmetries. Here, *in collaboration with Northwestern University, Evanston, USA,* we use scaling arguments and Kinetic Monte Carlo simulations to study the evolution of reversible aggregates in a solution of periodically irradiated photo-switchable nanoparticles. Scaling estimates of the characteristic size and the mean separation of aggregates agree with the simulations. The transition probabilities in the Kinetic Monte Carlo scheme are derived from a renormalized master equation of the diffusion process. Simulations on a system of nanoparticles, interacting through Lennard-Jones pair potentials that change their character from repulsive to attractive depending on the light

exposure, show that the slow diffusion of particles at low effective temperatures (where the attractions are much higher than the thermal energy) results in the formation of small, ‘‘kinetically frozen’’ aggregates. On the other hand, aggregation does not occur at high effective temperatures, where the attractions are comparable to the thermal energy. In the intermediate range of effective temperatures, ‘‘fluctuating’’ aggregates form that can be stabilized by applying light pulses of specific lengths and frequencies. The aggregate sizes increase by increasing the packing fraction and the aggregates undergo transition to a percolated ‘‘network’’ at high packing fractions. Light-control of inter-particle interactions can either inhibit or promote nucleation and growth, and can reduce gel and glass formation.

THE KINETIC MONTE CARLO SIMULATIONS OF FLOW-ASSISTED POLYMERIZATION

V.N. Kuzovkov,
Prateek K. Jha and M. Olvera de la Cruz (*Northwestern University, Evanston, USA*)

In collaboration with Northwestern University, Evanston, USA, we performed kinetic Monte Carlo simulations on a model of a polymerization process in the presence of a periodic oscillatory flow to explore the role of mixing in polymerization reactors. Application of an oscillatory flow field helps overcome the diffusive limitations that develop during a polymerization process due to an increase in the molecular weights of polymer chains, thereby giving rise to high rates of polymerization. A systematic increase in the flow strength results in a “dynamic” coil−stretch transition, leading to an elongation of polymer chains. Reactive ends of stretched (polymer) chains react more frequently than the reactive ends of coiled chains, which are screened by other monomers of the same chain. There exists a critical flow strength for the efficiency of polymerization processes. The kinetic Monte Carlo simulation scheme developed here exhibit great promise for the study of dynamic properties of polymer systems.

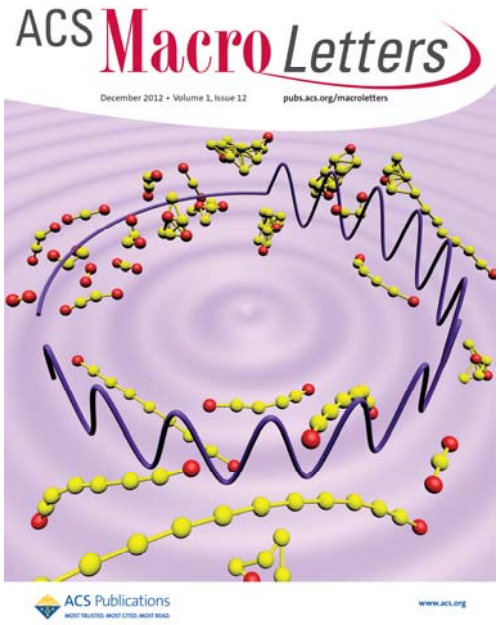

Fig.16. Cover page of the ACS Macro Letters with the presentation of this paper.

STATISTICAL ANALYSIS AND CELLULAR AUTOMATA MODELING OF VOID LATTICE FORMATION IN ELECTRON IRRADIATED CaF_2

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

Calcium fluoride (CaF_2) is widely used in both microlithography and as a deep UV window material. It is also known that electron beam irradiation creates a *superlattice* consisting of periodically distributed fluorine vacancy clusters (called a *void lattice*).

To perform a quantitative analysis of experimental TEM image data demonstrating void lattice formation under electron irradiation of CaF_2, we developed two distinct image filters. As a result, we can easily calculate vacancy concentration, cluster distribution function as well as average distance between clusters. In particular, an analysis of the consecutive experimental snapshots obtained by increasing irradiation dose, allows us to restore the void lattice formation process. The results for two suggested filters are similar and demonstrate that void cluster growth is accompanied with a slight increase of the superlattice parameter.

Despite numerous experiments, the void superlatticelattice formation in CaF_2 under electron irradiation still possesses open questions regarding the microscopic processes that govern the self-organization phenomenon. We propose a microscopic model that allows us to reproduce a macroscopic ordering in a form of void lattice, in agreement with experimental data and provide an explanation for existing theoretical and experimental contradictions. We consider fluorine sublattice, where irradiation produces correlated Frenkel defects – pairs of the F and H centers. Slow F center diffusion is accompanied with their nearest neighboring attractive interaction leading to the formation of F center clusters, i.e., voids. The driving forces for the long-range void ordering are H center planes. They are formed by highly mobile H centers due to three-atoms-in-a-line (trio) attractive interactions, see Fig. 17.

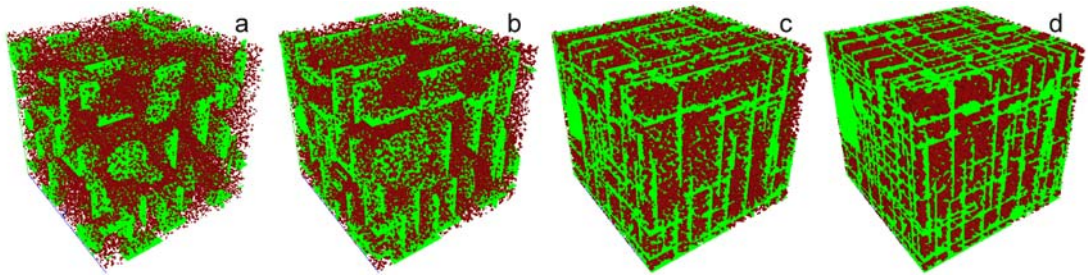

Fig. 17. 3D CA simulation snapshots at the following dimensionless F center 3D concentrations and CA simulation times (a) (0.02, 0.025 s), (b) (0.04, 0.057 s), (c) (0.10, 0.207 s), (d) (0.17, 0.542 s). The F centers are marked red, the H centers - light green.

Our cellular automata simulations demonstrate that global void lattice self-organization can occur only in a narrow parameter range where an average spacing between void clusters and H center planes is balanced. Moreover, we monitor also the kinetics of a void lattice ordering starting from an initial disordered stage, in agreement with the TEM experimental data.

C. Plasma Physics

BIFURCATION ANALYSIS IN A 3D SYSTEM MODELING OSCILLATING PHENOMENA IN FUSION PLASMA PHYSICS

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Max-Planck Institut für Plasmaphysik, Garching, Germany

The aim of this paper was a study of a 3D dynamical system which models some instabilities that occur in fusion plasma experiments in TOKAMAKs (toroidal devices for obtaining energy through controlled thermonuclear fusion). This model depends on three parameters. It was formulated for the description of a system with drive and relaxation processes which have different time scales. It has some properties analogue to Lorenz system, but it does not belong to the family of Lorenz-like systems. We systematically study the dynamics of the system for various values of the parameters and we provide analytical results concerning some bifurcations that occur in the parameters space. We theoretically analyze the fast-slow dynamics of the system and we apply the results in some situations which correspond to experimental data obtained in ASDEX-Upgrade tokamak.

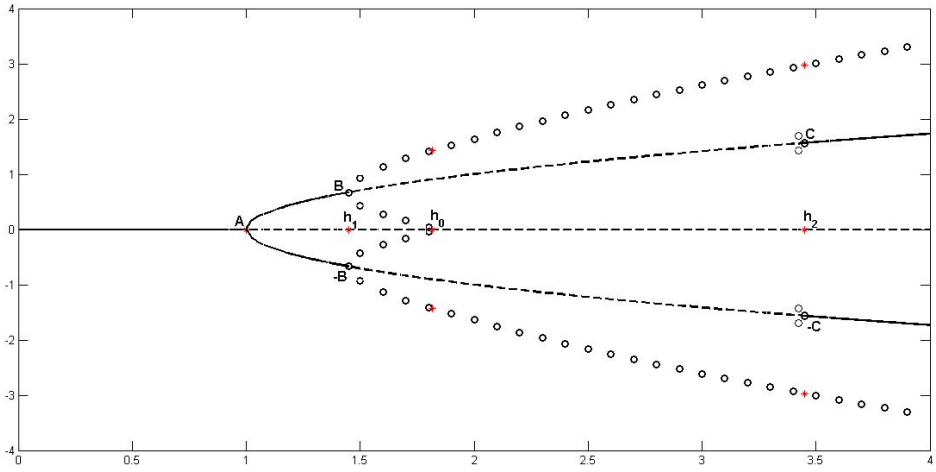

Fig.18. Bifurcation diagram for a fixed values of δ=0.2, η=0.2, pitchfork bifurcation (labelled A) in h=1, two pairs of Hopf bifurcations (labelled B, -B respectively C, -C) in h_1 and h_2, homoclinic bifurcation in h_0.

ANALYSIS OF AFTERCAVITY INTERACTION IN EUROPEAN ITER GYROTRONS AND IN THE COMPACT SUB-THZ GYROTRON FU CW-CI

O. Dumbrajs
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Possibilities of arising of aftercavity interaction are analyzed in the ITER 170 GHz 2 MW coaxial cavity gyrotron and the 170 GHz 1 MW cylindrical cavity gyrotron, as well as in the compact 394.5 GHz low power gyrotron FU CW-CI. Also, the simulations for the gyrotron efficiency in the presence of aftercavity interaction are performed in the cold cavity approximation. Results of the analysis illustrate the subtle interplay between the geometry of the output taper and the profile of the magnetic field.

REGIONS OF AZIMUTHAL INSTABILITY IN GYROTRONS

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This paper is devoted to the analysis of the instability of operating modes in high-power gyrotrons with cylindrically symmetric resonators. This instability manifests itself in destruction of the azimuthally uniform wave envelope rotating in a gyrotron resonator having a transverse size greatly exceeding the wavelength. The appearance of azimuthally nonuniform solutions can be interpreted as simultaneous excitation of modes with different azimuthal indices. This problem is studied self-consistently, i.e. taking into account the temporal evolution of both the azimuthal and axial structures of the wave envelope. The region of gyrotron operation free from this instability is identified. The efficiency achievable in this region can be only 1-2% lower than the maximum efficiency. It is also possible to address the difference between the theory of mode interaction developed under assumption that all modes have fixed axial structure and the self-consistent theory presented here. As known, for fixed axial mode profiles, single-mode high-efficiency oscillations remain stable no matter how dense is the spectrum of competing modes, while the self-consistent theory predicts stable high-efficiency operation only when the azimuthal index does not exceed a certain critical value. It is shown that the azimuthal instability found in the self-consistent theory is caused by excitation of modes having axial structures different from that of the desired central mode.

Defence of PhD Theses

The Doctoral Thesis D. Bocharov “First principles simulations on surface properties and reactivity of sustainable nitride nuclear fuels” was defended in January 2012 at the University of Latvia.

Scientific Publications

SCI publications

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1. D. Constantinescu, O. Dumbrajs, V. Igochine, K. Lackner, R. Meyer-Spasche, H. Zohm, and ASDEX Upgrade team, "A low-dimensional model system for quasi-periodic plasma perturbations". Abstracts: p. 5.

2. O. Lisovski, S. Piskunov, Yu.F. Zhukovskii, and J. Ozolins, „Quantum-chemical simulations of TiO_2 nanotubes for photocatalytic hydrogen generation." Abstracts: p. 7.

3. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, "Surface modeling of UN and other actinides: Current state and prospects". Abstracts: p. 16.

4. R.I. Eglitis, H. Shi, R. Jia, L. Yue, and X. He, "Ab initio calculations for the H centers in SrF_2 as well as surface H centers and F centers aggregation in BaF_2". Abstracts: p. 17.

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30. P. Zhgun, D. Bocharov, S. Piskunov, A. Kuzmin, and J. Purans, Electronic structure and lattice dynamics of ScF_3 from ab initio LCAO calculations. – Abstract: p. 125.

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41. P. Nazarov and V. Kashcheyevs, Finite temperature effects in single-parameter non-adiabatic electron pumps. – Abstract: p. 280.

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44. G. Zvejnieks, V.N. Kuzovkov, and E.A. Kotomin, Atomistic theory of messcopc pattern formation induced by bimolecular surface reactions between oppositely charged molecules. – Abstract: p. 283.

45. V.N. Kuzovkov, E.A. Kotomin, and M.O. de la Cruz, The non-equilibrium charge screening effects in diffusion-driven systems. – Abstract: p. 285.

46. V.N. Kuzovkov, The Anderson localization problem, the Fermi-Pasta-Ulam paradox and the generalized diffusion approach.– Abstract: p. 286.

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48. D. Bocharov, Yu.F. Zhukovskii, D. Gryaznov, and E.A. Kotomin, Ab initio modeling of uranium nitride grain boundary interfaces. – Abstract: p. 304.

49. F.U. Abuova, A.F. Fix, A.T. Akilbekov, S. Piskunov, E.A. Kotomin, and R.I. Eglitis, Ab initio calculations of bulk and surface defects in MgF_2 crystals. – Abstract: p. 305.

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51. R.A. Evarestov and Yu.F. Zhukovskii, Symmetry and properties of the rutile-based titania nanowires. – Abstract: p. 28.

52. F.U. Abuova, A.F. Fix, A.T. Akilbekov, E.A. Kotomin, and R.I. Eglitis, Ab initio calculations of bulk and surface color centers in MgF_2 crystals. – Abstract: p. 48.

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VII. 5th International Conference on Innovative Information Technologies, IIT-2012 (Vilnius, Lithuania, May, 2012).

54. Yu.N. Shunin, T. Lobanova-Shunina, N. Burlutskaya, and S. Bellucci, Novel carbon-based nanosensors for living and artificial complex systems. - Abstracts: p. 6.

55. Yu.N. Shunin, V.I. Gopeyenko, P.N. Dyachkov, N. Burlutskaya, Yu.F. Zhukovskii, and S. Bellucci, Simulation of dc- and ac-conductivity for armchair carbon nanotubes. - Abstracts: p. 7.

VIII. Spring European Materials Research Society (E-MRS) Meeting (Strasbourg, France, May, 2012).

56. 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 $La_{1-x}Sr_xCo_{1-y}Fe_yO_{3-\delta}$ perovskites. – Abstract: C7-2.

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59. R.I. Eglitis, Ab initio calculations of $SrTiO_3$, $BaTiO_3$, $PbTiO_3$, $CaTiO_3$, $BaZrO_3$, $SrZrO_3$ and $PbZrO_3$ (001), (011) and (111) surfaces as well as Nb impurity segregation towards the $SrTiO_3$ surface. – Abstract: CP12-1.

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62. E.A. Kotomin, D. Gryaznov, D. Bocharov, and Yu.F. Zhukovskii, Ab initio simulations of oxygen adsorption and migration upon uranium nitride surfaces. – Abstract: E2-2.

63. R.I. Eglitis, Ab initio calculations of $SrZrO_3$ and $PbZrO_3$ (001) and (011) surfaces as well as F center on ZrO_2-terminated $PbZrO_3$ (001) surface. – Abstract: L8P-17.

64. R.I. Eglitis, H. Shi, R. Jia, L. Yue, and X. He, Ab initio calculations for the H centers in SrF_2 as well as surface H centers and F centers aggregation in BaF_2. – Abstract: VO-3.

IX. International Conference on Fundamental and Applied NanoElectroMagnetics, FANEM'12 (Minsk, Belarus, May, 2012)

65. Yu.N. Shunin, Yu.F. Zhukovskii, N. Burlutskaya, T. Lobanova-Shunina, V.I. Gopeyenko, and S. Bellucci. Simulation of electromagnetic properties in CNT- and graphene-based nanostructures. - Abstract: p. 9.

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66. K.A. Avramides, A.K. Ram, O. Dumbrajs, S. Alberti, T.M. Tran, and S. Kern, On the numerical scheme employed in gyrotron interaction simulations.

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68. Yu.A. Mastrikov, P.V. Vladimirov, V.A. Borodin, Yu.F. Zhukovskii, E.A. Kotomin, and A. Möslang, Ab initio simulation of growth of vacancies formed clusters in α-Fe lattice.

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69. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M. Kuklja, D. Fuks, and J. Maier, First principles calculations on defects in ABO_3 perovskites: Applications for oxygen permeation membranes and SOFC cathodes. - Abstract: p.18.

70. F.U. Abuova, A.K. Dauletbekova, A.T. Akilbekov, E.A. Kotomin, and Zh.K. Yermekova, First principles calculations on radiation defects in MgF_2 crystals. - Abstract: p. 110.

XIV. "Nature Materials", Frontiers in Electronic Materials: Correlation Effects and Memristive Phenomena (Aachen, Germany, June, 2012).

71. R. Merkle, L. Wang, Y. A. Mastrikov, E. A. Kotomin, and J. Maier, Oxigen exchange kinetics on perovskite surfaces: importance of electronic and ionic defects.

XV. 10th international conference on Solid State Chemistry (Pardubice, Czech Republic, June, 2012).

72. R. Merkle, L.Wang, Yu.A. Mastrikov, A. Wedig, E.A. Kotomin, and J. Maier, Mechanistic insight into oxygen exchange SURFACE reaction on perovskites from experiments and DFT calculations.

XVI. 10th International Symposium on Systems with fast ionic transport (ISSFIT) (Chernogolovka, Russia, July, 2012).

73. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M. Kuklja, D. Fuks, and J. Maier, Ab initio modelling of oxygen transport in mixed conducting perovskites. - Abstract: p.14.

XVII. International Workshop on Nanocarbon Photonics and Optoelectronics, NPO-2012 (Huhmari-Polvijärvi, Finland, July-August, 2012).

74. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, Electromagnetic properties in carbon- and graphene-based monoperiodic nanostructures for nanosensor systems.

XVIII. E-MRS 2011 Fall Meeting (Warsaw, Poland, September, 2012).

75. R.I. Eglitis, Ab initio calculations of the ABO_3 perovskite (001), (011) and (111) surfaces including bulk and surface F centers and Nb impurity segregation towards the $SrTiO_3$ surface. – Abstract: C-VI-2.

76. D. Fuks, E.A. Kotomin, A. Weizman, Yu.A. Mastrikov, M.M. Kuklja, and J. Maier, Ab initio thermodynamic study of phase competition in ABO_3-type multicomponent solid solutions. – Abstract: C-XI-2.

77. E.A. Kotomin, R. Merkle, Yu.A. Mastrikov, M.M. Kuklja, D. Fuks, and J. Maier, First principles calculations of defects in ABO_3 perovskites: applications for oxygen permeation membranes and SOFC cathodes. – Abstract: C-XI-3.

78. A.I. Popov, V. Pankratov, E. Klotins, L. Shirmane, V. Dimza, M. Antonova, M. Livinsh, and A. Kotlov, VUV synchrotron radiation spectroscopy of PLZT ceramics. – Abstract: C-31.

79. A.I. Popov, V. Pankratov, V. Bratus, and A. Kotlov, Electronic excitation and luminescence of pure and neutron-irradiated 3C-SiC. – Abstract: E-23.

80. R.I. Eglitis, Towards a practical rechargeable 5 V Li ion battery. – Abstract: F-XII-5.

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82. Yu.F. Zhukovskii, J. Kazerovskis, S. Piskunov, and S. Bellucci, Ni filament encapsulated inside single-walled carbon nanotubes: Predictions from first principles. – Abstract: G-3.

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88. E. Klotins and G. Zvejnieks, Quantum chemical study of electron-phonon interactions in crystals. – Abstract: L-15.

XIX. 8th International Conference on Luminescent Detectors and Transformers of Ionizing Radiation (Halle, Germany, September, 2012).

89. V. Pankratov, A.I. Popov, L. Shirmane, A. Kotlov, G.A. Bizarri, A. Burger, P. Bhattacharya, E. Tupitsyn, E. Rowe, V.M. Buliga, and R.T. Williams, Luminescence of pure and europium doped SrI_2 and BaI_2, under VUV and x-ray excitation. - Abstracts: p. O-Mon-08.

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93. A. Weizman, D. Fuks, D. Gryaznov, E.A. Kotomin, Ab initio study of phase transformations in $(La_x,Sr_{1-x})CoO_3$: Beyond regular solid solutions.

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XXII. The XVIIIth International Seminar on Physics and Chemistry of Solids (Lviv, Ukraine, September, 2012).

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XXIII. XIII Ukrainian-Polish symposium Theoretical and Experimental Studies of Interfacial Phenomena and their Technological Applications (Kyiv, Ukraine, September, 2012).

96. O.I. Aksimentyeva, V.P. Savchyn, V.P. Dyakonov, S. Piechota, I.Ye. Opaynych, Yu.Yu. Horbenko, and A.I. Popov, Hybrid polymer-magnetic nanocomposites with conductive and luminescent functions.

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97. S. Piskunov, Yu.F. Zhukovskii, J. Kazerovskis, and S. Bellucci, First principles calculations of Ni filament encapsulated inside single-walled carbon nanotube. - Abstracts: p. 37-38.

98. Yu.N. Shunin, Yu.F. Zhukovskii, V.I. Gopeyenko, N. Burlutskaya, T. Lobanova-Shunina, and S. Bellucci, Nanocarbon electromagnetics for nanosensor applications. - Abstracts: p. 63-66.

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XXV. First Baltic School on Application of Neutron and Synchrotron Radiation in Solid State Physics and Material Science, BSANS-2012 (Riga, Latvia, October, 2012).

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107. I. Karbovnyk, I. Bolesta, V. Savchyn, M. Cestelli Guidi, and A.I. Popov, Infrared characterization of pure and doped cadium iodide crystals. - Abstracts: p. 37.

108. E. Klotins and G. Zvejnieks, Radiation field-electron-phonon interaction in the Hartree-Fock model. - Abstracts: p. 38.

109. A. Kuzmin, V. Pankratov, A. Kalinko, A. Kotlov, L. Shirmane, and A.I. Popov, UV-VUV synchrotron radiation spectroscopy of $NiWO_4$. - Abstracts: p. 42.

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115. A.I. Popov, J. Zimmermann, V. Pankratov, G.J. McIntyre, and H. von Seggern, Luminescent properties of neutron image plates. - Abstracts: p. 49.

116. A.I. Popov, V. Pankratov, E. Klotins, L. Shirmane, V. Dimza, M. Antonova, M. Livinsh, and A.Kotlov, VUV synchrotron radiation spectroscopy of PLTZ ceramics. - Abstracts: p. 50.

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121. P. Zhgun, D. Bocharov, S. Piskunov, A. Kuzmin, and J. Purans, Electronic structure and lattice dynamics of ScF_3 from firts-princiles LCAO calculations. - Abstracts: p. 58.

XXV. International Workshop „Hydrogen and Fuel Cells in Research and Applications: facing to Latvia" (Riga, Latvia, October 2012).

122. Yu.F. Zhukovskii and S. Piskunov, "Catalysts on the surface of the oxide nanotubes - calculations from the first principles".

XXVI. Fall MRS Meeting (Boston, USA, November, 2012)

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125. M. Kuklja, D. Fuks, O. Sharia, Yu.A. Mastrikov, and E.A. Kotomin, "Degradation and stability of complex perovskites for energy applications". Abstracts: I2.02.

DEPARTMENT OF PHOTONICS MATERIALS 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 experimental setups

The electronic properties of nanostructured materials were studied by time-resolved luminescence and absorbtion methods. Excitation sources: a pulsed electron beam accelerator (10 ns, 270 keV, 10^{12} electrons/pulse), YAG:Nd and nitrogen lasers (266 nm, 337 nm, 532 nm). X ray was used for steady state luminescence spectra and radiation defect creation.

FTIR absorption spectroscopy: EQUINOX 55 (10000-400 cm^{-1} and 22000-7000 cm^{-1} spectral regions) was developed for dispersed materials in wide temperature range.

VIS-UV spectrometer LABOMED for 190-1100 nm was used for absorbsion measurements.

Scientific Staff	**Students**
Dr.habil.phys. D.Millers	J.Rikveilis
Dr.habil.phys. L.Grigorjeva	V.Liepina
Dr.K.Smits	M.Vanks
	L.Puķina
	A.Zoloterjevs

Scientific Visits Abroad

1. Dr.habil.phys.L.Grigorjeva, Estonia (7 days)
2. Dr.K.Smits, USA, (7 days)
3. Dr.K.Smits, France (14 days)
4. Dr.Habil.phys. L.Grigorjeva, France (7 days)
5. Dr.Habil.phys. L.Grigorjeva, Greece (7 days)
6. Dr.Habil.phys. L.Grigorjeva, Germany (4 days)
7. Dr.Habil.phys. L.Grigorjeva, Germany (6 days)

Cooperation

Latvia

Riga Technical University, Institute of Inorganic Chemistry (Dr.habil.sc.ing. J.Grabis).
ZRF RITEC SIA (Dr.V.Ivanov).
LU Institute of Microbioligy (M.Gavare, J.Liepiņš)

Estonia
Institute of Physics, Tartu (Dr.S.Zazubovich)

Russia
GOI, St.Peterburg (Dr.L.Maksimov)

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)

Israel
Prof. A.Gedanken, Bar-Ilan University, Ramat Gan.

Main results

PHOTOCATALYTIC EFFICIENCY STUDIES OF TiO_2 NANOPOWDES

J.Rikveilis, L.Grigorjeva, D.Millers, K.Smits

Experimental results showed that for photocatalytic activity the ratio of anatase to rutile phase has more significant role than the anatase grain size. The smaller grain size does not lead to greater performance, possible due to high concentration of surface defects and electron-hole recombination on surface.
The doping of RE ions lead to anatase grain size decreasing and the photocatalytic activity decrease.

THE LUMINESCENCE PROPERTIES OF PERSISTENT STRONTIUM ALUMINATE PHOSPHOR PREPARED BY SOLAR INDUCES SOLID STATE SYNTHESIS

V.Liepina, K.Smits, D.Millers, L.Grigorjeva, C.Monty

A novel method –solar induced solid state synthesis was carried out and luminescence properties of aluminate phosphor doped with Eu and Dy were studied. The persistent phosphor was obtained and its properties were compared with prepared by conventional solid state reaction.

THE ELECTRON BEAM INDUCED SHORT LIVED ABSORPTION IN PLZT OPTICAL CERAMICS

D.Millers, V.Dimza, L.Grigorjeva, M.Antonova, K.Smits, M.Livins

The short lived absorption induced by a pulsed electron beam in the led-lanthanium-zirconate-titanate (PLZT) optical ceramic was studied. The measured absorption spectrum covers 1.1-2.9 eV energy range and consists of several strongly overlapping peaks. The rise of the absorption is delayed with respect to the excitation pulse, due to

charge carrier migration before trapping at centers responsible for the absorption. The formation rate of absorption centers and decay rate of absorption depend on the photon energy. The kinetics of short lived absorption varies over spectrum and can be approximated with a stretched exponent. The stretched exponent parameters indicate that the local disorder of a matrix is similar around all absorption centers.

NEAR-BAND LUMINESCENCE OF CdZnTe DETECTOR CRYSTALS

L.Grigorjeva, D.Millers, V.Ivanov, L.Aleksejeva

For the for nondestructive detector material selection the low temperature near-band luminescence measurements will be carried out and analyzed. It is shown that the complex of parameters such as presence and intensity of A and DAP luminescence bands, the decay kinetics in A^0Ex-1LO and DAP luminescence bands, the peak position and FWHM of D ^{0}Ex luminescence are more important characteristics. The A^0Ex-1LO and DAP luminescence peaks overlaps and conclusion about the DAP luminescence will be done from luminescence decay measurements. The DAP luminescence has non-exponential decay. Usually, acceptors – V_{cd}; donors – Te_{Cd} . The A^0Ex-1LO luminescence is fast with decay time 2-3 ns.

Zirconia nanocrystals as submicron level biological label

K.Smits, J.Liepins, M.Gavare, A.Patmalnieks, A.Gruduls, Dz.Janlovica

Inorganic nanocrystals are of increasing interest for their usage in biology and pharmatalogy research. We study the usage of ZrO_2 nanocrystals as submicron level biological label in baker's yest *Saccharomyces cerevisia* culture. The images with sub micro up-conversion luminescence particles in biologic media were made. A set of undoped as well as Er and Yb doped ZrO_2 nanopowders with different dopand concentration were prepared by sol-gel method. The up-conversion luminescence for free standing and for nanocrystals with baker's yeast cells was studied and the differences in up-conversion luminescence spectra were analyzed. In *vivo* toxic effects of ZrO_2 nanocrystals were tested by co-cultivation with baker's yest.

Scientific publications

1. Dorogov P., Ivanov V., Loutchanski A., **Grigorjeva L., Millers D**. Improving the performance of μ CdZnTe detectors using infrared stimulation. 2012, *IEEE Transactions on Nuclear Science* 59 (5 PART 3) , art. no. 6327737 , pp. 2375-2382.
2. **Zabels, R., Muktepavela F., Grigorjeva L**.Deformation behavior of nanostructured ZnO films on glass.. 2012, *Thin Solid Films* 520 (14) , pp. 4685-4688.
3. **Grigorjeva, L., Millers, D., Smits, K., Sarakovskis**, A., Lojkowski, W., Swiderska-Sroda A., Strek W., Gluchowski P.The time-resolved luminescence characteristics of Ce and Ce/Pr doped YAG ceramics obtained by high pressure technique. 2012, *Optical Materials* 34 (6) , pp. 986-989.
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5. **Grigorjeva L., Jankoviča D., Smits K., Millers D**., Zazubovich S.,Defect luminescence of YAG nanopowders and crystals. 2012, *Latvian Journal of Physics and Technical Sciences* 49 (4) , pp. 54-60
6. Alekseeva L., Dorogov P., Ivanov V., Loutchanski A., **Grigorjeva L., Millers D.** Investigation of the influence of light illumination on the characteristics of CdZnTe detectors. 2012, *IEEE Nuclear Science Symposium Conference Record* , art. no. 6154735 , pp. 4562-45667.
7. **V.Liepina, K.Smits, D.Millers, L.Grigorjeva**, C.Monty. The luminescence properties of persistent strontium aluminate phosphor prepared by solar induces solid state synthesis. *IOP Conf. Series:Materials Scienceand Engineering,* 2012, 38. 012045.
8. **L.Grigorjeva, D.Millers**. V.Ivanov, L.Alekseeva. Near band luminescence of CdZnTe detector crystal. *IOP Conf. Series: Materials Scienceand Engineering*, 2012, 38, 012037.
9. **K.Smits**, J.Liepins, M.Gavare, A.Patmalnieks, A.Grunduls, **Dz.Jankovica**. Zirconia nanocrystals as submicron level biological label. IOP Conf. Series: Materials Scienceand Engineering, 2012, 38,012050.
10. **K.Smits, D.Jankoviča, A.Sarakovskis, D.Millers.** Up-conversion luminescence dependence on structure in zirconia nanocrystals. *Optical Materials*, avaible online 24 Nov., 2012**.**

Lectures on Conferences

International Baltic Sea Region Conference "Functional materials and nanotechnologies 2012 (FM&NT)", April, 17-20, Riga, Latvia.

1. L.Grigorjeva, D.Millers. V.Ivanov, L.Alekseeva. Near band luminescence of CdZnTe detector crystal. PO-87
2. J.Liepins, K.Smits, M.Gavare, A.Patmalnieks, A.Grunduls, Dz.Jankovica. Zirconia nanocrystals as submicron level biological label. PO-128
3. V.Liepina, K.Smits, D.Millers, L.Grigorjeva, C.Monty. The luminescence properties of persistent strontium aluminate phosphor prepared by solar induces solid state synthesis. PO-112.
4. D.Millers, V.Dimza Induced short-lived absorption in PLZT electrooptical ceramics. PO-88.
5. K.Smits. Oxygen vacancies and RE ion agglomeration caused up-conversion luminescence quenching prevention in zirconia. PO-89.

4th International Symposium on Transparent Conductive Materials (TCM-2012) 17-21 Oct. Crete, Greece.

L.Grigorjeva, J.Rikveilis, D.Millers, K.Smits. Comparative study of photocatalytic activity of TiO_2-ZnO-WO_3 systems.

LU CFI 26th Scientific Conference, 2012, 17-19 Febr., Riga, Latvia

V.Liepina. K.Smits, L.Grigorjeva, D.Millers. The luminescent properties of rare earth doped aluminates. Thesis, p.38.

A.Zolotarjevs, K.Smits, D.Millers. Software and Hardware for TSL intensity and spectra measurements. Thesis, p.68.

J.Rikveilis, L.Grigorjeva, D.Millers, K.Smits. Photocatalytic efficiency studies of TiO_2 nanopowdes. Thesis, p. 69.

10th International Symposium on Ceramic Materials and Components for Energy and Environmental Applications. Dresden, Germany, May, 20-23, 2012.

L.Grigorjeva, D.Millers, K.Smits, S.Zazubovich. Fast luminescence of YAG ceramics and single crystals. Program and Abstract book, P.122.

8th International Conference on Luminescence detectors and Transformers of Ionizing Radiation, (LUMDETR2012), Halle (Saale), Germany, 10-14 Sept., 2012

1. L.Grigorjeva, D.Millers, A.Sarakovskis, J.Grube, K.Smits. Excitonic luminescence of ZnO ceramics. Book of Abstracts, P-Tue-21.

2012 International Conference on defects in insulating materiāls (ICDIM, 2012) Santa Fe, New Mexico, 24-29 June, 2012.

K.Smits, Defect luminescence in zirconia nanocrystals. Proceedings, p.60.

Bachelor Thesis

V.Liepina. The luminescence properties of rare earth doped aluminate and silicate phosphors.

LABORATORY OF AMORPHOUS MATERIALS SPECTROSCOPY

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

Research area

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.

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), 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.

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.

Staff

Dr.habil.phys. L.Skuja
Dr.habil.phys. A. Trukhin
Dr.Habil.Phys A.Siliņš

Scientific Visits Abroad

1. Dr. Hab. A. Trukhin France 5 days
2. Dr.Hab. L. Skuja France 5 days
3. Dr.habil. L.Skuja, Italy 3 days
4. Dr.habil. L.Skuja, Great Britain, 2 days

Cooperation

Latvia

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Main results

ABSORPTION AND LUMINESCENCE IN AMORPHOUS $Si_xGe_{1-x}O_2$ FILMS FABRICATED BY SPCVD

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Optical absorption and photoluminescence of Ge-doped silica films fabricated by the surface-plasma chemical vapor deposition (SPCVD) are studied in the 2-8 eV spectral band. The deposited on silica substrates films of about 10 microns in thickness are composed as Si_{1-x} Ge_xO_2 with x ranging from 0.02 to 1. It is found that all as deposited films do not luminesce under the excitation by a KrF (5 eV) excimer laser thus indicating lack of oxygen deficient centers (ODCs) in them. After subsequent fusion of silicon containing (x<1) films by a scanning focused CO_2 laser beam absorption band centered at 5 eV as well as two luminescence bands centered at blue (3.1 eV) and UV (4.3 eV) wavelengths arise highlighting the formation of the ODCs. The excitation of unfused SPCVD films by an ArF (6.4 eV) excimer laser yields a luminescence spectrum with two bands typical for the ODCs, but with a faster decay kinetics. Intensities of these bands grow up with samples cooling down to a temperature of 80 – 60 K. Unfused films excited by the ArF laser also demonstrate luminescence due to recombination of a trapped charge resulted from the excitation of localized electron states of the glass network. In the unfused GeO_2 filmluminescence related to a self-trapped exciton (STE) typical for GeO_2 crystals with α-quartz structure is observed. The observed STE luminescence can be indicative of the crystalline fraction availability in the film. Whereas GeO_2 crystals are known as not containing twofold coordinated germanium, a polycrystalline inclusion in the SPCVD GeO_2 film serves as a factor explaining the absence of any spectroscopic manifestation of this type of defects in it even after fusion. On the other hand, lack of STE luminescence in other unfused films with x< 1 testifies truly amorphous state of the matter in them.

LUMINESCENCE OF α-QUARTZ

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A short review of α-quartz crystal's luminescence properties are presented. Among the host material's luminescence the luminescence of the self-trapped exciton (STE) is reviewed. This luminescence, which band is situated at 2.6-2.7 eV, could be observed mainly under ionising radiation with energetic yield about 20 %. The STE does not participate in pure recombination processes and could not be used in dosimetry. Host material defect luminescence at 5 eV appears in α-quartz after heavy irradiation. It is constituted of permanent defect after neutron irradiation and transient defect after dens electron beam irradiation. This luminescence could be observed well at temperatures below 60 K. all another luminescence are of impurity nature. The Ge impurity luminescence in α-quartz explained as STE near Ge. The aluminium and alkali complexes in α-quartz provides at least three types of luminescence centers. One of

them is with UV band at 6 eV, appears at low temperatures and could be excited only in tunnelling recombination process between pairs [AlO_4 - Me^o], where Me^o is an alkali ion captured an electron and a hole remains on aluminium tetrahedron. Another luminescence with band at 3.4 eV is also luminescence of complexes [AlO_4/Me^+], which behaviour is similar to the luminescence of alkali alumo-silicate glass. The third luminescence with band at 3 eV could be observed mainly in natural α-quartz, bright at temperatures below 200 K and is interpreted as STE-like luminescence at alumo-silicate clasters. The exchange of alkali ions to noble ions of copper of silver reduces original luminescence of alumo – alkali complexes and luminescence of noble ions appears. The main band of copper related luminescence is at 3.4 eV and that of silver is at 4.75 eV, both could be observed up to 500 K. their nature could be well described in terms of intra-ions transition. Exchange of noble ions back to alkali ions renews initial luminescence of the samples.

LUMINESCENCE OF UNFUSED F-DOPED 95%SiO_2-5%GeO_2 AMORPHOUS FILMS FABRICATED BY SPCVD. ABSENCE OF GeODC(I) DEFECTS

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We have studied influence of fluorine on germanium oxygen deficient luminescence center (GeODC) in films (~100 μm) produced by the surface-plasma chemical vapor deposition (SPCVD). Two kinds of samples were studied: a sample with "high" 4.2 wt.% of F concentration of fluorine and a sample with "low" 0.5 wt. % of F concentration of fluorine. Main feature of the samples difference corresponds to difference in detection of GeODC luminescence. For the case of "high" level of fluorine a "normal" GeODC or so call GeODC(II) or twofold coordinated germanium is observable. That there is absorption band at 5 eV where luminescence of GeODC is excited. The effect of "high" fluorine thermally non treated sample is similar to the case of thermally treated germanium containing SPCVD sample without fluorine studied previously. So, we conclude that effect of "high" fluorine sample is related to diminishing of glass softening temperature. In the case of low fluorine concentration corresponds to the case of thermally non-treated SPCVD sample then we conclude that "low" fluorine case insufficiently diminishes softening temperature. the absorption band at 5 eV is not well expressed, and however luminescence of GeODC is observed there under 248 nm excimer laser (KrF), it intensity is much lower than in the case of high fluorine concentration. Most significant difference is observed for excitation with higher than 5 eV photons – that is excitation with 193 nm (ArF) and 157 nm (F2) of excimer lasers. The decay kinetics of luminescence for observed under these conditions is very different from usual GeODC, however luminescence bands positions are close to usual GeODC. Noticeable effect under both last cases of excitation is luminescence intensity growth during long time excitation (half an hour and more), therefore it was concluded that GeODC are produced by this irradiation.
In the case of "high" concentration of fluorine the yield of GeODC luminescence excited with 157 nm photons (F2 excimer laser) still is high. Therefore it was concluded that competitive absorption of SiODC(I) with 7.6 eV absorption band is diminished by fluorine. High yield of luminescence shows that analogous to the SiODC(I) a GeODC(I) does not exist. It is known from literature that SiODC(I) of pure silica glass could be passivated with fluorine with strong diminishing of famous 7.6 eV absorption band of oxygen deficient pure silica glass.

LUMINESCENCE OF FUSED AND UNFUSED Bi-DOPED AMORPHOUS SILICA FABRICATED BY SPCVD

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Bismuth-doped high purity silica samples synthesized by surface-plasma chemical vapor deposition (SPCVD) are studied to investigate the origin of Bi-associated defects responsible for near infrared (NIR) luminescence. Two types of samples are studied: unfused Bi-doped silica film immediately deposited on the inner surface of a substrate silica tube and the same material after fusion obtained as the result of the tube collapsing to a rod by external heating. Luminescence is excited by pulsed UV (ArF – 193 nm, KrF – 248 nm) and green (532 nm) lasers. Luminescence bands centered at 620-650 nm, 808 nm and 1400 nm wavelengths are observed in both fused and unfused samples. Orange and near-infrared luminescences excited by the green laser have decay time constant of about 3 μs for the 650 nm and of about 0.6 ms for the 1400 nm band at room temperature. Intensities of both bands do not depend on temperature in the 12 - 450 K range.

STUDY OF PHOSPHORUS DOPED CRYSTALLINE AND GLASSY SiO_2

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The main coordination of silicon in many materials, produced in "normal" pressure, is four. The α-quartz crystal, silica glass, different silicate glasses are example of those materials. However, in the case of glasses the density fluctuations with deviation of density to both directions higher and lower from "normal" are possible. Tetrahedron structure with sp^3 hybridization of silicon orbital allows wide range of fluctuations of density with creation of small rings. Example of dense tetrahedron structured silicon dioxide crystal is coesite with density gravity 2.915. Next modifications are related to principal change of silicon atomic orbital hybridization. High density fluctuation could be related to creation of sixfold-coordination silicon with d^2sp^3 hybridization. phosphosilicate crystal (SiP_2O_7), possesses mainly sixfold-coordinated silicon, then investigation of properties of that in phosphosilicate glasses should be performed for octahedron structure role clarification. Therefore we have studied samples of phosphosilicate glasses and samples of synthetic crystalline α-quartz doped with phosporus. Beside many differences in these samples we had found similar fast (40 – 60 ns) ultraviolet luminescence excited in the range of 7.6 eV in them showing similarity with oxygen deficient luminescence of silica. So the possible explanation is proposed: the defect responsible for this luminescence is phosphorus stimulated sixfold coordinated silicon. Further investigations are needed.

ABSORPTION AND LUMINESCENCE IN AMORPHOUS 95%SiO_2 5%GeO_2 FILMS WITH FLUORINE FABRICATED BY SPCVD. IF GeODC(I) EXIST

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We have studied influence of fluorine on germanium oxygen deficient luminescence center (GeODC) in films (~100 μm) produced by the surface-plasma chemical vapor deposition (SPCVD) without any consequent treatment, then corresponding to amorphous layer production at temperatures lower than temperature of glass softening. Two kinds of samples were studied: a sample with "high" concentration of fluorine and a sample with "low" concentration of fluorine. Main feature of the samples difference corresponds to difference in detection of GeODCluminescence. For the case of "high" level of fluorine a "normal" GeODC or so call GeODC(II) or twofold coordinated germanium is observable. That there is absorption band at 5 eVwere luminescence of GeODC is excited. In the case of low fluorine concentration the absorption band at 5 eV is not well expressed and however luminescence of GeODC is observed there under 248 nm excimer laser (KrF) it intensity is much lower than in the case of high fluorine concentration. Most significant difference is observed for excitation with higher than 5 eV photons – that is excitation with 193 nm (ArF) and 157 nm (F2) of excimer lasers. The decay kinetics of luminescence for observed under these conditions is very different from usual GeODC, however luminescence bands positions are close to usual GeODC. Noticeable effect under both last case of excitation is luminescence intensity growth during long time excitation (half an hour and more), therefore it was concluded that GeODC are produced by this irradiation.
In the case of "high" concentration of fluorine the yield of GeODC luminescence excited with 157 nm photons (F2 excimer laser) still be high and the absorption in the range of such excitation is high. Then is was concluded that hypoteticalGeODC(I) does not exist at least in the produced samples. It is known from literature that SiODC(I) of pure silica glass could be passivated with fluorine with strong diminishing of famous 7.6 eV absorption band of oxygen deficient pure silica glass.

^{18}O-LABELED INTERSTITIAL OXYGEN MOLECULES AS PROBES TO STUDY REACTIONS INVOLVING OXYGEN-RELATED SPECIES IN AMORPHOUS SiO_2

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Isotope labeling has been widely used to study reactions involving oxygen species in amorphous a-SiO_2. This article briefly describes recent progress in ^{18}O labeling techniques to study reactions involving interstitial oxygen molecules (O_2), which is one of the most important excess oxygen species in a-SiO_2. The primarily focus will be on the combination of the ^{18}O labeling with photoluminescence spectroscopy, which

enables sensitive and selective detection of interstitial O_2. Advantages of this method and results of evaluation of oxygen exchange between interstitial O_2 and the a-SiO_2 network are presented.

OXYGEN-EXCESS-RELATED POINT DEFECTS IN GLASSY/AMORPHOUS SiO_2 AND RELATED MATERIALS

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An insight is given into recent experimental advances in the spectroscopic studies of oxygen-excess intrinsic defects, in glassy SiO_2 and α-quartz. By controlling excess oxygen in a-SiO_2, and the conditions of F_2 -laser irradiation, SiO_2 glass samples can be obtained with optical absorption almost exclusively dominated by single defect, oxygen dangling bonds ("non-bridging oxygen hole centers" or NBOHCs), without the presence of complementary Si dangling bonds (generic "E'-centers"). This allows for a more accurate determination of the spectral shape of NBOHC optical absorption in UV and vacuum UV spectral regions. The temperature dependence of NBOHC electron paramagnetic resonance (EPR) signal intensity is stronger than predicted by Curie's law (1/T) even at temperatures at and below 77K. Dangling bonds are characteristic of an amorphous state and do not exist in a regular crystal lattice. However, site-selective luminescence shows that highly ordered NBOHCs exist in particle-irradiated α-quartz, evidently either on the border between the damage tracks and the crystalline phase or as a part of Si vacancies. They are different from the common "glass-like" NBOHCs in a-SiO_2 by giving distinct sharp zero-phonon lines with characteristic energies in luminescence spectra instead of a continuous distribution of lines. Two distinct types of luminescent NBOHCs, associated with the long and short Si-O bonds in α-quartz are suggested. EPR data corroborate the presence of oriented NBOHCs in neutron-irradiated α-quartz and confirm distinct NBOHCs at the sites of "long" and "short" Si-O bonds in α-quartz.

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5. **A. Trukhin**, K. Truhins, Luminescence of alpha-quartz, Conrnell University Library, arXiv:1209.4200 [cond-mat.mtrl-sci] (2012) (or arXiv:1209.4200v1 [cond-mat.mtrl-sci] for this version).

Lectures on Conferences

1. A.N. Trukhin, K.M. Golant, J. Teteris, Luminescence of unfused F-doped 95%SiO_2 - 5%GeO_2 amorphous films fabricated by SPCVD. Absence of GeODC(I) defects. SiO_2 -2012, 9-th Symposium "SiO_2: advanced dielectrics and related devices", Presqu'île de Giens–Hyères (France) (2012) p.16-17.
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3. L.Skuja, K.Kajihara, H.Hosono Thermostimulated luminescence of interstitial O_2 in F_2 laser-irradiated glassy SiO_2 Abstracts of 9th Symposium SiO_2, Advanced Dielectrics and Related Devices, Hyères, France June 17-20, 2012, p.12-13.
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LABORATORY OF OPTICAL RECORDING

Head of Laboratory Dr. phys. 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 lithoghraphy 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.

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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.

NANOSTUCTURED SURFACES FOR OPTICAL ANTIREFLECTION

J.Aleksejeva and J.Teteris

The demand for optically antireflective layers during last years has increased. Particularly such high demand is in the branches where large surfaces will be covered (greenhouses, solar cells etc.) At present work we show the results obtained for surface

patterning consisting of nano-structural elements smaller than incident light wavelength. The decreasing of light reflection for such structures results from light diffraction on above mentioned structures. Nanostructured antireflective elements are formed by holographic recording in chalcogenide photoresist. The next step is electrochemical growing of Ni shim used as a stamp for printing of nanostructures into organic polymer – laminate which can be pasted on glass surface. Nano-relief surface are transferred into transparent polymer films by hot embossing at 100-120^{0}C or UV curing.

The nanostructures with a sizes less than 100 nm were fabricated by immersion holography in amorphous chalcogenids, organic azobenzol and photopolymer films. For recording UV CW lasers with 325nm wavelength (He-Cd laser) and 266nm (frequency doubler pumped by Verdi-8 laser 532 nm radiation) and visible region lasers (442 and 532 nm) were used. The conventional photoresist technology and as well as direct relief fabrication method - surface relief formation in amorphous films during the holographic recording were used. For holographic grating forming was used Two-beam holographic setup for 1D, and three- and more beams holographic setup with possibility to change polarization state for each beam for 2D structural element recording were used.

Optical properties of nanostructures as transmission, reflection, diffraction efficiency and their spectral dependences were studied. The form and size of nanostructures were studied by AFM.

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.

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2. A.N.Truhins, J.Teteris, Fosfora dopētu kristālisko un stiklveida silīcija dioksīdu pētījumi (Study of phosphorus doped crystalline and glassy SiO_2), *LU CFI 28. zinātniskā konference*, Rīga, 2012.gada 8.-10.februāris*, 28th Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 8-10, 2012, Book of Abstracts, p.29.
3. V.Kolbjonoks, V.Gerbreders, J.Teteris, A.Bulanovs, Nanostrukturētas halkogenīdu As-Se-S plānas kārtiņas (Nanostructured chalcogenide As-Se-S thin films), *LU CFI 28. zinātniskā konference*, Rīga, 2012.gada 8.-10.februāris*, 28th Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 8-10, 2012, Book of Abstracts, p.37.
4. A.Kiseļova, J.Teteris, Hologrāfiskais ieraksts amorfās As-S-Se plānās kārtiņās (Holographic recording in amorphous As-S-Se thin layer), *LU CFI 28. zinātniskā konference*, Rīga, 2012.gada 8.-10.februāris*, 28th Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 8-10, 2012, Book of Abstracts, p.60.
5. K.Klismeta, J.Teteris, Azo-krāsvielu un želatīna sistēmas optiskās īpašības (Optical properties of azo dyes and gelatin system), *LU CFI 28. zinātniskā konference*, Rīga, 2012.gada 8.-10.februāris*, 28th Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 8-10, 2012, Book of Abstracts, p.61.
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8. M.Jirgensons, J.Teteris, Fotoinducētais dihroisms AS-s-Se plānās kārtiņās (Photoinduced dichroism in thin As-S-Se films), *LU CFI 28. zinātniskā konference*, Rīga, 2012.gada 8.-10.februāris*, 28th Scientific Conference of the Institute of Solid State Physics, University of Latvia,* February 8-10, 2012, Book of Abstracts, p.64.

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10. U.Gertners, J.Teteris, The Impact of Light Polarization on the Direct Relief Forming Processes in As_2S_3 Thin Films, *Intern. Conf. FM&NT2012 (Functional materials and nanotechnologies 2012,* Riga, Latvia, April 18-20, 2012, Book of abstracts,. p.176.
11. A.Gerbreders, O.Shimane, V.Kolbjonoks, J.Teteris, UV Optical Recorde and Electron Beam Lithography in Polymer Films, *Intern. Conf. FM&NT2012 (Functional materials and nanotechnologies 2012,* Riga, Latvia, April 18-20, 2012, Book of abstracts,. p.177.
12. J.Aleksejeva, J.Teteris, Photoinduced Phenomena in Azo-Dyed Gelatin Films, , *Intern. Conf. FM&NT2012 (Functional materials and nanotechnologies 2012,* Riga, Latvia, April 18-20, 2012, Book of abstracts,. p.178.
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15. V.Kolbjonoks, V.Gerbreders, J.Teteris, A.Bulanovs, Thin films chalcogenide As-Se-S glasses, *International Young Scientist Conference "Developments in Optics and Communications 2012",* Riga, Latvia, April 12-14, 2012, Book of abstracts, p. 96.
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17. E.Potanina, J.Teteris, Optical recording in Disperse Red 1 and Disperse Yellow 7 containing organic polymerts, *International Young Scientist Conference "Developments in Optics and Communications 2012",* Riga, Latvia, April 12-14, 2012, Book of abstracts, p. 104.
18. M.Reinfelde, Holography and its application, *International Young Scientist Conference "Developments in Optics and Communications 2012",* Riga, Latvia, April 12-14, 2012, Book of abstracts, p. 48.
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20. J.Aleksejeva, Volume and surface holographic grating recording in azo-dyed gelatine films, Intern. Conf. *Progress in Applied Surface, Interface and Thin Film Science 2012,* Florence, Italy, May 14-18, 2012, Book of abstracts, p.84.
21. A.Gerbreders, V.Kolbjonoks, O.Shimane, J.Teteris, Direct surface relief formation in polymer films, *2nd International Conf. on Materials and Applications for Sensors and Transducers,* Budapest, Hungary, May 24-28, 2012, Abstract book, p.211.
22. M.Reinfelde, J.Teteris, Photoinduced Mass Transport in Amorphous As-S-Se Films, *5th Intern.Conf. on Optical, Optoelectronic and Photonic Materials and Applications 2012,* Nara, Japan, 3-7 June, 2012,
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27. J.Teteris, Optical field-induced surface relief formation on chalcogenide and organic polymer films, *18th Intern. Symposium on Non Oxide and New Optical Glasses,* Saint Malo, France, 1-5 July, 2012, VI-3 O-5, p.167.
28. M.Reinfelde, J.Teteris, Photoinduced direct surface relief formation in amorphous As-S-Se films, *18th Intern. Symposium on Non Oxide and New Optical Glasses,* Saint Malo, France, 1-5 July, 2012, VI-3 O-6, p.169.
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30. U.Gertners, J.Teteris, Surface relief modulation phenomena by light induced interference, *18th Intern. Symposium on Non Oxide and New Optical Glasses,* Saint Malo, France, 1-5 July, 2012, II-P31, p.271.
31. J.Aleksejeva, J.Teteris, Azodyed gelatin films for holographic recording, *18th Intern. Symposium on Non Oxide and New Optical Glasses,* Saint Malo, France, 1-5 July, 2012, II-P35, p.275.
32. M.Reinfelde, J.Teteris, Surface relief depth dependence on holographic recording conditions. HOLOEXPO2012, *Proc.of 9th Intern.Conf. „HoloExpo-2012, September 17-21, 2012,32, Suzdal, Russia.*
33. J.Teteris, Optical field-induced surface relief formation on amorphous chalcogenide films, *13th International Conference on the Phyics of Non-Crystalline Solids,* Yichang, China, September 16-20, 2012, p.100-101.
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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 and micromechanical and optical properties of surfaces, interfaces and thin films of advanced tribological and optical materials, and materials for micro/nanotechnologies (e.g. metals and alloys, oxides, halides, fullerenes and composite systems). Research area includes development of the methods of surface modification and studies of surface and interface effects in indentation hardness, plasticity and adhesion. The research is based on methods of micro- and nanoindentation, AFM, SEM, XRD and optical microscopy.
Main research topics in 2012 were

- Modification processes of structures and micromechanical properties of functional materials, such as wide band-gap oxides (MgO), halogenides (LiF) and carbon materials (HOPG and polycrystalline graphite) under irradiation with high energy (MeV-GeV) ions.
- Micro- and nano-mechanical characterization of surface layers, thin films and interfaces of advanced materials.

Scientific Staff

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

PhD Students
Mg.phys. R.Zabels

Students
B.sc.R.Grants
L.Brauna

Technical Staff
A.Pētersons

Scientific visits abroad

1. R.Zabels, Warsaw, Poland (7 days).

Visitors from Abroad

1. Dr.A.Dauletbekova, ENU, Astana, Kazakhstan (6 days).
2. Prof.K.Schwartz, GSI, Darmstadt, Germany (6 days).

Cooperation

Latvia
Daugavpils University, Innovative Microscopy Centre (Dr. E.Tamanis).
Institute of Physics, University of Latvia (Dr.A.Shisko).

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

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

Israel
Technion, Haifa (Dr.S.Stolyarova).

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

Main Results

SHEAR BANDING MECHANISM OF PLASTIC DEFORMATION IN LiF IRRADIATED WITH SWIFT HEAVY IONS

J Maniks, R Zabels, I Manika

The effect of ion irradiation on the behavior of plastic deformation at micro- and nanoindentation on (001) face of LiF has been investigated. The irradiation was performed using heavy ions (U, Au, Ti and S) with energy in the range from 3 MeV to 2 GeV at fluences up to $5x10^{13}$ ions/cm^2. In non-irradiated LiF, the indentation produces dislocation gliding on the {110} planes along the <100> and <110> directions. At high fluence irradiation, the resource of the dislocation slip along the preferable directions becomes exhausted due to immobilization of dislocations by radiation defects and their aggregates. The present study demonstrates the change of the mechanism of plastic deformation from homogenous dislocation slip to localized shear banding in samples irradiated to high fluences. The factors facilitating of the localization of deformation have been analyzed

DEFORMATION BEHAVIOR OF NANOSTRUCTURED ZnO FILMS ON GLASS

R. Zabels, F. Muktepavela, L. Grigorjeva

Nanostructured ZnO films on glass substrate were studied by nanoindentation, scanning electron and atomic force microscopy. The films were obtained by a straightforward mechanoactivated oxidation method. The morphology of the obtained films was grained with a grain size in the range 50–100 nm and the thickness was approximately 2 μm. A detailed deformation behavior of ZnO films, critical parameters and indentation induced plastic deformation mechanisms were determined in correlation to bulk ZnO, Si single crystal and commercial ZnO films. In comparison to a single crystal ZnO, nanostructured films exhibit increased hardness (9 GPa); however, the Young's modulus is decreased (120 GPa). A directly detectable evidence of brittleness, “pop-in” and “pile-up” phenomena in ZnO films was not observed. The ZnO/glass interface is stable and exhibits high adhesion, no signs of delamination or presence of brittleness cracks were detected (even at load Pmax>2 N). The role of grain boundaries on the properties of deformation behavior of ZnO nanostructured films has been discussed.

Scientific publications

SCI publications

1. R**. Zabels, F. Muktepavela, L. Grigorjeva**. Deformation behavior of nanostructured ZnO films on glass. Thin Solid Films 520 (2012) 4685–4688.
2. **I. Manika, J. Maniks, R. Zabels, J. Gabrusenoks**, M. Krause, M. Tomut, K. Schwartz. Nanoindentation and Raman Spectroscopic Study of Graphite

Irradiated with Swift ^{238}U Ions. Fullerenes, Nanotubes, and Carbon Nanostructures, 20 (2012) 548–552.

3. **J. Maniks, I. Manika, R. Zabels, R. Grants**, E. Tamanis, K. Schwartz. Nanostructuring and strengthening of LiF crystals by swift heavy ions: AFM, XRD and nanoindentation study. Nuclear Instruments and Methods in Physics Research B 282 (2012) 81–84.
4. A. Dauletbekova, **J. Maniks, I. Manika, R. Zabels**, A.T. Aklibekov, M.V. Zdorovets, Y.Bikert, K. Schwartz, Color centers and nanodefects in LiF crystals irradiated with 150 MeV Kr ions, Nucl. Instr. and Meth. in Phys. Res. B 286 (2012) 56-60.
5. E. Platacis, A. Ziks, A. Poznjak, **F. Muktepavela**, A. Shisko, S. Sarada, P. Chakraborty, K. Sanjay, M. Vrushank, R. Fotedar, E. K. Rajendra and A. K. Suri. Investigation of the Li-Pb flow corrosion attack on the surface of P91 steel in the presence of magnetic field. Magnetohydrodynamics, 48, No.3 (2012) 343-350.
6. E. Platacis, **F. Muktepavela**, A. Shishko, A. Sobolev, A. Klyukin and A. Zik. Microstructural analysis of SS316L steel wetting in Lithium flow. Part I. Magnetohydrodymamics, 48, No.4 (2012) 667-676.
7. **F. Muktepavela, R. Zabels**, V. Sursajeva, **L. Grigorjeva, K. Kundzins**. The role of nanopowder particle surfaces and grain boundary defects in the sintering of ZnO ceramics. IOP Conf.Series:Materials Science and Engineering, 38 (2012) 01201.
8. **J. Maniks, R. Zabels, I. Manika**. Shear banding mechanism of plastic deformation in LiF irradiated with swift heavy ions. IOP Conf.Series:Materials Science and Engineering, 38 (2012) 012017.
9. A. Rusakova, **J. Maniks**, K. Schwartz, A. Dauletbekova, A Akilbekov,V.Lisitsin, M. Zdorovets. Color centers and structural damage in LiF induced by 150 MeV Kr ions IOP Conf.Series:Materials Science and Engineering, 38 (2012) 012040.
10. **M.Reinfelde, R.Grants, J.Teteris**. Photoinduced mass transport in amorphous As-S-Se filma. Phys.Status.Solidi C, 9, No.12 (2012) 2586-2589.

Other publications

11. **R. Zabels, I. Manika, R. Grants**. The impact of light on micromechanical properties of ZnSe. Program and materials of 4th International Conference on Radiation Interaction with Material and Its use in Technologies, Kaunas, Lithuania, 2012, pp. 490-493.
12. V.Sursajeva, **F.Muktepavela**. Experimental investigation of kinetic properties of equilibrium and nonequilibrium grain boundaries. Proc. of Intern Conf NMT -12, Sankt Petersburg , June 27-29, pp.120-126.

Lectures on Conferences

International Conference on Functional materials and Nanotechnologies FM&NT 2012, 17–20 April 2012, Riga, Latvia

1. F. Muktepavela, R. Zabels, V Sursajeva, L. Grigorjeva, K. Kundzins. The role of nanopowder particle surfaces and grain boundary defects in the sintering of ZnO ceramics. Abstracts, p.128.
2. J. Maniks, R. Zabels and I. Manika. Shear banding mechanism of plastic deformation in LiF irradiated with swift heavy ions. Abstracts 129.

3. A. Rusakova, J. Maniks, K. Schwartz, A. Dauletbekova, A. Akilbekov, V. Lisitsin and M. Zdorovets. Color centers and structural damage in LiF induced by 150 MeV Kr ions. Abstracts, p.207.

4th International Conference Radiation Interaction with Material and its use in technologies, May 14-17, 2012 Kaunas, Lithuania

4. R.Zabels, I.Manika, R.Grants. The impact of light on micromechanical properties of ZnSe.

E-MRS 2012 Fall Meeting, 17-21 September, 2012, Warsaw, Poland

5. R.Zabels, K.Schwartz, I.Manika Swift heavy ion induced structural damage and hardening of MgO.

8 th International Symposium on Swift Heavy Ions in Matter (SHIM-2012), October 24-27, Kyoto, Japan

6. I.Manika, J. Maniks, R. Zabels, A Akilbekov, A.Rusakova, A Dauletbekova Ion induced structural modifications in LiF crystals, Abstract Book, p.296.

International Conference NMT-12, June 27-29. 2012, Saint Petersburg, Russia

7. V.Sursajeva, F.Muktepavela. Experimental investigation of kinetic properties of equilibrium and nonequilibrium grain boundaries.

28th Scientific conference of ISSP, 8-10 February 2012, Riga, Latvia

8. R. Zabels, J. Maniks, R. Grants. High energy ion induced changes of structure and mechanical properties in polycrystalline graphite., Abstracts p.27.

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9. Zabels R. K.Kundziņš, L.Grigorjeva F.Muktepavela, ZnO nanopulveru morfoloģija un to ietekme uz ZnO keramikas saķepināšanas procesiem.

LABORATORY OF ORGANIC MATERIALS

Head of laboratory Dr. phys. M.Rutkis

Scientific Staff:		Students:	
Mārtiņš Rutkis	Dr.phys.	Kaspars Pudžs	BSc
Lilita Gerca	Dr.chem.	Raitis Gržibovskis	BSc
Oskars Vilītis	Dr.phys.	Eduards Titavs	BSc
Aivars Vembris	Dr.phys.	Mārtiņš Narels	
Andrejs Tokmakovs	MSc.	Santa Popova	
Jurģis Sīpols	MSc.	Zane Kalniņa	
Andrejs Jurģis		Igors Mihailovs	
Jānis Bussenbergs		Rolands Usāns	
		Arturs Bundulis	

PhD students:

Elīna Laizāne	MSc.
Jānis Latvels	MSc.
Edgars Nitišs	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;
- 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 and Kurtz powder methods and Mach – Zender interferometry.

Scientific projects of the Latvian Council of Sciences

09.1548	"Physical Processes in Multilayer and Multicomponental Structures" (2009-2012)
10.0032	„Development of research and technology potential for elaboration of new and nanostructured materials and related applications." subproject „Supramolecular nanostructuring of photonic materials – theoretical modeling and experimental investigations" (2010-2013)

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."

ERAF projects of the activity 2.1.1.1."Support of science and research"

No.2010/0308/2DP/2.1.1.1.0/10/APIA/VIAA/051, "Development of Polymer EO modulator prototype device"

No. 2010/0252/2DP/2.1.1.1.0/10/APIA/VIAA/009, "Materials and its tandem structure for solar cells" (2010-2013)

No. 2010/0275/2DP/2.1.1.1.0/10/ APIA/VIAA/124, „RTD for fabrication of diffractive optical elements" (2010-2013)

International projects

"Osmoze" – cooperation programme between France and Latvia for the development of science and technology: Project „Phthalocyanine architectures for sensor application" (2012-2013)

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).

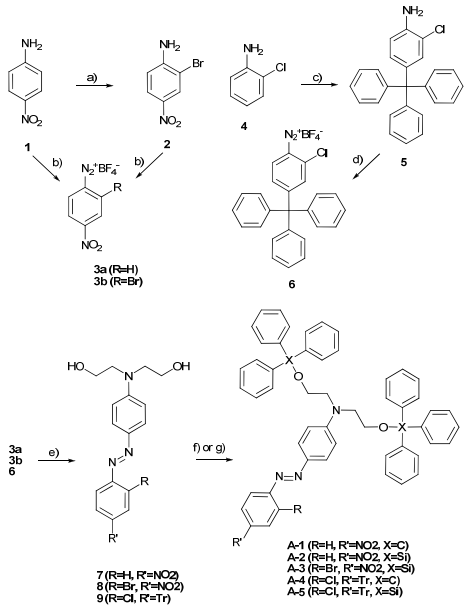
Main results

TRIPHENYL MOIETIES AS BUILDING BLOCKS FOR OBTAINING MOLECULAR GLASSES WITH NONLINEAR OPTICAL ACTIVITY

Kaspars Traskovskis,[a] **Igors Mihailovs,[a,b] Andrejs Tokmakovs,[b] Andrejs Jurgis,[b]** Valdis Kokars[a] and **Martins Rutkis[b]**

The incorporation of trityl and triphenylsilyl groups into low molecular weight molecules allows obtaining stable molecular glasses. Series of materials based on N-phenyldiethanolamine core were synthesized bearing different azobenzenes and benzylydene-1,3-indandione as active chromophores. Molecular hyperpolarizability of synthesized compounds was calculated by Restricted Hartree–Fock method with basis 6-31G and measured in solutions by hyper-Rayleight scattering. Non-linear optical (NLO) activity of thin glassy films was confirmed after corona polling procedure. Thermal sustainability of NLO response by up to 85° C was achieved. Quantum chemical calculations of compounds revealed increased sterical bulk and conformational freedom of triphenylsilyl moiety. While the presence of triphenylsilyl group results in more stable glasses and increased material nonlinearity, in the case of trityl groups, measured glass transition temperatures are higher.

In this paper, we have presented a new structural design of low molecular organic glasses suitable for photonics studies. Synthesized triaryl functionalized N-phenyldiethanolamine derivatives has shown excellent solubility in non-polar organic solvents and are able to form good optical quality glassy films without a mixing in a polymer matrix. Stability of the films was sufficient to undergo corona discharge poling at the elevated temperatures, making the materials NLO active.



Scheme 1 Synthesis of azobenzene containing molecular glasses

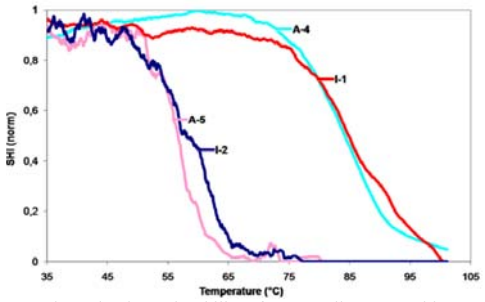
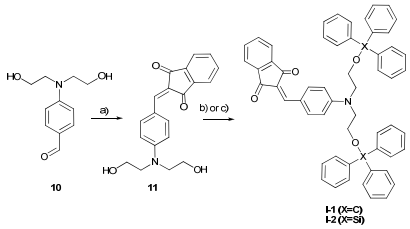


Fig. 4 Polar order thermal stability of structurally comparable chromophore pairs. Trityl group containing compounds show significantly higher thermal sustainability



Scheme 2 Synthesis of indane-1,3-dione fragment containing molecular glasses

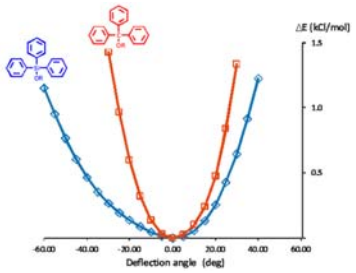


Fig.1 Trityl and triphenylsilyl group phenyl ring rotation potential energy wells according to RHF 6-31G(p,d) simulation. Deflection angle is CPh2-CPh1-C-O or CPh2-CPh1-Si-O torsion angle detune from equilibrium position

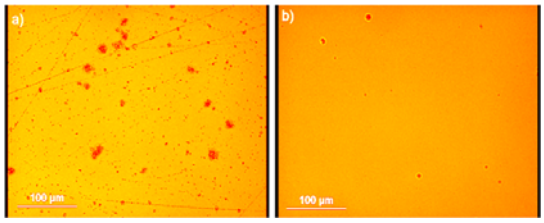


Fig. 5 Optical microscope images of corona poled samples for compounds I-1(a) and I-2 (b) after a month of storage. Sample (a) contains numerous growing crystals while sample (b) reveals no visible signs of crystallization.

Triphenyl moieties as crystallization preventing structural elements have shown no effect on electronic properties of push-pull NLO chromophores. QC calculations have revealed noticeable differences in the chosen triphenyl moieties structure regarding the conformational freedom and occupied volume. Due to these dissimilarities the replacement of carbon with silicon in triphenyl core has contradictory impact on the properties of investigated NLO active organic glasses. From one hand, the amorphous phase formation favours the presence of bulkier and conformationally less defined triphenylsilyl group what was most evidently demonstrated in the case of azochromophore containing compounds. At the same time this structural element reduces the thermal stability of polar order in corona poled films. For structurally comparable pairs (**A-4** and **A-5**, **I-1** and **I-2**) the temperature corresponding to the half vanished NLO activity is lowered by ~30° C. It is noteworthy that the presence of additional trityl group in the acceptor part of azochromophores enhanced amorphous phase stability and the polar order thermal stability of corona poled films. At the same time the increased rigidness of triphenyl groups resulted in lowered nonlinearity due to obstructed alignment of molecular dipoles along the external electrical field direction during corona discharge poling.

THERMAL AND OPTICAL PROPERTIES OF RED LUMINESCENT GLASS FORMING SYMMETRIC AND NON SYMMETRIC STYRYL-4H-PYRAN-4-YLIDENE FRAGMENT CONTAINING DERIVATIVES

Aivars Vembris[a], Elmars Zarins[b], Janis Jubels[b], Valdis Kokars[b], **Inta Muzikante**[a], Arunas Miasojedovas[c], Saulius Jursenas[c]

Dyes with amorphous structure deposited from organic solvents and having good fluorescence properties show potential for photonic device applications. Organic glass-forming symmetric and non symmetric styryl- derivatives of 2(2,6-substituted-4*H*-pyran-4-ylidene)-malononitrile (it has backbone of known laser dye 4-(dicyanomethylene)-2-methyl-6-[*p*-(dimethylamino)styryl]-4*H*-pyran), 2(2,6-substituted-4*H*-pyran-4-ylidene)-1*H*-indene-1,3(2*H*)-dione and 2(2,6-substituted-4*H*-pyran-4-ylidene)-pyrimidine-2,4,6(1*H*,3*H*,5*H*)-trione were synthesized and investigated. Glass transition temperatures higher than 110ºC were achieved. The absorption bands in dichloromethane solution cover the spectral region from 450 nm to 600 nm with fluorescence maxima between 580 nm and 690 nm. Photoluminescence quantum yields of the compounds in solution are between 0.3 and 0.55, which is reduced by one order in thin amorphous film prepared from volatile organic solvents. Incorporation of bulky trityloxyethyl groups in the derivatives results in significant reduction of aggregate formation. Thus fluorescence concentration quenching is reduced, enabling higher doping levels as compared to the unsubstituted 4-(dicyanomethylene)-2-methyl-6-[*p*-(dimethylamino)styryl]-4*H*-pyran dye.

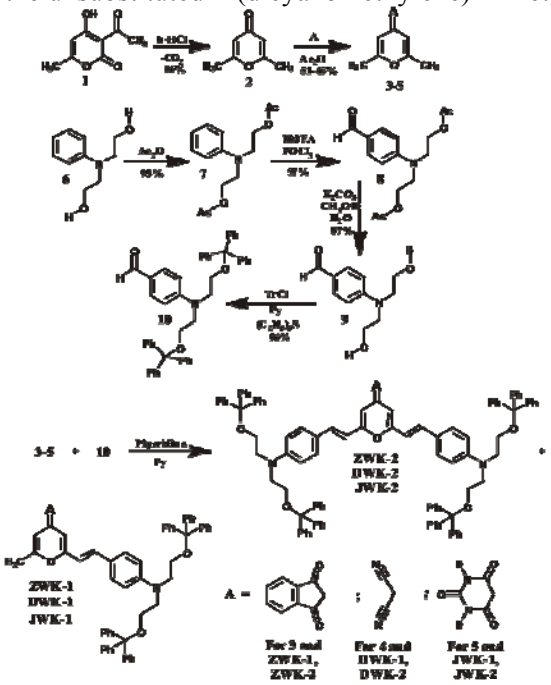


Figure 1. Synthesis of glass forming styryl-4H-pyran-4-ylidene fragment containing derivatives

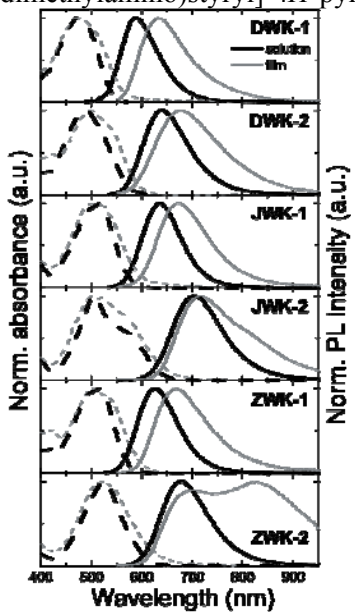


Figure 2. Absorption (dashed lines) and fluorescence (solid lines) spectra of compounds **DWK**, **JWK** and **ZWK** in dilute solutions and neat films.

Table 1. Thermal properties of synthesized compounds. T_g – glass transition temperature, T_m – melting temperature, T_d – decomposition temperature

	DWK		JWK		ZWK	
	1	2	1	2	1	2
T_g,	-	112	120	127	110	118
T_m,	250	148	146	144	212	144
T_d,	267	296	266	283	274	284

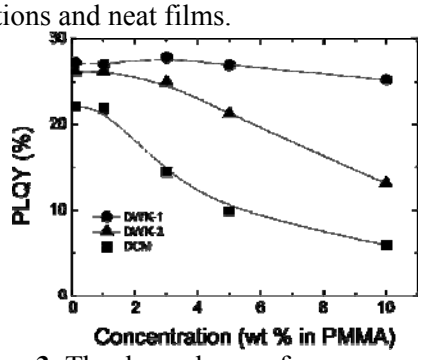


Figure 3. The dependence of photoluminescence PLQY on concentration of DWK-1 and DWK-2 and DCM dyes in PMMA matrix.

The synthesized compounds **ZWK-1, DWK-1, JWK-1** and **ZWK-2, DWK-2, JWK-2** form a glassy structure in the solid state from volatile organic solvents. The glass transition temperature of almost all compounds is higher than 110ºC. Absorption maxima lie between 450 nm to 550 nm, depending on electron acceptor and electron donor groups in the compound structure. The maximum of luminescence spectra is observed between 580 nm and 690 nm. In the case of two-donor groups (**ZWK-2, DWK-2, JWK-2)** the luminescence spectra consist of two bands in solid state compared to the solution. The second band is attributed to the excimer states. The photoluminescence quantum yield in solution is up to 0.54. It drops one order of magnitude in the solid state due to the closer intermolecular distance between molecules and probable formation of a high density of dimers, which results in a strong excitonic interaction in the thin solid films. Incorporation of bulky trityloxyethyl groups results in less aggregate formation of the dye molecules in the polymer films compared to the same type of molecules without the trityloxyethyl groups.

FLUORESCENCE AND AMPLIFIED SPONTANEOUS EMISSION OF GLASS FORMING COMPOUNDS CONTAINING STYRYL-4H-PYRAN-4-YLIDENE FRAGMENT

Aivars Vembris[1], **Inta Muzikante**[1], Renata Karpicz[2], Gytis Sliauzys[2], Arunas Miasojedovas[3], Saulius Jursenas[3] and Vidmantas Gulbinas[2]

Potential of glassy films of newly synthesised low molecular weight organic molecules for light amplification and lasing applications has been investigated by analysing fluorescence, transient differential absorption and amplified spontaneous emission properties. These non-symmetric and symmetric molecules contain styryl-4H-pyran-4-ylidene fragment with three different electron acceptor groups: dicyanomethylene, barbituric acid, indene-1,3-dione. Fluorescence quantum yields of the investigated compounds in solutions are between 0.32 and 0.54, while they drop down by an order of magnitude in thin solid films. Incorporation of bulky side groups reduced excitonic interactions enabling manifestation of amplified spontaneous emission in the neat films of the investigated derivatives.

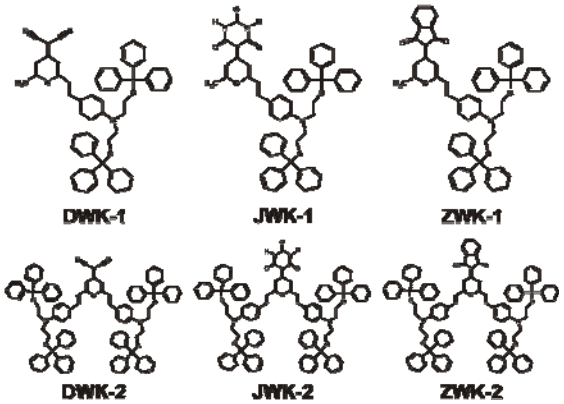


Figure 1. Styryl-4H-pyran-4-ylidene fragment containing derivatives **ZWK-1**, **ZWK-2**, **JWK-1**, **JWK-2**, **DWK-1**, **DWK-2**.

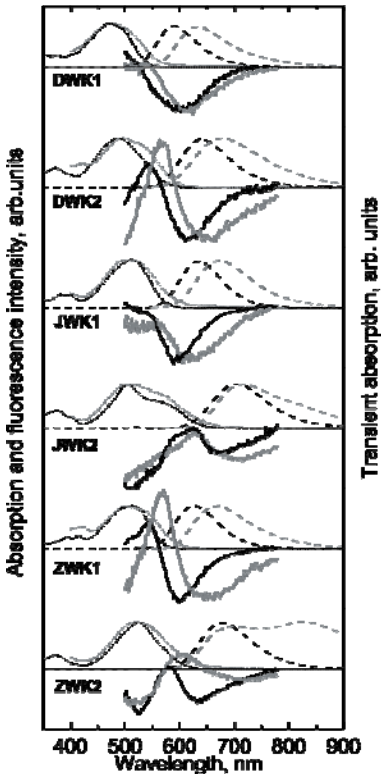


Figure 3. Absorption (thin solid line), fluorescence (dashed line) and differential absorption (thick solid line) spectra of all

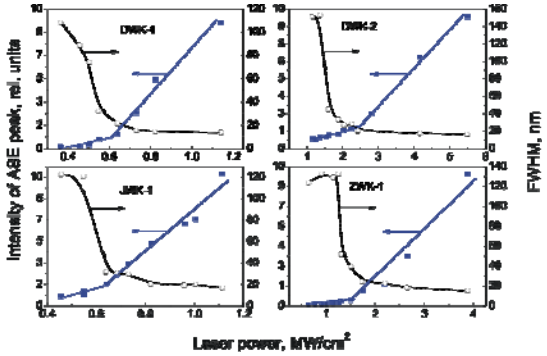


Figure 5. Full width at half maximum (circles) and ASE intensity (squares) as a function of irradiation intensity for **DWK-1**, **DWK-2**, **JWK-1**, **ZWK-1** compounds in thin solid film. Lines are guides for the eye.

investigated compounds in dilute dichloromethane solution (black lines) and neat films (gray lines).

The possibility of achieving amplified spontaneous emission in neat films of the glass forming **DCM** derivatives bearing bulky side groups demonstrates their applicability for the lasing applications despite a very low fluorescence quantum yield. However, a low fluorescence quantum yield caused by short excited state lifetimes of the molecules in films sets limitations on their applications. Such materials may be used for amplification or generation of short light pulses under their excitation with also short light pulses. However, these materials are not suitable for OLED fabrication or lasing under continuum wave excitation conditions.

All **DCM** derivatives bearing one donor group and different acceptor groups show similar spectroscopic and light amplification properties Attachment of two bulky donor groups negatively affects the light amplification properties of the compounds both in solutions and in neat solid films. This negative influence is less expressed for **DWK-2** compound, which shows light amplification properties similar to those of **DWK-1** compound. Amplification properties of two other compounds **ZWK-2** and **JWK-2** revealed by transient absorption investigations are much worse; consequently amplified spontaneous emission in neat films of these materials has not been achieved.

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2. **A.Vembris**, E.Zarins, J.Jubels, V.Kokars, **I.Muzikante**, A.Miasojedovas, S.Jursenas, Synthesis, thermal and optical properties of red luminescent glass forming symmetric and non symmetric styryl-4H-pyran-4-ylidene fragment containing derivatives, *Optical Materials*, 34, 2012, pp 1501 – 1506, doi: 10.1016/j.optmat.2012.02.051
3. **A.Vembris, I.Muzikante**, V.Gulbinas, R.Karpicz, G.Sliauzys, A.Miasojedovas, S.Jursenas, Fluorescence and amplified spontaneous emission properties of glass forming styryl-4H-pyran-4-ylidene fragment containing derivatives, *Journal of Luminescence*, 132, No 9, 2012, pp 2421–2426, doi: 10.1016/j.jlumin.2012.03.063
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5. **E. Nitišs**, R. Usans, **M. Rutkis**, Simple method for measuring bilayer system optical parameters, *SPIE Proceedings,* 8430, 84301C (2012), DOI: 10.1117/12.922317
6. E. Zarins, K. Siltane, E. Misina, V. Kokars, K. Lazdovica, **A. Vembris**, V. Kampars, **I. Muzikante, M. Rutkis**, Synthesis, optical and thermal properties of glassy trityl group containing luminescent derivatives of 2-*tert*-butyl-6-methyl-4*H*-pyran-4-one, *SPIE Proceedings,* 8435, 84351Q, (2012), DOI: 10.1117/12.921996

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Lectures on Conferences

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1. Santa Popova, Aivars Vembris, Inta Muzikante, Electroluminescence properties of organic compounds in amorphous state, Book of Abstracts, p.67
2. K.Pudzs, I.Muzikante, M.Rutkis, J.V.Grazulevicius, R.Reghu, Study of elektrical properties of thin film of perylene derivatives, Book of Abstracts, p.65
3. R.Gržibovskis, I.Muzikante, J.Latvels, B.Turovska, P.J.Pastors, V.Kampars, , Photoconductivity processes in polycrystalline films of DMABI derivatives, Book of Abstracts, p.66
4. E.Titavs, E.Nitišs, M.Rutkis, Study of internal structure of thin polymer layers after poling with corona triode, Book of Abstracts, p.23

International Young Scientist Conference "Developments in Optics and Communications 2012", Riga, Latvia, April 12-14

5. K.Pudzs, J.V.Grazulevicius, I.Muzikante, Determination of energy structure of bay substituted perylene bisimides in thin films, 2012, Book of Abstracts, p. 44
6. M.Narels, E.Laizane, I.Muzikante, Influence of temperature on photoisomerisation process of azobenzene molecules doped in polymer thin film, Book of Abstracts, p. 38
7. S.Popova, A.Vembris, I.Muzikante, Glassy forming low molecular weight organic compounds and their electroluminescent properties, Book of Abstracts, p. 40
8. R.Grzibovskis, J.Latvels, I.Muzikante, B.Turovska, Relation between energy levels and redox potential of DMABI derivatives, Book of Abstracts, p. 42
9. E. Titavs, E. Nitišs, M. Rutkis, Effect of corona poling parameters on polymer film poling efficiency, Book of Abstracts, p. 54
10. A.Vembris, S.Popova, K.Pudzs, I.Muzikante, Electrical and optical properties of glass forming indan-1,3-dione pyranderivatives, Book of Abstracts, p. 100
11. E. Nitišs, M. Rutkis, Basic principles of EO polymer waveguide modulator development, Book of Abstracts, p. 76

International Conference on Functional materials and Nanotechnologies FM&NT 2012, April 17 – 20, 2012, Riga, Latvia

12. I. Muzikante, M. Rutkis, V. Kampars, P.J. Pastors, B. Turovska, A. Jurģis, J. Sīpols, R. Gržibovskis, Assessment of quantum chemical and experimental methods for ionization energy and electron affinity evaluation of organic thin films. Book of Abstracts, p 111
13. I. Kaulachs, G. Shlihta, L. Gerca, P. Shipkovs, V. Grehovs, A. Murashov, J. Kalnachs, A. Cielavs, A. Ivanova, Non-Planar Phthalocyanine for Improved Optical Coverage in Bulk Heterojunction Solar Cell, Latvia, Book of Abstracts, p 180
14. K.Pudzs, J.Latvels, A.Vembris, I.Muzikante, Electrical properties and morphology of pentacene thin films evaporated on different temperature substrate, Book of Abstracts, p 187
15. A. Tokmakovs, M. Rutkis, K. Traskovskis, E. Zariņš, L. Laipniece, V. Kokars, V. Kampars, Nonlinear optical properties of low molecular organic glasses formed by triphenyl modified chromophores, Book of Abstracts, p 196
16. I. Mihailovs, J. Kreicberga, V. Kampars, S. Miasojedovas, S. Juršėnas, L. Skuja, M. Rutkis, Hyper-Rayleigh Scattering and Two-Photon Luminescence of Phenylamine–Indandione Chromophores, Book of Abstracts, p 197
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18. K. Traskovskis, I. Mihailovs, A. Tokmakovs, V. Kokars, M. A. Rutkis, An improved molecular design of obtaining NLO active molecular glasses using triphenyl moieties as amorphous phase formation enhancers, Technical summaries, p. 279
19. E. Zarins, K. Siltane, E. Misina, V. Kokars, K. Lazdovica, A. Vembris, V.Kampars, I. Muzikante, M. Rutkis, Synthesis, optical and thermal properties of glassy trityl group containing luminiscent derivatives of 2-tert-butyl-6-methyl-4H-pyran-4-one, Technical summaries, p. 295

20. A. Vembris, K. Pudzs, I. Muzikante, Light-emitting thin films of glassy forming organic compounds containing 2-tert-butyl-6-methyl-4H-pyran-4-one, Technical summaries, p. 299
21. E. Laizane, D. Gustina, I. Muzikante, M. Narels, Temperature influence on photoisomerisation kinetics in thin polymer films doped with carboxyl group azobenzene derivative, Belgium, Technical summaries, p. 299
22. E. Nitiss, R. Usans, M. Rutkis, Simple method for measuring bilayer system optical parameters, Technical summaries, p. 192
23. R. Grzibovskis, I. Muzikante, J. Latvels, M. Indrikova, V. Kampars, P. Pastors, Relation of energy levels in thin films of polar photoconductive molecules, Technical summaries, p. 298

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24. K. Pudzs, A. Vembris, R. Grzibovskis, B. Turovska, Electrical properties and energy structure of thin films of glass forming compounds containing styryl-4H-pyran-4-ylidene fragment, , Abstracts, p. 120
25. A. Vembris, K. Pudzs, I. Muzikante, Light emission properties of solution processed thin films from organic compounds containing pyranyliden fragment, , Abstracts, p. 136

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26. K. Pudzs, A. Vembris, R. Grzibovskis, B. Turovska, Energy Levels of Glass Forming Pyranyliden Derivatives and Their Electrical Properties in Amorphous Thin Films, Abstracts, p. 92
27. S. Popova, A.Vembris, Photoluminescence and Electroluminescence Properties of Glassy Forming Low Molecular Weight Organic Compounds, Abstracts, p. 88
28. M. Narels, E. Laizane, I. Muzikante, Impact of Temperature on Photoinduced Switching Effect of Azobenzene Molecules Doped in Polymer Thin Film, Abstracts, p. 83
29. R. Grzibovskis, J. Latvels, I. Muzikante, Correlation between Threshold Value and Optical Energy Gap in Thin Films of DMABI Derivatives, Abstracts, p. 141
30. Andrejs Tokmakovs, Martins Rutkis, Kaspars Traskovskis, Elmars Zarins, Lauma Laipniece, Valdis Kokars, Valdis Kampars, Properties of EO Active Molecular Glasses based on Indandione and Azobenzene chromophores, Abstracts, p. 63

Baltic Polymer Symposium, 2012, September 19-22, 2012, Liepaja, Latvia

31. A. Šternbergs, M. Spriņģis, M. Rutkis, Latvian National Research Program and Center as framework for polymer material development, Programme and Proceedings, p. 19

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 deposition

• Material characterization by spectroscopic methods (Raman scattering, Furrier IR, optical and Xray absorption, EXAFS), electrical and electrochemical impedances, 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

• Functional coatings and multi layer electrochemical systems

• Hydrogen absorption phenomena in metals, semiconductors and insulators

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

• New measurement technologies and instruments with artificial intellect (encl., eNose)

• Development methods and techniques for quality and reliability testing for lead – free joints of PCB

• Hydrogen technologies (production, storage, transportation, application); renewable energy technologies (solar, wind, static electricity, water, microbial fuel cells);

• Development of cathode materials for Lithium thin film batteries;

• Gas sensors and sensor arrays; odour removal with adsorbent and low temperature plasma discharge technologies.

• Tritium analysis

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.
- Application of electrical and electrochemical impedances for characterization of ionic systems, nanostructured and porous materials, composites.
- Development of nanostructuring methods 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.
- Development methods and techniques for quality and reliability testing for lead-free joints of printed circuit boards.
- 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 filtration.
- 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, wind, static electricity, water, algae and microorganisms);
- Gas sensors and sensor arrays for gas and odour monitoring; odour removal with adsorbents and corona discharge technologies;
- 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
- 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 EXAFS Spectroscopy – Head of Laboratory Dr. hab. phys.J.Purans

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Cooperation

Latvia

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2. University of Latvia, Faculty of Biology (Prof. I.Muiznieks, Prof. V. Nikolajeva) and Faculty of Economics and Management (Prof. B.Sloka)
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4. Riga Technical University - Institute of Inorganic Chemistry and Institute of Silicate Materials (Dr. J. Grabis, Dr. E.Palcevskis, Dr. A. Dindune, G.Mežinskis).
5. Riga Technical University, Institute of Idustrial Electronics and Energetics (Prof. L.Ribickis, Dr. O. Krievs).
6. Latvia University of Agriculture, Research Institute of Agricultural Machinery,
7. University of Latvia, Faculty of Physics and Mathematics.
8. University of Latvia, Faculty of Medicine
9. Latvian Electroindustry Business Innovation Centre (LEBIC).
10. Institute of Physical Energetics, Riga
11. Housing and Environment Department of Riga City Council, Riga,
12. Riga Energy Agency, Riga City Council

13. SIA „EMU PRIM”,
14. JSC „Riga Electric Machine Building Works”,
15. IC „Plazma PL”,
16. SIA “Adviser Union”
17. Latvian Hydrogen Association
18. JSC “Sidrabe”
19. JSC “Valmiera Glass Fiber”

France
1. Setaram Instrumentation

Czech Republic
University of Ostrava, Faculty of Science (Prof. Bogumil Horák)

Germany
1. Max-Planck-Institut für Festkörperforschung (Stuttgart, Germany) – Prof. J.Maier.
2. Kassel University (Prof. Jürgen Zick)
3. Institute of Solid State Research, Forschungszentrum Jülich (Jülich, Germany) – C. Lenser, Dr. R. Dittmann, Prof. K. Szot, Prof. R.Waser.

Italy
1. University of Trento (Trento, Italy) - Prof. G.Dalba, Prof. P.Fornasini
2. IFN-CNR CeFSA (Trento, Italy) - Dr. F. Rocca.
3. Universita della Calabria (Arcavacata di Rende, Italy) - Prof. E.Cazzanelli.

Lithuania
University of Vilnius - Department of Physics (Prof. A.Orliukas)
Lithuanian Institute of Energetic (Prof. D. Milcius)

Norway
Institute for Energy Technology, Kjeller, Prof. Volodimir Yartis

Russia
1. Joint Institute for Nuclear Research (Dubna, Russia) - Dr. S.I. Tjutjunnikov.
2. St. Petersburg University (St. Peterhof, Russia) - Prof. R.A. Evarestov
3. Moscow State Engineering Physics Institute (Moscow, Russia) – Prof. A.Menushenkov.

Spain
Instituto de Carboquímica (CSIC), Zaragoza, Spain (Dr. Wolfgang Maser)

Sweden
The Angstrom Laboratory, Uppsala University, Uppsala, Sweden – Prof. C.G.Granqvist.

Participation in Research Projects:

Latvian:
1. National Research Program “Innovative multifunctional materials, signal processing and informatic technologies -IMIS”, project No. 1 – Investigation functionalization of glass fiber fabrics.

2. Cooperation project of. Latvian Council of Science SP 10.0032 “Development of research and technology potential for elaboration of new and nanostructured materials

and related applications" -1.4. "Functional caoatings, processes and technologies for modification physicochemical properties of materials"

3. Cooperation project of. Latvian Council of Science SP 10.0040 "Investigation of Latvian renewable raw materials – flax and hemp products for development of innovative technologies and new functional materials".

4. National Research Program "Energy and Environment", Project No.4 "Research of methods for hydrogen production, storage and energy release, and development of prototypes for application in national economy"

5. Grant from Latvian Council of Science No. 09.1195 "Research and development of proton conducting PEEK polymer and composite membranes and catalysts for use in direct methanol and hydrogen fuel cells"

6. Grant from Latvian Council of Science No. 09.1192 "Research of properties and structure of nanosize composite materials for hydrogen storage and electrodes for water electrolysis"

7. "Structure of nano-oxide materials and self-organization in stochastic media "Latvian Government Grant Nr.09.1580 (2010-2012).

8. ESF Project "Nanomaterials for perspective energy effective solutions",. No 2009/0202/1DP/1.1.1.2.0/09/APIA/VIAA/141 (2009-2012).

9. "Structure of nano-oxide materials and self-organization in stochastic media" Latvian Government Grant Nr.09.1580, 2010-2012 (Head: J. Purans).

10. ESF Project "Nanomaterials for perspective energy effective solutions", 2009-2012 (Head: G. Zvejnieks , Responsible: A. Kuzmin, A. Anspoks).

11. Partners in ERAF Project Nr.2010/0243/2DP/2.1.1.1.0/10/APIA/VIAA/156, RTU PVS ID1524 „Solar thermal energy storage material development using sol-gel and vacuum coating technology" (Head A.Lusis)

International

1 .MNT ERA-NET Matera Project "Functional materials for resistive switching memories" (FMRSM), 2009-2012 (Head: R. Dittmann, Responsible: J. Purans).

2. Materials, Physical and Nanosciences COST Action MP0804: "Highly Ionised Pulse Plasma Processes", 2010 - 06.2013 (Head: J. Purans).

3. "Nano-structured test samples for a combined near-field and X-ray microscopy", "OSMOSE" collaboration France - Latvia, 2012 (Heads: J. Purans and D. Pailharey).

4**.** Mutual fundsTaiwan – Latvia – Lithuania cooperation project "Materials and processing development for advanced li ion batteries" (Head G.Bajars)
5.EFDA Fusion Technology task TW5-TTBB-006-D08 „Assessment of the effects of magnetic field, radiation and temperature on the tritium release from beryllium pebbles. Identification of chemical forms of tritium accumulated in the irradiated Be pebbles." (Principal investigator: Dr.chem. A. Vitins).

Didactic work at the University of Latvia

1. Master degree course "Solid State Ionics" at Faculty of Chemistry, UL – 4 credit points (G. Vaivars)
2. Course Fizi5028 "Structure and Description of Nanomaterials" at the Latvian University (A.Kuzmin).
4. Course Fizi7009 „Solid State Structure" at the Latvian University (A.Kuzmin).

Main results

Laboratory of Solid State Ionics

STUDY THE EFFECTS OF MOISTURE CONTENT ON THE ELECTRICAL PROPERTIES OF TECHNICAL TEXTILES BY IMPEDANCE SPECTROSCOPY

A Lusis[1], E Pentjuss, G Bajars, J Gabrusenoks , R Janeliukštis, L Jekabsone, J Zandersons

Application of metal coatings for the functionalization of technical fibres and fabrics faced with influence of moisture on functional properties, e.g., the impedance of the metal coated K-glass fabrics have strong dependence of content absorbed water or moisture. The stadies devoted to develop methodology for characterisation functional materials based on fabrics and model for interpretation of the electrical impedance spectra to obtained functional characteristics of technical textile fabrics. Model based on analyses of 3D plot of imaginary part of complex modulus spectra versus sample mass. Methodology helps to control content of adsorbed water in fabric and influence of moisture on the functional characteristics.

Electrochemical impedance and moisture content of glass fabric

The glass fiber fabrics have application at the wet conditions. Impedance measurements of sodium alumosilicate glass fabric in dependence on its moisture content are studied. The impact of pores of glass fibres and fabric components to electrochemical impedance of fabric are investigated.

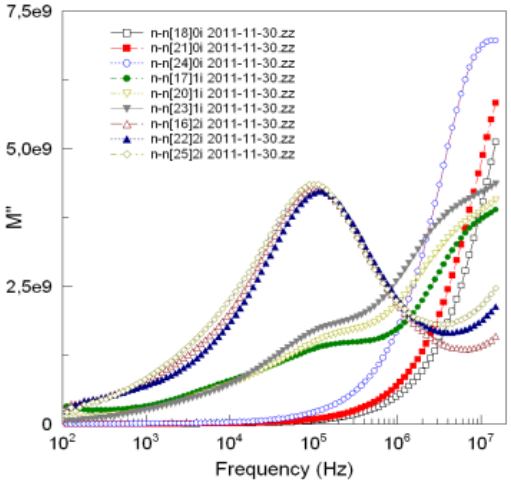

Fig. 1. M" spectra: moisture reduced 1% steps.

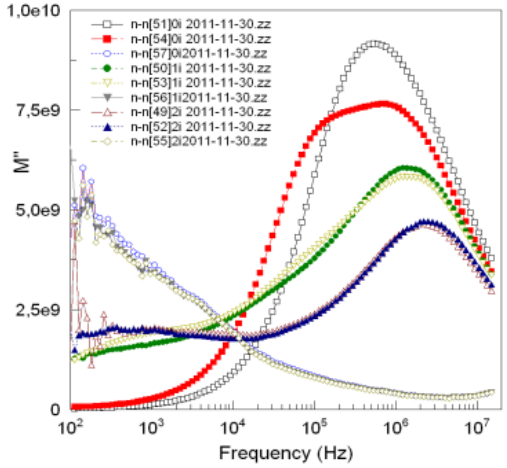

Fig. 2. Moisture reduced to dry state

The fabric samples can be characterized as mechanical mixture of ionically and electronically conducting phases. The water in such hetero system serves as electrolyte which involved in electrochemical reactions with sample fixture electrodes as well as with metal particles. The impedance such cases have components related to electrode reactions, ion transfer over double layer and bulk (yarn framework) as well as relaxation of dipoles, ions and electrons (polarization of ions and H_2O). The sample fixture electrodes can be turned as blocking electrodes by thin insulator film (PET 33 μm; fabric thickness 450-500 μm).The impedance characteristics of fabrics analyzed at different moisture content. The best presentation impedance data is modulus M" spectra (Fig.1- Fig. 2.) and for studies the role of moisture in the fabrics.

The complex modulus $M(M', M'')=j\omega C_0 Z(Z', Z'')$method for analyses impedance spectra has been used., where C_0 – geometric capacitance of fixture electrodes, $M'=\omega C_0 Z''$ and $M''= \omega C_0 Z'$. From the last formula followed $M''= (Cp/\varepsilon_0)\ \omega\tau/[1+ (\omega\tau)^2]$,

where ε_o – vacuum dielectric constant, τ=CpRp – Maxwell relaxation time of charge carriers in bulk of sample, Cp, Rp - parallel circuit elements. The results of this study are presented by 3D graphs in Fig.3.

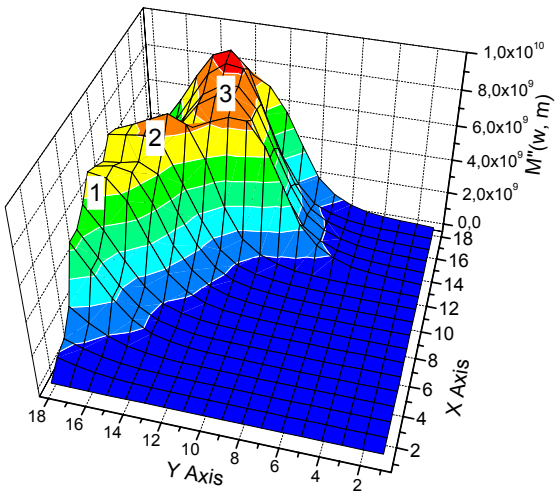

Fig.3a. M′′(ω, *m*) data 3D presentation for (0i) regions:
1-τ1=3E-8 sec
2-τ2=2E-7 sec
3-τ3=2E-6 sec

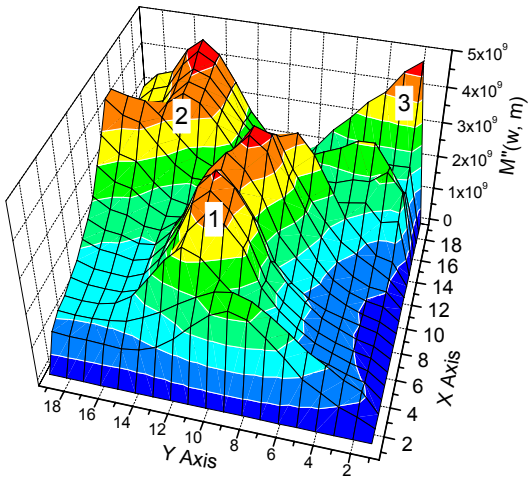

Fig.3b. M′′(ω, *m*) data 3D presentation for (2i) regions:
1-τ1=2E-5 sec
2-τ2=7E-7 sec
3-τ3=1E-4 sec

X Axis: matrix data for frequency 100 Hz – 15 MHz , Y Axis: matrix data for water content 0.35 – 0,08 g

The fixture electrode isolation method can helped to identify influence of moisture on the electrical properties of the fabrics based on glass fibers. The 3D plot of imaginary part complex modulus M′′(ω, m) can be good methodology to control water influence on electrical properties of metal coated and non coatd fabrics.
The Impedance spectroscopy is powerful tool for moisture control and to study the interaction of environment moisture with metal particles on the fibers and the influence on physical and chemical properties (corrosion of coatings) and functionality of technical textiles.). Moisture is the cause of the change in resistance time domain of fabrics in the form of electrochemical noise as result of moisture caused metal coating corrosion.

Flax and Hemp Fiber Functionalization Studies

A. Lusis, E. Pentjuss, J.Gabrusenoks , R.Janeliukštis, L.Veļķere, J.Zandersons, J. Balodis

Impedance spectroscopy of metal coated fabrics

Sustainable development of technical textiles is associated with natural fibers to replace the oil-producing fibers. In this context, it is necessary to carry out studies on the flax and hemp fiber and fabric functionalization for technical applications. The natural fibers (NF) as well as fabrics (FF) themselves are porous media. The porous media usually adsorbs some chemicals from environment. One of them is water and content of moisture in fabrics have to be controled.

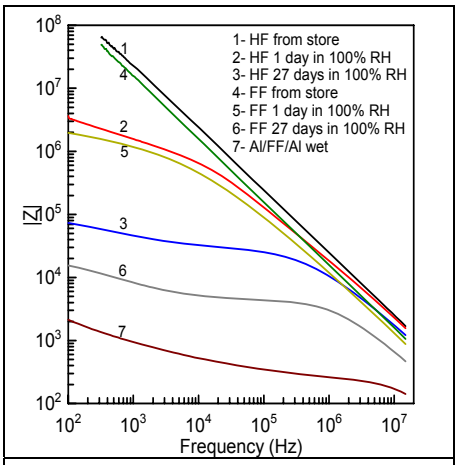

Fig.1.Impedance spectra of flax and hemp fabrics

Metal coatings are widely used for functionalization of fabrics for different technical applications. To characterize the metal coating is a problem in itself. First of all, to functionalize fibers or fabrics is to examine the content of moisture and its role on mechanical and physical properties. The impedance spectroscopy (IS) has been used to study moisture in FF and metal coated fabrics (M/FF/M). The impedance spectra of such samples are complicate due to heterogeneous and nonhomogeneous constitution.

The water content has strong influence on impedance modulus |Z| spectra (Fig.2). Analyses of |Z| spectra with simulation of equivalent circuit models, the best fit have been obtained with CPE for wet samples (Fig.2) and RC elements for dry samples. The value of capacitance C depends on water content and can be used for controle of moisture content in flax and hemp fabrics.

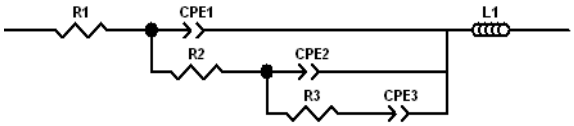

Fig.2. Equivalent circuit models for wet samples M/NF/M

R1= 0-2 Ohm R2≈R3=1-10 Ohm,
CPE1=0,1-100 μF CPE2= 50-1000 pF
CPE3=5-1000 nF L1=10-100 nH

Thermomechanical properties of metal coated hemp yarns

TGA shows two weight loss temperature areas of 30-110 ^{O}C (moisture retention) and 200-300 ^{O}C (hemp fiber carbonization). The thermo-mechanical strength of unmodified and modified hemp yarns is presented on Fig.3.

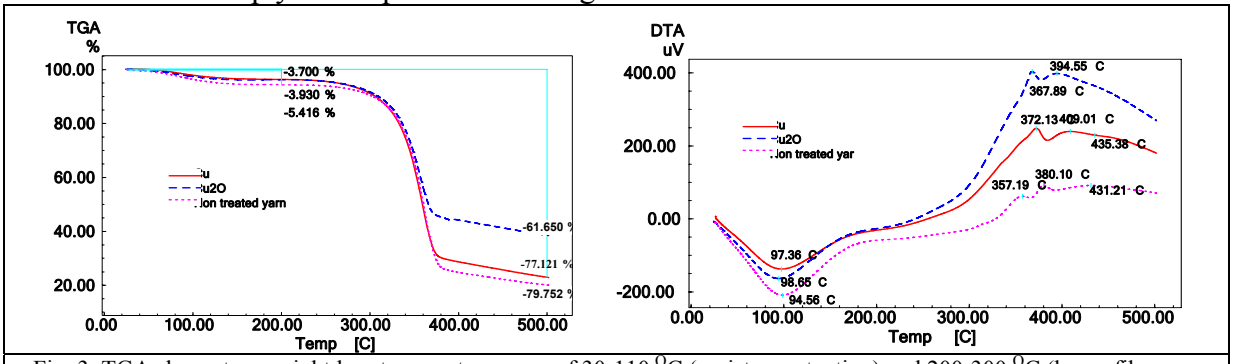

Fig. 3. TGA shows two weight loss temperature areas of 30-110 ^{O}C (moisture retention) and 200-300 ^{O}C (hemp fiber carbonization).

Modified yarn strength decreases by 30%, which correlated with the moisture content (6-12 %wt). Relative strength at 280 ^{O}C yarn with active particles respect to unmodified increased in the direction Cu, Cu_2O and CuO (fig.4; Fig.5).

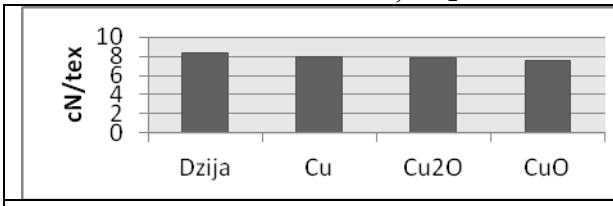

Fig. 4. Breaking load, 240^{o} C

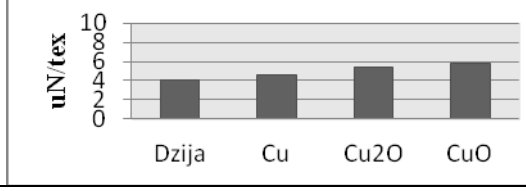

Fig. 5. Breaking load, 280^{o} C

PREPARATION OF TiO_2 THIN FILMS BY PARTICULATE SOL-ELECTROPHORETIC DEPOSITION

G.Bajars, I.Liepina, A. Lusis, J.Gabrusenoks, E. Pentjuss

Titanium dioxide thin films have been extensively studied because of their excellent properties for photocatalysis, gas sensors, ultrafiltration membranes, self-cleaning coatings, solar cells and photovoltaic applications. Many efforts have been made to improve their properties by preparing porous films with high surface area. There are a wide variety of preparation methods for TiO_2 thin films, e.g. sol-gel, doctor blade, spin coating, chemical vapor and sputter deposition. In this study nanocrystalline TiO_2 thin films have been prepared by sol-electrophoretic deposition process.

The first step was the preparation of TiO_2 sol. Titanium tetra-iso-butoxide (TTIB) was used as a precursor, hydrochloric acid as a catalyst for the peptization and deionized water as a dispersion media. A water-acid mixture was stabilized at 50 °C with continuous stirring. An appropriate amount of TTIB was added next forming the white precipitate that gradually peptized forming a clear sol.

For the electrophoresis growth, the Pt anode and cathode are placed parallel in an TiO_2 sol with a distance 1 cm in between. The cathodes used were metallic Cu and Ti, thin Pt layer on silicon, transparent indium tin oxide (ITO) on glass. A constant voltage of 0.5 – 0.6 V was applied by a dc power supply between the electrodes and held for 1 – 3 h. The as-deposited thin films were first dried at 100 °C for 24 h and then heated at a rate of 10 °C/min and were finally annealed at 500 °C for 2 h.

Obtained TiO_2 thin films were characterized by phase composition, morphology and their microstructures using X-ray diffraction, Raman spectroscopy, as well as transmission electron microscopy (TEM) and scanning electron microscopy (SEM). The optical properties of TiO_2 thin films were investigate by analyzing I – V curves. The possible correlations between the optical and structural properties of thin films are discussed.

TiO2 thin films have been obtained by a sol-electrophoretic deposition method on metallic Ti and Pt substrates. X-ray diffraction, Raman spectroscopy and scanning electron microscopy were used to investigate the structure and morphology of plated materials. Annealed TiO2 films mainly are formed in anatase structure with different morphology depending on substrate material. Light induced potential measurements indicate that the morphology substantially have an impact on photoactivity of TiO2 thin films.

CHARACTERIZATION OF LiFePO4/C COMPOSITE THIN FILMS USING ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY

G Bajars, G Kucinskis, J Smits, J Kleperis, A Lusis

The composite LiFePO4/C thin films were prepared on steel substrate by radio frequency (RF) magnetron sputtering. Electrochemical properties of the obtained thin films were investigated by cyclic voltammetry charge-discharge measurements and electrochemical impedance spectroscopy (EIS). The films annealed at 550 °C exhibited a couple of redox peaks at 3.45 V vs. Li/Li^+ characteristic for the electrochemical lithium insertion/extraction in $LiFePO_4$. At low current rate such composite thin film showed a discharge capacity of over 110 mAh g^{-1}. The dependence of charge transfer resistance, double layer capacitance and lithium diffusion coefficients on applied electrode potential were calculated from EIS data. Determined values of lithium diffusion coefficient were in the range from $8.3 \cdot 10^{-13}$ cm^2 s^{-1} to $1.2 \cdot 10^{-13}$ cm^2 s^{-1} at 3.4 V and 3.7 V, respectively.

DEVELOPMENT OF COATINGS ON BLACK ENAMEL AND METHOD FOR DETERMINATION RADIATION ABSORPTION AND EMISSION CHARACTERISTICS

J.Balodis, G.Bajars, J.Gabrusenoks, I.Liepiņa, A.Lūsis, G.Mežinskis[*],
[*]*Institute of Silicate Materials, Riga Technical University*

Selective absorption of solar radiation in the development of coatings is used enamel on iron-chromium oxide pigment base. The spectral characterization of the enamel was applied to infrared and visible light spectroscopy. The resulting black enamel samples show good enough solar radiation absorption properties in the visible spectrum and near-infrared region (300-1000 nm). This reflected radiation is less than 10% of the incident energy. Infrared region will remain the same level of reflection. It's not good enough to create low-emission coating. Such spectral properties does not provide minimal thermal energy emission in the infrared region (<2000 nm).

To enhance solar energy absorption and thermal emission parameters of concentrated solar radiation collector material are used multilayer thin film coatings. The metal and its oxide vacuum coating morphological and optical properties on the glass substrate and black enamel are studied on the circumstances of the deposition process (DC magnetron process). Copper oxide absorption studies showed that compared to CuO and Cu_2O light absorption graphs last graph peaks tend to move the most energy side. The X-ray diffraction graphs of NiO thin films obtained in DC magnetron process with gas mixture of Ar/O_2 80% / 20% and Ni target at different magnetron power supply voltages always showed the presence of NiO.

Preparation of TiO_2 thin coatings by particulate sol-electrophoretic deposition is carried out. Titanium tetra-iso-butoxide (TTIB) was used as a precursor and hydrochloric acid as a catalyst. For the electrophoresis growth, the Pt anode and cathode are placed parallel in an TiO_2 sol with a distance 1 cm in between. A constant voltage of 0.5 – 0.6 V was applied by a DC power supply between the electrodes. Obtained TiO_2 thin films were characterized by phase composition, morphology and their microstructures using X-ray diffraction, Raman spectroscopy, as well as transmission electron microscopy (TEM) and scanning electron microscopy (SEM). The optical properties of TiO_2 thin films were investigate by analyzing I – V curves.

APPLICATION IMPEDANCE SPECTROSCOPY TO STUDY ZINC AND NICKEL FERRITES

A. Lusis, A.Sutka*, G. Mezinskis*
**) Institute of Silicate Materials, Riga Technical University,*

For characterization of gas sensor material, synthesized by sol-gel auto combustion method the impedance spectroscopy were employed as well as to sdudy:

- Electric and dielectric properties of nanostructured stoichiometric and excess-iron Ni–Zn ferrites,
- Properties of Ni–Zn ferrite thin films deposited using spray pyrolysis,
- Influence of iron non-stoichiometry on spinel zinc ferrite gas sensing properties,
- An alternative method to modify the sensitivity of p-type NiFe2O4 gas sensor.

High DC resistivity and low dielectric losses of thin Ni1−xZnxFe2O4 films are explained by mixed n-p conductivity and nanograin structure of spray pyrolysis deposited coatings which are changing with the ratio of Ni/Zn.It has been shown that the DC resistivity, dielectric loss and optical band gap of deposited films are influenced by the zinc content. It was found that the sensors cooled with lower rate exhibited better sensing performance, due to increase of resistance. The influence of zinc ion concentration to the NiFe2O4 p-type semiconductor gas sensing characteristics is demonstrated. The change of sensitivity is deeply related to formation of small amount of the Fe2+ in compositions consisting zinc ion during sintering and surface conductance effects resulting with change type of conductivity for Ni-Zn ferrites. The impedance spectroscopy distinguishes influence on gas-sensing measurements different volatile organic compounds (VOCs) which were used as testing gases.The impedance spectroscopy helped to identify the contribution of the different sensing layer elements to the conduction.

Laboratory of EXAFS Spectroscopy

REVERSE MONTE CARLO MODELING OF THERMAL DISORDER IN CRYSTALLINE MATERIALS FROM EXAFS SPECTRA

J. Timoshenko, A. Kuzmin, J. Purans

In this work we propose the improved Reverse Monte Carlo (RMC) scheme for the analysis of the EXAFS spectra. In our approach, the difference between theoretical and experiment EXAFS signals is minimized during the RMC simulation simultaneously in k and R spaces by using the modified Morlet continuous wavelet transform of the EXAFS signal. Besides, to improve convergence during the simulation, we use slowly reducing “temperature” parameter in the Metropolis algorithm (the socalled simulated annealing method).

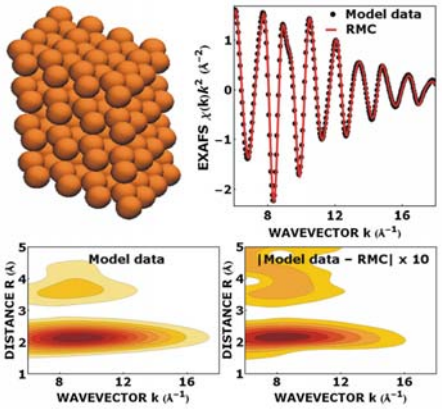

Fig.1. Upper panel: 4 × 4 ×4 supercell (128 atoms), used in the RMC simulations of crystalline germanium; model Ge K-edge EXAFS signal (dots) and EXAFS signal, obtained in RMC simulations (solid line). Bottom panel: WT moduli for model EXAFS signal and for difference between model and RMC EXAFS signals.

The use of the method is demonstrated on the example of the EXAFS spectra analysis for the model system and experimental data for crystalline germanium and rhenium trioxide. It is shown that the method allows one to reconstruct the 3D atomic structure of the compound taking into account the thermal disorder and to obtain the distributions of distances and bond angles describing the local structure around the absorber. Also the uncorrelated (MSD) and correlated (MSRD) thermal vibration amplitudes can be recovered with reasonable accuracy. The obtained results for Ge and ReO_3 are in good agreement with that previously found by conventional EXAFS analysis and molecular dynamics simulations.

PROBING THE OXYGEN VACANCY DISTRIBUTION IN RESISTIVE SWITCHING Fe-$SrTiO_3$ METAL-INSULATOR-METAL STRUCTURES BY MICRO-X-RAY ABSORPTION NEAR EDGE STRUCTURE

Ch. Lenser,[1,2] A. Kuzmin, J. Purans, A. Kalinko, R. Waser,[1,2,3] R. Dittmann[1,2]
[1] *Peter Grunberg Institute, Forschungszentrum Julich, Julich, Germany*
[2] *Julich-Aachen Research Alliance, Germany*
[3] *Institut fur Werkstoffe der Elektrotechnik, RWTH Aachen, Aachen, Germany*

Binary and ternary metal oxides as emergent materials for non-volatile memory applications are receiving an increasing amount of scientific attention due to the promising scalability, retention and switching characteristics of this material class. The key role of oxygen non-stoichiometry and oxygen-deficient oxide-phases as the underlying mechanism of the resistance change has been recognized for many different oxide systems. It is becoming widely accepted that the resistance switching process in SrTiO3 is related to the movement of oxygen vacancies and the associated electron doping. The mechanism of electroforming in Pt/Fe:SrTiO3/Nb:SrTiO3 MIM-structures proposes the local bypassing of the interfacial Schottky-type barrier by oxygen deficient filaments forming along extended defects. It is assumed that the films are already oxygen deficient after deposition. While this model is well supported by the electrical behaviour of the devices, direct experimental observation of the oxygen deficiency and the formation of the conducting filament has so far been reported for a few polycristalline, binary oxides, but not for single crystalline thin films of complex oxides.

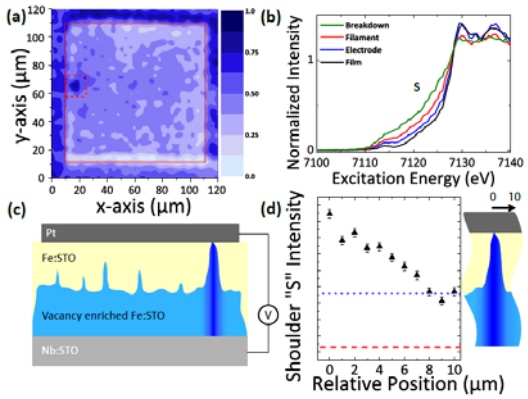

Fig.1. (a) XY-map of Fe Kα recorded on a 100x100 µm^2 MIM structure at 7122 eV excitation energy. The solid red line is a guide to the eye indicating the electrode area. (b) Fe K-edge XANES of the filament location (red), several different locations on the electrode area (blue), the as-deposited thin film (black), and a different electrode pad after "hard" dielectric breakdown (green). (c) Schematic model of the oxygen vacancy distribution in the switched memristor. (d) Profile of the conducting filament location, characterized by the fluorescence intensity at 7122 eV vs. the beam position.

In this study we examined µm-sized thin-film memristor devices with micro-XANES and utilize the sensitivity of the Fe K-edge to obtain information about the local changes around the Fe-dopant induced by resistive switching, and their spatial distribution in the MIM-structure. Ab initio full-multiple-scattering XANES calculations allowed us to interpret the observed changes in XANES to be due to the presence oxygen vacancies in the first coordination shell of iron. We found that the oxygen vacancy concentration increases dramatically at the location of the filament.

ATOMIC STRUCTURE RELAXATION IN NANOCRYSTALLINE NiO STUDIED BY EXAFS SPECTROSCOPY: ROLE OF NICKEL VACANCIES

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

Nanocrystalline NiO samples have been studied using the Ni *K*-edge extended x-ray absorption fine structure (EXAFS) spectroscopy and recently developed modeling technique, combining classical molecular dynamics with *ab initio* multiple-scattering EXAFS calculations (MD-EXAFS). Conventional analysis of the EXAFS signals from the first two coordination shells of nickel revealed that (i) the second shell average distance R(Ni–Ni$_2$) expands in nanocrystalline NiO compared to microcrystalline NiO, in agreement with overall unit cell volume expansion observed by x-ray diffraction; (ii) on the contrary, the first shell average distance R(Ni–O$_1$) in nanocrystalline NiO shrinks compared to microcrystalline NiO; (iii) the thermal contribution into the mean-square relative displacement σ^2 is close in both microcrystalline and nanocrystalline NiO and can be described by the Debye model; (iv) the static disorder is additionally present in nanocrystalline NiO in both the first Ni–O$_1$ and second Ni–Ni$_2$ shells due to nanocrystal structure relaxation.

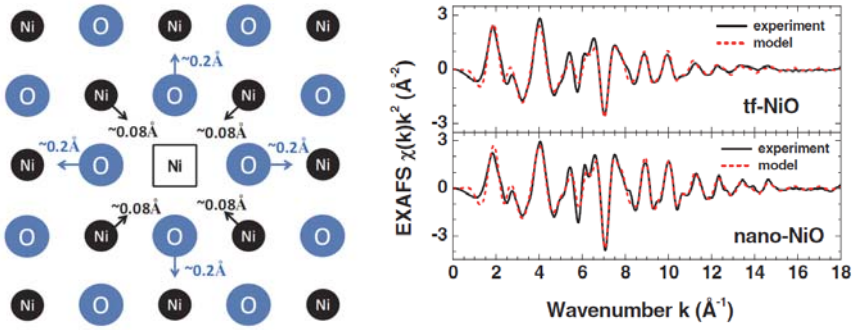

Fig.1. Left panel: Schematic view of the nearest-neighbor relaxation around nickel vacancy in the bulk of nickel oxide according to our molecular dynamics simulations. Note that oxygen atoms move outwards, but nickel atoms move inwards to the nickel vacancy. Right panel: Comparison of the experimental (solid lines) and configuration-averaged (dashed lines) Ni K-edge EXAFS spectra $\chi(k)k^2$ for nano-NiO and tf-NiO.

Within the MD-EXAFS method, the force-field potential models have been developed for nanosized NiO using as a criterion the agreement between the experimental and theoretical EXAFS spectra. The best solutions have been obtained for the 3D cubic-shaped nanoparticle models with nonzero Ni vacancy concentration C_{vac}: $C_{vac} \approx 0.4$–1.2% for NiO nanoparticles having the cube size of $L \approx 3.6$–4.2 nm and $C_{vac} \approx 1.6$–2.0% for NiO thin film composed of cubic nanograins with a size of $L \approx 1.3$–2.1 nm. Thus our results show that the Ni vacancies in nanosized NiO play important role in its atomic structure relaxation along with the size reduction effect.

Laboratory of Hydrogen Energy Materials

RESEARCH AND DEVELOPMENT OF MATERIALS AND DEVICES FOR HYDROGEN ENERGY TECHNOLOGIES

P. Aizpurietis, A.M. Alsbergs, G. Bajars, I. Dirba, L.Grinberga, J. Hodakovska, L. Jekabsons, J. Kleperis, J. Klavins, A. Krumina, A. Lusis, V. Nemcevs , A.Sivars, G. Vaivars, M. Vanags,
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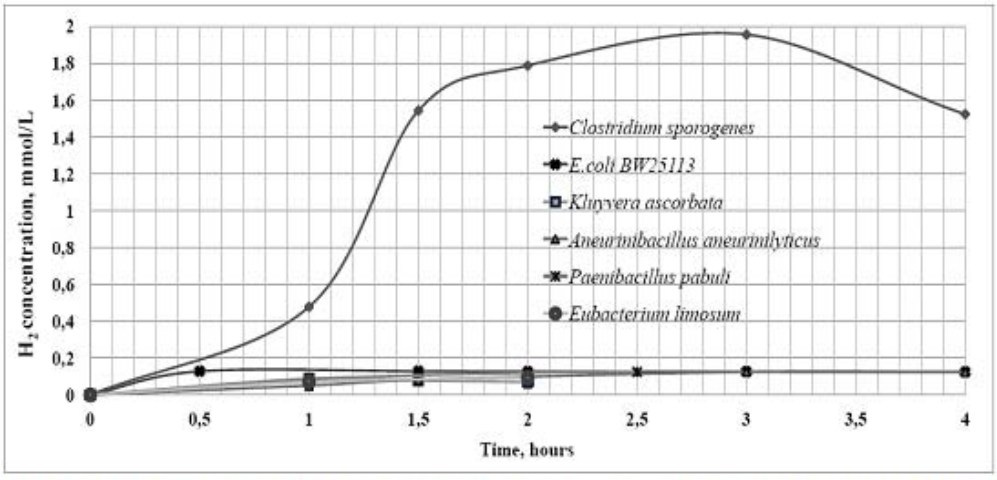
Hydrogen production: The Latvian Hydrogen Research Team at ISSP UL is developing inductive pulse power circuits for water electrolysis cell. The studies revealed a few significant differences compared to conventional DC electrolysis of water. New model is established and described, as well as the hypothesis is set that water molecule can split into hydrogen and oxygen on a single electrode (M.Vanags et all, 2012). There has been found and explained the principle of high efficiency electrolysis. A new type of power supply scheme based on inductive voltage pulse generator is designed for water electrolysis. Gases released in electrolysis process from electrodes for the first time are analyzed quantitatively and qualitatively using microsensors (dissolved gases in electrolyte solution nearby electrode) and masspectrometer (in atmosphere evolved gases). The hypothesis of hydrogen and oxygen evolution on a cathode during the process of pulse electrolysis is original, as well as interpretation of the process with relaxation mechanisms of electrons emitted by cathode and solvated in electrolyte (M.Vanags et all, 2012).

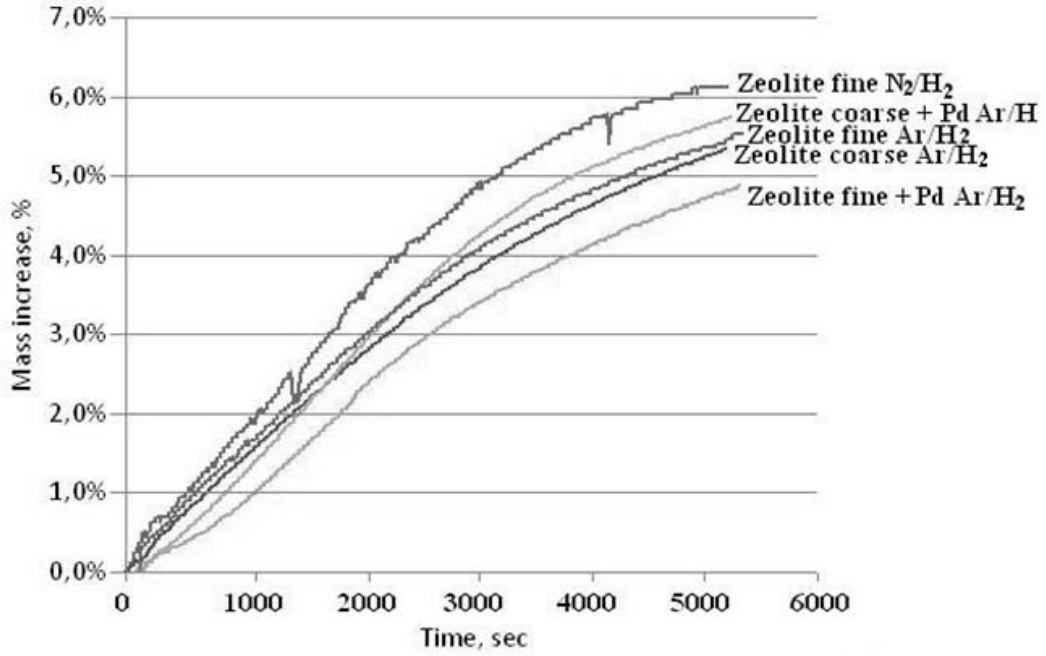
Hydrogen production via bacterial fermentation is perspective and environmentally viable because widely available renewable resources can be used as substrates (I.Diamanta et all, 2012). Biodisel production waste product, namely, crude glycerol can be effectively used for hydrogen production and large quantities of available crude glycerol are available in Latvia. Various bacterial isolates were tested for hydrogen gas production rates from glycerol with different test-systems. It was concluded that several of the isolated bacterial strains are suitable for bio-hydrogen production using crude glycerol as substrate (I. Dimanta et all, 2012).



Hydrogen production measurements in liquid phase on the sample with different bacterial strains using glycerol as substrate

Titania with anatase structure is investigated due to its photo-active properties that can be used in the water photocatalysis applications and in the organic photovoltaic devices (L.Grinberga et all, 2012). In this work the anodization conditions are described to obtain stable thin film TiO layers formed from vertically oriented nanotubes with approximate height 358 nm, inner tube diameter 48 nm and wall thickness 20 nm, but centre to centre distance 100 nm. Annealed at 500^{o}C TiO_2 layer mostly consists from oxide with anatase structure, though XRD spectroscopy shows rutile impurities as well. Obtained nanotube layers are sensitive mostly to UV light.

Hydrogen storage: Natural clinoptilolite is activated with palladium and tested for hydrogen adsorption capability at room temperatures (Lesnicenoks et all, 2012). Simple method is developed to measure hydrogen storage capability in solid materials with a commercial thermogravimeter. This method consists of two stages: material cleaning stage in inert gas (argon, nitrogen) flow, and hydrogen sorption stage where measured sample is cooled down from elevated to room temperature at hydrogen atmosphere. It is found that samples of finely grounded zeolite showed higher hydrogen adsorption capacity – up to 7 wt%.



Results of thermogravimetric measurements – mass increase during cooling down from +300 °C to room temperature in hydrogen atmosphere is shown only.

Slightly lower adsorption capability is observed for finely and course grounded zeolite samples that was activated with Pd.-. Hypothesis that the heating of zeolite in argon atmosphere activates the pore structure in zeolite material, where hydrogen encapsulation (trapping) can occur when cooling down to room temperature is proposed. An effect of catalyst (Pt) on hydrogen sorption capability is explained by spillover phenomena were less-porous fractions of natural clinoptilolite sample (quartz and muscovite) are involved in hydrogen transport.

Proton conducting membrane research: All studied composite Nafion 112 membranes impregnated with different hydroxyl ammonium ionic liquids showed similar behavior (V.Garaev et all, 2012). The conductivity decrease was not observed in a temperature range from 30 ^{o}C to 90 ^{o}C in ambient environment due to the potential water loss. Almost all composites have higher ion conductivity than a pure Nafion 112 at 90 ^{o}C. All ionic liquids increased the thermal stability of Nafion membrane approximately by 50 ^{o}C. The composite membrane of Nafion with ionic liquids has potential to be used in ionic devices at increased temperatures, especially acetates. However, the conductivity in a temperature range over 90 ^{o}C also should be studied. At

the same time, different ionic liquids with higher temperature stability should be selected for composite preparation. Such materials will find application in medium range PEM fuel cells. In this work, only biodegradable ionic liquids were used for composite preparation.

Hydrogen application research: Combined hydrogen, heat and power system is designed for Academic Centre of Natural Sciences (the territory of new Campus of University of Latvia), based on DFC300 power station (J.Dimants et all, 2012). Fuel supply to DFC300 is planned in three stages: 1) natural gas from city pipeline; 2) locally produced biogas mixed with natural gas from city pipeline; 3) only locally produced biogas mixed with synthesized on site methane.

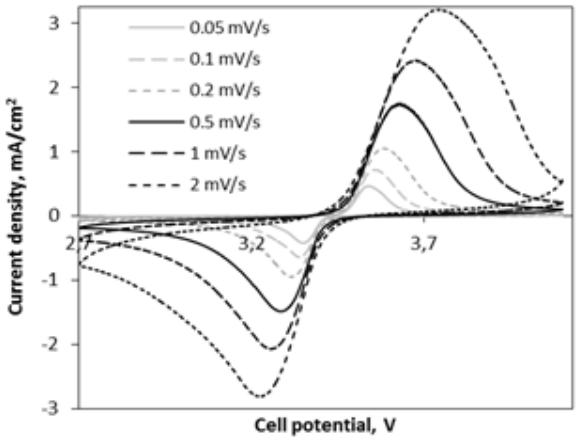
The site plan of University of Latvia Campus in Riga, Tornakalns, close to railway

Fuel cell power station as installed serves as the primary power source for Academic Centre of Natural Sciences, as an emergency power source for Academic Centre of Natural Sciences when the grid service is not online, as heat supplier to pre-heat the Academic Centre of Natural Sciences in winter season and hot water supplier to technical and service needs. Wind power and solar PV units are connected in grid and is powering electrolyser to generate additional hydrogen for CO_2+H_2 reactor to recover carbon dioxide from DFC300 exhaust. Hydrogen has a potential becoming a key factor in driving energy system to a sustainable trajectory. Hydrogen usage in stationary and mobile applications without damaging emissions is highly regarded. By using hydrogen energy, the end user can contribute in maintaining long-term energy stability. Public acceptance and knowledge expression is a substantial factor in order to implement renewable energy projects. Main results of survey show that majority of the respondents are very positive about renewable technology implementation idea in the University of Latvia Academic Centre Of Natural Sciences. Nevertheless many respondents are highly concerned about safety issues of the renewable energy technology. This means that safety education must be implemented and discussed more with society. As well as students and future students strongly agree that access to renewable energy technologies in the campus area during studies is an important part of student practical training. Students, academia as well as future students does support implementation of renewable technologies to improve the quality of learning, sustainable development of the university campus and green life style.

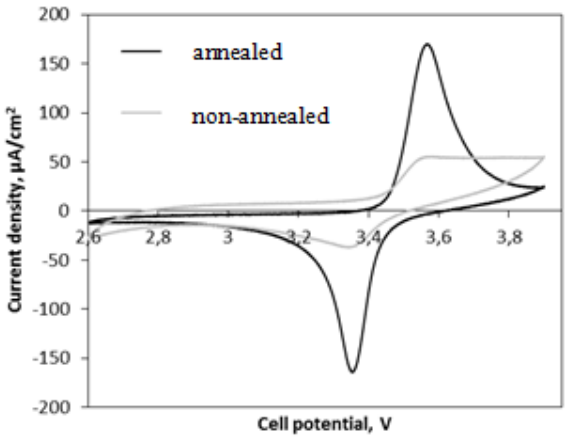
RESEARCH OF CATHODE MATERIALS FOR LITHIUM IRON PHOSPHATE THIN FILM BATTERIES

G. Kucinskis, G. Bajars, J. Kleperis, G. Čikvaidze, A. Lusis

$LiFePO_4$ is a promising olivine-type cathode material for lithium ion batteries. Structural and electrochemical analysis has been carried out for $LiFePO_4$ bulk material and thin films deposited by RF magnetron sputtering (G.Kucinskis et all, 2012). Thin films have lower effective surface area than bulk material samples due to their surface being smoother. Both bulk material and thin film electrochemical properties have been evaluated by cyclic voltammetry, chronopotentiometry and EIS. Bulk material gravimetric charge capacity was evaluated to be 135 mAh/g, thin film charge capacity corresponds to 45% of that determined for bulk material, and is 61 mAh/g. Lithium ion diffusion coefficients in $LiFePO_4$ bulk material and thin films have been determined at various states of charge and are observed to be lowest in equilibrium potential. The determined Li+ diffusion coefficient D_{Li} at cell equilibrium potential are $5.9 \cdot 10^{-14}$ and $9.7 \cdot 10^{-14}$ cm^2/s for bulk material and thin films accordingly.



Cyclic voltammetry of $LiFePO_4$ bulk material



Cyclic voltammetry of annealed and non-annealed $LiFePO_4$ thin film (scan rate 1 mV/s)

DIFFERENTIAL OPTICAL ABSORPTION SPECTROSCOPY AS A TOOL TO MEASURE EMISSIONS FROM SHIPS IN HARBOUR

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It is shown that the DOAS method with open light path is suitable for air pollution monitoring at the Riga Harbour. From monitoring data it is possible to track the source of emissions if average hourly concentrations of pollutants are analysed together with the meteorological data. As it is shown, sulphur dioxide sources in Harbour are mostly tankers manoeuvring through the river or standing at docks with powered engines during the handling of oil products. An open-beam DOAS system captures air pollution from a wider area and in case of observed high benzene emissions are from many different sources: rail cars, tankers, handling operations in the terminals, trucks and passenger cars, buses.

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37. **G. Kucinskis, G. Bajars, J. Kleperis**. Electrochemical properties of LiFePO4 thin films prepared by rf magnetron sputtering. International Scientific Journal for Alternative Energy and Ecology ISJAEE, No 9 (113) 2012, pp.72-77.
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2. 28th Conference of Institute of Solid State Physics, February 8 – 10, 2012, Riga

2. P. Lesnicenoks, L. Grinberga, J. Kleperis. Thermogravimetric Hydrogen Adsorption Studies of natural zeolite (clinoptilolite) material before and after activation.Abstracts, p.8.
3. J. Dimants, I. Dimanta, B. Sloka, J. Kleperis, Concept of implementation the hydrogen Technologies in academic center complex of University of Latvia. Abstracts, p.9.
4. K. Jurgelis, G. Vaivars. Preparation, properties and use in fuel cell of modified poly(etehretherketone) polymer membranes.Abstracts, p.10.
5. I. Dimanta, A. Gruduls, V. Nikolajeva, I. Muižnieks, J. Kleperis. Investigation of glycerol as substrate for hydrogen producers convertation dynamics and by-products identification. Abstracts, p.12.
6. A. Sivars, L. Grinberga, J. Kleperis, L. Kulikova, V. Serga. Studies on sorbed hydrogen amount in Pd modified clinoptilolite. Abstracts, p.13.
7. G. Kucinskis, G. Bajars, J. Kleperis. Synthesis and Structural Analysis of LiFeSiO4 Cathode Material for Lithium-ion Batteries. Abstracts, p.25.
8. P. Aizpurietis, M. Vanags, J. Kleperis. Electrolysis efficiency studies of steel electrodes with Raney nickel plating. Abstr., p.47.
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12. I. Dirnena, I. Dimanta, A. Gruduls, V. Nikolajeva. CO_2 Involmenet in the Formation of Methane Fermentation Reactor with Methane and Hydrogen-Producing Bacteria. Abstr., p.51.
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14. A. Sivars, L. Grinberga, J. Kleperis. Influence of Material Treatment on Hydrogen Sorption Kinetics. Abstr., p.53.

15. L. Grinberga, J. Kleperis. Functional Scheme of hydrogen storage tank. Abstr., p.54. RTU ERAF
16. I. Liepina, G. Bajars, L. Grinberga, J. Linitis, J. Kleperis, A. Lusis. Photocatalytic Properties of TiO2 Thin Films. Abstr., p.56.
17. S. Didrihsone, M. Kodols, J. Grabis. The Influence of Temperature and pH of Bi2WO6 Photocatalyst Nanopowder Formation. Abstr., p.76.
18. L. Grīnberga; nanostructured coating of electrodes for photo-catalytic water splitting, Abstr., p.14. LG ESF

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20. G. Bajars, J. Smits, G. Kucinskis, J. Kleperis, A. Lusis. Characterization of $LiFePO_4$/C Composite Thin Films Using Electrochemical Impedance Spectroscopy. Abstr. P.163.
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22. A. Knoks, I. Dirba, A. Sutka, M. Majorovs, J. Kleperis, G. Mezinskis. Magnetic and Electric Field Effects on the Growth of Ferrite Films in Spray Pyrolysis Process. Abstr. P. 289.
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24. L. Liepina, G. Bajars, J. Gabrusenoks, L. Grinberga, J. Kleperis, A. Lusis. Preparation and Photoactivity of Electrophoretic TiO_2 Coating Films. Abstr. P.291.
25. P. Lesnicenoks, A. Sivars, L. Grinberga, J. Kleperis. Hydrogen Adsorption in Zeolite Studied with Sievert and Thermogravimetric Methods. Abstr. P.293.
26. M. Vanags, P. Aizpurietis, J. Kleperis, G. Bajars. Comparison of Electrodes with Smooth and Nanostructured Surfaces in Pulse and D Electrolysis. Abstr., P.296.
27. J. Hodakovska, J. Kleperis. Measuring In-Plane and Through-Plane Conductivities of Polymer Electrolyte Membranes. Abstr. P.297.
28. V. Garaev, G. Vaivars, J. Kleperis, S. Pavlovica. Properties of the Nafion Membrane Impregnated With Hydroxyl Ammonium Based Ionic Liquids. Abstr. P.302.
29. Q. Naidoo, S. Naidoo, A. Nechaev, P. Ndungu, L. Petrik, G. Vaivars. Synthesis Tri-Metallic Platinum Group Metal Electrocatalysts Using Organometallic Chemical Vapour Deposition Technique for Methanol Oxidation. Abstr. P.190.

4. 10th Spring Meeting of the International Society of Electrochemistry: New approaches to nanostructuring electrodes for electroanalysis and energy storage, Perth, Australia, April 15-18, 2012

30. Gints Kucinskis, Gunars Bajars, Janis Kleperis, Liga Grinberga. Structure and Electrochemical Performance of Li2FeSiO4 Cathode Material. Book of Abstracts, p. 113
31. Liga Grinberga, Janis Linitis, Janis Kleperis, Gunars Bajars. Characteristics of Electrode with TiO_2 Nanostructured Layers for Photoelectric Hydrogen Production. Book of Abstracts, p. 311
32. G. Vaivars, J.Kleperis, A.Actins. Preparation of Phosphorized Zirconium Oxide Particles for Composite Electrode Materials. Book of Abstracts, p. 288

5. E-MRS 2012 Spring Meeting, Congress Center Strasbourg, France, May 14-18.

33. P. Lesnicenoks, A. Sivars, L. Grinberga, J. Kleperis. Research of Hydrogen Adsorption Dynamics in Natural Zeolite and Glass/Metal Hydride Composites. Programm and Book of Abstracts of E-MRS 2012 Spring Meeting, Congress Center Strasbourg, France, May 14-18, 012; C-18(Program): http://www.emrs-strasbourg.com/index.php?option=com_abstract&task=view&id=158&day=2012-05-16&year=2012&Itemid=99999999&id_season=6&PHPSESSID=01d0018706ba58f89cce142c495534a8

6. 10th International Symposium of Systems with Fast Ioon Transport, Chernogolovka, Russia, July 1-4, 2012.

34. J. Kleperis, L. Grinberga, P. Lesnicenoks, A. Sivars, G. Bajars. The study of hydrogen adsorption in natural zeolite. Book of Abstracts, p.97;
35. G. Kucinskis, G. Bajars, J. Kleperis, A. Lusis, A. Dindune, Z. Kanepe, J. Ronis. Preparation and electrochemical properties of Li2FeSiO4 bulk material and thin films. Book of Abstracts, p.76;

7. 14th International Conference-School „Advanced Materials and Tehnologies", August 27-31, Palanga (Lithuania)

36. P. Lesnicenoks, Hydrogen Sorption in Zeolite – Experimetal Results and Interpretation Version. Book of Abstracts, p.142.
37. G. Kucinskis, G. Bajars, J. Kleperis. Electrochemical Analysis of Li2FeSiO4 Cathode Material for Li-ion Batteries. Book of Abstracts, p.140.
38. A. Knoks, I. Dirba, M. Majorovs, J. Kleperis, G. Mezinskis, G. Kronkalns. Spray Pyrolysis Method to Obtain CoFe2O4 Thin Films: Optical, Magnetic an Morfological Properties. Book of Abstracts, p.51.

8. Invited talk in the Joint event of 11th Young Researchers' Conference: Materials Science and Engineering and the 1st European Early Stage Researcher's Conference on Hydrogen Storage, Belgrad, Serbia, Dec. 3-5,2012

L. Grinberga, J. Kleperis, Hydrogen storage in porous media at room temperature. http://www.mrs-serbia.org.rs/images/book_of_abstracts.pdf, Publisher: Materials Research Society of Serbia Institute of Technical Sciences of SASA Vinča Institute of Nuclear Sciences, University of Belgrade, 2012, p.13

9. 17th International Scientific Conference „EcoBalt 2012", Riga, Latvia, October 18-19, 2012

39. G. Vaivars. Membrane technologies in solving environmental problems. In: Abstr. 17th Int. sci. conf. Ecobalt 2012, Oct. 18-19, 2012. University of Latvia Press: 2012. P. 83.
40. J. Kleperis, K. Kundzins, L. Grinberga, A. Sarakovskis. Benzene Pollution in Riga Freeport – Monitoring and Opportunities. Abstr. P. 41.

10. International Workshop „Hydrogen and Fuel Cells in Research and Applications: facing to Latvia" October 4-5, Riga, Latvia

Informācija par semināru pieejama Web saitēs: www.cfi.lu.lv
http://www.h2lv.eu/galerija/notikumi/05-10-2012/
http://www.rea.riga.lv/jaunumi/aktualitasu-arhivs?id=550

PhD thesis

Aleksandr Kalinko, "Interpretation of x-ray absorption spectra using molecular dynamics simulations", Ph.D. Thesis, Latvian University, Riga, 2012.

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 department:
- 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.hab. M.Balodis
Dr.hab. V.Bondarenko
Dr. L.Simonova
Dr. T. Krasta
Dr. D.Riekstina
Dr. O.Veveris
Dr. J. Proskurins

Technical Staff
S.Afanasjeva

Students
Mag. students K. Bavrins

Scientific visits abroad
Dr. hab. J. Berzins, European Commission Euratom, Brussels,Belgium (8 days), 2012.
Dr. hab. J. Berzins, Cyclotron Workshop, Ispra, Italy 28-30 November 2012.
Dr. hab. J. Berzins, Insitut Laue Lagevin, Grenoble, 2-5 February 2012.
Dr. hab. J. Berzins, Insitut Laue Lagevin, Grenoble, 7-15 December 2012.

Cooperation

Latvia
1. Radiation Safety Center.
2. University of Latvia, Institute of Chemical Physics (Dr. G. Kizane)
3. Institute of Technical Physics, Rīga Technical University (Dr.J.Ruža).

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. J.Honzatko, Dr. I.Tomandl).

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

Main results

STUDY OF EFFECTS DUE TO NUCLEAR SHAPE CHANGE IN A~190 REGION NUCLEI

T.Krasta, M.Balodis, J.Bērziņš, Ļ.Simonova, V. Bondarenko

In the nuclear mass number A~190 region, one observes transition from the strong axially-symmetric prolate shape, characteristic to nuclei in the middle of deformation region, to the spherical shape at Z=82 and N=126 particle shell closures. Weakening of nuclear deformation results in the γ instability of nuclear shape, which notably affects nuclear properties, especially its low-energy decay scheme. In the case of non-axial deformation, intrinsic nuclear excitations lose their reflection symmetry along the nuclear core symmetry axis, and valence particle orbital momentum projection Ω, just like the total nuclear momentum projection K, are not good quantum numbers any more. As a result: a) for each nuclear spin I value, one has 2*I+1 states with projections K ranging from -I, -I+1,..., resulting in a considerably higher level density even at relatively low energy values; b) increased fragmentation of valence particle basis states manifests itself in the enhancement of single-particle transitions in comparison with collective intra-band transitions; c) one observes "inverted bands" - level sequences with different internal structure but connected with intense cascade γ-transitions.
Because of extreme level density, the development of nuclear level schemes in the A~190 region requires high precision data about γ-transition energies and intensities. Such data have been obtained via measurements of single and coincidence γ-spectra following thermal neutron capture reaction with enriched targets in the high-flux reactor of ILL (Grenoble, France). The single γ-spectra of odd-odd nuclei ^{186,188}Re have been measured in the energy range from 100 to 2000 keV employing the high precision crystal-diffraction spectrometer GAMS5. The energy and angular γγ-coincidence measurements for ^{188}Re in the energy range from 100 to 1200 keV have been performed in ILL at the PF1b polarized cold neutron guide using the multi-detector experimental set-up. These data, together with the results of our earlier high-low and low-low energy γγ-coincidence measurements [1] performed in Řež (Czech Republic), allowed to develop the level scheme of ^{188}Re nucleus up to 1.5 MeV energy. This level scheme includes more than 190 levels. The development of the level scheme for the neighboring odd-odd nucleus ^{186}Re is in progress.
The proposed model-independent ^{188}Re level scheme is strongly supported by γγ-coincidences. However, its model interpretation poses considerable difficulties. The Nilsson particle-plus-rotor model calculations have shown that, while one can reproduce most of the ^{188}Re low-lying levels assuming axially-symmetric core deformation with ε=0.18, and ε_4=0.05, then the experimentally observed level density above 400 keV is

much higher than that predicted by model calculations. Such increased level density indicates non-axial deformation, at least for some of ^{188}Re states. A possibility of non-axial deformation for nuclear states including neutron orbits with high orbital moment j values, e.g., 11/2[615] and 9/2[505], in A~190 region tungsten and osmium isotopes has been considered also in [2].

In order to resolve that problem, we have performed extensive model calculations employing the modified oscillator particle-plus-rotor model [3]. When $\gamma \neq 0$, particle's angular momentum j projection on the nuclear core symmetry axis Ω is not conserved, and the particle wave function includes all N shell oscillator state components $|Nljs\rangle$ with corresponding projections j_z. It means that one can employ the asymptotic quantum numbers $\Omega^{\pi}[Nn_z\Lambda]$ for nuclear state classification only approximately. Calculations have been performed both for the odd-odd nucleus ^{188}Re (Z=75,N=113), and for its odd neutron neighbor ^{187}W (Z=74,N=113). The dependence of quasiparticle energies and wave functions on the core non-axiality angle γ value have been studied for all low-lying valence proton and neutron orbits. The polarization energy and the γ stability for each particle state has been determined. It has been found that most orbits with high j values, e.g., $i_{13/2}$ neutron orbit 11/2[615], or $h_{11/2}$ proton orbit 9/2[514], are γ stable. On the contrary, the energy of neutron orbits 3/2[512] ($f_{5/2}$) and 9/2[505] ($h_{9/2}$) changes drastically. For some low j value states increased fragmentation results even in the change of particle orbit, e.g., the main component of the $p_{3/2}$ orbit 1/2[510] changes to that of the $f_{5/2}$ orbit 1/2[521] already at $\gamma=10^{\circ}$.

In the case of odd-odd nuclei, the resulting level scheme depends considerably also on the residual (i.e., not included in the nuclear mean field) NN-interaction between valence particles. Proton and neutron pairs form level multiplets with energy difference (Gallagher-Moszkowski (GM) splitting) depending on singlet or triplet orientation of particle spins. Other important effects of the residual NN-interaction are: a) the odd-even spin level energy shift (Newby shift) in K=0 rotational bands; b) the $\Delta K=0$ mixing between two-quasiparticle states. In the scope of our model calculations, we have studied the behavior of residual NN-interaction matrix elements on the nuclear non-axiality angle γ value. The values of corresponding V_{np} matrix elements have been calculated using expressions and parameter values given in [4]. It has been found that in order to reproduce the experimentally observed GM-splittings in ^{188}Re, one should include in the V_{np} both the short and the long range central interaction components, as well as the terms accounting for the polarization of nuclear core. Study of the γ-dependence of residual NN-interaction has shown that, because of increased fragmentation of particle wave functions, the values of most V_{np} matrix elements become smaller, though the well-known GM-rule (i.e., the spin triplet state has lower energy value in odd-odd nuclei) remains true also in the case of non-axial deformation. However, the behavior in dependence on γ of the matrix elements responsible for $\Delta K=0$ mixing is chaotic. Since the role of $\Delta K=0$ mixing in non-axial nuclei is greater than in axially-symmetric ones due to increased number of states with same K value, the resulting fragmentation of two-quasiparticle states in the case of non-axial deformation becomes very complex.

In general, our results show that the traditional particle-plus-rotor model interpretation of odd-odd transitional nuclei level schemes at energies above 500 keV is questionable. The only confident characteristics of excited levels are their energy, spin, and parity. If one intends to use for classification of nuclear levels the rotational bands based on Nilsson two-quasiparticle states, one should check for γ stability of involved states, as well as for possible fragmentation.

The results of our level energy and electromagnetic transition calculations in the case of odd ^{187}W have shown that one cannot regard the existence of positive parity “inverted bands”, observed in the level schemes of odd ^{183,185,187}W nuclei, as a firm indication of non-axial deformation. Observed levels can be interpreted as the band heads based on

different neutron orbits (11/2[615], 9/2[624], 7/2[633], 5/2[642], 3/2[651]) originating from the spherical orbit $i_{13/2}$. Very intense transitions between these levels are predicted also in the case of axially-symmetric core deformation. Though, in the case of ^{187}W, the possible non-axiality manifests itself as an increased level density, just like in neighboring odd-odd ^{188}Re. And, since there is no expected low Ω value positive parity orbits in that energy range, the experimentally observed $3/2^+$ and $5/2^+$ levels can be interpreted as the band-heads of 11/2[615] K+4, and 9/2[624] K-2 side (γ) bands.

1. M. Balodis, et al., Nucl.Phys. A 847 (2010) 121.
2. V. Bondarenko, et al, Nucl.Phys. A 856 (2011) 1.
3. S.E. Larsson, G. Leander and I. Ragnarsson, Nucl.Phys. A 307 (1978) 189.
4. J.P. Boisson, R. Piepenbring and W. Ogle, Phys. Rep. 26C (1976), 99.

MONITORING OF SOME CONTAMINATED TERRITORIES IN LATVIA

D. Riekstina, J. Berzins, 0. Veveris

Monitoring of artificial radionuclide Cs-137 in the soil and tritium in the groundwater around the potentially most contaminated areas of Latvia was carried out: the vicinity of the shut-down (1998) Salaspils research nuclear reactor and the radioactive waste repository “Radons”.

The aim of present work: 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 groundwater.

The concentrations of gamma radioactivity Cs-137 in different samples were determined using the high resolution HPGe gamma-spectrometers Ortec and Canberra within the energy range of 50-2000 keV. The uncertainty of measurements was within the range of 2%.

The tritium monitoring of groundwater in the 31 wells was performed since 1997. For particular years the results vary in certain wells within a wide range (5 – 8000 Bq/l) as well as seasonal changes are established there. The tritium concentration in the wells outside these territories was within limits 5 -18 Bq/l during last 5 years.

The results of Cs-137 monitoring in soils show, that the concentration varies in different points but it doesn’t exceed its average value in Latvia soil.

ASSESSMENT OF NATURAL RADIONUCLDES LEVEL IN BUILDING MATERIALS

D. Riekstina, J. Berzins, O.Veveris

Very different building materials are used today for the housing construction. The aim of this work was obtained data of natural radionuclides level for different building materials, put into practice in Latvia.

We present research data on the concentration of the natural radionuclides (K-40, Th-232 and U-238) in 155 building materials and products of different type, manufactured in Latvia as well as imported. We are subdivided all materials in the following groups: auxiliary materials (hydro-insulation, concrete additives, anti-corrosion, glues, and others); granite, marble; sand, gravel; cement, lime; putty, finishing materials; building ware (plumbing, ceramsite and concrete blocks; plastic boards).

The highest concentrations of natural radionuclides K-40 and the decay products of the Th-232 and U-238 (Ra-226) chains were detected in granite and its products. The maximally permitted concentrations of the radionuclides, Bq/kg (according to the

Regulation of the Cabinet of Ministers Latvia No.149, 09.04.2002) has been exceeding in particular plumbing and ceramsite products, and in some imported granite blocks.

Lectures on Conferences

1. J.Berzins, L.Simonova, M.Balodis, T.Krasta, V.Bondarenko, M.Jentschel, W.Urban, I.Tomandl. „Model interpretation possibilities for levels of the ^{188}Re nucleus up to about 2 MeV energy". 28th Scientific Conference Inst.of Solid State Physics, University of Latvia, Riga, February 8-10, 2012, p. 41.
2. D. Riekstina, J.Berzins, O. Veveris. "Possibilities to use cyclotron for activation analysis", 28th Scientific Conference Inst.of Solid State Physics, University of Latvia, Riga, February 8-10, 2012, p. 86.
3. D.Riekstina, J.Berzins, O.Veveris, Monitoring of some contaminated territories in Latvia, Abstract: 6th Int. Symposium on in Situ Nuclear Metrology as a Tool for Radioecology, 11-15 June 2012, Brussels, Belgium, p. 104.
4. V. Skvortsova, N. Mironova-Ulmane, L.Trinkler, D. Riekstina. Impurity defects in wide gap inorganic materials, 5th WSEAS Int. Conf. on Material Science (Materials 12), Sliema, Malta, Sept. 7-9, 2012, p. .
5. D.Riekstina, J.Berzins, O.Veveris, Assessment of natural radionuclide level in building material, Abstract: 17th Int. conf. "EcoBalt'2012", Riga, Oktober 18-19, 2012, p. 69.

LABORATORY OF ELECTRONIC ENGINEERING

Head of Laboratory Dr. phys. A. Kristins

Main Problems

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

Scientifical Staff

1. Dr. phys. A.Kristins

Technical Staff

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

Cooperation

Latvia

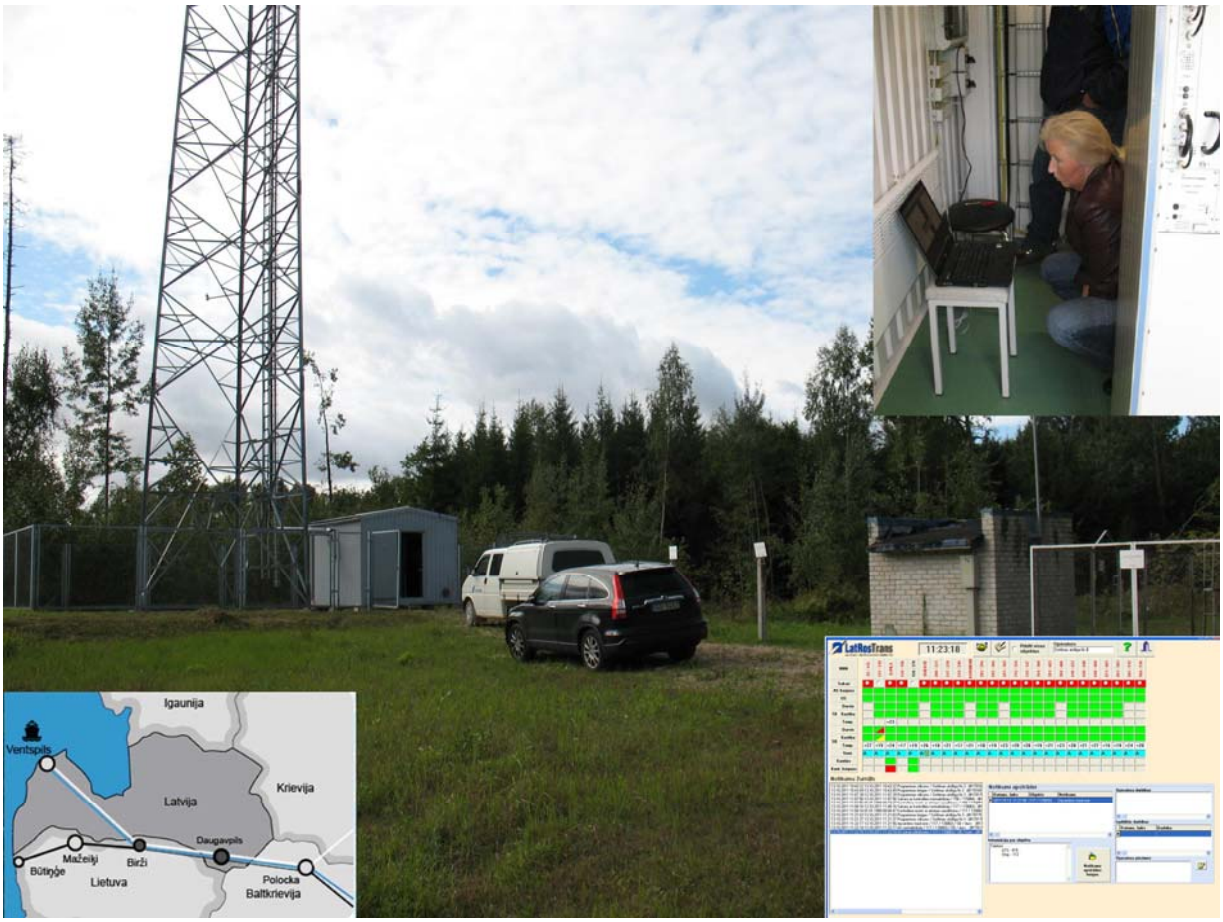
1. Joint-stock company *Augstsprieguma tīkls*
2. „*Fonons*” Ltd
3. Latvia Technology Park
4. Riga Technical University
5. *Loks* Ltd,
6. „*ADI Kartes*” Ltd
7. *GROG* Ltd
8. .*Energoremonts Rīga* Ltd

Estonia

1. Tallinn University of Technology
2. Competence Centre ELIKO

Main results

1. The system of the *LatRosTrans* Ltd for objects access, security, alarm, temperature monitoring and control were installed in 2004 – 2005 and modernized in 2011. The system serves 25 single or double block-boxes along the pipeline from the Belarus border to Ventspils.

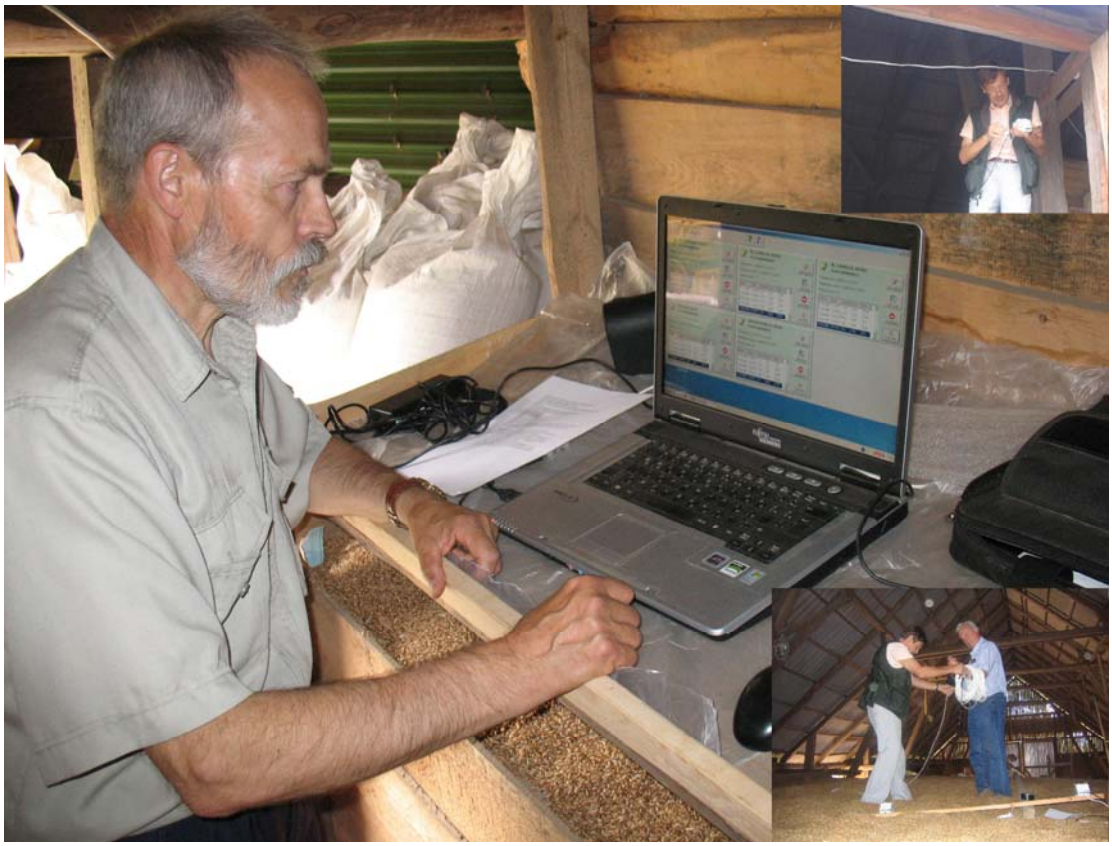


One of the *LatRosTrans* Ltd objects. Bottom left - the pipeline scheme. Right at the top - the leading programmer I. Gvardina performs the facility operational testing. Bottom right - *LatRosTrans* Ltd dispatcher service point program's main window.

2. For JSC *Augstsprieguma tīkls* and the *Energoremonts Riga* Ltd a number of testing equipment for high-voltage switches, automatic disconnecting switches, power transformer's step-switches were designed and produced in accordance with the customers' orders.

One of *Latvenergo* high voltage transformers. On the top – leading engineer Juris Veinbergs preparing for testing works. Bottom right - the test device *Koda-3M*.

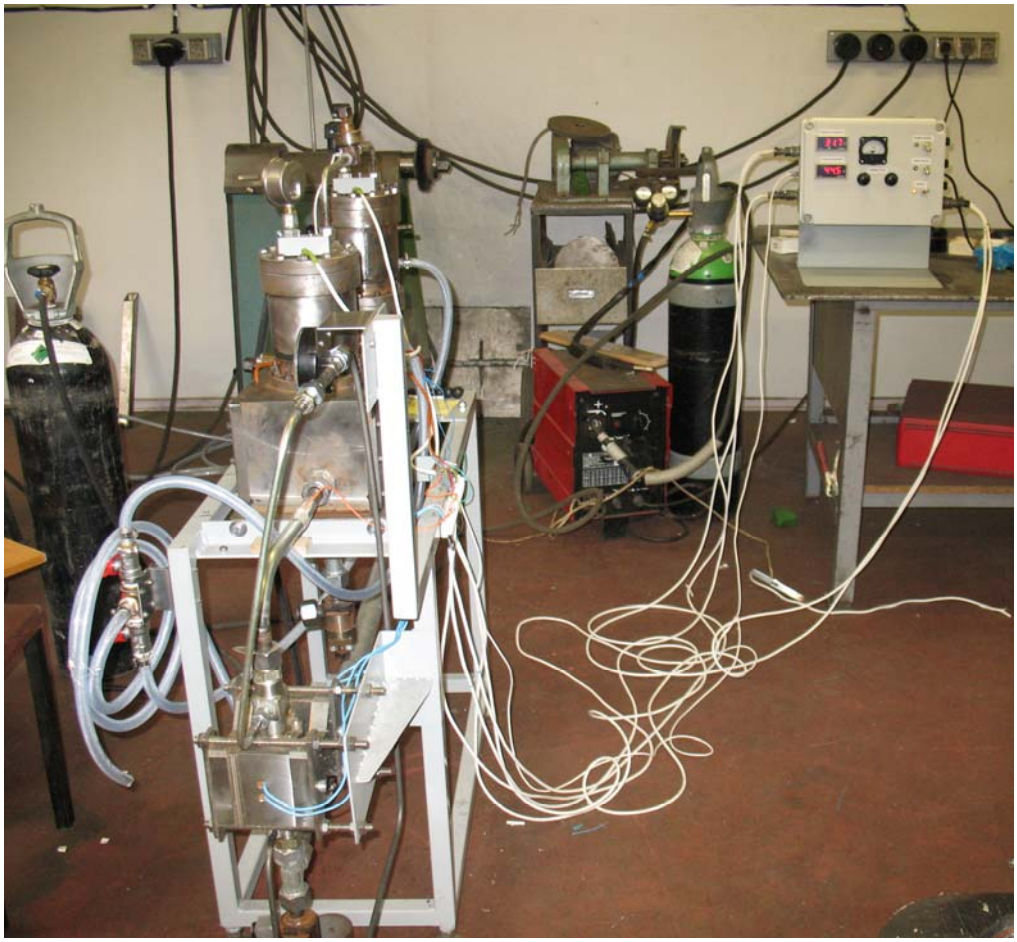
3. The grain drying computerized control equipment, monitoring temperature and humidity changes within four points of the dryer is developed and produced for one of Zemgale farms.



Dr. Alberts Kristins during installation and testing of the control device.

4. By orders of several organizations ("Latvian Shipping Company", "Latvian Gas", Vangazu industrial park, "Vaide", ISSP, etc.) checkpoints, access control and signaling computerized systems of various configuration and complexity were designed, manufactured and installed. The systems provide service for one or several buildings (may be in different locations), parking lots, gates and similar units.

Installation of the checkpoint system in the "Latvian Shipping Company" management.
From left - Jānis Straumēns, Alberts Kristiņš and Pēteris Kaļiņikovs



5. Device for preparation and testing of Na and Ca solution in propane-butane mixture is designed and manufactured for "Mesako" Ltd.

6. In accordance with a private enthusiast order an amusement device "swing" with pneumatic actuator is designed, manufactured and certified. The swing is designed for one person, and is 6m high, swinging duration - 3, 5, 10 or more minutes, roll angle of 30, 45, 60 and 75 degrees with the possibility of moving from one value to another during swinging time. The swing stops automatically after the period expires or upon pressing the "STOP" button. Special attention is paid to the customer's safety.

7. In cooperation with *FONONS* Ltd are developed several versions of control devices for compressors and heat pumps, three-phase soft starts for industrial equipments with current up to 400A, remote management and control system for air compressor station. (Financing was provided from *FONONS* Ltd, as well as from the ERDF and the TOP projects).

8. Dozens of visitor counters were designed, manufactured and installed in optical stores of Latvia and Lithuania in accordance with order of the Centre of Optometry, University of Latvia.

9. In accordance with an order of *Aqualogic* Ltd several product service dispensing machine control and limitation equipments were designed and manufactured.

10. Working time control systems (*Nienhaus & Lotz Lettland* Ltd, *Godske Latvian Textile* Ltd, *VAIDE* Ltd, *FONONS* Ltd, *FLEXOPLASTIC* Ltd).

Number of other projects are developed and implemented in addition to the abovementioned main results.

Our customers for 10 years: State JSC “Latvijas Pasts”, *LatRosTrans* Ltd, JSC Latvian Shipping Company, JSC Latvijas Gāze, Latvian Environmental Protection Agency, the Latvian Hydrometeorological Agency, Latvian Savings Bank, *Augstceltne* Ltd, CSDD (Road Traffic Safety Directorate), *Nienhaus & Lotz Lettland* Ltd, *Godske Latvian Textile* Ltd, *VAIDE* Ltd., *FLEXOPLASTIC* Ltd and others.

Partners: *Fonons* Ltd, Riga Technical University, Latvian Technology Park, *GROG* Ltd, JSC Augstsprieguma tīkls, *Energoremonts Riga* Ltd, *Augstceltne* Ltd, *ADI Card* Ltd, *Loks* Ltd, Competence Centre ELIKO, Estonia, Tallinn University of Technology Institute of Electronics, Estonia and others.

Publications. Despite the fact that due to the profile of the laboratory, the main evaluation criteria of the work is the developed and implemented projects, the staff of the Radioelectronics Laboratory has also published more than 60 scientific - technical articles. Patents applications are not filed due to economical considerations.
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. *Augstceltne* Ltd;
9. CSDD (Road Traffic Safety Directorate);
10. *Avantime Amusement Technology* Ltd;
11. Joint-stock company *Latvenergo;*
12. Latvia's Ministry of Foreign Affairs;
13. *Nienhaus & Lotz Lettland* Ltd;
14. *Godske Latvian Textile* Ltd;
15. *VAIDE* Ltd;
16. *Flexoplastic* Ltd

etc.

Lectures on Conferences

28th Scientific Meeting of Institute of Solid State physics, University of Latvia, Riga, February, 2012

1. I.Gvardina, A.Kristiņš, J.Melderis *"LatRosTrans" object security, alarm and control system functionality expansion*. Abstracts, p.88.
2. P.Annus, M.Rist, J Ojarand,, R.Land, A.Kristiņš. *Binary and ternary signals for wide band system identification*. Abstracts, p.90.
3. A.Kristiņš, J.Melderis. *Power controller for active load.* Abstracts, p.70.
4. I.Gvardina, A.Kristiņš, J.Melderis *ISSP checkpoint, access and alarm system.* Abstracts, p.89